JNC TN8400 2004-015

PHREEQCで取り扱うための C-S-Hゲルの熱力学データの検討

（研究報告）

２００４年７月

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（研究報告）

加藤　大生*，本田　明**

要　旨

TRU 廃棄物の処分施設においては，多量のセメント系材料を使用することが考えられており，処分施設の間隙水の化学的条件は，このセメント系材料の溶解／沈殿に強く影響されることが予想される。したがって，処分施設の化学的条件を評価するためには，セメント系材料に関連する鉱物の溶解／沈殿挙動を適切にモデル化し，評価に適用することが重要である。特に，低結晶性のカルシウム珪酸塩水和物である C-S-H ゲルは，セメントの水和において最も多量に生成する水和物であり，セメント系材料の力学的特性を決定している。また，主要構成鉱物という点で，C-S-H ゲルの溶解／沈殿が間隙率を介してセメント系材料の水理学的条件に強く影響する。さらに，長期的には C-S-H ゲルの溶解／沈殿が間隙水の化学的条件を支配する。このため，C-S-H ゲルの溶解／沈殿挙動の重要性は国際的にも認識されており，これまでいくつかのモデルが提案されている。C-S-H ゲルは，その構成元素であるカルシウム及びケイ素が非調和的に溶解／沈殿することが知られており，その挙動を表現することが，これらのモデルの主眼となっている。

一方，これまで放射性廃棄物の地層処分の分野における地球化学計算には，汎用の地球化学計算コードである PHREEQC がしばしば用いられている。PHREEQC では，評価したい系の化学反応式とその化学反応式の平衡定数の対数（log K）を与えることによって，系が到達する化学平衡状態を算定することができる。サイクル機構の高レベル放射性廃棄物処分におけるリファレンス地下水の組成は，この PHREEQC を用いて決定されている。TRU 廃棄物処分施設の化学的条件の評価においても，これと同じ組成の地下水を使用することが考えられており，セメント系材料とこの地下水との反応の評価には，PHREEQC を活用することが計画されている。そこで，本報では PHREEQC で使用することを前提として既往の C-S-H ゲルの溶解／沈殿モデルを調査し，それらのモデルの PHREEQC への適合性や，それらを用いて PHREEQC で計算した結果の妥当性について検討した。

既往の C-S-H ゲルの溶解／沈殿モデルを調査した結果，PHREEQC 上での取り扱いに相応しいモデルとして，Atkinson モデル及び Reardon モデルが選定された。選定されたモデルから導いた C-S-H ゲルの解離式及び log K を用いて C-S-H ゲルの溶解／沈殿反応を計算した結果，純水系の場合には，いずれのモデルも実験値に一致した非調和な C-S-H ゲルの溶解／沈殿反応を表現することができた。しかし，これら二つのモデルでは取り扱うことができる C-S-H ゲルの Ca/Si 比の範囲が異なり，炭酸イオン等の共存イオンの影響を考慮すると，より広範囲な Ca/Si 比の C-S-H ゲルの溶解／沈殿反応を取り扱うことができる Atkinson モデルの適用が推奨された。

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An Estimation of Applicable Thermodynamic Data for C-S-H Gel to PHREEQC (Research Document)

Hiroshige Kato*, Akira Honda**

ABSTRACT

Cementitious materials will be used extensively in the TRU waste repository. The dissolution/precipitation of cementitious materials will affect the chemical condition of pore water of TRU waste repository. Thus, it is important for estimation of chemical condition of pore water to apply the dissolution/precipitation of cementitious materials appropriately. A C-S-H gel (poorly crystallized calcium silicate hydrate) is a major component in cementitious materials which determined the mechanical characteristics of cementitious materials. The hydraulic condition of cementitious materials is strongly affected by the dissolution/precipitation of C-S-H gel due to the change of porosity accompanied with the dissolution/precipitation processes. Further, the chemical condition of pore water will be dominated by the dissolution/precipitation of C-S-H gel for a long period. Therefore, an importance of the dissolution/precipitation of C-S-H gel has been recognized internationally, and several dissolution/precipitation models of C-S-H gel have been proposed. The principal scopes of the C-S-H gel models are description of an incongruent dissolution/precipitation behavior of C-S-H gel.

On the other hand, PHREEQC is a computer program, which has been used generally for the geochemical calculation. PHREEQC can provide the state of chemical equilibrium of system defined by chemical equations and equilibrium constants (log K). In JNC, reference model groundwater determined by calculation using PHREEQC in HLW study will be also used in TRU waste study. In addition, PHREEQC will be used for calculation of the cement-water reaction. Therefore, applicability of the presented dissolution/precipitation models of C-S-H gel to PHREEQC was estimated.

As a result of estimation of the applicability, Atkinson model and Reardon model were selected as suitable models to the PHREEQC. The chemical equations and log K values of C-S-H gel were derived from these models and tested using PHREEQC. The calculation results using the data from both Atkinson model and Reardon model agreed to the experimental results measured in pure water system. However Atkinson model is preferable for considering the precipitation reaction with various species such as carbonate ion because of its capability of more extensive calcium silica ratio of C-S-H gel.

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1. はじめに

TRU 廃棄物の処分施設においては，多量のセメント系材料を使用することが考えられており，処分施設の間隙水の化学的条件は，このセメント系材料の溶解／沈殿に強く影響されることが予想される[1]。したがって，処分施設の化学的条件を評価するためには，セメント系材料に関連する鉱物の溶解／沈殿挙動を適切にモデル化し，評価に適用することが重要である。特に，C-S-H ゲルと呼ばれる低結晶性のカルシウム珪酸塩水和物（$CaO\text{-}SiO_2\text{-}H_2O$）は，セメントの水和において最も多量に生成する水和物であり，セメント系材料の力学的特性を決定している。また，主要構成鉱物という点で，C-S-H ゲルの溶解／沈殿が間隙率を介してセメント系材料の水理学的条件に強く影響する。さらに，長期的には C-S-H ゲルの溶解／沈殿が間隙水の化学的条件を支配する。このため，C-S-H ゲルの溶解／沈殿挙動の重要性は国際的にも認識されており，これまでいくつかのモデルが提案されている。C-S-H ゲルは，その構成元素であるカルシウム及びケイ素が非調和的に溶解／沈殿することが知られており，その挙動を表現することが，これらのモデルの主眼となっている。

一方，これまで放射性廃棄物の地層処分の分野における地球化学計算には，汎用の地球化学計算コードである PHREEQC [2]がしばしば用いられている。PHREEQC では，評価したい系の化学反応式とその化学反応式の平衡定数の対数（以下，log K と呼ぶ）を与えることによって，系が到達する化学平衡状態を算定することができる。また，ユーザーの設定により系の反応速度的評価や，一次元であれば物質輸送と化学平衡のカップリング計算も可能である。サイクル機構の高レベル放射性廃棄物処分におけるリファレンス地下水の組成は，この PHREEQC を用いて決定されている[3]。TRU 廃棄物処分施設の化学的条件の評価においても，これと同じ組成の地下水を使用することが考えられており，セメント系材料と地下水との反応の評価には，PHREEQC を活用することが計画されている。

そこで，本報では PHREEQC で使用することを前提として既往の C-S-H ゲルの溶解／沈殿モデルを調査し，それらのモデルの PHREEQC への適合性や，それらを用いて PHREEQC で計算した結果の妥当性について検討した。

2. C-S-H ゲルの解離式及び log K

2.1 既往の C-S-H ゲルの溶解／沈殿モデル

表-1 に，既往の C-S-H ゲルの溶解／沈殿モデルの特徴についてまとめる。既往の C-S-H ゲルの溶解／沈殿モデルには，ポルトランダイト（$Ca(OH)_2$），ある特定組成のカルシウム珪酸塩水和物，アモルファスシリカ（$SiO_2(am)$）を端成分とする固溶体モデルとして表現するものと，実験結果に基づく経験式を設定して非調和な溶解／沈殿を表現するものがある。これらのモデルについて，C-S-H ゲルの化学組成や溶解／沈殿反応の log K の与え方によって，大きく二つに分類できると考えられる。一方は，Ca/Si 比に応じて C-S-H ゲルの化学組成と，その化学組成に応じた溶解／沈殿反応の log K を与えるもので，Atkinson モデル[4]や Reardon モデル[5]がこれに該当する。もう一方は，C-S-H ゲル（固溶体）の化学組成を端成分の存在割合で表現し，その存在割合に応じて端成分の溶解／沈殿反応の log K を変化させるもので，Berner モデル[6]や Börjesson モデル[7]，杉山モデル[8]がこれに該当する。

前者のモデルでは，Ca/Si 比を少しづつ変化させたカルシウム珪酸塩水和物の化学組成を算出し，それぞれの化学組成に応じたカルシウム珪酸塩水和物の log K をモデルに従い与えることで，C-S-H ゲルを一連のカルシウム珪酸塩水和物群として表現することができる。この場合には PHREEQC の入力ファイルの中で C-S-H ゲルの溶解／沈殿モデルを設定することができる。一方，後者のように，同一鉱物（端成分）に対して，計算途中で Ca/Si 比に応じた異なる log K を与えているモデルを，PHREEQC の入力ファイルの中で設定することは困難であり，ソースコード自体を改造する必要がある。しかし，ソースコードの中を改造することは，プログラムの構成や内容を十分に理解した上で行わなければ，ソースコード自体の信頼性を損なうことになる。このため，PHREEQC の入力ファイルで設定可能な Atkinson モデル及び Reardon モデルを検討の対象とした。

2.2 Atkinson モデル

Atkinson らは， C-S-H ゲルを Ca/Si 比に応じて以下のような 2 種類の固相（端成分）から成る固溶体として表現している[4]。

・0<Ca/Si 比<n　　：SiO_2 (am)及び $nCaO.SiO_2.mH_2O$

・Ca/Si 比>n　　：$Ca(OH)_2$ 及び $nCaO.SiO_2.mH_2O$

Atkinson モデルでは，0 < Ca/Si 比 < n の C-S-H ゲルは Xs mol の $SiO_2(am)$と 1-Xs mol の $nCaO\text{-}SiO_2\text{-}mH_2O$ から成る固溶体として定義されており[4]，これを式にすると以下のように示すことができる。

$$Xs\ SiO_2(am) + (1\text{-}Xs)\ (nCaO.SiO_2.mH_2O) = n\ (1\text{-}Xs)\ CaO.SiO_2.m\ (1\text{-}Xs)\ H_2O \quad \cdots ①$$

この C-S-H ゲルの解離式は以下のように示すことができる。

$$n\ (1-Xs)\ CaO.SiO_2.m\ (1-Xs)\ H_2O = n(1\text{-}Xs)Ca^{2+} + H_4SiO_4 + \{(n+m)(1-Xs)\text{-}2\}H_2O - 2n(1-Xs)H^+ \quad \cdots ②$$

一方，Ca/Si 比> n の C-S-H ゲルに対しては，Xp mol の $Ca(OH)_2$ と(1-Xp)/n mol の $nCaO.SiO_2.mH_2O$ から成る固溶体として定義しており[4]，これを式にすると以下のように示すことができる。

$$Xp\ Ca(OH)_2 + \left(\frac{1-Xp}{n}\right)(nCaO.SiO_2.mH_2O)$$

$$= CaO.\left(\frac{1-Xp}{n}\right)SiO_2.\left\{\frac{m(1-Xp)}{n}+Xp\right\}H_2O \quad \cdots ③$$

この C-S-H ゲルの解離式は以下のように示すことができる。

$$CaO.\left(\frac{1-Xp}{n}\right)SiO_2.\left\{\frac{m(1-Xp)}{n}+Xp\right\}H2O = Ca^{2+} + \left(\frac{1-Xp}{n}\right)H_4SiO_4$$

$$+ \left\{\frac{(m-2)(1-Xp)}{n}+Xp+1\right\}H_2O - 2H^+ \quad \cdots ④$$

さらに，Atkinson モデルでは，①及び③式に示す C-S-H ゲルに対して，それぞれ次式に示す標準生成自由エネルギー ΔG^0_f を与えている[4]。

$$\Delta G^0_{f(0<Ca/Si<n)} = Xs\,\Delta G^o_{fs} + (1-Xs)\,\Delta G^0_{fx} + RT\{Xs \ln Xs + (1-Xs)\ln(1-Xs)\}$$
$$+ Lsx\ Xs + Asx\ Xs(1-Xs) \quad \cdots ⑤$$

$$\Delta G^0_{f(0<Ca/Si<n)} = Xp\,\Delta G^0_{fp} + \left(\frac{1-Xp}{n}\right)\Delta G^0_{fx} + RT\left\{Xp\ln Xp + \left(\frac{1-Xp}{n}\right)\ln\left(\frac{1-Xp}{n}\right)\right\}$$

$$+ Lpx\ Xp + Apx\ Xp\left(\frac{1-Xp}{n}\right) \quad \cdots ⑥$$

ここで，

$\Delta G^0_{f(0<Ca/Si<n)}$	: 0 < Ca/Si 比 < n の C-S-H ゲルの標準生成自由エネルギー
$\Delta G^0_{f(Ca/Si>n)}$	: Ca/Si 比 > n の C-S-H ゲルの標準生成自由エネルギー
ΔG^0_{fs}	: SiO_2(am)の標準生成自由エネルギー
ΔG^0_{fx}	: $nCaO.SiO_2.mH_2O$ の標準生成自由エネルギー
ΔG^0_{fp}	: $Ca(OH)_2$ の標準生成自由エネルギー
Xs	: SiO_2(am)のモルフラクション
Xp	: $Ca(OH)_2$ のモルフラクション
Lsx，Lpx	: lattice stability term を決定するパラメーター
Asx, Apx	: regular solution term を決定するパラメーター
R	: 気体定数
T	: 温度

である。

Atkinson モデルでは，②式及び④式が解離反応の一般式と考えることができ，⑤式及び⑥式から算出した C-S-H ゲルの標準生成自由エネルギー及び C-S-H ゲルの解離式から log K を求めることができる。Atkinson らは，端成分の一つである $nCaO.SiO_2.mH_2O$ をトバモライトと同じ組成である $0.833CaO\text{-}SiO_2\text{-}0.917H_2O$ とした場合と，$0.5CaO\text{-}SiO_2\text{-}1.5H_2O$（仮想の鉱物）とした場合のパラメーターLsx, Lpx, Asx, Apx, ΔG^0_{fx} を決定し，C-S-H ゲルの溶解反応を計算した結果，両者に大きな違いがなく，実験結果によく一致したことを報告している[4]。そこで，本報では，端成分 $nCaO.SiO_2.mH_2O$ の組成を $0.833CaO\text{-}SiO_2\text{-}0.917H_2O$（CSH(0.833)）としたときの C-S-H ゲルの解離式及び log K を Ca/Si 比 0.1 刻みで導いた。

表-2，3 に C-S-H ゲルの解離式及び log K の導出に用いた標準生成自由エネルギー ΔG^0_f 及びパラメーターをそれぞれ示す。また，表-4，5 に C-S-H ゲルの解離式及び log K をそれぞれ示す。現在，サイクル機構においては JNC-TDB として熱力学データの整備が進められており，その中で，$Ca(OH)_2$ の ΔG^0_f については-897,498J･mol^{-1} もしくは-898,426 J･mol^{-1} のいずれかで検討されている。また，表-2 に示すように，JNC-TDB と Atkinson らの報告とでは，ΔG^0_f がわずかに異なる部分がある。このため，Atkinson モデルからは，①Atkinson らの報告に記されているオリジナルの ΔG^0_f を使用したケース（Atkinson ケース），②$Ca(OH)_2$ の ΔG^0_f を-897,498J･mol^{-1} としたときの JNC-TDB の ΔG^0_f を使用したケース（JNC-TDB(1)ケース），③$Ca(OH)_2$ の ΔG^0_f を-898,426J･mol^{-1} としたときの JNC-TDB の ΔG^0_f を使用したケース（JNC-TDB(2)ケース）の計 3 ケースで C-S-H ゲルの log K を算出した。

2.3 Reardon モデル

Reardon モデルでは，実験結果に基づき，以下の経験式を設定して C-S-H ゲルの解離式及び log K を定義している[5]。

$$xCaO.SiO_2.xH_2O + H_2O = xCa^{2+} + H_3SiO_4^- + (2x - 1)OH^- \quad \cdots ⑦$$

$$\log K = -9.044 + 0.568R - 0.193R^2 \quad \cdots ⑧$$

$$Ca/Si = 0.88 + 0.03e^{0.513R} \quad \cdots ⑨$$

ここで，$R = \log ([Ca]^{2+}_{aq} / [H_4SiO_4]_{aq})$である。

⑦～⑨式を用いて，Ca/Si 比が 0.9～1.8 の C-S-H ゲルについて，Ca/Si 比を 0.1 刻みで解離式及び log K を導いた。表-6 にその結果を示す。

3. 計算条件及び検証方法

3.1 計算条件

表-7 に計算条件をまとめる。ここでは，純水 1kg に対し，ある一つの Ca/Si 比の C-S-H ゲルを 1mol 添加したときの溶解／沈殿反応を PHREEQC で計算した。PHREEQC は，米国地質調査所（USGS：U. S. Geological Survey）の WEB サイト（http://www.usgs.gov/）からダウンロードした。バージョンは，PHREEQC Interactive 2.8 である。また，データベースには，Arthur らがまとめた SPRON. JNC Database[9]を PHREEQC に適用できるように変換したものを使用した。

Atkinson モデルから導いた熱力学データを用いた計算においては，EQUILIBRIUM PHASE（反応に寄与する固相）に C-S-H ゲル（Ca/Si=0.1~1.8）及び 3 種類の端成分（SiO_2(am), CSH(0.833), $Ca(OH)_2$）を設定した。また，前項で述べたように Atkinson モデルからは①Atkinson ケース，②JNC-TDB(1)ケース，③JNC-TDB(2)ケースの 3 ケースの log K を算出した。このため，それぞれのケースについて計算を行なった。

Reardon モデルから導いた熱力学データを用いた計算においては，EQUILIBRIUMU PHASE に Ca/Si 比が 1.0～1.8 の C-S-H ゲル及び $Ca(OH)_2$ を設定した。ここで，Reardon モデルからは表-6 に示すように Ca/Si 比が 0.9 の C-S-H ゲル（CSH(0.9)）の log K を算出することができる。しかし，この CSH(0.9)を EQUILIBRIUMU PHASE に加えて計算すると，初期固相の Ca/Si 比によらず，CSH(0.9)が支配的な沈殿固相となり，液相の Ca 濃度，Si 濃度，pH が一定の値となってしまう。このため，EQUILIBRIUM PHASE から CSH(0.9)を外して計算した。なお，$Ca(OH)_2$ については，Reardon の報告に記載されているデータ[5]を用いた。

3.2 検証方法

Berner は，C-S-H ゲルの溶解に関するデータをコンパイルしている[10]。図-1 に，Berner のコンパイルしたデータ[11-16]をもとに作成した CaO-SiO_2-H_2O 系における固相の Ca/Si 比と液相の Ca，Si 濃度，pH との関係を示す。

図-1 に示すように，液相の Ca 濃度については，固相（C-S-H ゲル）の Ca/Si 比が 0 から 0.5 の領域では Ca/Si 比の増加にともない緩やかに高くなり，0.5 から 0.8 にかけてわずかに低くなる。Ca/Si 比が 0.9 から 1.5 にかけては，Ca/Si 比の増加にともない再び液相の Ca 濃度が高くなり，Ca/Si 比が 1.5 を超えるあたりからほぼ一定の値となる。

一方，Si の濃度については，固相の Ca/Si 比が 0～0.5 までは変化がなく，0.5 を超えるあたりから Ca/Si 比の増加にともない低下している。また，Ca/Si 比が 1.5 以上の領域になると再び一定の値を示している。

pH については， Ca/Si 比<1.0 の領域において，Ca/Si 比が高くなるにともない上昇し，Ca/Si 比が 1.0 で pH は 12 に達する。Ca/Si 比が 1.0 を超えると pH の上昇は緩やかになり，Ca/Si 比 1.7 において pH が 12.5 に達した後は，Ca/Si 比が高くなっても pH に変化は見られず一定の値を示している。

本報では，各モデルから得られた C-S-H ゲルの解離式及び log K をインプットデータとして C-S-H ゲルの溶解／沈殿反応を PHREEQC を用いて計算し，それらの計算結果と Berner のコンパイルした実験データを比較することにより，各モデルから得られた C-S-H ゲルの解離式及び log K のインプットデータとしての妥当性について検証した。

4. 計算結果

4.1 Atkinson モデルから導いた熱力学データによる計算結果

表-8～10 に Atkinson モデルから導いた解離式及び log K を用いて計算した結果を示す。なお，計算のアウトプットを巻末に添付する（付録 1～3)。Atkinson モデルにおいては，①Atkinson ケース，②JNC-TDB(1)ケース，及び③JNC-TDB(2)ケースの 3 ケースについて，それぞれ計算を行なった。表-8～10 に示すように，全てのケースにおいて，Ca/Si 比が 0.1 の C-S-H ゲルの溶解反応で初期固相の一部が溶解し，二次固相として SiO_2(am)が沈殿した。また，Ca/Si 比が 0.2～0.3 の C-S-H ゲルの溶解反応では，初期固相の一部が溶解し，二次固相として初期固相の Ca/Si 比より 0.1 低い Ca/Si 比の C-S-H ゲルが沈殿し，Ca/Si 比が 0.4～0.9 の C-S-H ゲルの溶解反応では，初期 Ca/Si 比より 0.1 高い Ca/Si 比の C-S-H ゲルが沈殿した。Ca/Si 比が 1.0 の C-S-H ゲルの溶解反応では，初期固相の一部が溶解し，初期固相以外の固相は沈殿しなかった。Ca/Si 比が 1.1～1.8 の C-S-H ゲルの溶解反応では，二次固相として初期 Ca/Si 比より 0.1 低い Ca/Si 比の C-S-H ゲルが沈殿した。SiO_2(am)以外の端成分である CSH(0.833)及び $Ca(OH)_2$ の沈殿は示されなかった。

図-2 に計算結果と実験値との比較を示す。ほとんどの Ca/Si 比において 2 種類の固相が沈殿する結果が示されたため（表-8～10 参照)，この場合には，その 2 種類の固相を 1 つの固相とみなし，両固相に含まれる Ca の和と Si の和の比を固相の Ca/Si 比とした。

図-2 に示すように，上記①～③の全てのケースにおいて，液相の Ca 濃度，Si 濃度及び pH ともに実験値に一致する計算結果が得られた。この結果から，今回検討した範囲では，log K の算出に使用した関連液相種及び端成分の標準生成自由エネルギーの相違が計算結果に大きな影響を及ぼさないことが分かった。

4.2 Reardon モデルから導いた熱力学データによる計算結果

表-11 に Reardon モデルから導いた解離式及び log K を用いて計算した結果をまとめる。なお，計算のアウトプットを巻末に添付する（付録-4)。表-11 に示すように，Ca/Si 比が 1.0 の C-S-H ゲルの溶解反応では，Atkinson モデルの計算結果と同様に，初期固相の一部が溶解し，初期固相以外の固相は沈殿しなかった。Ca/Si 比が 1.1～1.6 の C-S-H ゲルの溶解反応では，二次固相として初期 Ca/Si 比より 0.1 低い Ca/Si 比の C-S-H ゲルが沈殿した。しかし，Ca/Si 比が 1.6 以上の C-S-H ゲルの溶解反応では，初期 Ca/Si 比によらず，初期固相は全量溶解し，二次固相として CSH(1.5)及び $Ca(OH)_2$ が沈殿した。

図-3 に計算値と実験値との比較を示す。Reardon モデルでの計算においても，2 種類の固相が沈殿する結果が示されたため，この 2 種類の固相を 1 つの固相とみなし，それぞれの固相に含まれる Ca の和と Si の和の比を固相の Ca/Si 比とした。

図-3 に示すように，液相の Ca 濃度，Si 濃度及び pH の計算値は，一定の値となる Ca/Si 比が 1.6 以上の領域も含めて，実験値に一致する結果となった。

5. 考察

図-4 に, Atkinson モデルから導いた熱力学データを用いて計算した場合の固相の Ca/Si 比（Ca/Si_{solid}）に対する液相の Ca/Si 比（Ca/Si_{liquid}）を示す。図中の調和直線（congruent line）と交差する点が調和溶解点（congruent point），すなわち $Ca/Si_{solid} = Ca/Si_{liquid}$ となる箇所である。この図に示すように，純水の場合での計算においては，Ca/Si 比が 0.4 付近及び 1.0 の 2 点が調和溶解点となり，それを境に $Ca/Si_{solid} < Ca/Si_{liquid}$ と $Ca/Si_{solid} > Ca/Si_{liquid}$ の非調和溶解区間が交互に存在した。これらの区間のうち，$Ca/Si_{solid} < Ca/Si_{liquid}$ の区間では，Ca 成分が優先的に溶け，初期固相より Ca/Si_{solid} の低い C-S-H ゲルの沈殿が生じる。一方，$Ca/Si_{solid} > Ca/Si_{liquid}$ の区間では，C-S-H ゲルの Si 成分が優先的に溶け，初期固相より Ca/Si_{solid} の高い C-S-H ゲルの沈殿が生じる。このことは，表-8～10 に示す計算結果にも示されている。

この図から，$Ca/Si_{solid}>1.0$ の C-S-H ゲルの溶解／沈殿反応について考えると，Ca/Si_{solid} が 1.0 になるまでは Ca が優先的に溶解する非調和溶解挙動を示し，Ca/Si_{solid} が 1.0 に到達した後は，調和溶解することが分かる。一方，$0.4< Ca/Si_{solid} <1.0$ の C-S-H ゲルについては， Si が優先的に溶解する非調和溶解により Ca/Si_{solid} が 1.0 に近づき，Ca/Si_{solid} が 1.0 に到達した後は，調和溶解することが分かる。普通ポルトランドセメント（OPC）の水和反応により生成する C-S-H ゲルの Ca/Si_{solid} は 1.5 以上であることから，OPC 水和物相に含まれる C-S-H ゲルの溶解／沈殿を評価するためには，純水の場合には Ca/Si_{solid} が 1.0 以上の C-S-H ゲルの熱力学データ（解離式及び log K）を揃えておけば十分である。

しかし，地下水の場合には様々な共存イオンを考慮する必要がある。そこで，回分方式による液相のみを交換していく平衡計算により，純水及び炭酸イオンが共存した溶液での C-S-H ゲルの Ca/Si_{solid} の変化について評価を行った。図-5 に計算のフローを示す。この計算における初期固相は CSH(1.8), 1 バッチあたりの液固比は 100 とした。炭酸イオンの濃度は $NaHCO_3$ として $2x10^{-3}$mol/L とした。C-S-H ゲルのデータには，Atkinson モデルから導いたもの（Atkinson ケース）を使用した。

図-6 に純水と炭酸イオン共存時の C-S-H ゲルの Ca/Si_{solid} の変化の比較を示す。この図の横軸は初期固相に対する積算液固比（（反応させた液相の積算重量）／（初期固相の重量））を示している。図-6 に示すように，純水の場合には液を交換するごとに Ca/Si_{solid} が低下し，Ca/Si_{solid} が調和溶解点である 1.0 に到達した後は一定であることが分かる。しかし，炭酸イオンが共存した場合には，Ca/Si_{solid} が 1.0 に到達した後も Ca/Si_{solid} は低下し続けている。これは，液相に溶けた Ca がカルサイトとして沈殿するため, その消費分を補うように C-S-H ゲルから更に Ca が溶出するためである。したがって，地下水のように様々な共存溶液種の影響を考慮する必要がある場合には，Ca/Si_{solid} が 1.0 未満の C-S-H ゲルの熱力学データ（解離式及び log K）が必要となる。しかし，Reardon モデルからは Ca/Si_{solid} が 1.0 未満の C-S-H ゲルの熱力学データを導くことができない。このため，Ca/Si_{solid} が 0.1～1.0 の C-S-H ゲルの熱力学データを導くことができ，その範囲の C-S-H ゲルの溶解／沈殿を取り扱うことができる Atkinson モデルの適用が推奨される。

6. おわりに

PHREEQC で使用することを前提として，既往の C-S-H ゲルの溶解／沈殿モデルを調査した。それぞれのモデルの特性から PHREEQC 上での取扱いに相応しいモデルとして，PHREEQC の入力ファイルの範囲内で設定可能な Atkinson モデル及び Reardon モデルを選定した。PHREEQC 上では C-S-H ゲルを一連のカルシウムケイ酸塩水和物群として表現することとし，選定したモデルに従い Ca/Si 比を 0.1 づつ変化させた C-S-H ゲルの化学組成を算定し，その化学組成に応じた解離式と log K を決定した。各モデルから導いた C-S-H ゲルの解離式及び log K の妥当性を検証するため，PHREEQC で C-S-H ゲルの溶解／沈殿反応を計算した。その結果，純水系の場合には，Atkinson モデルで Ca/Si 比が 0.1～1.8 の範囲の実験値を再現することができた。また Reardon モデルでは 1.0～1.8 の範囲の実験値を再現することができた。このため，両者ともに PHREEQC に適合することが示された。

一方，Atkinson モデルから導いた解離式及び log K を用いて炭酸イオンが共存した系を PHREEQC で計算した結果，Ca/Si 比が 1.0 未満の C-S-H ゲルの解離式及び log K が重要であることが示された。しかしながら，Reardon モデルではこの範囲を取り扱うことができないため，炭酸イオン等の共存イオンの影響を考慮するためには，より広範囲な Ca/Si 比の C-S-H ゲルの溶解／沈殿反応を取り扱うことができる Atkinson モデルの適用が推奨された。

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表- 1　既往の C-S-H ゲルの溶解／沈殿モデルの特徴

モデル	特徴
Atkinson モデル	・固溶体モデルで C-S-H ゲルを表現している。 ・Ca/Si 比を少しづつ変化させた一連のカルシウムケイ酸塩水和物群として C-S-H ゲルを表現することができ，各 Ca/Si 比に応じた log K をモデルに従い導くことができる。 ・PHREEQC の入力ファイルで設定できる。 ・Ca/Si 比が 0.1～1.8 までの溶解／沈殿反応を再現でき，炭酸イオン等の影響を考慮した評価ができる。
Reardon モデル	・実験結果に基づく経験式を設定して C-S-H ゲルの解離式及び log K を定義している。 ・Ca/Si 比を少しづつ変化させた一連のカルシウムケイ酸塩水和物群として C-S-H ゲルを表現することができ，各 Ca/Si 比に応じた log K をモデルに従い導くことができる。 ・PHREEQC の入力ファイルで設定できる。 ・Ca/Si 比が 1.0～1.8 までの溶解反応を再現できるが，炭酸イオン等の影響を評価するにあたり，計算条件によっては Ca/Si 比の範囲が不十分となることが想定される。
杉山モデル Berner モデル Börjesson モデル	・固溶体モデルで C-S-H ゲルを表現している。 ・同一の鉱物（端成分）に対して，計算途中で固溶体の Ca/Si 比に応じた log K を設定する必要があるため，PHREEQC に適用するためには，別途プログラムを組み込む必要がある。

表- 2　Atkinson モデルから C-S-H ゲルの解離式及び log K を導く際に使用した標準生成自由エネルギー

[単位：$J \cdot mol^{-1}$]

	Atkinson ケース	JNC-TDB (1)ケース	JNC-TDB (2)ケース
H_2O	－237,160	－237,140	－237,140
Ca^{2+}	－552,806	－552,806	－552,806
H_4SiO_4	－1,307,788	－1,307,735	－1,307,735
$SiO_2(am)$	－848,530	－848,900	－848,900
$Ca(OH)_2$	－897,498	－897,498	－898,426

（備考）

Atkinson ケース：全て Atkinson らの報告[4]の値を使用した。

JNC-TDB (1)ケース，JNC-TDB (2)ケース：現在整備が進められている JNC-TDB の値を使用した。なお，現時点においては，$Ca(OH)_2$ の標準生成自由エネルギーΔG^0_fについて－897,498$J \cdot mol^{-1}$ もしくは－898,426 $J \cdot mol^{-1}$ のいずれかで検討されている。

表- 3　Atkinson モデルから C-S-H ゲルの解離式及び log K を導く際に使用したパラメーター

ΔG^0_f Tobermorite	−1,643,708	[J・mol^{-1}]
n	0.833	
m	0.917	
Lsx	0	[J・mol^{-1} Si]
Lpx	9,000	[J・mol^{-1} Ca]
Asx	2,000	[J・mol^{-1} Si]
Apx	−29,000	[J・mol^{-1} Ca]
R	8.31451	[J・mol^{-1}・K^{-1}]
T	298.15	[K]

（表中の値は全て Atkinson らの報告[4]を引用）

表- 4　Atkinson モデルから導いた C-S-H ゲル及び端成分の解離式

Ca/Si 比	固相名	解離式
0.0	SiO_2(am)	$SiO_2(am) = H_4SiO_4 - 2H_2O$
0.1	CSH(0.1)	$Ca_{0.100}Si_{1.000}O_{2.100}\cdot 0.110\ H_2O = 0.100\ Ca^{2+} + 1.000\ H_4SiO_4 - 1.790\ H_2O - 0.200\ H^+$
0.2	CSH(0.2)	$Ca_{0.200}Si_{1.000}O_{2.200}\cdot 0.220\ H_2O = 0.200\ Ca^{2+} + 1.000\ H_4SiO_4 - 1.580\ H_2O - 0.400\ H^+$
0.3	CSH(0.3)	$Ca_{0.300}Si_{1.000}O_{2.300}\cdot 0.330\ H_2O = 0.300\ Ca^{2+} + 1.000\ H_4SiO_4 - 1.370\ H_2O - 0.600\ H^+$
0.4	CSH(0.4)	$Ca_{0.400}Si_{1.000}O_{2.400}\cdot 0.440\ H_2O = 0.400\ Ca^{2+} + 1.000\ H_4SiO_4 - 1.160\ H_2O - 0.800\ H^+$
0.5	CSH(0.5)	$Ca_{0.500}Si_{1.000}O_{2.500}\cdot 0.550\ H_2O = 0.500\ Ca^{2+} + 1.000\ H_4SiO_4 - 0.950\ H_2O - 1.000\ H^+$
0.6	CSH(0.6)	$Ca_{0.600}Si_{1.000}O_{2.600}\cdot 0.661\ H_2O = 0.600\ Ca^{2+} + 1.000\ H_4SiO_4 - 0.739\ H_2O - 1.200\ H^+$
0.7	CSH(0.7)	$Ca_{0.700}Si_{1.000}O_{2.700}\cdot 0.771\ H_2O = 0.700\ Ca^{2+} + 1.000\ H_4SiO_4 - 0.529\ H_2O - 1.400\ H^+$
0.8	CSH(0.8)	$Ca_{0.800}Si_{1.000}O_{2.800}\cdot 0.881\ H_2O = 0.800\ Ca^{2+} + 1.000\ H_4SiO_4 - 0.319\ H_2O - 1.600\ H^+$
0.833	CSH(0.833)	$Ca_{0.833}Si_{1.000}O_{2.833}\cdot 0.917\ H_2O = 0.833\ Ca^{2+} + 1.000\ H_4SiO_4 - 0.250\ H_2O - 1.666\ H^+$
0.9	CSH(0.9)	$Ca_{1.000}Si_{1.111}O_{3.222}\cdot 1.093\ H_2O = 1.000\ Ca^{2+} + 1.111\ H_4SiO_4 - 0.129\ H_2O - 0.200\ H^+$
1.0	CSH(1.0)	$Ca_{1.000}Si_{1.000}O_{3.000}\cdot 1.084\ H_2O = 1.000\ Ca^{2+} + 1.000\ H_4SiO_4 + 0.084\ H_2O - 0.200\ H^+$
1.1	CSH(1.1)	$Ca_{1.000}Si_{0.909}O_{2.818}\cdot 1.076\ H_2O = 1.000\ Ca^{2+} + 0.909\ H_4SiO_4 + 0.258\ H_2O - 0.200\ H^+$
1.2	CSH(1.2)	$Ca_{1.000}Si_{0.833}O_{2.666}\cdot 1.070\ H_2O = 1.000\ Ca^{2+} + 0.833\ H_4SiO_4 + 0.404\ H_2O - 0.200\ H^+$
1.3	CSH(1.3)	$Ca_{1.000}Si_{0.769}O_{2.538}\cdot 1.065\ H_2O = 1.000\ Ca^{2+} + 0.769\ H_4SiO_4 + 0.527\ H_2O - 0.200\ H^+$
1.4	CSH(1.4)	$Ca_{1.000}Si_{0.714}O_{2.428}\cdot 1.060\ H_2O = 1.000\ Ca^{2+} + 0.714\ H_4SiO_4 + 0.632\ H_2O - 0.200\ H^+$
1.5	CSH(1.5)	$Ca_{1.000}Si_{0.667}O_{2.334}\cdot 1.056\ H_2O = 1.000\ Ca^{2+} + 0.667\ H_4SiO_4 + 0.722\ H_2O - 0.200\ H^+$
1.6	CSH(1.6)	$Ca_{1.000}Si_{0.625}O_{2.250}\cdot 1.053\ H_2O = 1.000\ Ca^{2+} + 0.625\ H_4SiO_4 + 0.803\ H_2O - 0.200\ H^+$
1.7	CSH(1.7)	$Ca_{1.000}Si_{0.588}O_{2.176}\cdot 1.049\ H_2O = 1.000\ Ca^{2+} + 0.588\ H_4SiO_4 + 0.873\ H_2O - 0.200\ H^+$
1.8	CSH(1.8)	$Ca_{1.000}Si_{0.556}O_{2.112}\cdot 1.047\ H_2O = 1.000\ Ca^{2+} + 0.556\ H_4SiO_4 + 0.935\ H_2O - 0.200\ H^+$
∞	$Ca(OH)_2$	$Ca(OH)_2 = Ca^{2+} + 2\ H_2O - 2H^+$

表- 5　Atkinson モデルから導いた C-S-H ゲルの log K

固相名	Atkinson ケース	JNC-TDB(1) ケース	JNC-TDB(2) ケース
SiO_2(am)	－2.639	－2.706	－2.706
CSH(0.1)	－1.071	－1.132	－1.132
CSH(0.2)	0.565	0.512	0.512
CSH(0.3)	2.227	2.181	2.181
CSH(0.4)	3.907	3.868	3.868
CSH(0.5)	5.601	5.569	5.569
CSH(0.6)	7.312	7.288	7.288
CSH(0.7)	9.045	9.027	9.027
CSH(0.8)	10.819	10.809	10.809
CSH(0.833)	11.436	11.428	11.428
CSH(0.9)	14.061	14.051	14.039
CSH(1.0)	14.514	14.504	14.477
CSH(1.1)	14.983	14.974	14.935
CSH(1.2)	15.439	15.430	15.381
CSH(1.3)	15.870	15.861	15.803
CSH(1.4)	16.272	16.263	16.197
CSH(1.5)	16.643	16.635	16.562
CSH(1.6)	16.987	16.978	16.900
CSH(1.7)	17.304	17.296	17.213
CSH(1.8)	17.597	17.589	17.502
$Ca(OH)_2$	22.710	22.703	22.540

表- 6　Reardon モデルから導いた C-S-H ゲルの解離式及び log K

固相名	Ca/Si 比	解離式	R	log K
CSH(0.9)	0.9	$Ca_{0.9}Si_{1.0}O_{2.9}\cdot 0.9\,H_2O + H_2O = 0.9\,Ca^{2+} + H_3SiO_4^- + 0.8\,OH^-$	−0.790	−9.614
CSH(1.0)	1.0	$Ca_{1.0}Si_{1.0}O_{3.0}\cdot 1.0\,H_2O + H_2O = 1.0\,Ca^{2+} + H_3SiO_4^- + 1.0\,OH^-$	2.702	−8.918
CSH(1.1)	1.1	$Ca_{1.1}Si_{1.0}O_{3.1}\cdot 1.1\,H_2O + H_2O = 1.1\,Ca^{2+} + H_3SiO_4^- + 1.2\,OH^-$	3.884	−9.749
CSH(1.2)	1.2	$Ca_{1.2}Si_{1.0}O_{3.2}\cdot 1.2\,H_2O + H_2O = 1.2\,Ca^{2+} + H_3SiO_4^- + 1.4\,OH^-$	4.614	−10.532
CSH(1.3)	1.3	$Ca_{1.3}Si_{1.0}O_{3.3}\cdot 1.3\,H_2O + H_2O = 1.3\,Ca^{2+} + H_3SiO_4^- + 1.6\,OH^-$	5.144	−11.230
CSH(1.4)	1.4	$Ca_{1.4}Si_{1.0}O_{3.4}\cdot 1.4\,H_2O + H_2O = 1.4\,Ca^{2+} + H_3SiO_4^- + 1.8\,OH^-$	5.561	−11.853
CSH(1.5)	1.5	$Ca_{1.5}Si_{1.0}O_{3.5}\cdot 1.5\,H_2O + H_2O = 1.5\,Ca^{2+} + H_3SiO_4^- + 2.0\,OH^-$	5.904	−12.417
CSH(1.6)	1.6	$Ca_{1.6}Si_{1.0}O_{3.6}\cdot 1.6\,H_2O + H_2O = 1.6\,Ca^{2+} + H_3SiO_4^- + 2.2\,OH^-$	6.195	−12.932
CSH(1.7)	1.7	$Ca_{1.7}Si_{1.0}O_{3.7}\cdot 1.7\,H_2O + H_2O = 1.7\,Ca^{2+} + H_3SiO_4^- + 2.4\,OH^-$	6.449	−13.407
CSH(1.8)	1.8	$Ca_{1.8}Si_{1.0}O_{3.8}\cdot 1.8\,H_2O + H_2O = 1.8\,Ca^{2+} + H_3SiO_4^- + 2.6\,OH^-$	6.673	−13.848

表- 7　計算条件

計算コード	PHREEQC Interactive 2.8
データベース	SPRON. JNC Database を PHREEQC 用に変換したデータベース
液　相	純水
C-S-H ゲルの添加量	純水 1kg に対し C-S-H ゲル 1mol を添加
EQUILIBRIUM PHASE	①Atkinson モデル ・表-3 に示す C-S-H ゲル及び 3 種類の端成分 ②Reardon モデル ・表-4 に示す C-S-H ゲル（ただし，Ca/Si 比=0.9 を除く） ・$Ca(OH)_2$*　［$Ca(OH)_2 = Ca^{2+} + 2\ OH^-$　　log K = －5.19］

* Reardon モデルから導いた熱力学データを使用した計算では，表中に示す Reardon の報告[5]に記載されているデータを使用した。

表- 8　Atkinson モデルから導いた C-S-H ゲルの解離式及び log K を用いて C-S-H ゲルの溶解反応を PHREEQC で計算した結果　Atkinson ケース

初期の Ca/Si 比	反応後の固相					反応後の液相		
	沈殿固相	沈殿量 (mol)	Ca_{total} (mol)	Si_{total} (mol)	Ca/Si 比	pH	$[Ca]_{aq}$ (mol/L)	$[Si]_{aq}$ (mol/L)
0.1	SiO_2(am) CSH(0.1)	4.269E-03 9.918E-01	9.918E-02	9.961E-01	0.100	9.433	8.168E-04	3.899E-03
0.2	CSH(0.1) CSH(0.2)	3.855E-03 9.917E-01	1.987E-01	9.956E-01	0.200	9.687	1.277E-03	4.464E-03
0.3	CSH(0.2) CSH(0.3)	8.188E-04 9.946E-01	2.985E-01	9.954E-01	0.300	9.793	1.457E-03	4.584E-03
0.4	CSH(0.4) CSH(0.5)	9.937E-01 1.828E-03	3.984E-01	9.955E-01	0.400	9.936	1.591E-03	4.436E-03
0.5	CSH(0.5) CSH(0.6)	9.909E-01 4.959E-03	4.984E-01	9.959E-01	0.500	10.020	1.599E-03	4.190E-03
0.6	CSH(0.6) CSH(0.7)	9.891E-01 7.104E-03	5.984E-01	9.962E-01	0.601	10.136	1.557E-03	3.778E-03
0.7	CSH(0.7) CSH(0.8)	9.902E-01 6.783E-03	6.986E-01	9.970E-01	0.701	10.366	1.404E-03	2.975E-03
0.8	CSH(0.8) CSH(0.9)	9.944E-01 3.316E-03	7.988E-01	9.981E-01	0.800	10.701	1.175E-03	1.930E-03
0.9	CSH(0.9) CSH(1.0)	9.960E-01 2.891E-03	9.960E-01	1.109E+00	0.898	10.832	1.111E-03	1.555E-03
1.0	CSH(1.0)	9.989E-01	9.989E-01	9.989E-01	1.000	11.003	1.068E-03	1.068E-03
1.1	CSH(1.0) CSH(1.1)	9.344E-03 9.893E-01	9.986E-01	9.087E-01	1.099	11.329	1.379E-03	4.036E-04
1.2	CSH(1.1) CSH(1.2)	2.473E-02 9.729E-01	9.976E-01	8.332E-01	1.197	11.613	2.393E-03	1.137E-04
1.3	CSH(1.2) CSH(1.3)	4.751E-02 9.485E-01	9.960E-01	7.692E-01	1.295	11.830	4.001E-03	3.559E-05
1.4	CSH(1.3) CSH(1.4)	7.642E-02 9.177E-01	9.941E-01	7.143E-01	1.392	11.987	5.907E-03	1.435E-05
1.5	CSH(1.4) CSH(1.5)	1.223E-01 8.691E-01	9.914E-01	6.668E-01	1.487	12.137	8.627E-03	5.557E-06
1.6	CSH(1.5) CSH(1.6)	1.542E-01 8.355E-01	9.897E-01	6.250E-01	1.584	12.208	1.036E-02	3.410E-06
1.7	CSH(1.6) CSH(1.7)	2.055E-01 7.815E-01	9.870E-01	5.881E-01	1.678	12.293	1.294E-02	1.818E-06
1.8	CSH(1.7) CSH(1.8)	3.133E-01 6.687E-01	9.820E-01	5.558E-01	1.767	12.420	1.803E-02	6.765E-07

表- 9　Atkinson モデルから導いた C-S-H ゲルの解離式及び log K を用いて C-S-H ゲルの溶解反応を PHREEQC で計算した結果　JNC-TDB(1)ケース

初期の Ca/Si 比	反応後の固相					反応後の液相		
	沈殿固相	沈殿量 (mol)	Ca_{total} (mol)	Si_{total} (mol)	Ca/Si 比	pH	$[Ca]_{aq}$ (mol/L)	$[Si]_{aq}$ (mol/L)
0.1	SiO_2(am) CSH(0.1)	4.232E-03 9.923E-01	9.923E-02	9.965E-01	0.100	9.477	7.708E-04	3.476E-03
0.2	CSH(0.1) CSH(0.2)	4.105E-03 9.918E-01	1.988E-01	9.959E-01	0.200	9.736	1.222E-03	4.056E-03
0.3	CSH(0.2) CSH(0.3)	1.302E-03 9.945E-01	2.986E-01	9.958E-01	0.300	9.837	1.386E-03	4.186E-03
0.4	CSH(0.4) CSH(0.5)	9.948E-01 1.169E-03	3.985E-01	9.960E-01	0.400	9.981	1.515E-03	4.079E-03
0.5	CSH(0.5) CSH(0.6)	9.921E-01 4.043E-03	4.985E-01	9.961E-01	0.500	10.069	1.524E-03	3.856E-03
0.6	CSH(0.6) CSH(0.7)	9.902E-01 6.252E-03	5.985E-01	9.965E-01	0.601	10.174	1.489E-03	3.524E-03
0.7	CSH(0.7) CSH(0.8)	9.914E-01 5.871E-03	6.987E-01	9.973E-01	0.701	10.408	1.344E-03	2.758E-03
0.8	CSH(0.8) CSH(0.9)	9.947E-01 3.118E-03	7.989E-01	9.982E-01	0.800	10.709	1.158E-03	1.881E-03
0.9	CSH(0.9) CSH(1.0)	9.960E-01 2.874E-03	9.960E-01	1.109E+00	0.898	10.829	1.102E-03	1.543E-03
1.0	CSH(1.0)	9.989E-01	9.989E-01	9.989E-01	1.000	11.000	1.060E-03	1.060E-03
1.1	CSH(1.0) CSH(1.1)	9.422E-03 9.892E-01	9.986E-01	9.087E-01	1.099	11.329	1.377E-03	3.943E-04
1.2	CSH(1.1) CSH(1.2)	2.454E-02 9.731E-01	9.976E-01	8.332E-01	1.197	11.610	2.375E-03	1.129E-04
1.3	CSH(1.2) CSH(1.3)	4.714E-02 9.489E-01	9.960E-01	7.692E-01	1.295	11.827	3.970E-03	3.570E-05
1.4	CSH(1.3) CSH(1.4)	7.580E-02 9.183E-01	9.941E-01	7.142E-01	1.392	11.984	5.859E-03	1.423E-05
1.5	CSH(1.4) CSH(1.5)	1.230E-01 8.683E-01	9.913E-01	6.667E-01	1.487	12.139	8.676E-03	5.323E-06
1.6	CSH(1.5) CSH(1.6)	1.508E-01 8.391E-01	9.899E-01	6.250E-01	1.584	12.199	1.014E-02	3.518E-06
1.7	CSH(1.6) CSH(1.7)	2.071E-01 7.799E-01	9.870E-01	5.882E-01	1.678	12.296	1.303E-02	1.722E-06
1.8	CSH(1.7) CSH(1.8)	3.109E-01 6.712E-01	9.821E-01	5.558E-01	1.767	12.417	1.789E-02	6.706E-07

表- 10　Atkinson モデルから導いた C-S-H ゲルの解離式及び log K を用いて C-S-H ゲルの溶解反応を PHREEQC で計算した結果　JNC-TDB(2)ケース

初期の Ca/Si 比	反応後の固相					反応後の液相		
	沈殿固相	沈殿量 (mol)	Ca_{total} (mol)	Si_{total} (mol)	Ca/Si 比	pH	$[Ca]_{aq}$ (mol/L)	$[Si]_{aq}$ (mol/L)
0.1	SiO_2(am) CSH(0.1)	4.232E-03 9.923E-01	9.923E-02	9.965E-01	0.100	9.477	7.708E-04	3.476E-03
0.2	CSH(0.1) CSH(0.2)	4.105E-03 9.918E-01	1.988E-01	9.959E-01	0.200	9.736	1.222E-03	4.056E-03
0.3	CSH(0.2) CSH(0.3)	1.302E-03 9.945E-01	2.986E-01	9.958E-01	0.300	9.837	1.386E-03	4.186E-03
0.4	CSH(0.4) CSH(0.5)	9.948E-01 1.169E-03	3.985E-01	9.960E-01	0.400	9.981	1.515E-03	4.079E-03
0.5	CSH(0.5) CSH(0.6)	9.921E-01 4.043E-03	4.985E-01	9.961E-01	0.500	10.069	1.524E-03	3.856E-03
0.6	CSH(0.6) CSH(0.7)	9.902E-01 6.252E-03	5.985E-01	9.965E-01	0.601	10.174	1.489E-03	3.524E-03
0.7	CSH(0.7) CSH(0.8)	9.914E-01 5.871E-03	6.987E-01	9.973E-01	0.701	10.408	1.344E-03	2.758E-03
0.8	CSH(0.8) CSH(0.9)	9.936E-01 3.916E-03	7.988E-01	9.980E-01	0.800	10.661	1.183E-03	2.029E-03
0.9	CSH(0.9) CSH(1.0)	9.944E-01 4.518E-03	9.944E-01	1.109E+00	0.896	10.743	1.125E-03	1.752E-03
1.0	CSH(1.0)	9.990E-01	9.990E-01	9.990E-01	1.000	10.991	1.036E-03	1.036E-03
1.1	CSH(1.0) CSH(1.1)	7.402E-03 9.913E-01	9.987E-01	9.086E-01	1.099	11.268	1.250E-03	4.626E-04
1.2	CSH(1.1) CSH(1.2)	2.113E-02 9.768E-01	9.979E-01	8.332E-01	1.198	11.554	2.088E-03	1.332E-04
1.3	CSH(1.2) CSH(1.3)	4.065E-02 9.559E-01	9.966E-01	7.692E-01	1.296	11.769	3.438E-03	4.256E-05
1.4	CSH(1.3) CSH(1.4)	6.507E-02 9.299E-01	9.950E-01	7.143E-01	1.393	11.924	5.036E-03	1.700E-05
1.5	CSH(1.4) CSH(1.5)	1.050E-01 8.876E-01	9.926E-01	6.667E-01	1.489	12.077	7.409E-03	6.351E-06
1.6	CSH(1.5) CSH(1.6)	1.309E-01 8.603E-01	9.912E-01	6.250E-01	1.586	12.145	8.801E-03	3.981E-06
1.7	CSH(1.6) CSH(1.7)	1.776E-01 8.112E-01	9.888E-01	5.882E-01	1.681	12.237	1.118E-02	1.991E-06
1.8	CSH(1.7) CSH(1.8)	2.673E-01 7.174E-01	9.847E-01	5.558E-01	1.772	12.360	1.538E-02	7.559E-07

表- 11　Reardon モデルから導いた C-S-H ゲルの解離式及び log K を用いて C-S-H ゲルの溶解反応を PHREEQC で計算した結果

初期の Ca/Si 比	反応後の固相					反応後の液相		
	沈殿固相	沈殿量 (mol)	Ca_{total} (mol)	Si_{total} (mol)	Ca/Si 比	pH	$[Ca]_{aq}$ (mol/L)	$[Si]_{aq}$ (mol/L)
1.0	CSH(1.0)	9.988E-01	9.988E-01	9.988E-01	1.000	11.061	1.253E-03	1.235E-03
1.1	CSH(1.0) CSH(1.1)	8.102E-03 9.913E-01	1.099E-01	9.994E-01	1.099	11.322	1.456E-03	5.870E-04
1.2	CSH(1.1) CSH(1.2)	1.627E-02 9.853E-01	1.198E+00	9.998E-01	1.198	11.509	1.952E-03	2.707E-04
1.3	CSH(1.2) CSH(1.3)	3.788E-02 9.621E-01	1.296E+00	1.000E+00	1.296	11.815	3.860E-03	5.490E-05
1.4	CSH(1.3) CSH(1.4)	7.486E-02 9.251E-01	1.392E+00	1.000E+00	1.393	12.082	7.502E-03	1.163E-05
1.5	CSH(1.4) CSH(1.5)	1.297E-01 8.702E-01	1.487E+00	9.999E-01	1.487	12.295	1.298E-02	3.119E-06
1.6	CSH(1.5) $Ca(OH)_2$	1.000E+00 7.998E-02	1.580E+00	1.000E+00	1.580	12.459	2.002E-02	1.067E-06
1.7	CSH(1.5) $Ca(OH)_2$	1.000E+00 1.800E-01	1.680E+00	1.000E+00	1.680	12.459	2.002E-02	1.067E-06
1.8	CSH(1.5) $Ca(OH)_2$	1.000E+00 2.800E-01	1.780E+0	1.000E+00	1.780	12.459	2.002E-02	1.067E-06

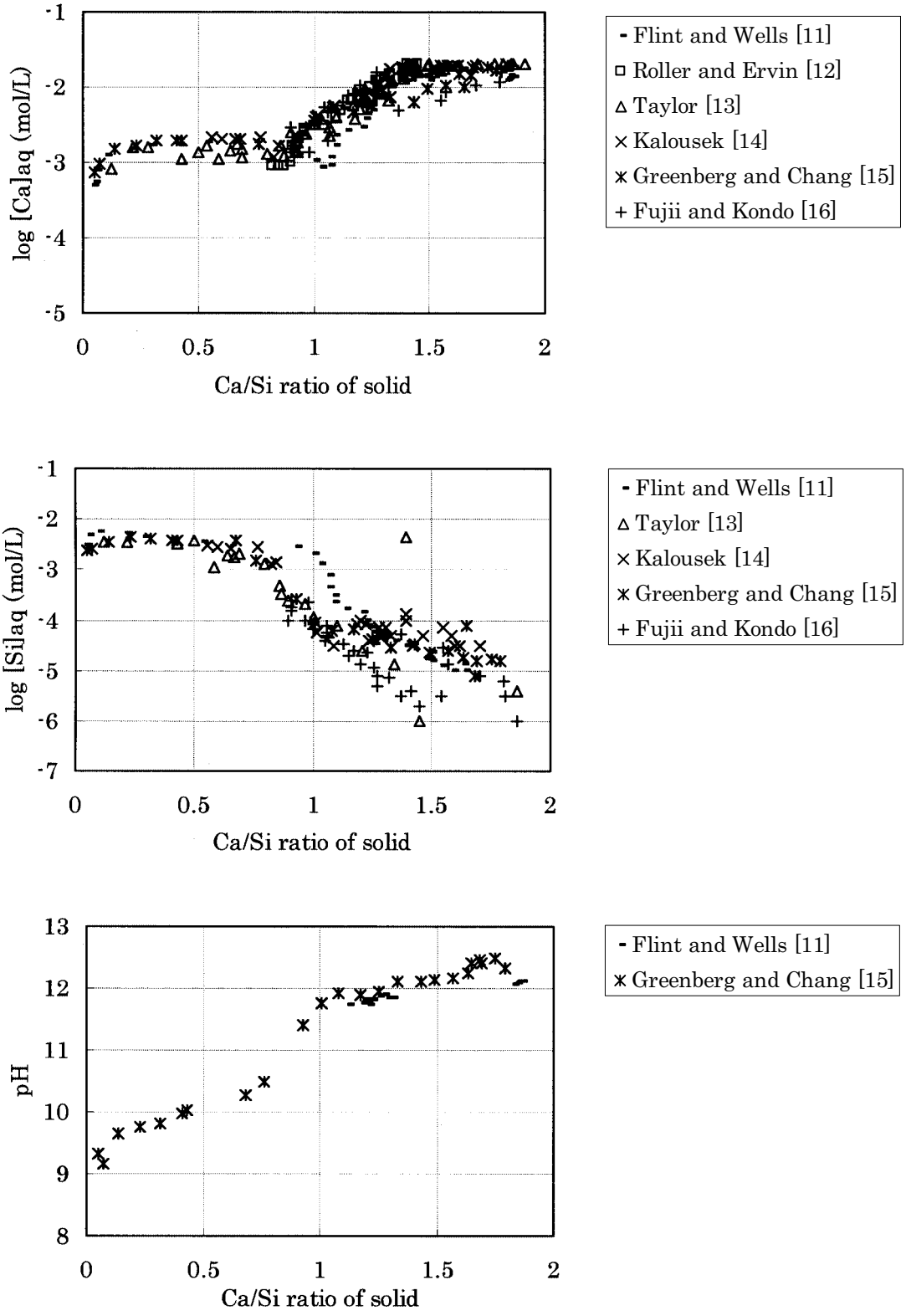

図- 1　$CaO\text{-}SiO_2\text{-}H_2O$ 系における固相の Ca/Si 比と液相のカルシウム濃度，シリカ濃度及び pH との関係
Berner がコンパイルした実験データ[10]をもとに作成した。

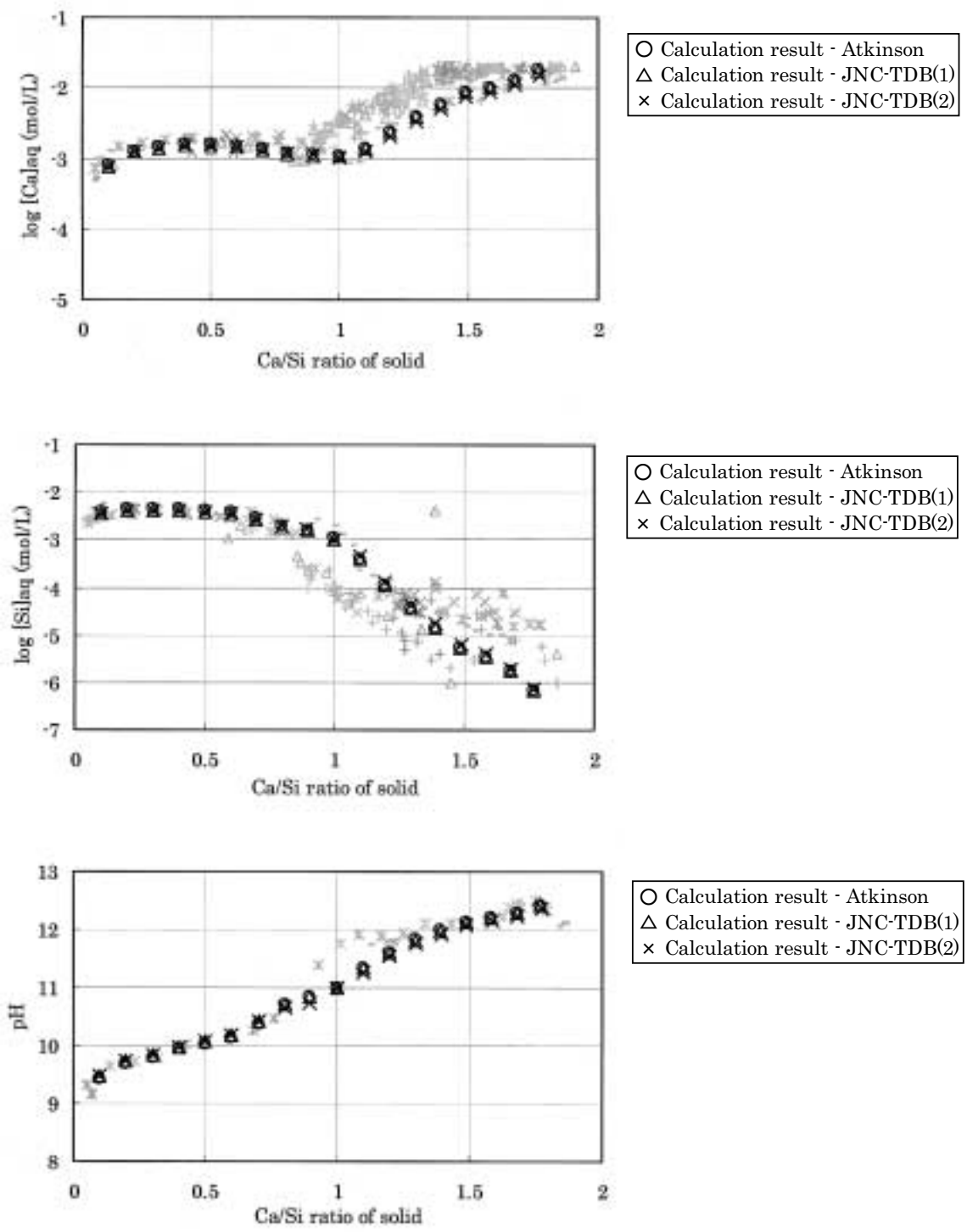

図- 2　Atkinson モデルから導いた熱力学データによる C-S-H ゲルの溶解反応の計算結果と実験結果との比較
Berner がコンパイルした実験データ[10]をもとに作成した図-1 に PHREEQC による計算結果をプロットした。

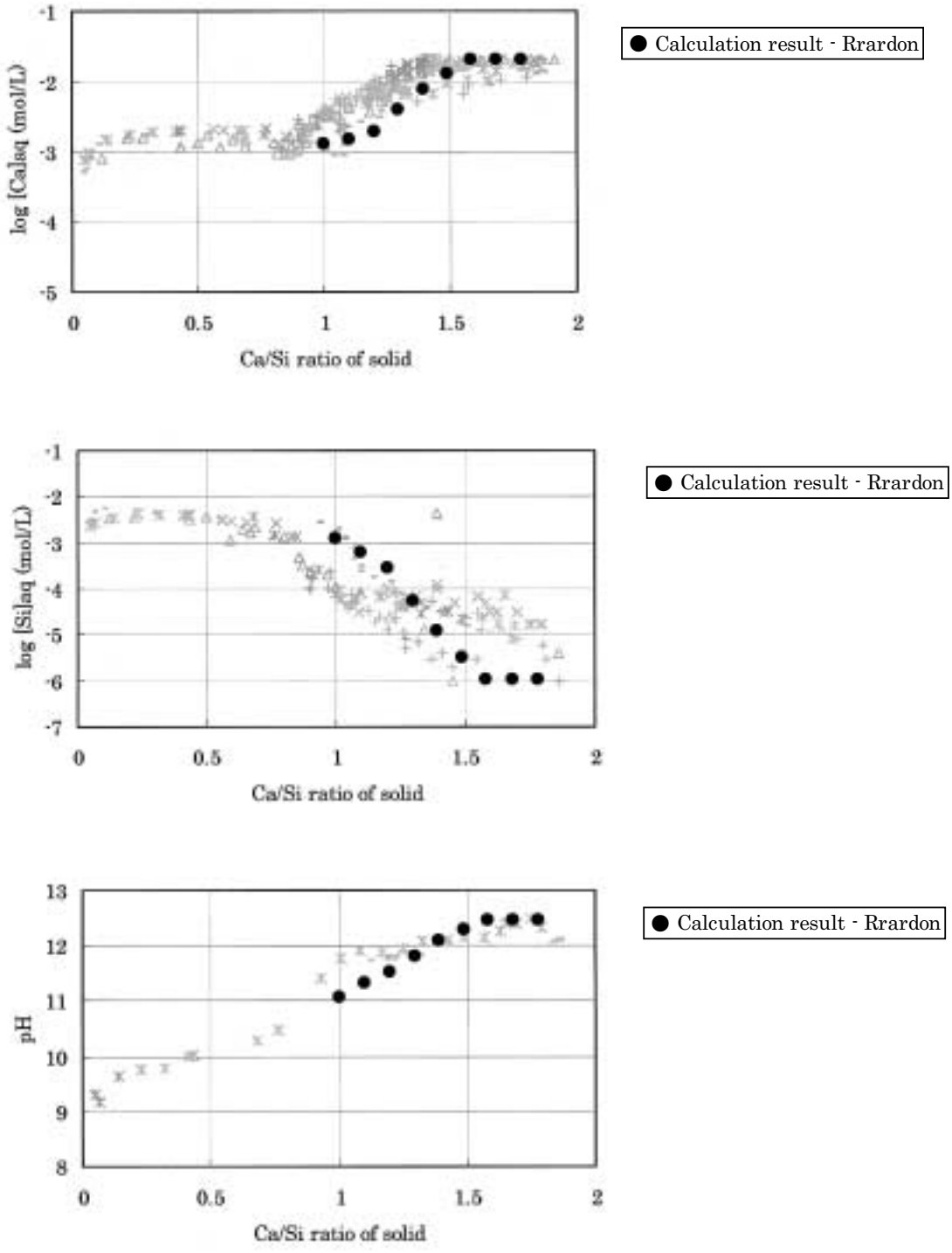

図- 3　Reardon モデルから導いた熱力学データによる C-S-H ゲルの溶解反応の計算結果と実験結果との比較
Berner がコンパイルした実験データ[10]をもとに作成した図-1 に PHREEQC による計算結果をプロットした。

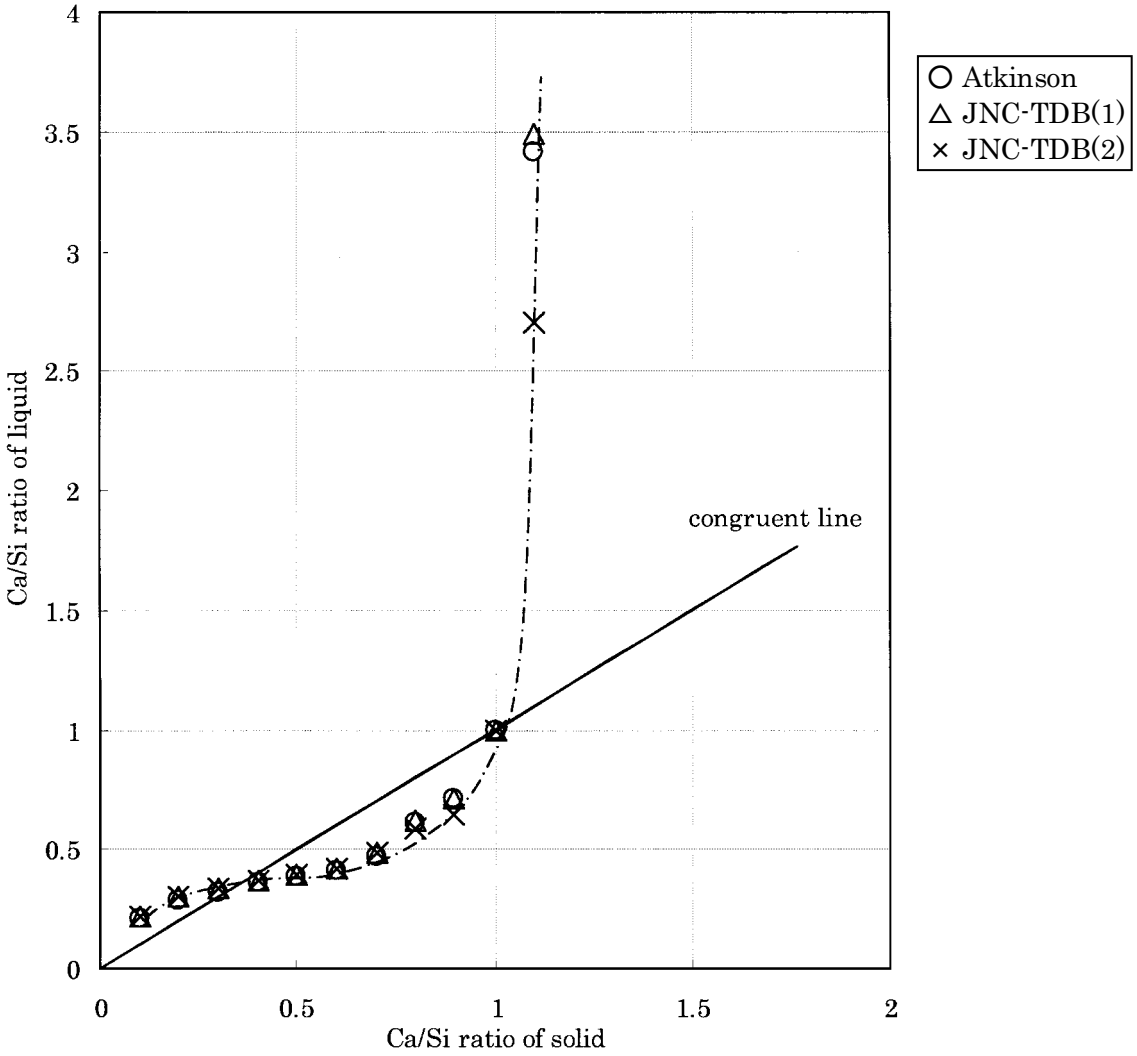

図- 4　Atkinson モデルから導いた熱力学データを用いて計算した場合の固相の Ca/Si 比に対する液相の Ca/Si 比

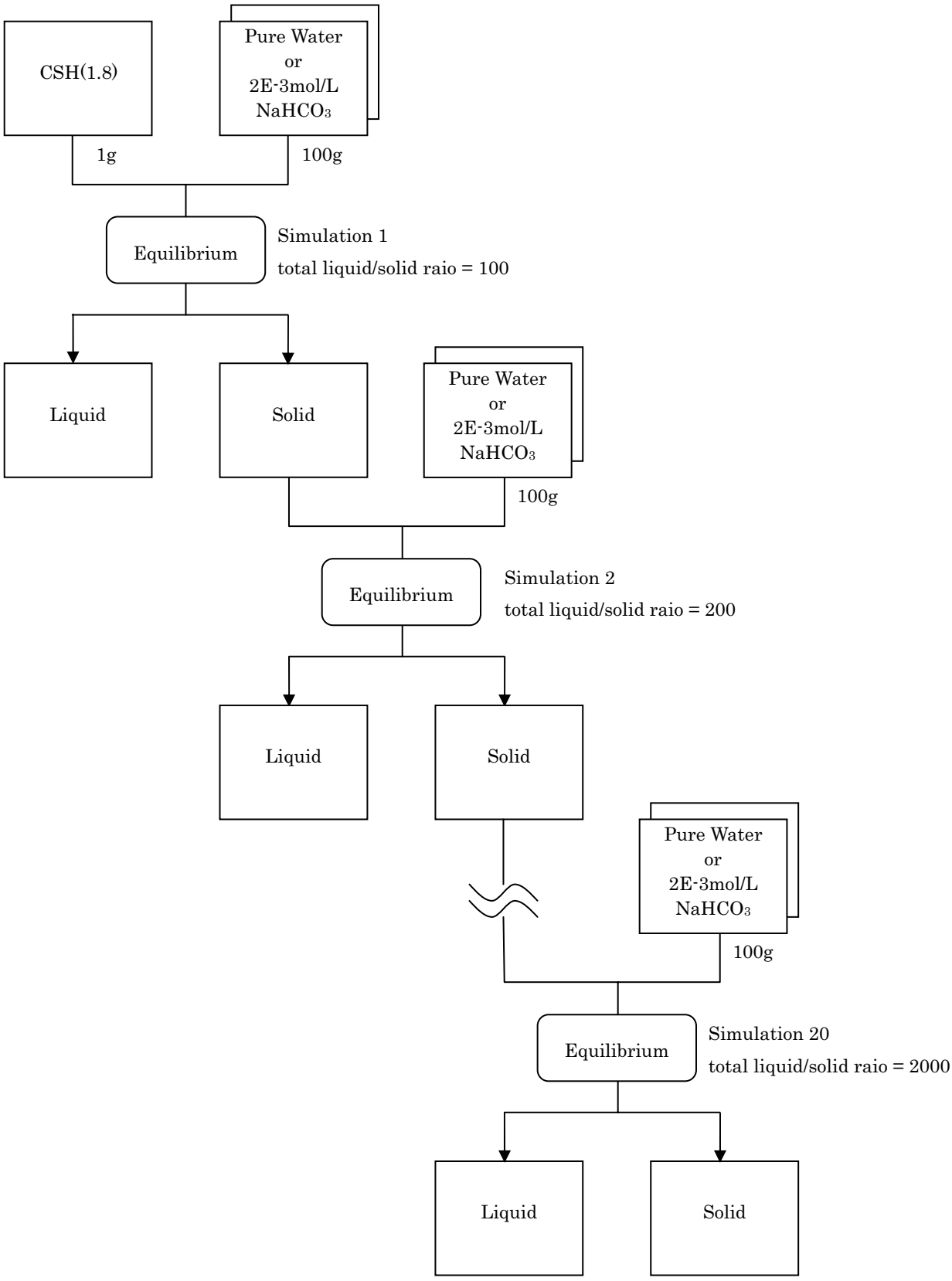

図- 5　回分方式で液相を交換する平衡計算のフロー

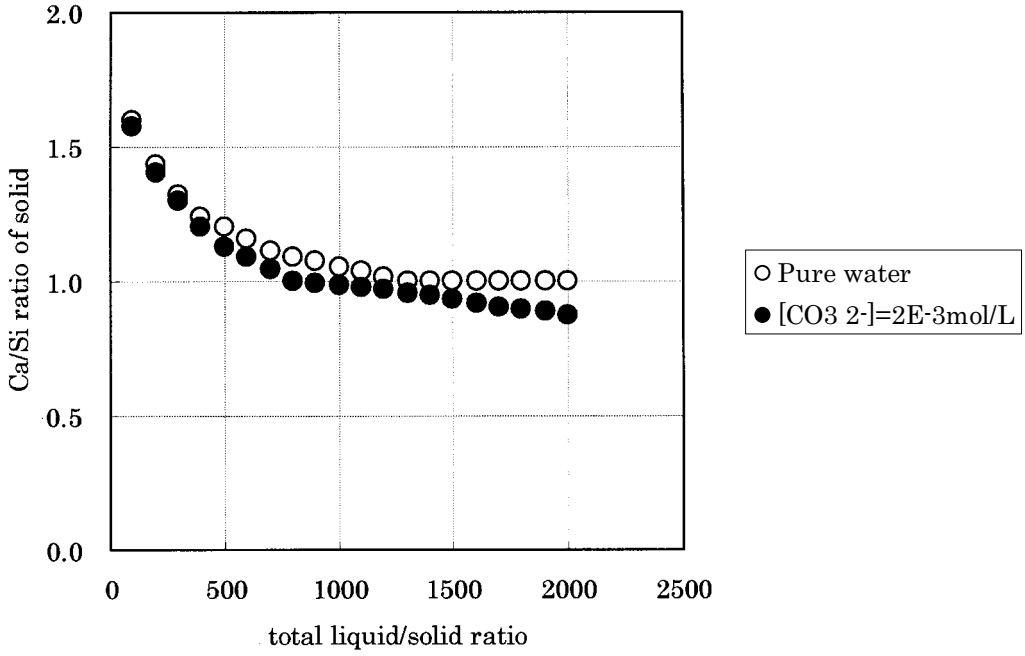

図- 6　回分方式で液相を交換する平衡計算における純水系と炭酸イオン共存系の C-S-H ゲルの溶解挙動の比較

初期固相：Ca/Si 比 1.8 の C-S-H ゲル

1 バッチ当たりの液固比：100

炭酸イオン：2E-3mol/L $NaHCO_3$

使用データ：Atkinson モデルから導いたデータ（Atkinson ケース）

付録- 1　Atkinson モデルから導いた解離式及び log K を用いて C-S-H ゲルの溶解／沈殿反応を PHREEQC で計算した結果（アウトプット）　Atkinson ケース

```
Input file: Atkinson Model Input(Atkinson case).pqi
Output file: Atkinson Model Input(Atkinson case).pqo
Database file: spron_phc_kai.txt

------------------
Reading data base.
------------------

        SOLUTION_MASTER_SPECIES
        SOLUTION_SPECIES
        PHASES
        END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

        DATABASE: spron_phc_kai.txt
        Title C-S-H dissolution using data from Atkinson model - case:Atkinson
        PHASES
        CSH(0.1)
            Ca 0.100 Si 1.000 O 2.100 : 0.110 H2O = 0.100 Ca+2 + 1.000 H4SiO4 -1.790 H2O - 0.200 H+
            log_K -1.071
        CSH(0.2)
            Ca 0.200 Si 1.000 O 2.200 : 0.220 H2O = 0.200 Ca+2 + 1.000 H4SiO4 -1.580 H2O - 0.400 H+
            log_K 0.565
        CSH(0.3)
            Ca 0.300 Si 1.000 O 2.300 : 0.330 H2O = 0.300 Ca+2 + 1.000 H4SiO4 -1.370 H2O - 0.600 H+
            log_K 2.227
        CSH(0.4)
            Ca 0.400 Si 1.000 O 2.400 : 0.440 H2O = 0.400 Ca+2 + 1.000 H4SiO4 -1.160 H2O - 0.800 H+
            log_K 3.907
        CSH(0.5)
            Ca 0.500 Si 1.000 O 2.500 : 0.550 H2O = 0.500 Ca+2 + 1.000 H4SiO4 -0.950 H2O - 1.000 H+
            log_K 5.601
        CSH(0.6)
            Ca 0.600 Si 1.000 O 2.600 : 0.661 H2O = 0.600 Ca+2 + 1.000 H4SiO4 -0.739 H2O - 1.200 H+
            log_K 7.312
        CSH(0.7)
            Ca 0.700 Si 1.000 O 2.700 : 0.771 H2O = 0.700 Ca+2 + 1.000 H4SiO4 -0.529 H2O - 1.400 H+
            log_K 9.045
        CSH(0.8)
            Ca 0.800 Si 1.000 O 2.800 : 0.881 H2O = 0.800 Ca+2 + 1.000 H4SiO4 -0.319 H2O - 1.600 H+
            log_K 10.819
        CSH(0.9)
            Ca 1.000 Si 1.111 O 3.222 : 1.093 H2O = 1.000 Ca+2 + 1.111 H4SiO4 -0.129 H2O - 2.000 H+
            log_K 14.061
        CSH(1.0)
            Ca 1.000 Si 1.000 O 3.000 : 1.084 H2O = 1.000 Ca+2 + 1.000 H4SiO4 + 0.084 H2O - 2.000 H+
            log_K 14.514
        CSH(1.1)
            Ca 1.000 Si 0.909 O 2.818 : 1.076 H2O = 1.000 Ca+2 + 0.909 H4SiO4 + 0.258 H2O - 2.000 H+
            log_K 14.983
        CSH(1.2)
            Ca 1.000 Si 0.833 O 2.666 : 1.070 H2O = 1.000 Ca+2 + 0.833 H4SiO4 + 0.404 H2O - 2.000 H+
            log_K 15.439
        CSH(1.3)
            Ca 1.000 Si 0.769 O 2.538 : 1.065 H2O = 1.000 Ca+2 + 0.769 H4SiO4 + 0.527 H2O - 2.000 H+
            log_K 15.870
        CSH(1.4)
            Ca 1.000 Si 0.714 O 2.428 : 1.060 H2O = 1.000 Ca+2 + 0.714 H4SiO4 + 0.632 H2O - 2.000 H+
            log_K 16.272
        CSH(1.5)
            Ca 1.000 Si 0.667 O 2.334 : 1.056 H2O = 1.000 Ca+2 + 0.667 H4SiO4 + 0.722 H2O - 2.000 H+
            log_K 16.643
        CSH(1.6)
            Ca 1.000 Si 0.625 O 2.250 : 1.053 H2O = 1.000 Ca+2 + 0.625 H4SiO4 + 0.803 H2O - 2.000 H+
            log_K 16.987
        CSH(1.7)
            Ca 1.000 Si 0.588 O 2.176 : 1.049 H2O = 1.000 Ca+2 + 0.588 H4SiO4 + 0.873 H2O - 2.000 H+
            log_K 17.304
```

```
        CSH(1.8)
            Ca 1.000 Si 0.556 O 2.112 : 1.047 H2O = 1.000 Ca+2 + 0.556 H4SiO4 + 0.935 H2O - 2.000 H+
            log_K 17.597
        Ca(OH)2
            Ca(OH)2 = Ca+2 + 2H2O - 2 H+
            log_k 22.710
        SiO2(am)
            Si 1.000 O 2.000 = 1.000 H4SiO4 - 2.000 H2O
            log_K -2.639
        CSH(0.833)
            Ca 0.833 Si 1.000 O 2.833 : 0.917 H2O = 0.833 Ca+2 + 1.000 H4SiO4 -0.250 H2O - 1.666 H+
           log_K 11.436
        Title 1 CSH(0.1)
        SOLUTION 1 DW
        units mol/L
        pH 7
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  1
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 2
        END
-----
TITLE
-----

 1 CSH(0.1)

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.       DW

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Pure water

----------------------------Description of solution----------------------------

                                pH =   7.000
                                pe =   4.000
                  Activity of water =   1.000
                     Ionic strength =  1.009e-007
                 Mass of water (kg) =  1.000e+000
            Total alkalinity (eq/kg) =  1.715e-009
              Total carbon (mol/kg) =  0.000e+000
                 Total CO2 (mol/kg) =  0.000e+000
               Temperature (deg C) =  25.000
             Electrical balance (eq) = -1.715e-009
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.85
                         Iterations  =   0
                           Total H  = 1.110124e+002
                           Total O  = 5.550622e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            1.018e-007  1.017e-007   -6.992   -6.993   -0.000
        H+             1.001e-007  1.000e-007   -7.000   -7.000   -0.000
        H2O            5.551e+001  1.000e+000    1.744    0.000    0.000
H(0)          1.565e-025
        H2             7.823e-026  7.823e-026  -25.107  -25.107    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -42.012  -42.012    0.000

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        H2            -22.00  -22.00   -0.00  H2
        O2            -39.13   44.00   83.13  O2

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -7.03   15.68   22.71 0.000e+000          0.000e+000
        CSH(0.1)        0.00   -1.07   -1.07 1.000e+000 9.918e-001-8.167e-003
        CSH(0.2)       -0.07    0.50    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.16    2.06    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.27    3.63    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.40    5.20    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.54    6.77    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.71    8.34    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.91    9.90   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -1.01   10.42   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -1.31   12.75   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -1.47   13.04   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -1.70   13.28   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -1.96   13.48   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -2.22   13.65   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -2.48   13.80   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -2.72   13.92   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -2.96   14.03   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -3.18   14.13   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -3.38   14.21   17.60 0.000e+000          0.000e+000
        SiO2(am)        0.00   -2.64   -2.64 0.000e+000 4.269e-003 4.269e-003

------------------------------Solution composition-----------------------------

        Elements         Molality     Moles

        Ca             8.168e-004  8.167e-004
        Si             3.899e-003  3.898e-003

----------------------------Description of solution----------------------------

                                pH  =   9.433     Charge balance
```

```
                                  pe =  8.461     Adjusted to redox equilibrium
                        Activity of water =  1.000
                           Ionic strength =  2.431e-003
                        Mass of water (kg) =  9.999e-001
                  Total alkalinity (eq/kg) =  1.634e-003
                     Total carbon (mol/kg) =  0.000e+000
                       Total CO2 (mol/kg) =  0.000e+000
                      Temperature (deg C) =  25.000
                   Electrical balance (eq) = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.00
                             Iterations =  15
                               Total H  = 1.110142e+002
                               Total O  = 5.551573e+001

----------------------------Distribution of species-----------------------------

                                                 Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            2.911e-005  2.756e-005    -4.536    -4.560    -0.024
         H+             3.882e-010  3.691e-010    -9.411    -9.433    -0.022
         H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
Ca            8.168e-004
         Ca+2           8.068e-004  6.520e-004    -3.093    -3.186    -0.093
         CaSiH3O4+       9.734e-006  9.220e-006    -5.012    -5.035    -0.024
         CaHO+          2.729e-007  2.585e-007    -6.564    -6.588    -0.024
H(0)          2.545e-039
         H2             1.273e-039  1.273e-039   -38.895   -38.895     0.000
O(0)          7.330e-015
         O2             3.665e-015  3.667e-015   -14.436   -14.436     0.000
Si            3.899e-003
         H4SiO4          2.294e-003  2.296e-003    -2.639    -2.639     0.000
         SiH3O4-         1.594e-003  1.510e-003    -2.797    -2.821    -0.024
         CaSiH3O4+       9.734e-006  9.220e-006    -5.012    -5.035    -0.024
         SiH2O4-2        2.028e-007  1.633e-007    -6.693    -6.787    -0.094

------------------------------Saturation indices--------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite    0.79   -2.64   -3.43  SiO2
         b-Cristobalite    0.34   -2.64   -2.98  SiO2
         Ca(OH)2         -7.03   15.68   22.71  Ca(OH)2
         Chalcedony       1.10   -2.64   -3.74  SiO2
         CSH(0.1)         0.00   -1.07   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)        -0.07    0.50    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)        -0.16    2.06    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)        -0.27    3.63    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)        -0.40    5.20    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)        -0.54    6.77    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)        -0.71    8.34    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)        -0.91    9.90   10.82  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)      -1.01   10.42   11.44  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)        -1.31   12.75   14.06  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)        -1.47   13.04   14.51  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)        -1.70   13.28   14.98  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)        -1.96   13.48   15.44  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)        -2.22   13.65   15.87  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)        -2.48   13.80   16.27  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)        -2.72   13.92   16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)        -2.96   14.03   16.99  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)        -3.18   14.13   17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)        -3.38   14.21   17.60  Ca1.000Si0.556O2.112:1.047H2O
         H2            -35.78  -35.79   -0.00  H2
         Lime          -16.88   15.68   32.56  CaO
         O2            -11.55   71.58   83.13  O2
         Quartz          1.39   -2.64   -4.03  SiO2
         SiO2(am)         0.00   -2.64   -2.64  Si1.000O2.000
         Wollastonite    -0.74   13.04   13.78  CaSiO3

-----------------
```

```
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 2.
-----------------------------------

        Title 2 CSH(0.2)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  1
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 3
        END
-----
TITLE
-----

 2 CSH(0.2)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -6.35   16.36   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -0.00   -1.07   -1.07 0.000e+000 3.855e-003 3.855e-003
        CSH(0.2)       -0.00    0.56    0.56 1.000e+000 9.917e-001-8.319e-003
        CSH(0.3)       -0.03    2.20    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.07    3.84    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.13    5.47    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.20    7.11    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.30    8.74    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.44   10.38   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.52   10.92   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.71   13.35   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.86   13.65   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -1.08   13.90   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -1.33   14.11   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -1.59   14.28   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -1.84   14.43   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -2.09   14.55   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -2.32   14.67   16.99 0.000e+000          0.000e+000
```

```
        CSH(1.7)       -2.54   14.77   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -2.74   14.85   17.60 0.000e+000          0.000e+000
        SiO2(am)       -0.07   -2.71   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca            1.278e-003  1.278e-003
        Si            4.464e-003  4.463e-003

----------------------------Description of solution----------------------------

                                pH  =   9.687     Charge balance
                                pe  =   8.108     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.789e-003
                   Mass of water (kg)  =  9.999e-001
              Total alkalinity (eq/kg)  =  2.557e-003
                 Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
               Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  85
                            Total H  = 1.110152e+002
                            Total O  = 5.551783e+001

---------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            5.296e-005  4.951e-005   -4.276   -4.305   -0.029
        H+             2.184e-010  2.054e-010   -9.661   -9.687   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.278e-003
        Ca+2           1.255e-003  9.670e-004   -2.901   -3.015   -0.113
        CaSiH3O4+       2.245e-005  2.101e-005   -4.649   -4.678   -0.029
        CaHO+          7.363e-007  6.888e-007   -6.133   -6.162   -0.029
H(0)         4.018e-039
        H2             2.009e-039  2.011e-039  -38.697  -38.697    0.000
O(0)         2.938e-015
        O2             1.469e-015  1.470e-015  -14.833  -14.833    0.000
Si           4.464e-003
        SiH3O4-         2.479e-003  2.319e-003   -2.606   -2.635   -0.029
        H4SiO4         1.961e-003  1.963e-003   -2.707   -2.707    0.000
        CaSiH3O4+       2.245e-005  2.101e-005   -4.649   -4.678   -0.029
        SiH2O4-2        5.883e-007  4.506e-007   -6.230   -6.346   -0.116

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.73  -2.71  -3.43  SiO2
        b-Cristobalite    0.27  -2.71  -2.98  SiO2
        Ca(OH)2         -6.35   16.36   22.71  Ca(OH)2
        Chalcedony       1.03  -2.71  -3.74  SiO2
        CSH(0.1)        -0.00  -1.07  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.00   0.56   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.03   2.20   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.07   3.84   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.13   5.47   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.20   7.11   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.30   8.74   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.44  10.38  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.52  10.92  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.71  13.35  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.86  13.65  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -1.08  13.90  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -1.33  14.11  15.44  Ca1.000Si0.833O2.666:1.070H2O
```

```
        CSH(1.3)        -1.59   14.28   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -1.84   14.43   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -2.09   14.55   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -2.32   14.67   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -2.54   14.77   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -2.74   14.85   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.59  -35.59   -0.00  H2
        Lime          -16.20   16.36   32.56  CaO
        O2            -11.95   71.18   83.13  O2
        Quartz          1.32   -2.71   -4.03  SiO2
        SiO2(am)       -0.07   -2.71   -2.64  Si1.000O2.000
        Wollastonite    -0.13   13.65   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 3.
-----------------------------------

        Title 3 CSH(0.3)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  1
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 4
        END
-----
TITLE
-----

 3 CSH(0.3)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase           SI log IAP  log KT   Initial     Final     Delta
```

```
        Ca(OH)2        -6.09   16.62   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -0.03   -1.10   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        0.00    0.56    0.56 0.000e+000 8.188e-004 8.188e-004
        CSH(0.3)        0.00    2.23    2.23 1.000e+000 9.946e-001-5.403e-003
        CSH(0.4)       -0.02    3.89    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.05    5.55    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.10    7.21    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.17    8.87    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.28   10.54   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.35   11.09   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.51   13.55   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.65   13.86   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.87   14.11   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -1.12   14.32   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -1.37   14.50   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -1.62   14.65   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -1.86   14.78   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -2.09   14.90   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -2.31   15.00   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -2.51   15.09   17.60 0.000e+000          0.000e+000
        SiO2(am)       -0.12   -2.76   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.457e-003  1.457e-003
        Si             4.584e-003  4.584e-003

----------------------------Description of solution---------------------------

                                pH  =   9.793     Charge balance
                                pe  =   8.087     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.313e-003
                    Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  2.914e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.712e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  20
                             Total H  = 1.110156e+002
                             Total O  = 5.551844e+001

----------------------------Distribution of species---------------------------

                                                Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            6.780e-005  6.311e-005   -4.169   -4.200   -0.031
        H+             1.719e-010  1.611e-010   -9.765   -9.793   -0.028
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.457e-003
        Ca+2           1.428e-003  1.083e-003   -2.845   -2.965   -0.120
        CaSiH3O4+       2.855e-005  2.660e-005   -4.544   -4.575   -0.031
        CaHO+          1.055e-006  9.832e-007   -5.977   -6.007   -0.031
H(0)         2.721e-039
        H2             1.361e-039  1.362e-039  -38.866  -38.866    0.000
O(0)         6.405e-015
        O2             3.202e-015  3.206e-015  -14.495  -14.494    0.000
Si           4.584e-003
        SiH3O4-         2.815e-003  2.623e-003   -2.550   -2.581   -0.031
        H4SiO4         1.740e-003  1.741e-003   -2.760   -2.759    0.000
        CaSiH3O4+       2.855e-005  2.660e-005   -4.544   -4.575   -0.031
        SiH2O4-2        8.621e-007  6.496e-007   -6.064   -6.187   -0.123

----------------------------Saturation indices--------------------------------
```

```
        Phase            SI log IAP  log KT

        a-Cristobalite    0.67  -2.76  -3.43  SiO2
        b-Cristobalite    0.22  -2.76  -2.98  SiO2
        Ca(OH)2         -6.09  16.62  22.71  Ca(OH)2
        Chalcedony       0.98  -2.76  -3.74  SiO2
        CSH(0.1)        -0.03  -1.10  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         0.00   0.56   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         0.00   2.23   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.02   3.89   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.05   5.55   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.10   7.21   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.17   8.87   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.28  10.54  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.35  11.09  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.51  13.55  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.65  13.86  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.87  14.11  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -1.12  14.32  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -1.37  14.50  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -1.62  14.65  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -1.86  14.78  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -2.09  14.90  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -2.31  15.00  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -2.51  15.09  17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.76 -35.76  -0.00  H2
        Lime           -15.94  16.62  32.56  CaO
        O2             -11.61  71.52  83.13  O2
        Quartz           1.27  -2.76  -4.03  SiO2
        SiO2(am)        -0.12  -2.76  -2.64  Si1.000O2.000
        Wollastonite     0.08  13.86  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 4.
------------------------------------

        Title 4 CSH(0.4)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  1
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2  0.0  0.0
        Save Solution 5
        END
-----
TITLE
-----

 4 CSH(0.4)
```

```
----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase             SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2         -5.77   16.94   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -0.10   -1.18   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -0.05    0.52    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -0.01    2.21    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -0.00    3.91    3.91 1.000e+000 9.937e-001-6.263e-003
        CSH(0.5)        -0.00    5.60    5.60 0.000e+000 1.828e-003 1.828e-003
        CSH(0.6)        -0.02    7.29    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.06    8.99    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.14   10.68   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.19   11.24   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.31   13.75   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.44   14.07   14.51 0.000e+000          0.000e+000
        CSH(1.1)        -0.65   14.33   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.89   14.55   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -1.14   14.73   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -1.38   14.89   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -1.62   15.03   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -1.84   15.15   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -2.05   15.25   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -2.25   15.34   17.60 0.000e+000          0.000e+000
        SiO2(am)        -0.23   -2.87   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.591e-003  1.591e-003
        Si             4.436e-003  4.435e-003

----------------------------Description of solution----------------------------

                                pH  =   9.936     Charge balance
                                pe  =   8.079     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.706e-003
                    Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  3.183e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                             Iterations  =  46
                               Total H  = 1.110159e+002
                               Total O  = 5.551843e+001

----------------------------Distribution of species----------------------------

                                            Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            9.465e-005  8.785e-005   -4.024   -4.056   -0.032
        H+             1.238e-010  1.158e-010   -9.907   -9.936   -0.029
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.591e-003
        Ca+2           1.556e-003  1.168e-003   -2.808   -2.933   -0.125
```

```
        CaSiH3O4+       3.336e-005  3.099e-005   -4.477   -4.509   -0.032
        CaHO+           1.589e-006  1.476e-006   -5.799   -5.831   -0.032
H(0)         1.457e-039
        H2              7.283e-040  7.291e-040   -39.138  -39.137    0.000
O(0)         2.235e-014
        O2              1.117e-014  1.119e-014   -13.952  -13.951    0.000
Si           4.436e-003
        SiH3O4-         3.051e-003  2.834e-003    -2.516   -2.548   -0.032
        H4SiO4          1.350e-003  1.352e-003    -2.870   -2.869    0.000
        CaSiH3O4+       3.336e-005  3.099e-005    -4.477   -4.509   -0.032
        SiH2O4-2        1.311e-006  9.769e-007    -5.882   -6.010   -0.128

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.56  -2.87  -3.43  SiO2
        b-Cristobalite    0.11  -2.87  -2.98  SiO2
        Ca(OH)2         -5.77  16.94  22.71  Ca(OH)2
        Chalcedony        0.87  -2.87  -3.74  SiO2
        CSH(0.1)         -0.10  -1.18  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -0.05   0.52   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.01   2.21   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.00   3.91   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.00   5.60   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.02   7.29   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.06   8.99   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.14  10.68  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.19  11.24  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.31  13.75  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.44  14.07  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.65  14.33  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.89  14.55  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -1.14  14.73  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -1.38  14.89  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -1.62  15.03  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -1.84  15.15  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -2.05  15.25  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -2.25  15.34  17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -36.03 -36.03   -0.00  H2
        Lime           -15.62  16.94  32.56  CaO
        O2             -11.06  72.06  83.13  O2
        Quartz           1.16  -2.87  -4.03  SiO2
        SiO2(am)        -0.23  -2.87  -2.64  Si1.000O2.000
        Wollastonite     0.29  14.07  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 5.
------------------------------------

        Title 5 CSH(0.5)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  1
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
```

```
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 6
        END
-----
TITLE
-----

 5 CSH(0.5)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2         -5.60   17.11   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -0.17   -1.24   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -0.10    0.47    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -0.05    2.18    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -0.02    3.89    3.91 0.000e+000          0.000e+000
        CSH(0.5)         0.00    5.60    5.60 1.000e+000 9.909e-001-9.149e-003
        CSH(0.6)        -0.00    7.31    7.31 0.000e+000 4.959e-003 4.959e-003
        CSH(0.7)        -0.02    9.02    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.08   10.73   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.14   11.30   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.23   13.83   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.36   14.16   14.51 0.000e+000          0.000e+000
        CSH(1.1)        -0.56   14.42   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.79   14.65   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -1.03   14.84   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -1.27   15.00   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -1.50   15.14   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -1.72   15.26   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -1.93   15.37   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -2.13   15.47   17.60 0.000e+000          0.000e+000
        SiO2(am)        -0.32   -2.95   -2.64 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.599e-003  1.599e-003
        Si             4.190e-003  4.190e-003

-----------------------------Description of solution-----------------------------

                                pH  =  10.020     Charge balance
                                pe  =   7.859     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.728e-003
                    Mass of water (kg)  =  9.999e-001
               Total alkalinity (eq/kg)  =  3.198e-003
```

```
                Total carbon (mol/kg)  =  0.000e+000
                  Total CO2 (mol/kg)  =  0.000e+000
                 Temperature (deg C)  =  25.000
               Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                        Iterations  =  71
                          Total H  = 1.110159e+002
                          Total O  = 5.551795e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            1.149e-004  1.066e-004   -3.940   -3.972   -0.032
        H+             1.020e-010  9.539e-011   -9.991  -10.020   -0.029
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.599e-003
        Ca+2           1.564e-003  1.172e-003   -2.806   -2.931   -0.125
        CaSiH3O4+       3.344e-005  3.106e-005   -4.476   -4.508   -0.032
        CaHO+          1.936e-006  1.799e-006   -5.713   -5.745   -0.032
H(0)         2.724e-039
        H2             1.362e-039  1.363e-039  -38.866  -38.865    0.000
O(0)         6.391e-015
        O2             3.196e-015  3.199e-015  -14.495  -14.495    0.000
Si           4.190e-003
        SiH3O4-         3.045e-003  2.828e-003   -2.516   -2.548   -0.032
        H4SiO4         1.110e-003  1.112e-003   -2.955   -2.954    0.000
        CaSiH3O4+       3.344e-005  3.106e-005   -4.476   -4.508   -0.032
        SiH2O4-2        1.590e-006  1.183e-006   -5.799   -5.927   -0.128

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.48   -2.95   -3.43  SiO2
        b-Cristobalite    0.03   -2.95   -2.98  SiO2
        Ca(OH)2         -5.60   17.11   22.71  Ca(OH)2
        Chalcedony        0.78   -2.95   -3.74  SiO2
        CSH(0.1)         -0.17   -1.24   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -0.10    0.47    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.05    2.18    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.02    3.89    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)          0.00    5.60    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.00    7.31    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.02    9.02    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.08   10.73   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.14   11.30   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.23   13.83   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.36   14.16   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.56   14.42   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.79   14.65   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -1.03   14.84   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -1.27   15.00   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -1.50   15.14   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -1.72   15.26   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -1.93   15.37   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -2.13   15.47   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.76  -35.76   -0.00  H2
        Lime           -15.45   17.11   32.56  CaO
        O2             -11.61   71.52   83.13  O2
        Quartz           1.07   -2.95   -4.03  SiO2
        SiO2(am)        -0.32   -2.95   -2.64  Si1.000O2.000
        Wollastonite      0.37   14.16   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 6.
```

```
-----------------------------------

        Title 6 CSH(0.6)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  1
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 7
        END
-----
TITLE
-----

 6 CSH(0.6)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase              SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -5.38   17.33   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -0.28   -1.35   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -0.18    0.38    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -0.11    2.11    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -0.06    3.85    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.02    5.58    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.00    7.31    7.31 1.000e+000 9.891e-001-1.088e-002
        CSH(0.7)         0.00    9.04    9.04 0.000e+000 7.104e-003 7.104e-003
        CSH(0.8)        -0.04   10.78   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.09   11.35   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.16   13.90   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.27   14.24   14.51 0.000e+000          0.000e+000
        CSH(1.1)        -0.46   14.52   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.68   14.76   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.91   14.96   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -1.15   15.13   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -1.37   15.27   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -1.59   15.40   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -1.79   15.52   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.98   15.61   17.60 0.000e+000          0.000e+000
        SiO2(am)        -0.45   -3.09   -2.64 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------
```

```
        Elements         Molality     Moles

        Ca            1.557e-003  1.556e-003
        Si            3.778e-003  3.778e-003

----------------------------Description of solution----------------------------

                                pH  =  10.136     Charge balance
                                pe  =   7.655     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.604e-003
                    Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  3.113e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.709e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  25
                             Total H  = 1.110159e+002
                             Total O  = 5.551705e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-           1.496e-004  1.390e-004   -3.825   -3.857   -0.032
        H+            7.821e-011  7.319e-011  -10.107  -10.136   -0.029
        H2O           5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.557e-003
        Ca+2          1.523e-003  1.146e-003   -2.817   -2.941   -0.124
        CaSiH3O4+      3.139e-005  2.918e-005   -4.503   -4.535   -0.032
        CaHO+         2.463e-006  2.290e-006   -5.608   -5.640   -0.032
H(0)         4.097e-039
        H2            2.049e-039  2.051e-039  -38.689  -38.688    0.000
O(0)         2.825e-015
        O2            1.413e-015  1.414e-015  -14.850  -14.850    0.000
Si           3.778e-003
        SiH3O4-        2.926e-003  2.720e-003   -2.534   -2.565   -0.032
        H4SiO4         8.193e-004  8.202e-004   -3.087   -3.086    0.000
        CaSiH3O4+      3.139e-005  2.918e-005   -4.503   -4.535   -0.032
        SiH2O4-2       1.985e-006  1.483e-006   -5.702   -5.829   -0.127

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   0.35  -3.09  -3.43  SiO2
        b-Cristobalite  -0.10  -3.09  -2.98  SiO2
        Ca(OH)2        -5.38  17.33  22.71  Ca(OH)2
        Chalcedony      0.65  -3.09  -3.74  SiO2
        CSH(0.1)       -0.28  -1.35  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)       -0.18   0.38   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)       -0.11   2.11   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)       -0.06   3.85   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)       -0.02   5.58   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)       -0.00   7.31   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        0.00   9.04   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)       -0.04  10.78  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)     -0.09  11.35  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)       -0.16  13.90  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)       -0.27  14.24  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)       -0.46  14.52  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)       -0.68  14.76  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)       -0.91  14.96  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)       -1.15  15.13  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)       -1.37  15.27  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)       -1.59  15.40  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)       -1.79  15.52  17.30  Ca1.000Si0.588O2.176:1.049H2O
```

```
        CSH(1.8)       -1.98   15.61   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.58  -35.58   -0.00  H2
        Lime          -15.23   17.33   32.56  CaO
        O2            -11.96   71.16   83.13  O2
        Quartz          0.94   -3.09   -4.03  SiO2
        SiO2(am)       -0.45   -3.09   -2.64  Si1.000O2.000
        Wollastonite    0.46   14.24   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 7.
-----------------------------------

        Title 7 CSH(0.7)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  1
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 8
        END
-----
TITLE
-----

 7 CSH(0.7)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

WARNING: Maximum iterations exceeded, 200

Numerical method failed with this set of convergence parameters.
WARNING: Trying diagonal scaling ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase           SI log IAP  log KT   Initial     Final     Delta
```

```
        Ca(OH)2        -4.97   17.74   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -0.53   -1.60   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.39    0.18    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.28    1.95    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.18    3.72    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.10    5.50    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.04    7.27    7.31 0.000e+000          0.000e+000
        CSH(0.7)        0.00    9.05    9.04 1.000e+000 9.902e-001-9.758e-003
        CSH(0.8)        0.00   10.82   10.82 0.000e+000 6.783e-003 6.783e-003
        CSH(0.833)     -0.03   11.40   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.07   13.99   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.15   14.37   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.31   14.67   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.51   14.93   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.72   15.15   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.94   15.33   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -1.15   15.49   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -1.36   15.63   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.55   15.76   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.73   15.86   17.60 0.000e+000          0.000e+000
        SiO2(am)       -0.73   -3.37   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.404e-003  1.404e-003
        Si             2.975e-003  2.975e-003

----------------------------Description of solution---------------------------

                                pH  =  10.360     Charge balance
                                pe  =   7.553     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.158e-003
                     Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  2.808e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  77
                             Total H  = 1.110155e+002
                             Total O  = 5.551512e+001

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            2.499e-004  2.329e-004   -3.602   -3.633   -0.031
        H+             4.653e-011  4.367e-011  -10.332  -10.360   -0.028
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.404e-003
        Ca+2           1.376e-003  1.048e-003   -2.862   -2.980   -0.118
        CaSiH3O4+       2.478e-005  2.311e-005   -4.606   -4.636   -0.030
        CaHO+          3.765e-006  3.512e-006   -5.424   -5.454   -0.030
H(0)         2.332e-039
        H2             1.166e-039  1.167e-039  -38.933  -38.933    0.000
O(0)         8.726e-015
        O2             4.363e-015  4.367e-015  -14.360  -14.360    0.000
Si           2.975e-003
        SiH3O4-         2.524e-003  2.355e-003   -2.598   -2.628   -0.030
        H4SiO4         4.232e-004  4.236e-004   -3.373   -3.373    0.000
        CaSiH3O4+       2.478e-005  2.311e-005   -4.606   -4.636   -0.030
        SiH2O4-2        2.842e-006  2.152e-006   -5.546   -5.667   -0.121

----------------------------Saturation indices--------------------------------
```

```
        Phase            SI log IAP  log KT

        a-Cristobalite   0.06  -3.37  -3.43  SiO2
        b-Cristobalite  -0.39  -3.37  -2.98  SiO2
        Ca(OH)2        -4.97  17.74  22.71  Ca(OH)2
        Chalcedony      0.37  -3.37  -3.74  SiO2
        CSH(0.1)       -0.53  -1.60  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)       -0.39   0.18   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)       -0.28   1.95   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)       -0.18   3.72   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)       -0.10   5.50   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)       -0.04   7.27   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        0.00   9.05   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        0.00  10.82  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)     -0.03  11.40  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)       -0.07  13.99  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)       -0.15  14.37  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)       -0.31  14.67  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)       -0.51  14.93  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)       -0.72  15.15  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)       -0.94  15.33  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)       -1.15  15.49  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)       -1.36  15.63  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)       -1.55  15.76  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)       -1.73  15.86  17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.82 -35.83  -0.00  H2
        Lime          -14.82  17.74  32.56  CaO
        O2            -11.47  71.65  83.13  O2
        Quartz          0.66  -3.37  -4.03  SiO2
        SiO2(am)       -0.73  -3.37  -2.64  Si1.000O2.000
        Wollastonite    0.58  14.37  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 8.
------------------------------------

        Title 8 CSH(0.8)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  1
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 9
        END
-----
TITLE
-----

 8 CSH(0.8)
```

```
----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -4.35   18.36   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -0.96   -2.03   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.76   -0.19    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.59    1.64    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.43    3.48    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.29    5.31    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.16    7.15    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.06    8.98    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.00   10.82   10.82 1.000e+000 9.944e-001-5.613e-003
        CSH(0.833)     -0.01   11.42   11.44 0.000e+000          0.000e+000
        CSH(0.9)        0.00   14.06   14.06 0.000e+000 3.316e-003 3.316e-003
        CSH(1.0)       -0.02   14.49   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.14   14.84   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.30   15.14   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.49   15.38   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.68   15.60   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.87   15.78   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -1.05   15.94   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.22   16.08   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.39   16.21   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.23   -3.87   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.175e-003  1.175e-003
        Si             1.930e-003  1.930e-003

----------------------------Description of solution----------------------------

                                pH  =  10.701     Charge balance
                                pe  =   7.119     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.486e-003
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.350e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  28
                             Total H  = 1.110151e+002
                             Total O  = 5.551257e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            5.454e-004  5.111e-004   -3.263   -3.291   -0.028
        H+             2.111e-011  1.990e-011  -10.676  -10.701   -0.026
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.175e-003
        Ca+2           1.153e-003  8.970e-004   -2.938   -3.047   -0.109
```

```
          CaSiH3O4+       1.491e-005  1.398e-005   -4.827   -4.855   -0.028
          CaHO+           7.034e-006  6.597e-006   -5.153   -5.181   -0.028
H(0)           3.578e-039
          H2              1.789e-039  1.790e-039  -38.747  -38.747    0.000
O(0)           3.708e-015
          O2              1.854e-015  1.855e-015  -14.732  -14.732    0.000
Si            1.930e-003
          SiH3O4-         1.774e-003  1.664e-003   -2.751   -2.779   -0.028
          H4SiO4          1.363e-004  1.364e-004   -3.866   -3.865    0.000
          CaSiH3O4+       1.491e-005  1.398e-005   -4.827   -4.855   -0.028
          SiH2O4-2        4.314e-006  3.337e-006   -5.365   -5.477   -0.111

-----------------------------Saturation indices-------------------------------

          Phase            SI log IAP  log KT

          a-Cristobalite   -0.43   -3.87   -3.43  SiO2
          b-Cristobalite   -0.88   -3.87   -2.98  SiO2
          Ca(OH)2         -4.35   18.36   22.71  Ca(OH)2
          Chalcedony       -0.13   -3.87   -3.74  SiO2
          CSH(0.1)         -0.96   -2.03   -1.07  Ca0.100Si1.000O2.100:0.110H2O
          CSH(0.2)         -0.76   -0.19    0.56  Ca0.200Si1.000O2.200:0.220H2O
          CSH(0.3)         -0.59    1.64    2.23  Ca0.300Si1.000O2.300:0.330H2O
          CSH(0.4)         -0.43    3.48    3.91  Ca0.400Si1.000O2.400:0.440H2O
          CSH(0.5)         -0.29    5.31    5.60  Ca0.500Si1.000O2.500:0.550H2O
          CSH(0.6)         -0.16    7.15    7.31  Ca0.600Si1.000O2.600:0.661H2O
          CSH(0.7)         -0.06    8.98    9.04  Ca0.700Si1.000O2.700:0.771H2O
          CSH(0.8)         -0.00   10.82   10.82  Ca0.800Si1.000O2.800:0.881H2O
          CSH(0.833)       -0.01   11.42   11.44  Ca0.833Si1.000O2.833:0.917H2O
          CSH(0.9)          0.00   14.06   14.06  Ca1.000Si1.111O3.222:1.093H2O
          CSH(1.0)         -0.02   14.49   14.51  Ca1.000Si1.000O3.000:1.084H2O
          CSH(1.1)         -0.14   14.84   14.98  Ca1.000Si0.909O2.818:1.076H2O
          CSH(1.2)         -0.30   15.14   15.44  Ca1.000Si0.833O2.666:1.070H2O
          CSH(1.3)         -0.49   15.38   15.87  Ca1.000Si0.769O2.538:1.065H2O
          CSH(1.4)         -0.68   15.60   16.27  Ca1.000Si0.714O2.428:1.060H2O
          CSH(1.5)         -0.87   15.78   16.64  Ca1.000Si0.667O2.334:1.056H2O
          CSH(1.6)         -1.05   15.94   16.99  Ca1.000Si0.625O2.250:1.053H2O
          CSH(1.7)         -1.22   16.08   17.30  Ca1.000Si0.588O2.176:1.049H2O
          CSH(1.8)         -1.39   16.21   17.60  Ca1.000Si0.556O2.112:1.047H2O
          H2              -35.64  -35.64   -0.00  H2
          Lime            -14.21   18.36   32.56  CaO
          O2              -11.85   71.28   83.13  O2
          Quartz            0.16   -3.87   -4.03  SiO2
          SiO2(am)         -1.23   -3.87   -2.64  Si1.000O2.000
          Wollastonite      0.71   14.49   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 9.
------------------------------------

          Title 9 CSH(0.9)
          USE SOLUTION 1 DW
          EQUILIBRIUM_PHASES
          CSH(0.1)  0.0  0.0
          CSH(0.2)  0.0  0.0
          CSH(0.3)  0.0  0.0
          CSH(0.4)  0.0  0.0
          CSH(0.5)  0.0  0.0
          CSH(0.6)  0.0  0.0
          CSH(0.7)  0.0  0.0
          CSH(0.8)  0.0  0.0
          CSH(0.9)  0.0  1
          CSH(1.0)  0.0  0.0
          CSH(1.1)  0.0  0.0
          CSH(1.2)  0.0  0.0
          CSH(1.3)  0.0  0.0
          CSH(1.4)  0.0  0.0
```

```
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 10
        END
-----
TITLE
-----

 9 CSH(0.9)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -4.11   18.60   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -1.15   -2.22   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.93   -0.36    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.73    1.50    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.55    3.36    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.38    5.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.24    7.08    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.11    8.94    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.02   10.79   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.03   11.41   11.44 0.000e+000          0.000e+000
        CSH(0.9)        0.00   14.06   14.06 1.000e+000 9.960e-001-4.002e-003
        CSH(1.0)        0.00   14.51   14.51 0.000e+000 2.891e-003 2.891e-003
        CSH(1.1)       -0.10   14.89   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.24   15.20   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.41   15.46   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.59   15.68   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.77   15.87   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.94   16.04   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.11   16.20   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.27   16.33   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.44   -4.08   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca            1.111e-003  1.111e-003
        Si            1.555e-003  1.555e-003

----------------------------Description of solution----------------------------

                                pH  =  10.832     Charge balance
                                pe  =   6.652     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.296e-003
                   Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.222e-003
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
```

```
                          Iterations  =  17
                            Total H  = 1.110149e+002
                            Total O  = 5.551168e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            7.358e-004  6.908e-004   -3.133   -3.161   -0.027
        H+             1.560e-011  1.472e-011   -10.807  -10.832   -0.025
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.111e-003
        Ca+2           1.090e-003  8.535e-004   -2.962   -3.069   -0.106
        CaSiH3O4+       1.164e-005  1.093e-005   -4.934   -4.961   -0.027
        CaHO+          9.029e-006  8.482e-006   -5.044   -5.071   -0.027
H(0)         1.685e-038
        H2             8.423e-039  8.429e-039   -38.075  -38.074    0.000
O(0)         1.673e-016
        O2             8.364e-017  8.370e-017   -16.078  -16.077    0.000
Si           1.555e-003
        SiH3O4-         1.456e-003  1.368e-003   -2.837   -2.864   -0.027
        H4SiO4          8.290e-005  8.296e-005   -4.081   -4.081    0.000
        CaSiH3O4+       1.164e-005  1.093e-005   -4.934   -4.961   -0.027
        SiH2O4-2        4.760e-006  3.707e-006   -5.322   -5.431   -0.109

----------------------------Saturation indices---------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.65   -4.08   -3.43  SiO2
        b-Cristobalite   -1.10   -4.08   -2.98  SiO2
        Ca(OH)2         -4.11   18.60   22.71  Ca(OH)2
        Chalcedony       -0.34   -4.08   -3.74  SiO2
        CSH(0.1)         -1.15   -2.22   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -0.93   -0.36    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.73    1.50    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.55    3.36    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.38    5.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.24    7.08    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.11    8.94    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.02   10.79   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.03   11.41   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)          0.00   14.06   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)          0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.10   14.89   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.24   15.20   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.41   15.46   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.59   15.68   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.77   15.87   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.94   16.04   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -1.11   16.20   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -1.27   16.33   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -34.96  -34.97   -0.00  H2
        Lime           -13.97   18.60   32.56  CaO
        O2             -13.19   69.94   83.13  O2
        Quartz           -0.05   -4.08   -4.03  SiO2
        SiO2(am)         -1.44   -4.08   -2.64  Si1.000O2.000
        Wollastonite      0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 10.
------------------------------------

        Title 10 CSH(1.0)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
```

```
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  1
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 11
        END
-----
TITLE
-----

 10 CSH(1.0)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -3.79  18.92   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -1.44  -2.52   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -1.19  -0.62    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.96   1.27    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.75   3.16    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.55   5.05    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.37   6.95    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.21   8.84    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.09  10.73   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.08  11.35   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.04  14.02   14.06 0.000e+000          0.000e+000
        CSH(1.0)        0.00  14.51   14.51 1.000e+000 9.989e-001-1.068e-003
        CSH(1.1)       -0.07  14.92   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.19  15.25   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.34  15.53   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.50  15.77   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.66  15.98   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.82  16.17   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.97  16.33   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.13  16.47   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.77  -4.41   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Ca             1.068e-003  1.068e-003
        Si             1.068e-003  1.068e-003
```

----------Description of solution----------

```
                                pH  =  11.003     Charge balance
                                pe  =   6.787     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.168e-003
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.137e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  15
                             Total H  = 1.110147e+002
                             Total O  = 5.551058e+001
```

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	1.090e-003	1.024e-003	-2.963	-2.990	-0.027
H+	1.051e-011	9.932e-012	-10.978	-11.003	-0.025
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
Ca	1.068e-003				
Ca+2	1.048e-003	8.236e-004	-2.980	-3.084	-0.104
CaHO+	1.290e-005	1.213e-005	-4.889	-4.916	-0.027
CaSiH3O4+	7.841e-006	7.374e-006	-5.106	-5.132	-0.027
H(0)	4.107e-039				
H2	2.053e-039	2.055e-039	-38.688	-38.687	0.000
O(0)	2.815e-015				
O2	1.407e-015	1.408e-015	-14.852	-14.851	0.000
Si	1.068e-003				
SiH3O4-	1.016e-003	9.559e-004	-2.993	-3.020	-0.027
H4SiO4	3.909e-005	3.911e-005	-4.408	-4.408	0.000
CaSiH3O4+	7.841e-006	7.374e-006	-5.106	-5.132	-0.027
SiH2O4-2	4.910e-006	3.841e-006	-5.309	-5.416	-0.107

----------Saturation indices----------

Phase	SI	log IAP	log KT	
a-Cristobalite	-0.97	-4.41	-3.43	SiO2
b-Cristobalite	-1.43	-4.41	-2.98	SiO2
Ca(OH)2	-3.79	18.92	22.71	Ca(OH)2
Chalcedony	-0.67	-4.41	-3.74	SiO2
CSH(0.1)	-1.44	-2.52	-1.07	Ca0.100Si1.000O2.100:0.110H2O
CSH(0.2)	-1.19	-0.62	0.56	Ca0.200Si1.000O2.200:0.220H2O
CSH(0.3)	-0.96	1.27	2.23	Ca0.300Si1.000O2.300:0.330H2O
CSH(0.4)	-0.75	3.16	3.91	Ca0.400Si1.000O2.400:0.440H2O
CSH(0.5)	-0.55	5.05	5.60	Ca0.500Si1.000O2.500:0.550H2O
CSH(0.6)	-0.37	6.95	7.31	Ca0.600Si1.000O2.600:0.661H2O
CSH(0.7)	-0.21	8.84	9.04	Ca0.700Si1.000O2.700:0.771H2O
CSH(0.8)	-0.09	10.73	10.82	Ca0.800Si1.000O2.800:0.881H2O
CSH(0.833)	-0.08	11.35	11.44	Ca0.833Si1.000O2.833:0.917H2O
CSH(0.9)	-0.04	14.02	14.06	Ca1.000Si1.111O3.222:1.093H2O
CSH(1.0)	0.00	14.51	14.51	Ca1.000Si1.000O3.000:1.084H2O
CSH(1.1)	-0.07	14.92	14.98	Ca1.000Si0.909O2.818:1.076H2O
CSH(1.2)	-0.19	15.25	15.44	Ca1.000Si0.833O2.666:1.070H2O
CSH(1.3)	-0.34	15.53	15.87	Ca1.000Si0.769O2.538:1.065H2O
CSH(1.4)	-0.50	15.77	16.27	Ca1.000Si0.714O2.428:1.060H2O
CSH(1.5)	-0.66	15.98	16.64	Ca1.000Si0.667O2.334:1.056H2O
CSH(1.6)	-0.82	16.17	16.99	Ca1.000Si0.625O2.250:1.053H2O
CSH(1.7)	-0.97	16.33	17.30	Ca1.000Si0.588O2.176:1.049H2O
CSH(1.8)	-1.13	16.47	17.60	Ca1.000Si0.556O2.112:1.047H2O
H2	-35.58	-35.58	-0.00	H2
Lime	-13.64	18.92	32.56	CaO
O2	-11.96	71.16	83.13	O2
Quartz	-0.38	-4.41	-4.03	SiO2

```
        SiO2(am)       -1.77   -4.41   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 11.
------------------------------------

        Title 11 CSH(1.1)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  1
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 12
        END
-----
TITLE
-----

 11 CSH(1.1)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -3.04   19.67   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -2.12   -3.19   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -1.79   -1.22    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -1.48    0.75    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -1.19    2.71    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.92    4.68    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.67    6.65    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.43    8.61    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.24   10.58   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.21   11.23   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.12   13.94   14.06 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.51   14.51 0.000e+000 9.344e-003 9.344e-003
        CSH(1.1)        0.00   14.98   14.98 1.000e+000 9.893e-001-1.072e-002
        CSH(1.2)       -0.06   15.37   15.44 0.000e+000          0.000e+000
```

```
        CSH(1.3)        -0.17   15.70   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.28   15.99   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.41   16.23   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.54   16.45   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -0.67   16.64   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.79   16.80   17.60 0.000e+000          0.000e+000
        SiO2(am)        -2.51   -5.15   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.379e-003  1.379e-003
        Si             4.036e-004  4.036e-004

----------------------------Description of solution---------------------------

                                pH  =  11.329     Charge balance
                                pe  =   6.604     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.067e-003
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  2.759e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  20
                             Total H  = 1.110153e+002
                             Total O  = 5.550981e+001

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            2.324e-003  2.168e-003    -2.634    -2.664    -0.030
        H+             4.997e-012  4.692e-012   -11.301   -11.329    -0.027
        H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
Ca           1.379e-003
        Ca+2           1.341e-003  1.025e-003    -2.872    -2.989    -0.117
        CaHO+          3.424e-005  3.196e-005    -4.465    -4.495    -0.030
        CaSiH3O4+      3.732e-006  3.484e-006    -5.428    -5.458    -0.030
H(0)         2.129e-039
        H2             1.064e-039  1.065e-039   -38.973   -38.973     0.000
O(0)         1.047e-014
        O2             5.235e-015  5.240e-015   -14.281   -14.281     0.000
Si           4.036e-004
        SiH3O4-        3.888e-004  3.629e-004    -3.410    -3.440    -0.030
        H4SiO4         7.010e-006  7.016e-006    -5.154    -5.154     0.000
        SiH2O4-2       4.066e-006  3.087e-006    -5.391    -5.510    -0.120
        CaSiH3O4+      3.732e-006  3.484e-006    -5.428    -5.458    -0.030

----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -1.72   -5.15   -3.43  SiO2
        b-Cristobalite   -2.17   -5.15   -2.98  SiO2
        Ca(OH)2         -3.04   19.67   22.71  Ca(OH)2
        Chalcedony       -1.42   -5.15   -3.74  SiO2
        CSH(0.1)         -2.12   -3.19   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -1.79   -1.22    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -1.48    0.75    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -1.19    2.71    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.92    4.68    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.67    6.65    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.43    8.61    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.24   10.58   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.21   11.23   11.44  Ca0.833Si1.000O2.833:0.917H2O
```

```
        CSH(0.9)        -0.12   13.94   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.06   15.37   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.17   15.70   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.28   15.99   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.41   16.23   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.54   16.45   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.67   16.64   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.79   16.80   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.86  -35.87   -0.00  H2
        Lime          -12.89   19.67   32.56  CaO
        O2            -11.39   71.73   83.13  O2
        Quartz         -1.13   -5.15   -4.03  SiO2
        SiO2(am)       -2.51   -5.15   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 12.
------------------------------------

        Title 12 CSH(1.2)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  1
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 13
        END
-----
TITLE
-----

 12 CSH(1.2)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1.DW
Using pure phase assemblage 1.
```

```
-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -2.27  20.44  22.71 0.000e+000          0.000e+000
        CSH(0.1)       -2.89  -3.96  -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -2.48  -1.91   0.56 0.000e+000          0.000e+000
        CSH(0.3)       -2.10   0.13   2.23 0.000e+000          0.000e+000
        CSH(0.4)       -1.73   2.17   3.91 0.000e+000          0.000e+000
        CSH(0.5)       -1.38   4.22   5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.05   6.26   7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.74   8.31   9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.47  10.35  10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.41  11.02  11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.29  13.77  14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.08  14.44  14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.00  14.98  14.98 0.000e+000 2.473e-002 2.473e-002
        CSH(1.2)        0.00  15.44  15.44 1.000e+000 9.729e-001-2.713e-002
        CSH(1.3)       -0.05  15.82  15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.12  16.15  16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.21  16.44  16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.30  16.69  16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.39  16.91  17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.50  17.10  17.60 0.000e+000          0.000e+000
        SiO2(am)       -3.36  -6.00  -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             2.393e-003  2.393e-003
        Si             1.137e-004  1.137e-004

----------------------------Description of solution-----------------------------

                                pH  =  11.613     Charge balance
                                pe  =   6.257     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  6.965e-003
                   Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  4.786e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  = 169
                            Total H  = 1.110173e+002
                            Total O  = 5.551125e+001

---------------------------Distribution of species-----------------------------

                                              Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            4.565e-003  4.175e-003   -2.341   -2.379   -0.039
        H+             2.635e-012  2.436e-012  -11.579  -11.613   -0.034
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           2.393e-003
        Ca+2           2.285e-003  1.624e-003   -2.641   -2.790   -0.148
        CaHO+          1.065e-004  9.753e-005   -3.973   -4.011   -0.038
        CaSiH3O4+      1.654e-006  1.515e-006   -5.781   -5.820   -0.038
H(0)         2.834e-039
        H2             1.417e-039  1.419e-039  -38.849  -38.848    0.001
O(0)         5.896e-015
        O2             2.948e-015  2.953e-015  -14.530  -14.530    0.001
Si           1.137e-004
        SiH3O4-        1.088e-004  9.962e-005   -3.964   -4.002   -0.038
        SiH2O4-2       2.319e-006  1.632e-006   -5.635   -5.787   -0.153
        CaSiH3O4+      1.654e-006  1.515e-006   -5.781   -5.820   -0.038
```

```
        H4SiO4          9.982e-007  9.998e-007   -6.001   -6.000    0.001

-----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -2.57   -6.00   -3.43  SiO2
        b-Cristobalite   -3.02   -6.00   -2.98  SiO2
        Ca(OH)2          -2.27   20.44   22.71  Ca(OH)2
        Chalcedony       -2.26   -6.00   -3.74  SiO2
        CSH(0.1)         -2.89   -3.96   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -2.48   -1.91    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -2.10    0.13    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -1.73    2.17    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -1.38    4.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -1.05    6.26    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.74    8.31    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.47   10.35   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.41   11.02   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.29   13.77   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.08   14.44   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)          0.00   15.44   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.05   15.82   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.12   16.15   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.21   16.44   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.30   16.69   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.39   16.91   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.50   17.10   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.74  -35.74   -0.00  H2
        Lime           -12.12   20.44   32.56  CaO
        O2             -11.64   71.48   83.13  O2
        Quartz          -1.97   -6.00   -4.03  SiO2
        SiO2(am)        -3.36   -6.00   -2.64  Si1.000O2.000
        Wollastonite     0.65   14.44   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 13.
------------------------------------

        Title 13 CSH(1.3)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  1
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 14
        END
-----
```

```
TITLE
-----

 13 CSH(1.3)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -1.66   21.05   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -3.56   -4.63   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -3.09   -2.52    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -2.65   -0.42    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -2.22    1.69    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -1.81    3.79    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.42    5.89    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -1.05    8.00    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.71   10.10   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.64   10.80   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.49   13.57   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.20   14.31   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.06   14.93   14.98 0.000e+000          0.000e+000
        CSH(1.2)        0.00   15.44   15.44 0.000e+000 4.751e-002 4.751e-002
        CSH(1.3)       -0.00   15.87   15.87 1.000e+000 9.485e-001-5.152e-002
        CSH(1.4)       -0.03   16.24   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.09   16.56   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.15   16.84   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.22   17.09   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.29   17.30   17.60 0.000e+000          0.000e+000
        SiO2(am)       -4.10   -6.73   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             4.001e-003  4.001e-003
        Si             3.599e-005  3.599e-005

----------------------------Description of solution----------------------------

                                pH  =  11.830     Charge balance
                                pe  =   6.038     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.146e-002
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  8.002e-003
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  48
                              Total H  = 1.110205e+002
                              Total O  = 5.551431e+001

---------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            7.695e-003  6.881e-003   -2.114   -2.162   -0.049
```

```
        H+            1.626e-012  1.478e-012  -11.789  -11.830   -0.041
        H2O           5.551e+001  9.998e-001    1.744   -0.000    0.000
Ca           4.001e-003
        Ca+2          3.730e-003  2.444e-003   -2.428   -2.612   -0.184
        CaHO+         2.700e-004  2.420e-004   -3.569   -3.616   -0.048
        CaSiH3O4+     7.729e-007  6.929e-007   -6.112   -6.159   -0.048
H(0)         2.867e-039
        H2            1.433e-039  1.437e-039  -38.844  -38.843    0.001
O(0)         5.742e-015
        O2            2.871e-015  2.879e-015  -14.542  -14.541    0.001
Si           3.599e-005
        SiH3O4-       3.377e-005  3.027e-005   -4.472   -4.519   -0.048
        SiH2O4-2      1.266e-006  8.173e-007   -5.898   -6.088   -0.190
        CaSiH3O4+     7.729e-007  6.929e-007   -6.112   -6.159   -0.048
        H4SiO4        1.838e-007  1.843e-007   -6.736   -6.735    0.001

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -3.30  -6.73  -3.43  SiO2
        b-Cristobalite  -3.75  -6.73  -2.98  SiO2
        Ca(OH)2        -1.66  21.05  22.71  Ca(OH)2
        Chalcedony      -3.00  -6.73  -3.74  SiO2
        CSH(0.1)        -3.56  -4.63  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -3.09  -2.52   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -2.65  -0.42   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -2.22   1.69   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -1.81   3.79   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -1.42   5.89   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -1.05   8.00   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.71  10.10  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.64  10.80  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.49  13.57  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.20  14.31  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.06  14.93  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         0.00  15.44  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.00  15.87  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.03  16.24  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.09  16.56  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.15  16.84  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.22  17.09  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.29  17.30  17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.73 -35.74  -0.00  H2
        Lime          -11.51  21.05  32.56  CaO
        O2            -11.65  71.47  83.13  O2
        Quartz         -2.71  -6.73  -4.03  SiO2
        SiO2(am)       -4.10  -6.73  -2.64  Si1.000O2.000
        Wollastonite    0.53  14.31  13.78  CaSiO3

-----------------
End of simulation.
-----------------

------------------------------------
Reading input data for simulation 14.
------------------------------------

        Title 14 CSH(1.4)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
```

```
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  1
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 15
        END
-----
TITLE
-----

 14 CSH(1.4)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -1.22   21.49   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -4.09   -5.16   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -3.58   -3.01    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -3.09   -0.86    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -2.62    1.29    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -2.16    3.44    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.73    5.59    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -1.31    7.73    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.94    9.88   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.84   10.59   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.69   13.37   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.33   14.18   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.14   14.85   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.04   15.40   15.44 0.000e+000          0.000e+000
        CSH(1.3)        0.00   15.87   15.87 0.000e+000 7.642e-002 7.642e-002
        CSH(1.4)        0.00   16.27   16.27 1.000e+000 9.177e-001-8.233e-002
        CSH(1.5)       -0.03   16.62   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.06   16.92   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.11   17.19   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.17   17.43   17.60 0.000e+000          0.000e+000
        SiO2(am)       -4.67   -7.31   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             5.907e-003  5.907e-003
        Si             1.435e-005  1.435e-005

----------------------------Description of solution----------------------------

                                pH  =  11.987     Charge balance
                                pe  =   5.636     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.666e-002
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  1.181e-002
                  Total carbon (mol/kg)  =  0.000e+000
```

```
                  Total CO2 (mol/kg)  =  0.000e+000
                Temperature (deg C)  =  25.000
              Electrical balance (eq)  = -1.714e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                        Iterations  =  82
                          Total H  = 1.110242e+002
                          Total O  = 5.551803e+001

----------------------------Distribution of species----------------------------

                                                 Log      Log       Log
         Species          Molality   Activity  Molality  Activity    Gamma

         HO-            1.127e-002  9.877e-003   -1.948   -2.005   -0.057
         H+             1.149e-012  1.030e-012  -11.940  -11.987   -0.048
         H2O            5.551e+001  9.997e-001    1.744   -0.000    0.000
Ca            5.907e-003
         Ca+2           5.376e-003  3.283e-003   -2.270   -2.484   -0.214
         CaHO+          5.303e-004  4.665e-004   -3.275   -3.331   -0.056
         CaSiH3O4+       4.042e-007  3.556e-007   -6.393   -6.449   -0.056
H(0)          8.817e-039
         H2             4.409e-039  4.425e-039  -38.356  -38.354    0.002
O(0)          6.047e-016
         O2             3.023e-016  3.035e-016  -15.520  -15.518    0.002
Si            1.435e-005
         SiH3O4-         1.315e-005  1.156e-005   -4.881   -4.937   -0.056
         SiH2O4-2        7.486e-007  4.483e-007   -6.126   -6.348   -0.223
         CaSiH3O4+       4.042e-007  3.556e-007   -6.393   -6.449   -0.056
         H4SiO4          4.887e-008  4.905e-008   -7.311   -7.309    0.002

------------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -3.88   -7.31   -3.43  SiO2
         b-Cristobalite   -4.33   -7.31   -2.98  SiO2
         Ca(OH)2         -1.22   21.49   22.71  Ca(OH)2
         Chalcedony       -3.57   -7.31   -3.74  SiO2
         CSH(0.1)         -4.09   -5.16   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -3.58   -3.01    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -3.09   -0.86    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -2.62    1.29    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -2.16    3.44    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -1.73    5.59    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -1.31    7.73    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -0.94    9.88   10.82  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -0.84   10.59   11.44  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)         -0.69   13.37   14.06  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)         -0.33   14.18   14.51  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)         -0.14   14.85   14.98  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.04   15.40   15.44  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)          0.00   15.87   15.87  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)          0.00   16.27   16.27  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.03   16.62   16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -0.06   16.92   16.99  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)         -0.11   17.19   17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)         -0.17   17.43   17.60  Ca1.000Si0.556O2.112:1.047H2O
         H2             -35.24  -35.25   -0.00  H2
         Lime           -11.07   21.49   32.56  CaO
         O2             -12.63   70.49   83.13  O2
         Quartz          -3.28   -7.31   -4.03  SiO2
         SiO2(am)        -4.67   -7.31   -2.64  Si1.000O2.000
         Wollastonite     0.40   14.18   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 15.
------------------------------------
```

```
        Title 15 CSH(1.5)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  1
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 16
        END
-----
TITLE
-----

 15 CSH(1.5)

-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase              SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -0.80   21.91   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -4.63   -5.70   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -4.08   -3.51    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -3.55   -1.32    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -3.04    0.87    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -2.54    3.06    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -2.06    5.25    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -1.60    7.44    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -1.19    9.63   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -1.08   10.36   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.92   13.14   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.50   14.01   14.51 0.000e+000          0.000e+000
        CSH(1.1)        -0.25   14.73   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.11   15.33   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.03   15.84   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.00   16.27   16.27 0.000e+000 1.223e-001 1.223e-001
        CSH(1.5)        -0.00   16.64   16.64 1.000e+000 8.691e-001-1.309e-001
        CSH(1.6)        -0.01   16.97   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -0.04   17.27   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.08   17.52   17.60 0.000e+000          0.000e+000
        SiO2(am)        -5.25   -7.89   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------
```

```
        Elements         Molality      Moles

        Ca             8.627e-003  8.627e-003
        Si             5.557e-006  5.557e-006

----------------------------Description of solution----------------------------

                                pH  =  12.137     Charge balance
                                pe  =   5.403     Adjusted to redox equilibrium
                     Activity of water  =  1.000
                        Ionic strength  =  2.388e-002
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  1.725e-002
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  64
                             Total H  = 1.110297e+002
                             Total O  = 5.552348e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            1.625e-002  1.393e-002   -1.789   -1.856   -0.067
        H+             8.267e-013  7.300e-013  -12.083  -12.137   -0.054
        H2O            5.551e+001  9.996e-001    1.744   -0.000    0.000
Ca           8.627e-003
        Ca+2           7.624e-003  4.315e-003   -2.118   -2.365   -0.247
        CaHO+          1.003e-003  8.648e-004   -2.999   -3.063   -0.065
        CaSiH3O4+      1.990e-007  1.716e-007   -6.701   -6.766   -0.065
H(0)         1.294e-038
        H2             6.471e-039  6.507e-039  -38.189  -38.187    0.002
O(0)         2.792e-016
        O2             1.396e-016  1.404e-016  -15.855  -15.853    0.002
Si           5.557e-006
        SiH3O4-        4.925e-006  4.245e-006   -5.308   -5.372   -0.065
        SiH2O4-2       4.204e-007  2.321e-007   -6.376   -6.634   -0.258
        CaSiH3O4+      1.990e-007  1.716e-007   -6.701   -6.766   -0.065
        H4SiO4         1.270e-008  1.277e-008   -7.896   -7.894    0.002

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -4.46   -7.89   -3.43  SiO2
        b-Cristobalite   -4.91   -7.89   -2.98  SiO2
        Ca(OH)2          -0.80   21.91   22.71  Ca(OH)2
        Chalcedony       -4.16   -7.89   -3.74  SiO2
        CSH(0.1)         -4.63   -5.70   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -4.08   -3.51    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -3.55   -1.32    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.04    0.87    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -2.54    3.06    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.06    5.25    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.60    7.44    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.19    9.63   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.08   10.36   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.92   13.14   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.50   14.01   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.25   14.73   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.11   15.33   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.03   15.84   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.00   16.27   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.00   16.64   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.01   16.97   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.04   17.27   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.08   17.52   17.60  Ca1.000Si0.556O2.112:1.047H2O
```

```
        H2           -35.08  -35.08   -0.00  H2
        Lime         -10.65   21.91   32.56  CaO
        O2           -12.97   70.16   83.13  O2
        Quartz        -3.87   -7.89   -4.03  SiO2
        SiO2(am)      -5.25   -7.89   -2.64  Si1.000O2.000
        Wollastonite   0.23   14.01   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 16.
------------------------------------

        Title 16 CSH(1.6)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  1
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 17
        END
-----
TITLE
-----

 16 CSH(1.6)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase              SI log IAP  log KT    Initial      Final      Delta

        Ca(OH)2         -0.60   22.11   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -4.91   -5.98   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -4.33   -3.77    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -3.79   -1.56    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -3.26    0.65    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -2.74    2.86    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -2.24    5.07    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -1.76    7.28    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -1.32    9.49   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -1.21   10.22   11.44 0.000e+000          0.000e+000
```

```
        CSH(0.9)        -1.05   13.01   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.60   13.92   14.51 0.000e+000          0.000e+000
        CSH(1.1)        -0.32   14.66   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.16   15.28   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.06   15.81   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.01   16.26   16.27 0.000e+000          0.000e+000
        CSH(1.5)         0.00   16.64   16.64 0.000e+000 1.542e-001 1.542e-001
        CSH(1.6)         0.00   16.99   16.99 1.000e+000 8.355e-001-1.645e-001
        CSH(1.7)        -0.01   17.29   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.04   17.55   17.60 0.000e+000          0.000e+000
        SiO2(am)        -5.55   -8.19   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Ca             1.036e-002  1.036e-002
        Si             3.410e-006  3.410e-006

----------------------------Description of solution----------------------------

                                pH  =  12.208     Charge balance
                                pe  =   5.698     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  2.838e-002
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  2.073e-002
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                            Iterations  =  22
                               Total H  = 1.110333e+002
                               Total O  = 5.552704e+001

----------------------------Distribution of species----------------------------

                                            Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            1.937e-002  1.641e-002   -1.713   -1.785   -0.072
        H+             7.067e-013  6.194e-013  -12.151  -12.208   -0.057
        H2O            5.551e+001  9.995e-001    1.744   -0.000    0.000
Ca           1.036e-002
        Ca+2           9.007e-003  4.902e-003   -2.045   -2.310   -0.264
        CaHO+          1.357e-003  1.158e-003   -2.867   -2.936   -0.069
        CaSiH3O4+      1.359e-007  1.159e-007   -6.867   -6.936   -0.069
H(0)         2.390e-039
        H2             1.195e-039  1.203e-039  -38.923  -38.920    0.003
O(0)         8.157e-015
        O2             4.079e-015  4.105e-015  -14.389  -14.387    0.003
Si           3.410e-006
        SiH3O4-        2.960e-006  2.525e-006   -5.529   -5.598   -0.069
        SiH2O4-2       3.074e-007  1.627e-007   -6.512   -6.789   -0.276
        CaSiH3O4+      1.359e-007  1.159e-007   -6.867   -6.936   -0.069
        H4SiO4         6.401e-009  6.443e-009   -8.194   -8.191    0.003

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -4.76  -8.19  -3.43  SiO2
        b-Cristobalite  -5.21  -8.19  -2.98  SiO2
        Ca(OH)2         -0.60  22.11  22.71  Ca(OH)2
        Chalcedony      -4.45  -8.19  -3.74  SiO2
        CSH(0.1)        -4.91  -5.98  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -4.33  -3.77   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -3.79  -1.56   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -3.26   0.65   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -2.74   2.86   5.60  Ca0.500Si1.000O2.500:0.550H2O
```

```
        CSH(0.6)        -2.24    5.07    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -1.76    7.28    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -1.32    9.49   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -1.21   10.22   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -1.05   13.01   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.60   13.92   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.32   14.66   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.16   15.28   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.06   15.81   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.01   16.26   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         0.00   16.64   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         0.00   16.99   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.01   17.29   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.04   17.55   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.81  -35.81   -0.00  H2
        Lime          -10.46   22.11   32.56  CaO
        O2            -11.50   71.63   83.13  O2
        Quartz         -4.16   -8.19   -4.03  SiO2
        SiO2(am)       -5.55   -8.19   -2.64  Si1.000O2.000
        Wollastonite    0.13   13.92   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 17.
------------------------------------

        Title 17 CSH(1.7)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  1
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 18
        END
-----
TITLE
-----

 17 CSH(1.7)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------
```

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca(OH)2	-0.37	22.34	22.71	0.000e+000		0.000e+000
CSH(0.1)	-5.26	-6.33	-1.07	0.000e+000		0.000e+000
CSH(0.2)	-4.66	-4.10	0.56	0.000e+000		0.000e+000
CSH(0.3)	-4.09	-1.87	2.23	0.000e+000		0.000e+000
CSH(0.4)	-3.54	0.37	3.91	0.000e+000		0.000e+000
CSH(0.5)	-3.00	2.60	5.60	0.000e+000		0.000e+000
CSH(0.6)	-2.47	4.84	7.31	0.000e+000		0.000e+000
CSH(0.7)	-1.97	7.07	9.04	0.000e+000		0.000e+000
CSH(0.8)	-1.51	9.31	10.82	0.000e+000		0.000e+000
CSH(0.833)	-1.39	10.04	11.44	0.000e+000		0.000e+000
CSH(0.9)	-1.24	12.82	14.06	0.000e+000		0.000e+000
CSH(1.0)	-0.74	13.77	14.51	0.000e+000		0.000e+000
CSH(1.1)	-0.43	14.55	14.98	0.000e+000		0.000e+000
CSH(1.2)	-0.23	15.20	15.44	0.000e+000		0.000e+000
CSH(1.3)	-0.12	15.75	15.87	0.000e+000		0.000e+000
CSH(1.4)	-0.05	16.22	16.27	0.000e+000		0.000e+000
CSH(1.5)	-0.02	16.63	16.64	0.000e+000		0.000e+000
CSH(1.6)	0.00	16.99	16.99	0.000e+000	2.055e-001	2.055e-001
CSH(1.7)	0.00	17.30	17.30	1.000e+000	7.815e-001	-2.185e-001
CSH(1.8)	-0.02	17.58	17.60	0.000e+000		0.000e+000
SiO2(am)	-5.93	-8.57	-2.64	0.000e+000		0.000e+000

----------Solution composition----------

Elements	Molality	Moles
Ca	1.294e-002	1.294e-002
Si	1.818e-006	1.818e-006

----------Description of solution----------

pH = 12.293 Charge balance
pe = 5.352 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 3.492e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = 2.587e-002
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.715e-009
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 84
Total H = 1.110379e+002
Total O = 5.553190e+001

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	2.392e-002	1.998e-002	-1.621	-1.699	-0.078
H+	5.860e-013	5.089e-013	-12.232	-12.293	-0.061
H2O	5.551e+001	9.994e-001	1.744	-0.000	0.000
Ca	1.294e-002				
Ca+2	1.099e-002	5.695e-003	-1.959	-2.245	-0.286
CaHO+	1.945e-003	1.637e-003	-2.711	-2.786	-0.075
CaSiH3O4+	8.171e-008	6.878e-008	-7.088	-7.163	-0.075
H(0)	7.953e-039				
H2	3.976e-039	4.009e-039	-38.401	-38.397	0.003
O(0)	7.334e-016				
O2	3.667e-016	3.697e-016	-15.436	-15.432	0.003
Si	1.818e-006				
SiH3O4-	1.532e-006	1.290e-006	-5.815	-5.890	-0.075
SiH2O4-2	2.015e-007	1.011e-007	-6.696	-6.995	-0.299
CaSiH3O4+	8.171e-008	6.878e-008	-7.088	-7.163	-0.075
H4SiO4	2.682e-009	2.703e-009	-8.572	-8.568	0.003

```
-----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -5.13   -8.57   -3.43  SiO2
        b-Cristobalite   -5.59   -8.57   -2.98  SiO2
        Ca(OH)2         -0.37   22.34   22.71  Ca(OH)2
        Chalcedony       -4.83   -8.57   -3.74  SiO2
        CSH(0.1)         -5.26   -6.33   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -4.66   -4.10    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -4.09   -1.87    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.54    0.37    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -3.00    2.60    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.47    4.84    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.97    7.07    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.51    9.31   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.39   10.04   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -1.24   12.82   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.74   13.77   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.43   14.55   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.23   15.20   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.12   15.75   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.05   16.22   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.02   16.63   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)          0.00   16.99   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)          0.00   17.30   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.02   17.58   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.29  -35.29   -0.00  H2
        Lime           -10.22   22.34   32.56  CaO
        O2             -12.55   70.58   83.13  O2
        Quartz          -4.54   -8.57   -4.03  SiO2
        SiO2(am)        -5.93   -8.57   -2.64  Si1.000O2.000
        Wollastonite    -0.01   13.77   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 18.
------------------------------------

        Title 18 CSH(1.8)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  1
        SiO2(am)  0.0  0.0
        CSH(0.833)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 19
-----
TITLE
-----
```

```
 18 CSH(1.8)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -0.02   22.69   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -5.82   -6.89   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -5.18   -4.62    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -4.58   -2.35    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -3.99   -0.08    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -3.41    2.19    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -2.86    4.46    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -2.32    6.73    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -1.82    8.99   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -1.69    9.74   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -1.55   12.52   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.98   13.53   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.62   14.36   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.38   15.06   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.22   15.65   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.12   16.15   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.06   16.58   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.02   16.97   16.99 0.000e+000          0.000e+000
        CSH(1.7)        0.00   17.30   17.30 0.000e+000 3.133e-001 3.133e-001
        CSH(1.8)        0.00   17.60   17.60 1.000e+000 6.687e-001-3.313e-001
        SiO2(am)       -6.52   -9.16   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Ca             1.803e-002  1.803e-002
        Si             6.765e-007  6.765e-007

----------------------------Description of solution----------------------------

                                pH  =  12.420     Charge balance
                                pe  =   5.419     Adjusted to redox equilibrium
                    Activity of water  =   0.999
                       Ionic strength  =  4.751e-002
                   Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  3.607e-002
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  30
                             Total H  = 1.110489e+002
                             Total O  = 5.554250e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            3.277e-002  2.671e-002   -1.485   -1.573   -0.089
        H+             4.445e-013  3.805e-013  -12.352  -12.420   -0.068
        H2O            5.551e+001  9.991e-001    1.744   -0.000    0.000
```

```
Ca            1.803e-002
        Ca+2           1.474e-002  7.067e-003    -1.832    -2.151    -0.319
        CaHO+          3.295e-003  2.716e-003    -2.482    -2.566    -0.084
        CaSiH3O4+       3.569e-008  2.942e-008    -7.447    -7.531    -0.084
H(0)          3.251e-039
        H2             1.626e-039  1.644e-039   -38.789   -38.784     0.005
O(0)          4.348e-015
        O2             2.174e-015  2.198e-015   -14.663   -14.658     0.005
Si            6.765e-007
        SiH3O4-         5.392e-007  4.445e-007    -6.268    -6.352    -0.084
        SiH2O4-2        1.010e-007  4.662e-008    -6.996    -7.331    -0.336
        CaSiH3O4+       3.569e-008  2.942e-008    -7.447    -7.531    -0.084
        H4SiO4          6.891e-010  6.967e-010    -9.162    -9.157     0.005

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -5.72   -9.16   -3.43  SiO2
        b-Cristobalite   -6.17   -9.16   -2.98  SiO2
        Ca(OH)2         -0.02   22.69   22.71  Ca(OH)2
        Chalcedony       -5.42   -9.16   -3.74  SiO2
        CSH(0.1)         -5.82   -6.89   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -5.18   -4.62    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -4.58   -2.35    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.99   -0.08    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -3.41    2.19    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.86    4.46    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -2.32    6.73    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.82    8.99   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.69    9.74   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -1.55   12.52   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.98   13.53   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.62   14.36   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.38   15.06   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.22   15.65   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.12   16.15   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.06   16.58   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.02   16.97   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)          0.00   17.30   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)          0.00   17.60   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.67  -35.68   -0.00  H2
        Lime            -9.87   22.69   32.56  CaO
        O2             -11.77   71.35   83.13  O2
        Quartz          -5.13   -9.16   -4.03  SiO2
        SiO2(am)        -6.52   -9.16   -2.64  Si1.000O2.000
        Wollastonite    -0.25   13.53   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 19.
------------------------------------

-----------
End of run.
-----------
```

付録- 2　Atkinson モデルから導いた解離式及び log K を用いて C-S-H ゲルの溶解／沈殿反応を PHREEQC で計算した結果（アウトプット）　JNC-TDB (1) ケース

```
Input file: Atkinson Model JNCtdb(1) Input.pqi
Output file: Atkinson Model JNCtdb(1) Input.pqo
Database file: spron_phc_kai.txt

------------------
Reading data base.
------------------

        SOLUTION_MASTER_SPECIES
        SOLUTION_SPECIES
        PHASES
        END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

        DATABASE: spron_phc_kai.txt
        Title C-S-H dissolution using data from Atkinson model - case:JNCtdb(1)
        PHASES
        CSH(0.1)
            Ca 0.100 Si 1.000 O 2.100 : 0.110 H2O = 0.100 Ca+2 + 1.000 H4SiO4 -1.790 H2O - 0.200 H+
            log_K -1.132
        CSH(0.2)
            Ca 0.200 Si 1.000 O 2.200 : 0.220 H2O = 0.200 Ca+2 + 1.000 H4SiO4 -1.580 H2O - 0.400 H+
            log_K 0.512
        CSH(0.3)
            Ca 0.300 Si 1.000 O 2.300 : 0.330 H2O = 0.300 Ca+2 + 1.000 H4SiO4 -1.370 H2O - 0.600 H+
            log_K 2.181
        CSH(0.4)
            Ca 0.400 Si 1.000 O 2.400 : 0.440 H2O = 0.400 Ca+2 + 1.000 H4SiO4 -1.160 H2O - 0.800 H+
            log_K 3.868
        CSH(0.5)
            Ca 0.500 Si 1.000 O 2.500 : 0.550 H2O = 0.500 Ca+2 + 1.000 H4SiO4 -0.950 H2O - 1.000 H+
            log_K 5.569
        CSH(0.6)
            Ca 0.600 Si 1.000 O 2.600 : 0.661 H2O = 0.600 Ca+2 + 1.000 H4SiO4 -0.739 H2O - 1.200 H+
            log_K 7.288
        CSH(0.7)
            Ca 0.700 Si 1.000 O 2.700 : 0.771 H2O = 0.700 Ca+2 + 1.000 H4SiO4 -0.529 H2O - 1.400 H+
            log_K 9.027
        CSH(0.8)
            Ca 0.800 Si 1.000 O 2.800 : 0.881 H2O = 0.800 Ca+2 + 1.000 H4SiO4 -0.319 H2O - 1.600 H+
            log_K 10.809
        CSH(0.9)
            Ca 1.000 Si 1.111 O 3.222 : 1.093 H2O = 1.000 Ca+2 + 1.111 H4SiO4 -0.129 H2O - 2.000 H+
            log_K 14.051
        CSH(1.0)
            Ca 1.000 Si 1.000 O 3.000 : 1.084 H2O = 1.000 Ca+2 + 1.000 H4SiO4 + 0.084 H2O - 2.000 H+
            log_K 14.504
        CSH(1.1)
            Ca 1.000 Si 0.909 O 2.818 : 1.076 H2O = 1.000 Ca+2 + 0.909 H4SiO4 + 0.258 H2O - 2.000 H+
            log_K 14.974
        CSH(1.2)
            Ca 1.000 Si 0.833 O 2.666 : 1.070 H2O = 1.000 Ca+2 + 0.833 H4SiO4 + 0.404 H2O - 2.000 H+
            log_K 15.430
        CSH(1.3)
            Ca 1.000 Si 0.769 O 2.538 : 1.065 H2O = 1.000 Ca+2 + 0.769 H4SiO4 + 0.527 H2O - 2.000 H+
            log_K 15.861
        CSH(1.4)
            Ca 1.000 Si 0.714 O 2.428 : 1.060 H2O = 1.000 Ca+2 + 0.714 H4SiO4 + 0.632 H2O - 2.000 H+
            log_K 16.263
        CSH(1.5)
            Ca 1.000 Si 0.667 O 2.334 : 1.056 H2O = 1.000 Ca+2 + 0.667 H4SiO4 + 0.722 H2O - 2.000 H+
            log_K 16.635
        CSH(1.6)
            Ca 1.000 Si 0.625 O 2.250 : 1.053 H2O = 1.000 Ca+2 + 0.625 H4SiO4 + 0.803 H2O - 2.000 H+
            log_K 16.978
        CSH(1.7)
            Ca 1.000 Si 0.588 O 2.176 : 1.049 H2O = 1.000 Ca+2 + 0.588 H4SiO4 + 0.873 H2O - 2.000 H+
            log_K 17.296
```

```
        CSH(1.8)
            Ca 1.000 Si 0.556 O 2.112 : 1.047 H2O = 1.000 Ca+2 + 0.556 H4SiO4 + 0.935 H2O - 2.000 H+
            log_K 17.589
        SiO2(am)
            Si 1.000 O 2.000 = 1.000 H4SiO4 - 2.000 H2O
            log_K -2.706
        CSH(0.833)
            Ca 0.833 Si 1.000 O 2.833 : 0.917 H2O = 0.833 Ca+2 + 1.000 H4SiO4 -0.250 H2O - 1.666 H+
           log_K 11.428
        Ca(OH)2
            Ca(OH)2 = Ca+2 + 2H2O - 2 H+
            log_k 22.703
        Title 1 CSH(0.1)
        SOLUTION 1 DW
        units mol/L
        pH 7
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  1
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 2
        END
-----
TITLE
-----

 1 CSH(0.1)

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.       DW

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Pure water

----------------------------Description of solution----------------------------

                                pH =   7.000
                                pe =   4.000
                  Activity of water =   1.000
                     Ionic strength =  1.009e-007
                 Mass of water (kg) =  1.000e+000
            Total alkalinity (eq/kg) =  1.715e-009
               Total carbon (mol/kg) =  0.000e+000
                  Total CO2 (mol/kg) =  0.000e+000
                 Temperature (deg C) =  25.000
           Electrical balance (eq)  = -1.715e-009
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.85
                         Iterations  =   0
                           Total H  = 1.110124e+002
                           Total O  = 5.550622e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.018e-007  1.017e-007   -6.992   -6.993   -0.000
        H+             1.001e-007  1.000e-007   -7.000   -7.000   -0.000
        H2O            5.551e+001  1.000e+000    1.744    0.000    0.000
H(0)          1.565e-025
        H2             7.823e-026  7.823e-026  -25.107  -25.107    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -42.012  -42.012    0.000

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        H2            -22.00  -22.00   -0.00  H2
        O2            -39.13   44.00   83.13  O2

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -6.96   15.74   22.70 0.000e+000          0.000e+000
        CSH(0.1)        -0.00   -1.13   -1.13 1.000e+000 9.923e-001-7.707e-003
        CSH(0.2)        -0.07    0.44    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -0.17    2.02    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -0.28    3.59    3.87 0.000e+000          0.000e+000
        CSH(0.5)        -0.41    5.16    5.57 0.000e+000          0.000e+000
        CSH(0.6)        -0.55    6.74    7.29 0.000e+000          0.000e+000
        CSH(0.7)        -0.72    8.31    9.03 0.000e+000          0.000e+000
        CSH(0.8)        -0.92    9.89   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -1.02   10.41   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -1.32   12.73   14.05 0.000e+000          0.000e+000
        CSH(1.0)        -1.47   13.03   14.50 0.000e+000          0.000e+000
        CSH(1.1)        -1.69   13.28   14.97 0.000e+000          0.000e+000
        CSH(1.2)        -1.94   13.49   15.43 0.000e+000          0.000e+000
        CSH(1.3)        -2.20   13.66   15.86 0.000e+000          0.000e+000
        CSH(1.4)        -2.46   13.81   16.26 0.000e+000          0.000e+000
        CSH(1.5)        -2.70   13.94   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -2.93   14.05   16.98 0.000e+000          0.000e+000
        CSH(1.7)        -3.15   14.15   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -3.35   14.24   17.59 0.000e+000          0.000e+000
        SiO2(am)         0.00   -2.71   -2.71 0.000e+000 4.232e-003 4.232e-003

-----------------------------Solution composition-----------------------------

        Elements         Molality     Moles

        Ca             7.708e-004  7.707e-004
        Si             3.476e-003  3.475e-003

----------------------------Description of solution---------------------------

                                pH  =   9.474     Charge balance
```

```
                                pe =  8.422     Adjusted to redox equilibrium
                     Activity of water =  1.000
                        Ionic strength =  2.295e-003
                    Mass of water (kg) =  9.999e-001
               Total alkalinity (eq/kg) =  1.542e-003
                  Total carbon (mol/kg) =  0.000e+000
                     Total CO2 (mol/kg) =  0.000e+000
                   Temperature (deg C) =  25.000
                Electrical balance (eq) = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.00
                          Iterations =  15
                             Total H  = 1.110141e+002
                             Total O  = 5.551479e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
         Species          Molality    Activity Molality Activity    Gamma

         HO-            3.196e-005  3.030e-005   -4.495   -4.518   -0.023
         H+             3.525e-010  3.356e-010   -9.453   -9.474   -0.021
         H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca            7.708e-004
         Ca+2           7.618e-004  6.191e-004   -3.118   -3.208   -0.090
         CaSiH3O4+       8.698e-006  8.251e-006   -5.061   -5.083   -0.023
         CaHO+          2.846e-007  2.699e-007   -6.546   -6.569   -0.023
H(0)          2.522e-039
         H2             1.261e-039  1.261e-039  -38.899  -38.899    0.000
O(0)          7.470e-015
         O2             3.735e-015  3.737e-015  -14.428  -14.427    0.000
Si            3.476e-003
         H4SiO4          1.967e-003  1.968e-003   -2.706   -2.706    0.000
         SiH3O4-         1.500e-003  1.423e-003   -2.824   -2.847   -0.023
         CaSiH3O4+       8.698e-006  8.251e-006   -5.061   -5.083   -0.023
         SiH2O4-2        2.090e-007  1.692e-007   -6.680   -6.772   -0.092

------------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite    0.73  -2.71  -3.43  SiO2
         b-Cristobalite    0.28  -2.71  -2.98  SiO2
         Ca(OH)2         -6.96   15.74   22.70  Ca(OH)2
         Chalcedony       1.03  -2.71  -3.74  SiO2
         CSH(0.1)        -0.00  -1.13  -1.13  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)        -0.07   0.44   0.51  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)        -0.17   2.02   2.18  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)        -0.28   3.59   3.87  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)        -0.41   5.16   5.57  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)        -0.55   6.74   7.29  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)        -0.72   8.31   9.03  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)        -0.92   9.89  10.81  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)      -1.02  10.41  11.43  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)        -1.32  12.73  14.05  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)        -1.47  13.03  14.50  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)        -1.69  13.28  14.97  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)        -1.94  13.49  15.43  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)        -2.20  13.66  15.86  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)        -2.46  13.81  16.26  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)        -2.70  13.94  16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)        -2.93  14.05  16.98  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)        -3.15  14.15  17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)        -3.35  14.24  17.59  Ca1.000Si0.556O2.112:1.047H2O
         H2            -35.79 -35.79  -0.00  H2
         Lime          -16.82  15.74  32.56  CaO
         O2            -11.54  71.58  83.13  O2
         Quartz          1.32  -2.71  -4.03  SiO2
         SiO2(am)        0.00  -2.71  -2.71  Si1.000O2.000
         Wollastonite    -0.75  13.03  13.78  CaSiO3

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```

```
End of simulation.
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------------------------------------
Reading input data for simulation 2.
------------------------------------

        Title 2 CSH(0.2)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  1
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 3
        END
-----
TITLE
-----

 2 CSH(0.2)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -6.26   16.44   22.70 0.000e+000          0.000e+000
        CSH(0.1)        0.00   -1.13   -1.13 0.000e+000 4.105e-003 4.105e-003
        CSH(0.2)        0.00    0.51    0.51 1.000e+000 9.918e-001-8.161e-003
        CSH(0.3)       -0.02    2.16    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.07    3.80    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.13    5.44    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.20    7.09    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.30    8.73    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.43   10.38   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.51   10.92   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.70   13.36   14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.84   13.66   14.50 0.000e+000          0.000e+000
        CSH(1.1)       -1.06   13.92   14.97 0.000e+000          0.000e+000
        CSH(1.2)       -1.30   14.13   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -1.56   14.31   15.86 0.000e+000          0.000e+000
        CSH(1.4)       -1.81   14.46   16.26 0.000e+000          0.000e+000
        CSH(1.5)       -2.05   14.59   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -2.27   14.71   16.98 0.000e+000          0.000e+000
```

```
        CSH(1.7)        -2.49   14.81   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -2.69   14.90   17.59 0.000e+000          0.000e+000
        SiO2(am)        -0.07   -2.78   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.222e-003  1.222e-003
        Si             4.056e-003  4.056e-003

----------------------------Description of solution----------------------------

                                pH  =   9.736     Charge balance
                                pe  =   8.063     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.623e-003
                      Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  2.444e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  =  94
                            Total H  = 1.110151e+002
                            Total O  = 5.551689e+001

---------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            5.914e-005  5.536e-005   -4.228   -4.257   -0.029
        H+             1.951e-010  1.837e-010   -9.710   -9.736   -0.026
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.222e-003
        Ca+2           1.200e-003  9.297e-004   -2.921   -3.032   -0.111
        CaSiH3O4+       2.057e-005  1.927e-005   -4.687   -4.715   -0.028
        CaHO+          7.905e-007  7.405e-007   -6.102   -6.130   -0.028
H(0)         3.943e-039
        H2             1.972e-039  1.973e-039  -38.705  -38.705    0.000
O(0)         3.052e-015
        O2             1.526e-015  1.527e-015  -14.816  -14.816    0.000
Si           4.056e-003
        SiH3O4-         2.362e-003  2.213e-003   -2.627   -2.655   -0.028
        H4SiO4         1.673e-003  1.675e-003   -2.776   -2.776    0.000
        CaSiH3O4+       2.057e-005  1.927e-005   -4.687   -4.715   -0.028
        SiH2O4-2        6.241e-007  4.806e-007   -6.205   -6.318   -0.113

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.66   -2.78   -3.43  SiO2
        b-Cristobalite    0.21   -2.78   -2.98  SiO2
        Ca(OH)2         -6.26   16.44   22.70  Ca(OH)2
        Chalcedony       0.96   -2.78   -3.74  SiO2
        CSH(0.1)         0.00   -1.13   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         0.00    0.51    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.02    2.16    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.07    3.80    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.13    5.44    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.20    7.09    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.30    8.73    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.43   10.38   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.51   10.92   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.70   13.36   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.84   13.66   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -1.06   13.92   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -1.30   14.13   15.43  Ca1.000Si0.833O2.666:1.070H2O
```

```
        CSH(1.3)        -1.56   14.31   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -1.81   14.46   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -2.05   14.59   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -2.27   14.71   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -2.49   14.81   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -2.69   14.90   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.59  -35.60   -0.00  H2
        Lime          -16.12   16.44   32.56  CaO
        O2            -11.93   71.20   83.13  O2
        Quartz          1.25   -2.78   -4.03  SiO2
        SiO2(am)       -0.07   -2.78   -2.71  Si1.000O2.000
        Wollastonite    -0.12   13.66   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 3.
------------------------------------

        Title 3 CSH(0.3)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  1
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 4
        END
-----
TITLE
-----

 3 CSH(0.3)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

WARNING: Maximum iterations exceeded, 200

Numerical method failed with this set of convergence parameters.
WARNING: Trying diagonal scaling ...

Using solution 1.DW
Using pure phase assemblage 1.
```

```
-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -6.01   16.69   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -0.03   -1.16   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.00    0.51    0.51 0.000e+000 1.302e-003 1.302e-003
        CSH(0.3)       -0.00    2.18    2.18 1.000e+000 9.945e-001-5.487e-003
        CSH(0.4)       -0.02    3.85    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.05    5.52    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.10    7.19    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.17    8.86    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.28   10.53   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.35   11.08   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.50   13.55   14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.64   13.86   14.50 0.000e+000          0.000e+000
        CSH(1.1)       -0.85   14.12   14.97 0.000e+000          0.000e+000
        CSH(1.2)       -1.09   14.34   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -1.34   14.52   15.86 0.000e+000          0.000e+000
        CSH(1.4)       -1.59   14.67   16.26 0.000e+000          0.000e+000
        CSH(1.5)       -1.83   14.81   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -2.05   14.92   16.98 0.000e+000          0.000e+000
        CSH(1.7)       -2.27   15.03   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -2.47   15.12   17.59 0.000e+000          0.000e+000
        SiO2(am)       -0.12   -2.83   -2.71 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.386e-003  1.386e-003
        Si             4.186e-003  4.186e-003

-----------------------------Description of solution-----------------------------

                                pH  =   9.837     Charge balance
                                pe  =   8.049     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.105e-003
                   Mass of water (kg)  =  9.999e-001
               Total alkalinity (eq/kg)  =  2.772e-003
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  75
                              Total H  = 1.110155e+002
                              Total O  = 5.551750e+001

----------------------------Distribution of species----------------------------

                                            Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            7.497e-005  6.990e-005   -4.125   -4.156   -0.030
        H+             1.550e-010  1.455e-010   -9.810   -9.837   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.386e-003
        Ca+2           1.359e-003  1.037e-003   -2.867   -2.984   -0.117
        CaSiH3O4+       2.592e-005  2.418e-005   -4.586   -4.616   -0.030
        CaHO+          1.118e-006  1.043e-006   -5.952   -5.982   -0.030
H(0)         2.646e-039
        H2             1.323e-039  1.324e-039  -38.878  -38.878    0.000
O(0)         6.775e-015
        O2             3.388e-015  3.391e-015  -14.470  -14.470    0.000
Si           4.186e-003
        SiH3O4-         2.668e-003  2.490e-003   -2.574   -2.604   -0.030
        H4SiO4         1.491e-003  1.493e-003   -2.826   -2.826    0.000
```

```
        CaSiH3O4+       2.592e-005  2.418e-005   -4.586   -4.616   -0.030
        SiH2O4-2        9.006e-007  6.830e-007   -6.045   -6.166   -0.120

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.61   -2.83   -3.43  SiO2
        b-Cristobalite    0.16   -2.83   -2.98  SiO2
        Ca(OH)2          -6.01   16.69   22.70  Ca(OH)2
        Chalcedony        0.91   -2.83   -3.74  SiO2
        CSH(0.1)         -0.03   -1.16   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -0.00    0.51    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.00    2.18    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.02    3.85    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.05    5.52    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.10    7.19    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.17    8.86    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.28   10.53   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.35   11.08   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.50   13.55   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.64   13.86   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.85   14.12   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -1.09   14.34   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -1.34   14.52   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -1.59   14.67   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -1.83   14.81   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -2.05   14.92   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -2.27   15.03   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -2.47   15.12   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.77  -35.77   -0.00  H2
        Lime           -15.87   16.69   32.56  CaO
        O2             -11.58   71.54   83.13  O2
        Quartz           1.20   -2.83   -4.03  SiO2
        SiO2(am)        -0.12   -2.83   -2.71  Si1.000O2.000
        Wollastonite     0.08   13.86   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 4.
------------------------------------

        Title 4 CSH(0.4)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  1
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 5
        END
```

```
-----
TITLE
-----

 4 CSH(0.4)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -5.69   17.01   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -0.10   -1.24   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.05    0.47    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.01    2.17    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.00    3.87    3.87 1.000e+000 9.948e-001-5.248e-003
        CSH(0.5)       -0.00    5.57    5.57 0.000e+000 1.169e-003 1.169e-003
        CSH(0.6)       -0.02    7.27    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.06    8.97    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.14   10.67   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.19   11.23   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.30   13.75   14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.43   14.07   14.50 0.000e+000          0.000e+000
        CSH(1.1)       -0.63   14.34   14.97 0.000e+000          0.000e+000
        CSH(1.2)       -0.87   14.56   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -1.11   14.75   15.86 0.000e+000          0.000e+000
        CSH(1.4)       -1.35   14.91   16.26 0.000e+000          0.000e+000
        CSH(1.5)       -1.58   15.05   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -1.80   15.18   16.98 0.000e+000          0.000e+000
        CSH(1.7)       -2.01   15.28   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -2.21   15.38   17.59 0.000e+000          0.000e+000
        SiO2(am)       -0.23   -2.94   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.515e-003  1.515e-003
        Si             4.079e-003  4.079e-003

----------------------------Description of solution----------------------------

                                pH  =   9.981     Charge balance
                                pe  =   7.947     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.481e-003
                    Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  3.029e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                            Iterations  =  15
                               Total H  = 1.110158e+002
                               Total O  = 5.551755e+001

---------------------------Distribution of species----------------------------

                                            Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma
```

```
        HO-            1.046e-004  9.726e-005   -3.980   -4.012   -0.032
        H+             1.117e-010  1.046e-010   -9.952   -9.981   -0.028
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.515e-003
        Ca+2           1.483e-003  1.119e-003   -2.829   -2.951   -0.122
        CaSiH3O4+       3.029e-005  2.819e-005   -4.519   -4.550   -0.031
        CaHO+          1.683e-006  1.566e-006   -5.774   -5.805   -0.031
H(0)         2.182e-039
        H2             1.091e-039  1.092e-039  -38.962  -38.962    0.000
O(0)         9.963e-015
        O2             4.981e-015  4.987e-015  -14.303  -14.302    0.000
Si           4.079e-003
        SiH3O4-         2.890e-003  2.689e-003   -2.539   -2.570   -0.031
        H4SiO4         1.157e-003  1.159e-003   -2.937   -2.936    0.000
        CaSiH3O4+       3.029e-005  2.819e-005   -4.519   -4.550   -0.031
        SiH2O4-2        1.369e-006  1.026e-006   -5.864   -5.989   -0.125

-----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   0.50  -2.94  -3.43  SiO2
        b-Cristobalite   0.05  -2.94  -2.98  SiO2
        Ca(OH)2        -5.69  17.01  22.70  Ca(OH)2
        Chalcedony      0.80  -2.94  -3.74  SiO2
        CSH(0.1)       -0.10  -1.24  -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)       -0.05   0.47   0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)       -0.01   2.17   2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)       -0.00   3.87   3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)       -0.00   5.57   5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)       -0.02   7.27   7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)       -0.06   8.97   9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)       -0.14  10.67  10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)     -0.19  11.23  11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)       -0.30  13.75  14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)       -0.43  14.07  14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)       -0.63  14.34  14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)       -0.87  14.56  15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)       -1.11  14.75  15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)       -1.35  14.91  16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)       -1.58  15.05  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)       -1.80  15.18  16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)       -2.01  15.28  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)       -2.21  15.38  17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2           -35.85 -35.86  -0.00  H2
        Lime         -15.55  17.01  32.56  CaO
        O2           -11.42  71.71  83.13  O2
        Quartz         1.09  -2.94  -4.03  SiO2
        SiO2(am)       -0.23  -2.94  -2.71  Si1.000O2.000
        Wollastonite    0.29  14.07  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 5.
------------------------------------

        Title 5 CSH(0.5)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  1
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
```

```
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 6
        END
-----
TITLE
-----

 5 CSH(0.5)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -5.51   17.19   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -0.18   -1.31   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.10    0.41    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.05    2.13    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.02    3.85    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.00    5.57    5.57 1.000e+000 9.921e-001-7.898e-003
        CSH(0.6)        0.00    7.29    7.29 0.000e+000 4.043e-003 4.043e-003
        CSH(0.7)       -0.02    9.01    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.08   10.73   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.13   11.29   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.22   13.83   14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.34   14.16   14.50 0.000e+000          0.000e+000
        CSH(1.1)       -0.53   14.44   14.97 0.000e+000          0.000e+000
        CSH(1.2)       -0.76   14.67   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -1.00   14.86   15.86 0.000e+000          0.000e+000
        CSH(1.4)       -1.23   15.03   16.26 0.000e+000          0.000e+000
        CSH(1.5)       -1.46   15.17   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -1.68   15.30   16.98 0.000e+000          0.000e+000
        CSH(1.7)       -1.89   15.41   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -2.08   15.51   17.59 0.000e+000          0.000e+000
        SiO2(am)       -0.32   -3.03   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca            1.524e-003  1.524e-003
        Si            3.856e-003  3.856e-003

----------------------------Description of solution----------------------------

                                pH  =  10.069     Charge balance
                                pe  =   7.810     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.508e-003
                    Mass of water (kg)  =  9.999e-001
               Total alkalinity (eq/kg)  =  3.047e-003
```

```
                Total carbon (mol/kg)  =  0.000e+000
                  Total CO2 (mol/kg)  =  0.000e+000
                Temperature (deg C)  =  25.000
              Electrical balance (eq)  = -1.713e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                        Iterations  =  53
                          Total H  = 1.110158e+002
                          Total O  = 5.551712e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            1.284e-004  1.194e-004   -3.891   -3.923   -0.032
        H+             9.100e-011  8.521e-011  -10.041  -10.069   -0.029
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.524e-003
        Ca+2           1.491e-003  1.125e-003   -2.826   -2.949   -0.122
        CaSiH3O4+       3.038e-005  2.826e-005   -4.517   -4.549   -0.031
        CaHO+          2.076e-006  1.932e-006   -5.683   -5.714   -0.031
H(0)         2.725e-039
        H2             1.362e-039  1.364e-039  -38.866  -38.865    0.000
O(0)         6.389e-015
        O2             3.194e-015  3.198e-015  -14.496  -14.495    0.000
Si           3.856e-003
        SiH3O4-         2.883e-003  2.682e-003   -2.540   -2.571   -0.031
        H4SiO4          9.407e-004  9.417e-004   -3.027   -3.026    0.000
        CaSiH3O4+       3.038e-005  2.826e-005   -4.517   -4.549   -0.031
        SiH2O4-2        1.677e-006  1.256e-006   -5.776   -5.901   -0.125

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.41   -3.03   -3.43  SiO2
        b-Cristobalite   -0.04   -3.03   -2.98  SiO2
        Ca(OH)2         -5.51   17.19   22.70  Ca(OH)2
        Chalcedony       0.71   -3.03   -3.74  SiO2
        CSH(0.1)        -0.18   -1.31   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.10    0.41    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.05    2.13    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.02    3.85    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.00    5.57    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         0.00    7.29    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.02    9.01    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.08   10.73   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.13   11.29   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.22   13.83   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.34   14.16   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.53   14.44   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.76   14.67   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -1.00   14.86   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -1.23   15.03   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -1.46   15.17   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -1.68   15.30   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.89   15.41   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -2.08   15.51   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.76  -35.76   -0.00  H2
        Lime          -15.37   17.19   32.56  CaO
        O2            -11.61   71.52   83.13  O2
        Quartz          1.00   -3.03   -4.03  SiO2
        SiO2(am)       -0.32   -3.03   -2.71  Si1.000O2.000
        Wollastonite     0.38   14.16   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 6.
```

```
        Title 6 CSH(0.6)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  1
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 7
        END
-----
TITLE
-----

 6 CSH(0.6)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase              SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -5.31   17.39   22.70 0.000e+000          0.000e+000
        CSH(0.1)        -0.27   -1.41   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        -0.18    0.33    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -0.11    2.07    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -0.06    3.81    3.87 0.000e+000          0.000e+000
        CSH(0.5)        -0.02    5.55    5.57 0.000e+000          0.000e+000
        CSH(0.6)         0.00    7.29    7.29 1.000e+000 9.902e-001-9.776e-003
        CSH(0.7)         0.00    9.03    9.03 0.000e+000 6.252e-003 6.252e-003
        CSH(0.8)        -0.04   10.77   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -0.09   11.34   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.16   13.89   14.05 0.000e+000          0.000e+000
        CSH(1.0)        -0.26   14.24   14.50 0.000e+000          0.000e+000
        CSH(1.1)        -0.44   14.53   14.97 0.000e+000          0.000e+000
        CSH(1.2)        -0.66   14.77   15.43 0.000e+000          0.000e+000
        CSH(1.3)        -0.89   14.97   15.86 0.000e+000          0.000e+000
        CSH(1.4)        -1.12   15.14   16.26 0.000e+000          0.000e+000
        CSH(1.5)        -1.34   15.29   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -1.55   15.42   16.98 0.000e+000          0.000e+000
        CSH(1.7)        -1.76   15.54   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.95   15.64   17.59 0.000e+000          0.000e+000
        SiO2(am)        -0.44   -3.15   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------
```

```
        Elements         Molality     Moles

        Ca            1.489e-003  1.489e-003
        Si            3.524e-003  3.523e-003

----------------------------Description of solution----------------------------

                                pH  =  10.174     Charge balance
                                pe  =   7.602     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.406e-003
                    Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  2.978e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.716e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  85
                             Total H  = 1.110157e+002
                             Total O  = 5.551639e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-           1.631e-004  1.518e-004   -3.787   -3.819   -0.031
        H+            7.152e-011  6.701e-011  -10.146  -10.174   -0.028
        H2O           5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.489e-003
        Ca+2          1.458e-003  1.103e-003   -2.836   -2.958   -0.121
        CaSiH3O4+      2.870e-005  2.672e-005   -4.542   -4.573   -0.031
        CaHO+         2.586e-006  2.408e-006   -5.587   -5.618   -0.031
H(0)         4.393e-039
        H2            2.197e-039  2.199e-039  -38.658  -38.658    0.000
O(0)         2.457e-015
        O2            1.229e-015  1.230e-015  -14.911  -14.910    0.000
Si           3.524e-003
        SiH3O4-        2.779e-003  2.588e-003   -2.556   -2.587   -0.031
        H4SiO4         7.136e-004  7.144e-004   -3.147   -3.146    0.000
        CaSiH3O4+      2.870e-005  2.672e-005   -4.542   -4.573   -0.031
        SiH2O4-2       2.051e-006  1.541e-006   -5.688   -5.812   -0.124

----------------------------Saturation indices---------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   0.29  -3.15  -3.43  SiO2
        b-Cristobalite  -0.16  -3.15  -2.98  SiO2
        Ca(OH)2        -5.31  17.39  22.70  Ca(OH)2
        Chalcedony      0.59  -3.15  -3.74  SiO2
        CSH(0.1)       -0.27  -1.41  -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)       -0.18   0.33   0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)       -0.11   2.07   2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)       -0.06   3.81   3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)       -0.02   5.55   5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        0.00   7.29   7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        0.00   9.03   9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)       -0.04  10.77  10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)     -0.09  11.34  11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)       -0.16  13.89  14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)       -0.26  14.24  14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)       -0.44  14.53  14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)       -0.66  14.77  15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)       -0.89  14.97  15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)       -1.12  15.14  16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)       -1.34  15.29  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)       -1.55  15.42  16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)       -1.76  15.54  17.30  Ca1.000Si0.588O2.176:1.049H2O
```

```
        CSH(1.8)       -1.95   15.64   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.55  -35.55   -0.00  H2
        Lime          -15.17   17.39   32.56  CaO
        O2            -12.02   71.10   83.13  O2
        Quartz          0.88   -3.15   -4.03  SiO2
        SiO2(am)       -0.44   -3.15   -2.71  Si1.000O2.000
        Wollastonite    0.46   14.24   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 7.
-----------------------------------

        Title 7 CSH(0.7)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  1
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 8
        END
-----
TITLE
-----

 7 CSH(0.7)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.88   17.82   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -0.53   -1.66   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.39    0.12    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.28    1.90    2.18 0.000e+000          0.000e+000
```

```
        CSH(0.4)        -0.19    3.68    3.87 0.000e+000          0.000e+000
        CSH(0.5)        -0.11    5.46    5.57 0.000e+000          0.000e+000
        CSH(0.6)        -0.04    7.25    7.29 0.000e+000          0.000e+000
        CSH(0.7)        -0.00    9.03    9.03 1.000e+000 9.914e-001-8.629e-003
        CSH(0.8)        -0.00   10.81   10.81 0.000e+000 5.871e-003 5.871e-003
        CSH(0.833)      -0.03   11.40   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.06   13.99   14.05 0.000e+000          0.000e+000
        CSH(1.0)        -0.13   14.37   14.50 0.000e+000          0.000e+000
        CSH(1.1)        -0.29   14.69   14.97 0.000e+000          0.000e+000
        CSH(1.2)        -0.48   14.95   15.43 0.000e+000          0.000e+000
        CSH(1.3)        -0.69   15.17   15.86 0.000e+000          0.000e+000
        CSH(1.4)        -0.90   15.36   16.26 0.000e+000          0.000e+000
        CSH(1.5)        -1.11   15.52   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -1.31   15.67   16.98 0.000e+000          0.000e+000
        CSH(1.7)        -1.50   15.79   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.69   15.90   17.59 0.000e+000          0.000e+000
        SiO2(am)        -0.74   -3.45   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Ca             1.344e-003  1.344e-003
        Si             2.758e-003  2.758e-003

----------------------------Description of solution----------------------------

                                pH  =  10.408     Charge balance
                                pe  =   7.497     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.981e-003
                       Mass of water (kg)  =  9.999e-001
                 Total alkalinity (eq/kg)  =  2.687e-003
                    Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  53
                             Total H  = 1.110154e+002
                             Total O  = 5.551456e+001

---------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            2.789e-004  2.603e-004    -3.555    -3.585    -0.030
        H+             4.159e-011  3.907e-011   -10.381   -10.408    -0.027
        H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
Ca           1.344e-003
        Ca+2           1.317e-003  1.009e-003    -2.880    -2.996    -0.116
        CaSiH3O4+       2.245e-005  2.097e-005    -4.649    -4.678    -0.030
        CaHO+          4.045e-006  3.778e-006    -5.393    -5.423    -0.030
H(0)         2.418e-039
        H2             1.209e-039  1.210e-039   -38.918   -38.917     0.000
O(0)         8.117e-015
        O2             4.059e-015  4.062e-015   -14.392   -14.391     0.000
Si           2.758e-003
        SiH3O4-         2.376e-003  2.219e-003    -2.624    -2.654    -0.030
        H4SiO4         3.569e-004  3.572e-004    -3.447    -3.447     0.000
        CaSiH3O4+       2.245e-005  2.097e-005    -4.649    -4.678    -0.030
        SiH2O4-2        2.978e-006  2.267e-006    -5.526    -5.645    -0.118

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.01   -3.45   -3.43  SiO2
        b-Cristobalite   -0.47   -3.45   -2.98  SiO2
        Ca(OH)2         -4.88   17.82   22.70  Ca(OH)2
```

```
        Chalcedony       0.29   -3.45   -3.74  SiO2
        CSH(0.1)        -0.53   -1.66   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.39    0.12    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.28    1.90    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.19    3.68    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.11    5.46    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.04    7.25    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.00    9.03    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.00   10.81   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.03   11.40   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.06   13.99   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.13   14.37   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.29   14.69   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.48   14.95   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.69   15.17   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.90   15.36   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -1.11   15.52   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -1.31   15.67   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.50   15.79   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.69   15.90   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.81  -35.81   -0.00  H2
        Lime          -14.74   17.82   32.56  CaO
        O2            -11.50   71.62   83.13  O2
        Quartz          0.58   -3.45   -4.03  SiO2
        SiO2(am)       -0.74   -3.45   -2.71  Si1.000O2.000
        Wollastonite    0.59   14.37   13.78  CaSiO3

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End of simulation.
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Reading input data for simulation 8.
-----------------------------------

        Title 8 CSH(0.8)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  1
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 9
        END
-----
TITLE
-----

 8 CSH(0.8)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------
```

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca(OH)2	-4.34	18.37	22.70	0.000e+000	0.000e+000	
CSH(0.1)	-0.91	-2.05	-1.13	0.000e+000	0.000e+000	
CSH(0.2)	-0.72	-0.21	0.51	0.000e+000	0.000e+000	
CSH(0.3)	-0.55	1.63	2.18	0.000e+000	0.000e+000	
CSH(0.4)	-0.41	3.46	3.87	0.000e+000	0.000e+000	
CSH(0.5)	-0.27	5.30	5.57	0.000e+000	0.000e+000	
CSH(0.6)	-0.15	7.14	7.29	0.000e+000	0.000e+000	
CSH(0.7)	-0.05	8.97	9.03	0.000e+000	0.000e+000	
CSH(0.8)	0.00	10.81	10.81	1.000e+000	9.947e-001	-5.345e-003
CSH(0.833)	-0.01	11.42	11.43	0.000e+000	0.000e+000	
CSH(0.9)	-0.00	14.05	14.05	0.000e+000	3.118e-003	3.118e-003
CSH(1.0)	-0.02	14.48	14.50	0.000e+000	0.000e+000	
CSH(1.1)	-0.14	14.84	14.97	0.000e+000	0.000e+000	
CSH(1.2)	-0.30	15.13	15.43	0.000e+000	0.000e+000	
CSH(1.3)	-0.48	15.38	15.86	0.000e+000	0.000e+000	
CSH(1.4)	-0.67	15.59	16.26	0.000e+000	0.000e+000	
CSH(1.5)	-0.86	15.78	16.64	0.000e+000	0.000e+000	
CSH(1.6)	-1.04	15.94	16.98	0.000e+000	0.000e+000	
CSH(1.7)	-1.21	16.08	17.30	0.000e+000	0.000e+000	
CSH(1.8)	-1.38	16.21	17.59	0.000e+000	0.000e+000	
SiO2(am)	-1.18	-3.88	-2.71	0.000e+000	0.000e+000	

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Ca	1.158e-003	1.158e-003
Si	1.881e-003	1.881e-003

----------------------------Description of solution----------------------------

pH = 10.709 Charge balance
pe = 7.111 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 3.437e-003
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = 2.317e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.715e-009
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 42
Total H = 1.110150e+002
Total O = 5.551244e+001

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	5.549e-004	5.203e-004	-3.256	-3.284	-0.028
H+	2.073e-011	1.955e-011	-10.683	-10.709	-0.025
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
Ca	1.158e-003				
Ca+2	1.137e-003	8.859e-004	-2.944	-3.053	-0.108
CaSiH3O4+	1.437e-005	1.348e-005	-4.843	-4.870	-0.028
CaHO+	7.068e-006	6.632e-006	-5.151	-5.178	-0.028
H(0)	3.576e-039				
H2	1.788e-039	1.790e-039	-38.748	-38.747	0.000
O(0)	3.711e-015				

```
        O2            1.855e-015  1.857e-015   -14.732   -14.731    0.000
Si           1.881e-003
        SiH3O4-        1.732e-003  1.625e-003    -2.761    -2.789    -0.028
        H4SiO4         1.308e-004  1.309e-004    -3.883    -3.883     0.000
        CaSiH3O4+       1.437e-005  1.348e-005    -4.843    -4.870    -0.028
        SiH2O4-2        4.281e-006  3.318e-006    -5.368    -5.479    -0.111

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.45   -3.88   -3.43  SiO2
        b-Cristobalite   -0.90   -3.88   -2.98  SiO2
        Ca(OH)2         -4.34   18.37   22.70  Ca(OH)2
        Chalcedony       -0.14   -3.88   -3.74  SiO2
        CSH(0.1)         -0.91   -2.05   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -0.72   -0.21    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.55    1.63    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.41    3.46    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.27    5.30    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.15    7.14    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.05    8.97    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)          0.00   10.81   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.01   11.42   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.00   14.05   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.02   14.48   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.14   14.84   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.30   15.13   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.48   15.38   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.67   15.59   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.86   15.78   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -1.04   15.94   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -1.21   16.08   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -1.38   16.21   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2              -35.64  -35.64   -0.00  H2
        Lime            -14.20   18.37   32.56  CaO
        O2              -11.84   71.28   83.13  O2
        Quartz            0.15   -3.88   -4.03  SiO2
        SiO2(am)         -1.18   -3.88   -2.71  Si1.000O2.000
        Wollastonite      0.70   14.48   13.78  CaSiO3

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End of simulation.
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------------------------------------
Reading input data for simulation 9.
------------------------------------

        Title 9 CSH(0.9)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  1
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
```

```
        CSH(0.833) 0.0 0.0
        Ca(OH)2  0.0  0.0
        Save Solution 10
        END
-----
TITLE
-----

 9 CSH(0.9)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.12   18.59   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -1.09   -2.22   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.88   -0.36    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.69    1.49    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.52    3.35    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.36    5.21    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.22    7.07    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.10    8.93    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.02   10.79   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.03   11.40   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.00   14.05   14.05 1.000e+000 9.960e-001-3.975e-003
        CSH(1.0)       -0.00   14.50   14.50 0.000e+000 2.874e-003 2.874e-003
        CSH(1.1)       -0.10   14.88   14.97 0.000e+000          0.000e+000
        CSH(1.2)       -0.24   15.19   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -0.41   15.45   15.86 0.000e+000          0.000e+000
        CSH(1.4)       -0.59   15.67   16.26 0.000e+000          0.000e+000
        CSH(1.5)       -0.77   15.86   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.94   16.03   16.98 0.000e+000          0.000e+000
        CSH(1.7)       -1.11   16.19   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.27   16.32   17.59 0.000e+000          0.000e+000
        SiO2(am)       -1.38   -4.08   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.102e-003  1.102e-003
        Si             1.543e-003  1.543e-003

----------------------------Description of solution----------------------------

                                pH  =  10.829     Charge balance
                                pe  =   6.657     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.269e-003
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  2.204e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  17
                             Total H  = 1.110149e+002
                             Total O  = 5.551163e+001

---------------------------Distribution of species-----------------------------
```

```
                                        Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            7.298e-004  6.853e-004   -3.137   -3.164   -0.027
        H+             1.572e-011  1.484e-011  -10.804  -10.829   -0.025
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.102e-003
        Ca+2           1.081e-003  8.473e-004   -2.966   -3.072   -0.106
        CaSiH3O4+       1.146e-005  1.077e-005   -4.941   -4.968   -0.027
        CaHO+           8.892e-006  8.355e-006   -5.051   -5.078   -0.027
H(0)         1.674e-038
        H2             8.370e-039  8.377e-039  -38.077  -38.077    0.000
O(0)         1.694e-016
        O2             8.469e-017  8.475e-017  -16.072  -16.072    0.000
Si           1.543e-003
        SiH3O4-         1.444e-003  1.357e-003   -2.840   -2.867   -0.027
        H4SiO4          8.290e-005  8.296e-005   -4.081   -4.081    0.000
        CaSiH3O4+       1.146e-005  1.077e-005   -4.941   -4.968   -0.027
        SiH2O4-2        4.681e-006  3.649e-006   -5.330   -5.438   -0.108

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.65   -4.08   -3.43  SiO2
        b-Cristobalite   -1.10   -4.08   -2.98  SiO2
        Ca(OH)2         -4.12   18.59   22.70  Ca(OH)2
        Chalcedony       -0.34   -4.08   -3.74  SiO2
        CSH(0.1)         -1.09   -2.22   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -0.88   -0.36    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.69    1.49    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.52    3.35    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.36    5.21    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.22    7.07    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.10    8.93    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.02   10.79   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.03   11.40   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.00   14.05   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.00   14.50   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.10   14.88   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.24   15.19   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.41   15.45   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.59   15.67   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.77   15.86   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.94   16.03   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -1.11   16.19   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -1.27   16.32   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2             -34.97  -34.97   -0.00  H2
        Lime           -13.98   18.59   32.56  CaO
        O2             -13.19   69.94   83.13  O2
        Quartz           -0.05   -4.08   -4.03  SiO2
        SiO2(am)         -1.38   -4.08   -2.71  Si1.000O2.000
        Wollastonite      0.72   14.50   13.78  CaSiO3

------------------
End of simulation.
------------------

--------------------------------------
Reading input data for simulation 10.
--------------------------------------

        Title 10 CSH(1.0)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
```

```
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  1
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 11
        END
-----
TITLE
-----

 10 CSH(1.0)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase              SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -3.79   18.91   22.70 0.000e+000          0.000e+000
        CSH(0.1)        -1.38   -2.52   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        -1.14   -0.63    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -0.92    1.27    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -0.71    3.16    3.87 0.000e+000          0.000e+000
        CSH(0.5)        -0.52    5.05    5.57 0.000e+000          0.000e+000
        CSH(0.6)        -0.35    6.94    7.29 0.000e+000          0.000e+000
        CSH(0.7)        -0.20    8.83    9.03 0.000e+000          0.000e+000
        CSH(0.8)        -0.09   10.72   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -0.08   11.35   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.04   14.01   14.05 0.000e+000          0.000e+000
        CSH(1.0)         0.00   14.50   14.50 1.000e+000 9.989e-001-1.060e-003
        CSH(1.1)        -0.07   14.91   14.97 0.000e+000          0.000e+000
        CSH(1.2)        -0.19   15.24   15.43 0.000e+000          0.000e+000
        CSH(1.3)        -0.34   15.52   15.86 0.000e+000          0.000e+000
        CSH(1.4)        -0.50   15.76   16.26 0.000e+000          0.000e+000
        CSH(1.5)        -0.66   15.97   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.82   16.16   16.98 0.000e+000          0.000e+000
        CSH(1.7)        -0.98   16.32   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.13   16.46   17.59 0.000e+000          0.000e+000
        SiO2(am)        -1.70   -4.41   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.060e-003  1.060e-003
        Si             1.060e-003  1.060e-003

----------------------------Description of solution----------------------------

                                pH  =  11.000     Charge balance
                                pe  =   6.791     Adjusted to redox equilibrium
```

```
                    Activity of water =  1.000
                      Ionic strength =  3.143e-003
                   Mass of water (kg) =  1.000e+000
                Total alkalinity (eq/kg) =  2.119e-003
                  Total carbon (mol/kg) =  0.000e+000
                    Total CO2 (mol/kg) =  0.000e+000
                  Temperature (deg C) =  25.000
               Electrical balance (eq) = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.00
                         Iterations =  15
                           Total H  = 1.110147e+002
                           Total O  = 5.551054e+001

----------------------------Distribution of species-----------------------------

                                                Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            1.081e-003  1.016e-003    -2.966    -2.993    -0.027
         H+             1.059e-011  1.001e-011   -10.975   -11.000    -0.024
         H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
Ca            1.060e-003
         Ca+2           1.039e-003  8.177e-004    -2.983    -3.087    -0.104
         CaHO+          1.271e-005  1.196e-005    -4.896    -4.922    -0.027
         CaSiH3O4+       7.719e-006  7.261e-006    -5.112    -5.139    -0.027
H(0)          4.106e-039
         H2             2.053e-039  2.055e-039   -38.688   -38.687     0.000
O(0)          2.815e-015
         O2             1.408e-015  1.409e-015   -14.852   -14.851     0.000
Si            1.060e-003
         SiH3O4-         1.008e-003  9.481e-004    -2.997    -3.023    -0.027
         H4SiO4         3.906e-005  3.909e-005    -4.408    -4.408     0.000
         CaSiH3O4+       7.719e-006  7.261e-006    -5.112    -5.139    -0.027
         SiH2O4-2        4.828e-006  3.781e-006    -5.316    -5.422    -0.106

------------------------------Saturation indices--------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -0.97   -4.41   -3.43  SiO2
         b-Cristobalite   -1.43   -4.41   -2.98  SiO2
         Ca(OH)2         -3.79   18.91   22.70  Ca(OH)2
         Chalcedony       -0.67   -4.41   -3.74  SiO2
         CSH(0.1)         -1.38   -2.52   -1.13  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -1.14   -0.63    0.51  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -0.92    1.27    2.18  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -0.71    3.16    3.87  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -0.52    5.05    5.57  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -0.35    6.94    7.29  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -0.20    8.83    9.03  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -0.09   10.72   10.81  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -0.08   11.35   11.43  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)         -0.04   14.01   14.05  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)          0.00   14.50   14.50  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)         -0.07   14.91   14.97  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.19   15.24   15.43  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.34   15.52   15.86  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)         -0.50   15.76   16.26  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.66   15.97   16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -0.82   16.16   16.98  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)         -0.98   16.32   17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)         -1.13   16.46   17.59  Ca1.000Si0.556O2.112:1.047H2O
         H2             -35.58  -35.58   -0.00  H2
         Lime           -13.65   18.91   32.56  CaO
         O2             -11.96   71.16   83.13  O2
         Quartz           -0.38   -4.41   -4.03  SiO2
         SiO2(am)         -1.70   -4.41   -2.71  Si1.000O2.000
         Wollastonite      0.72   14.50   13.78  CaSiO3

------------------
End of simulation.
```

```
------------------

------------------------------------
Reading input data for simulation 11.
------------------------------------

        Title 11 CSH(1.1)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  1
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 12
        END
-----
TITLE
-----

 11 CSH(1.1)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                 Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -3.03   19.67   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -2.07   -3.20   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -1.74   -1.23    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -1.45    0.74    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -1.17    2.70    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.90    4.67    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.65    6.64    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.42    8.60    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.24   10.57   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.21   11.22   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.12   13.93   14.05 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.50   14.50 0.000e+000 9.422e-003 9.422e-003
        CSH(1.1)        0.00   14.97   14.97 1.000e+000 9.892e-001-1.080e-002
        CSH(1.2)       -0.06   15.37   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -0.16   15.70   15.86 0.000e+000          0.000e+000
        CSH(1.4)       -0.28   15.98   16.26 0.000e+000          0.000e+000
        CSH(1.5)       -0.41   16.22   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.54   16.44   16.98 0.000e+000          0.000e+000
        CSH(1.7)       -0.66   16.63   17.30 0.000e+000          0.000e+000
```

```
        CSH(1.8)        -0.79   16.80   17.59 0.000e+000          0.000e+000
        SiO2(am)        -2.46   -5.16   -2.71 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.377e-003  1.377e-003
        Si             3.943e-004  3.943e-004

----------------------------Description of solution---------------------------

                                pH  =  11.329     Charge balance
                                pe  =   6.603     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.059e-003
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.754e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  =  22
                            Total H  = 1.110152e+002
                            Total O  = 5.550979e+001

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            2.328e-003  2.172e-003   -2.633   -2.663   -0.030
        H+             4.987e-012  4.683e-012  -11.302  -11.329   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.377e-003
        Ca+2           1.339e-003  1.023e-003   -2.873   -2.990   -0.117
        CaHO+          3.425e-005  3.197e-005   -4.465   -4.495   -0.030
        CaSiH3O4+      3.640e-006  3.398e-006   -5.439   -5.469   -0.030
H(0)         2.129e-039
        H2             1.064e-039  1.065e-039  -38.973  -38.973    0.000
O(0)         1.047e-014
        O2             5.235e-015  5.240e-015  -14.281  -14.281    0.000
Si           3.943e-004
        SiH3O4-        3.798e-004  3.546e-004   -3.420   -3.450   -0.030
        H4SiO4         6.834e-006  6.841e-006   -5.165   -5.165    0.000
        SiH2O4-2       3.979e-006  3.021e-006   -5.400   -5.520   -0.120
        CaSiH3O4+      3.640e-006  3.398e-006   -5.439   -5.469   -0.030

----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -1.73   -5.16   -3.43  SiO2
        b-Cristobalite   -2.18   -5.16   -2.98  SiO2
        Ca(OH)2          -3.03   19.67   22.70  Ca(OH)2
        Chalcedony       -1.43   -5.16   -3.74  SiO2
        CSH(0.1)         -2.07   -3.20   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -1.74   -1.23    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -1.45    0.74    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -1.17    2.70    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.90    4.67    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.65    6.64    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.42    8.60    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.24   10.57   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.21   11.22   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.12   13.93   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)          0.00   14.50   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)          0.00   14.97   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.06   15.37   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.16   15.70   15.86  Ca1.000Si0.769O2.538:1.065H2O
```

```
        CSH(1.4)        -0.28   15.98   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.41   16.22   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.54   16.44   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.66   16.63   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.79   16.80   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.86  -35.87   -0.00  H2
        Lime           -12.89   19.67   32.56  CaO
        O2             -11.39   71.73   83.13  O2
        Quartz          -1.14   -5.16   -4.03  SiO2
        SiO2(am)        -2.46   -5.16   -2.71  Si1.000O2.000
        Wollastonite     0.72   14.50   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 12.
------------------------------------

        Title 12 CSH(1.2)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  1
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 13
        END
-----
TITLE
-----

 12 CSH(1.2)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase              SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -2.27   20.43   22.70 0.000e+000          0.000e+000
        CSH(0.1)        -2.83   -3.96   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        -2.43   -1.91    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -2.05    0.13    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -1.70    2.17    3.87 0.000e+000          0.000e+000
```

```
        CSH(0.5)        -1.35    4.21    5.57 0.000e+000          0.000e+000
        CSH(0.6)        -1.03    6.26    7.29 0.000e+000          0.000e+000
        CSH(0.7)        -0.73    8.30    9.03 0.000e+000          0.000e+000
        CSH(0.8)        -0.47   10.34   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -0.41   11.02   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.29   13.76   14.05 0.000e+000          0.000e+000
        CSH(1.0)        -0.08   14.43   14.50 0.000e+000          0.000e+000
        CSH(1.1)         0.00   14.97   14.97 0.000e+000 2.454e-002 2.454e-002
        CSH(1.2)         0.00   15.43   15.43 1.000e+000 9.731e-001-2.692e-002
        CSH(1.3)        -0.05   15.81   15.86 0.000e+000          0.000e+000
        CSH(1.4)        -0.12   16.14   16.26 0.000e+000          0.000e+000
        CSH(1.5)        -0.21   16.43   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.30   16.68   16.98 0.000e+000          0.000e+000
        CSH(1.7)        -0.40   16.90   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.50   17.09   17.59 0.000e+000          0.000e+000
        SiO2(am)        -3.29   -6.00   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             2.375e-003  2.375e-003
        Si             1.129e-004  1.129e-004

----------------------------Description of solution----------------------------

                                pH  =  11.610     Charge balance
                                pe  =   6.272     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  6.913e-003
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  4.750e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  37
                              Total H  = 1.110172e+002
                              Total O  = 5.551121e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            4.531e-003  4.145e-003   -2.344   -2.383   -0.039
        H+             2.654e-012  2.454e-012  -11.576  -11.610   -0.034
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           2.375e-003
        Ca+2           2.268e-003  1.614e-003   -2.644   -2.792   -0.148
        CaHO+          1.050e-004  9.622e-005   -3.979   -4.017   -0.038
        CaSiH3O4+       1.631e-006  1.495e-006   -5.787   -5.826   -0.038
H(0)         2.693e-039
        H2             1.347e-039  1.349e-039  -38.871  -38.870    0.001
O(0)         6.526e-015
        O2             3.263e-015  3.268e-015  -14.486  -14.486    0.001
Si           1.129e-004
        SiH3O4-         1.080e-004  9.890e-005   -3.967   -4.005   -0.038
        SiH2O4-2        2.283e-006  1.608e-006   -5.641   -5.794   -0.152
        CaSiH3O4+       1.631e-006  1.495e-006   -5.787   -5.826   -0.038
        H4SiO4          9.982e-007  9.998e-007   -6.001   -6.000    0.001

----------------------------Saturation indices---------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -2.57   -6.00   -3.43  SiO2
        b-Cristobalite   -3.02   -6.00   -2.98  SiO2
        Ca(OH)2         -2.27   20.43   22.70  Ca(OH)2
        Chalcedony       -2.26   -6.00   -3.74  SiO2
```

```
        CSH(0.1)        -2.83   -3.96   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -2.43   -1.91    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -2.05    0.13    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -1.70    2.17    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -1.35    4.21    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -1.03    6.26    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.73    8.30    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.47   10.34   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.41   11.02   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.29   13.76   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.08   14.43   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         0.00   14.97   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         0.00   15.43   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.05   15.81   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.12   16.14   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.21   16.43   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.30   16.68   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.40   16.90   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.50   17.09   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.76  -35.76   -0.00  H2
        Lime          -12.13   20.43   32.56  CaO
        O2            -11.60   71.53   83.13  O2
        Quartz         -1.97   -6.00   -4.03  SiO2
        SiO2(am)       -3.29   -6.00   -2.71  Si1.000O2.000
        Wollastonite    0.64   14.43   13.78  CaSiO3

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End of simulation.
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------------------------------------
Reading input data for simulation 13.
------------------------------------

        Title 13 CSH(1.3)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  1
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 14
        END
-----
TITLE
-----

 13 CSH(1.3)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.
```

```
Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -1.66   21.04   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -3.50   -4.63   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -3.04   -2.53    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -2.60   -0.42    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -2.19    1.68    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -1.78    3.79    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -1.40    5.89    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -1.03    7.99    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.71   10.10   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.64   10.79   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.49   13.56   14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.20   14.31   14.50 0.000e+000          0.000e+000
        CSH(1.1)       -0.06   14.92   14.97 0.000e+000          0.000e+000
        CSH(1.2)        0.00   15.43   15.43 0.000e+000 4.714e-002 4.714e-002
        CSH(1.3)        0.00   15.86   15.86 1.000e+000 9.489e-001-5.111e-002
        CSH(1.4)       -0.03   16.23   16.26 0.000e+000          0.000e+000
        CSH(1.5)       -0.09   16.55   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.15   16.83   16.98 0.000e+000          0.000e+000
        CSH(1.7)       -0.22   17.08   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.29   17.30   17.59 0.000e+000          0.000e+000
        SiO2(am)       -4.03   -6.73   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             3.970e-003  3.970e-003
        Si             3.570e-005  3.570e-005

----------------------------Description of solution----------------------------

                                pH  =  11.827     Charge balance
                                pe  =   6.031     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  1.138e-002
                      Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  7.940e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  61
                             Total H  = 1.110204e+002
                             Total O  = 5.551425e+001

---------------------------Distribution of species----------------------------

                                                Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            7.637e-003  6.831e-003   -2.117   -2.165   -0.048
        H+             1.637e-012  1.489e-012  -11.786  -11.827   -0.041
        H2O            5.551e+001  9.998e-001    1.744   -0.000    0.000
Ca           3.970e-003
        Ca+2           3.703e-003  2.429e-003   -2.431   -2.615   -0.183
        CaHO+          2.663e-004  2.388e-004   -3.575   -3.622   -0.047
        CaSiH3O4+       7.624e-007  6.836e-007   -6.118   -6.165   -0.047
H(0)         2.992e-039
        H2             1.496e-039  1.500e-039  -38.825  -38.824    0.001
O(0)         5.271e-015
        O2             2.636e-015  2.643e-015  -14.579  -14.578    0.001
```

```
Si           3.570e-005
        SiH3O4-        3.351e-005  3.005e-005   -4.475   -4.522   -0.047
        SiH2O4-2       1.246e-006  8.055e-007   -5.905   -6.094   -0.189
        CaSiH3O4+      7.624e-007  6.836e-007   -6.118   -6.165   -0.047
        H4SiO4         1.838e-007  1.843e-007   -6.736   -6.735    0.001

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -3.30  -6.73  -3.43  SiO2
        b-Cristobalite  -3.75  -6.73  -2.98  SiO2
        Ca(OH)2        -1.66  21.04  22.70  Ca(OH)2
        Chalcedony      -3.00  -6.73  -3.74  SiO2
        CSH(0.1)        -3.50  -4.63  -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -3.04  -2.53   0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -2.60  -0.42   2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -2.19   1.68   3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -1.78   3.79   5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -1.40   5.89   7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -1.03   7.99   9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.71  10.10  10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.64  10.79  11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.49  13.56  14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.20  14.31  14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.06  14.92  14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         0.00  15.43  15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         0.00  15.86  15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.03  16.23  16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.09  16.55  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.15  16.83  16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.22  17.08  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.29  17.30  17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.71 -35.72  -0.00  H2
        Lime          -11.52  21.04  32.56  CaO
        O2            -11.69  71.43  83.13  O2
        Quartz         -2.71  -6.73  -4.03  SiO2
        SiO2(am)       -4.03  -6.73  -2.71  Si1.000O2.000
        Wollastonite    0.52  14.31  13.78  CaSiO3

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End of simulation.
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------------------------------------
Reading input data for simulation 14.
------------------------------------

        Title 14 CSH(1.4)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  1
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
```

```
        Ca(OH)2   0.0  0.0
        Save Solution 15
        END
-----
TITLE
-----

 14 CSH(1.4)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -1.22  21.48  22.70 0.000e+000          0.000e+000
        CSH(0.1)       -4.03  -5.16  -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -3.52  -3.01   0.51 0.000e+000          0.000e+000
        CSH(0.3)       -3.05  -0.86   2.18 0.000e+000          0.000e+000
        CSH(0.4)       -2.58   1.28   3.87 0.000e+000          0.000e+000
        CSH(0.5)       -2.14   3.43   5.57 0.000e+000          0.000e+000
        CSH(0.6)       -1.71   5.58   7.29 0.000e+000          0.000e+000
        CSH(0.7)       -1.30   7.73   9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.93   9.88  10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.84  10.59  11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.69  13.36  14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.33  14.17  14.50 0.000e+000          0.000e+000
        CSH(1.1)       -0.14  14.84  14.97 0.000e+000          0.000e+000
        CSH(1.2)       -0.04  15.39  15.43 0.000e+000          0.000e+000
        CSH(1.3)        0.00  15.86  15.86 0.000e+000 7.580e-002 7.580e-002
        CSH(1.4)        0.00  16.26  16.26 1.000e+000 9.183e-001-8.166e-002
        CSH(1.5)       -0.03  16.61  16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.06  16.91  16.98 0.000e+000          0.000e+000
        CSH(1.7)       -0.11  17.18  17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.17  17.42  17.59 0.000e+000          0.000e+000
        SiO2(am)       -4.60  -7.31  -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             5.859e-003  5.859e-003
        Si             1.423e-005  1.423e-005

----------------------------Description of solution----------------------------

                                pH  =  11.984     Charge balance
                                pe  =   5.463     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.653e-002
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  1.172e-002
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.723e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  21
                             Total H  = 1.110241e+002
                             Total O  = 5.551794e+001

---------------------------Distribution of species----------------------------
```

```
                                                Log      Log       Log
          Species          Molality   Activity  Molality  Activity    Gamma

          HO-            1.118e-002  9.804e-003    -1.952    -2.009    -0.057
          H+             1.157e-012  1.037e-012   -11.937   -11.984    -0.047
          H2O            5.551e+001  9.997e-001     1.744    -0.000     0.000
Ca             5.859e-003
          Ca+2           5.336e-003  3.263e-003    -2.273    -2.486    -0.214
          CaHO+          5.230e-004  4.603e-004    -3.281    -3.337    -0.055
          CaSiH3O4+      3.987e-007  3.508e-007    -6.399    -6.455    -0.055
H(0)           1.984e-038
          H2             9.920e-039  9.958e-039   -38.003   -38.002     0.002
O(0)           1.194e-016
          O2             5.972e-017  5.995e-017   -16.224   -16.222     0.002
Si             1.423e-005
          SiH3O4-        1.304e-005  1.148e-005    -4.885    -4.940    -0.055
          SiH2O4-2       7.364e-007  4.417e-007    -6.133    -6.355    -0.222
          CaSiH3O4+      3.987e-007  3.508e-007    -6.399    -6.455    -0.055
          H4SiO4         4.887e-008  4.905e-008    -7.311    -7.309     0.002

-----------------------------Saturation indices-------------------------------

          Phase            SI log IAP  log KT

          a-Cristobalite   -3.88   -7.31   -3.43  SiO2
          b-Cristobalite   -4.33   -7.31   -2.98  SiO2
          Ca(OH)2          -1.22   21.48   22.70  Ca(OH)2
          Chalcedony       -3.57   -7.31   -3.74  SiO2
          CSH(0.1)         -4.03   -5.16   -1.13  Ca0.100Si1.000O2.100:0.110H2O
          CSH(0.2)         -3.52   -3.01    0.51  Ca0.200Si1.000O2.200:0.220H2O
          CSH(0.3)         -3.05   -0.86    2.18  Ca0.300Si1.000O2.300:0.330H2O
          CSH(0.4)         -2.58    1.28    3.87  Ca0.400Si1.000O2.400:0.440H2O
          CSH(0.5)         -2.14    3.43    5.57  Ca0.500Si1.000O2.500:0.550H2O
          CSH(0.6)         -1.71    5.58    7.29  Ca0.600Si1.000O2.600:0.661H2O
          CSH(0.7)         -1.30    7.73    9.03  Ca0.700Si1.000O2.700:0.771H2O
          CSH(0.8)         -0.93    9.88   10.81  Ca0.800Si1.000O2.800:0.881H2O
          CSH(0.833)       -0.84   10.59   11.43  Ca0.833Si1.000O2.833:0.917H2O
          CSH(0.9)         -0.69   13.36   14.05  Ca1.000Si1.111O3.222:1.093H2O
          CSH(1.0)         -0.33   14.17   14.50  Ca1.000Si1.000O3.000:1.084H2O
          CSH(1.1)         -0.14   14.84   14.97  Ca1.000Si0.909O2.818:1.076H2O
          CSH(1.2)         -0.04   15.39   15.43  Ca1.000Si0.833O2.666:1.070H2O
          CSH(1.3)          0.00   15.86   15.86  Ca1.000Si0.769O2.538:1.065H2O
          CSH(1.4)          0.00   16.26   16.26  Ca1.000Si0.714O2.428:1.060H2O
          CSH(1.5)         -0.03   16.61   16.64  Ca1.000Si0.667O2.334:1.056H2O
          CSH(1.6)         -0.06   16.91   16.98  Ca1.000Si0.625O2.250:1.053H2O
          CSH(1.7)         -0.11   17.18   17.30  Ca1.000Si0.588O2.176:1.049H2O
          CSH(1.8)         -0.17   17.42   17.59  Ca1.000Si0.556O2.112:1.047H2O
          H2             -34.89  -34.90   -0.00  H2
          Lime           -11.08   21.48   32.56  CaO
          O2             -13.34   69.79   83.13  O2
          Quartz          -3.28   -7.31   -4.03  SiO2
          SiO2(am)        -4.60   -7.31   -2.71  Si1.000O2.000
          Wollastonite     0.39   14.17   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 15.
------------------------------------

          Title 15 CSH(1.5)
          USE SOLUTION 1 DW
          EQUILIBRIUM_PHASES
          CSH(0.1)  0.0  0.0
          CSH(0.2)  0.0  0.0
          CSH(0.3)  0.0  0.0
          CSH(0.4)  0.0  0.0
          CSH(0.5)  0.0  0.0
          CSH(0.6)  0.0  0.0
```

```
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  1
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 16
        END
-----
TITLE
-----

 15 CSH(1.5)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -0.79   21.91   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -4.59   -5.72   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -4.04   -3.53    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -3.52   -1.34    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -3.02    0.85    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -2.53    3.04    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -2.05    5.23    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -1.60    7.43    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -1.19    9.62   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -1.09   10.34   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.93   13.12   14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.50   14.00   14.50 0.000e+000          0.000e+000
        CSH(1.1)       -0.25   14.72   14.97 0.000e+000          0.000e+000
        CSH(1.2)       -0.11   15.32   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -0.03   15.83   15.86 0.000e+000          0.000e+000
        CSH(1.4)        0.00   16.26   16.26 0.000e+000 1.230e-001 1.230e-001
        CSH(1.5)        0.00   16.64   16.64 1.000e+000 8.683e-001-1.317e-001
        CSH(1.6)       -0.01   16.97   16.98 0.000e+000          0.000e+000
        CSH(1.7)       -0.04   17.26   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.08   17.51   17.59 0.000e+000          0.000e+000
        SiO2(am)       -5.21   -7.91   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             8.676e-003  8.676e-003
        Si             5.323e-006  5.323e-006
```

----------Description of solution----------

```
                                pH  =  12.139     Charge balance
                                pe  =   5.465     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  2.400e-002
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  1.735e-002
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.731e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  65
                             Total H  = 1.110298e+002
                             Total O  = 5.552357e+001
```

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	1.633e-002	1.400e-002	-1.787	-1.854	-0.067
H+	8.226e-013	7.262e-013	-12.085	-12.139	-0.054
H2O	5.551e+001	9.996e-001	1.744	-0.000	0.000
Ca	8.676e-003				
Ca+2	7.663e-003	4.333e-003	-2.116	-2.363	-0.248
CaHO+	1.013e-003	8.727e-004	-2.994	-3.059	-0.065
CaSiH3O4+	1.913e-007	1.648e-007	-6.718	-6.783	-0.065
H(0)	9.657e-039				
H2	4.828e-039	4.855e-039	-38.316	-38.314	0.002
O(0)	5.014e-016				
O2	2.507e-016	2.521e-016	-15.601	-15.598	0.002
Si	5.323e-006				
SiH3O4-	4.715e-006	4.063e-006	-5.327	-5.391	-0.065
SiH2O4-2	4.049e-007	2.232e-007	-6.393	-6.651	-0.259
CaSiH3O4+	1.913e-007	1.648e-007	-6.718	-6.783	-0.065
H4SiO4	1.209e-008	1.215e-008	-7.918	-7.915	0.002

----------Saturation indices----------

Phase	SI	log IAP	log KT	
a-Cristobalite	-4.48	-7.91	-3.43	SiO2
b-Cristobalite	-4.93	-7.91	-2.98	SiO2
Ca(OH)2	-0.79	21.91	22.70	Ca(OH)2
Chalcedony	-4.18	-7.91	-3.74	SiO2
CSH(0.1)	-4.59	-5.72	-1.13	Ca0.100Si1.000O2.100:0.110H2O
CSH(0.2)	-4.04	-3.53	0.51	Ca0.200Si1.000O2.200:0.220H2O
CSH(0.3)	-3.52	-1.34	2.18	Ca0.300Si1.000O2.300:0.330H2O
CSH(0.4)	-3.02	0.85	3.87	Ca0.400Si1.000O2.400:0.440H2O
CSH(0.5)	-2.53	3.04	5.57	Ca0.500Si1.000O2.500:0.550H2O
CSH(0.6)	-2.05	5.23	7.29	Ca0.600Si1.000O2.600:0.661H2O
CSH(0.7)	-1.60	7.43	9.03	Ca0.700Si1.000O2.700:0.771H2O
CSH(0.8)	-1.19	9.62	10.81	Ca0.800Si1.000O2.800:0.881H2O
CSH(0.833)	-1.09	10.34	11.43	Ca0.833Si1.000O2.833:0.917H2O
CSH(0.9)	-0.93	13.12	14.05	Ca1.000Si1.111O3.222:1.093H2O
CSH(1.0)	-0.50	14.00	14.50	Ca1.000Si1.000O3.000:1.084H2O
CSH(1.1)	-0.25	14.72	14.97	Ca1.000Si0.909O2.818:1.076H2O
CSH(1.2)	-0.11	15.32	15.43	Ca1.000Si0.833O2.666:1.070H2O
CSH(1.3)	-0.03	15.83	15.86	Ca1.000Si0.769O2.538:1.065H2O
CSH(1.4)	0.00	16.26	16.26	Ca1.000Si0.714O2.428:1.060H2O
CSH(1.5)	0.00	16.64	16.64	Ca1.000Si0.667O2.334:1.056H2O
CSH(1.6)	-0.01	16.97	16.98	Ca1.000Si0.625O2.250:1.053H2O
CSH(1.7)	-0.04	17.26	17.30	Ca1.000Si0.588O2.176:1.049H2O
CSH(1.8)	-0.08	17.51	17.59	Ca1.000Si0.556O2.112:1.047H2O
H2	-35.20	-35.21	-0.00	H2
Lime	-10.65	21.91	32.56	CaO
O2	-12.71	70.41	83.13	O2
Quartz	-3.89	-7.91	-4.03	SiO2
SiO2(am)	-5.21	-7.91	-2.71	Si1.000O2.000

```
        Wollastonite     0.22   14.00   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 16.
------------------------------------

        Title 16 CSH(1.6)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  1
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 17
        END
-----
TITLE
-----

 16 CSH(1.6)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -0.62   22.08   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -4.83   -5.96   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -4.26   -3.75    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -3.72   -1.54    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -3.20    0.67    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -2.69    2.87    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -2.21    5.08    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -1.74    7.29    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -1.31    9.50   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -1.20   10.23   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -1.04   13.01   14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.59   13.92   14.50 0.000e+000          0.000e+000
        CSH(1.1)       -0.32   14.66   14.97 0.000e+000          0.000e+000
        CSH(1.2)       -0.15   15.28   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -0.06   15.80   15.86 0.000e+000          0.000e+000
```

```
        CSH(1.4)        -0.01   16.25   16.26 0.000e+000          0.000e+000
        CSH(1.5)         0.00   16.64   16.64 0.000e+000 1.508e-001 1.508e-001
        CSH(1.6)        -0.00   16.98   16.98 1.000e+000 8.391e-001-1.609e-001
        CSH(1.7)        -0.02   17.28   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.05   17.54   17.59 0.000e+000          0.000e+000
        SiO2(am)        -5.46   -8.17   -2.71 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.014e-002  1.014e-002
        Si             3.518e-006  3.518e-006

----------------------------Description of solution---------------------------

                                pH  =  12.199     Charge balance
                                pe  =   5.710     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  2.779e-002
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.027e-002
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  78
                              Total H  = 1.110329e+002
                              Total O  = 5.552658e+001

----------------------------Distribution of species---------------------------

                                                Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.896e-002  1.609e-002   -1.722   -1.793   -0.071
        H+             7.202e-013  6.318e-013  -12.143  -12.199   -0.057
        H2O            5.551e+001  9.995e-001    1.744   -0.000    0.000
Ca           1.014e-002
        Ca+2           8.827e-003  4.828e-003   -2.054   -2.316   -0.262
        CaHO+          1.309e-003  1.118e-003   -2.883   -2.952   -0.069
        CaSiH3O4+       1.384e-007  1.182e-007   -6.859   -6.927   -0.069
H(0)         2.363e-039
        H2             1.181e-039  1.189e-039  -38.928  -38.925    0.003
O(0)         8.353e-015
        O2             4.177e-015  4.203e-015  -14.379  -14.376    0.003
Si           3.518e-006
        SiH3O4-         3.062e-006  2.615e-006   -5.514   -5.583   -0.069
        SiH2O4-2        3.105e-007  1.652e-007   -6.508   -6.782   -0.274
        CaSiH3O4+       1.384e-007  1.182e-007   -6.859   -6.927   -0.069
        H4SiO4          6.763e-009  6.806e-009   -8.170   -8.167    0.003

----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -4.73   -8.17   -3.43  SiO2
        b-Cristobalite   -5.19   -8.17   -2.98  SiO2
        Ca(OH)2         -0.62   22.08   22.70  Ca(OH)2
        Chalcedony       -4.43   -8.17   -3.74  SiO2
        CSH(0.1)        -4.83   -5.96   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -4.26   -3.75    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -3.72   -1.54    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -3.20    0.67    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -2.69    2.87    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -2.21    5.08    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -1.74    7.29    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -1.31    9.50   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.20   10.23   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -1.04   13.01   14.05  Ca1.000Si1.111O3.222:1.093H2O
```

```
        CSH(1.0)        -0.59   13.92   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.32   14.66   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.15   15.28   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.06   15.80   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.01   16.25   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         0.00   16.64   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.00   16.98   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.02   17.28   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.05   17.54   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.81  -35.82   -0.00  H2
        Lime          -10.48   22.08   32.56  CaO
        O2            -11.49   71.64   83.13  O2
        Quartz         -4.14   -8.17   -4.03  SiO2
        SiO2(am)       -5.46   -8.17   -2.71  Si1.000O2.000
        Wollastonite    0.13   13.92   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 17.
------------------------------------

        Title 17 CSH(1.7)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  1
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 18
        END
-----
TITLE
-----

 17 CSH(1.7)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase              SI log IAP  log KT    Initial      Final      Delta

        Ca(OH)2         -0.35   22.35   22.70 0.000e+000          0.000e+000
```

```
        CSH(0.1)        -5.23   -6.36   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        -4.64   -4.12    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -4.07   -1.89    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -3.52    0.35    3.87 0.000e+000          0.000e+000
        CSH(0.5)        -2.99    2.58    5.57 0.000e+000          0.000e+000
        CSH(0.6)        -2.47    4.82    7.29 0.000e+000          0.000e+000
        CSH(0.7)        -1.98    7.05    9.03 0.000e+000          0.000e+000
        CSH(0.8)        -1.52    9.29   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -1.41   10.02   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -1.25   12.80   14.05 0.000e+000          0.000e+000
        CSH(1.0)        -0.75   13.76   14.50 0.000e+000          0.000e+000
        CSH(1.1)        -0.44   14.54   14.97 0.000e+000          0.000e+000
        CSH(1.2)        -0.24   15.19   15.43 0.000e+000          0.000e+000
        CSH(1.3)        -0.12   15.74   15.86 0.000e+000          0.000e+000
        CSH(1.4)        -0.05   16.21   16.26 0.000e+000          0.000e+000
        CSH(1.5)        -0.02   16.62   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.00   16.98   16.98 0.000e+000 2.071e-001 2.071e-001
        CSH(1.7)        -0.00   17.30   17.30 1.000e+000 7.799e-001-2.201e-001
        CSH(1.8)        -0.02   17.57   17.59 0.000e+000          0.000e+000
        SiO2(am)        -5.89   -8.59   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.303e-002  1.303e-002
        Si             1.722e-006  1.722e-006

----------------------------Description of solution----------------------------

                                pH  =  12.296     Charge balance
                                pe  =   5.426     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  3.516e-002
                       Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  2.607e-002
                    Total carbon (mol/kg)  =  0.000e+000
                       Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.768e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                            Iterations  =  18
                              Total H  = 1.110381e+002
                              Total O  = 5.553210e+001

---------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            2.410e-002  2.011e-002   -1.618   -1.697   -0.079
        H+             5.824e-013  5.055e-013  -12.235  -12.296   -0.061
        H2O            5.551e+001  9.994e-001    1.744   -0.000    0.000
Ca           1.303e-002
        Ca+2           1.106e-002  5.723e-003   -1.956   -2.242   -0.286
        CaHO+          1.968e-003  1.656e-003   -2.706   -2.781   -0.075
        CaSiH3O4+       7.771e-008  6.538e-008   -7.110   -7.185   -0.075
H(0)         5.580e-039
        H2             2.790e-039  2.812e-039  -38.554  -38.551    0.004
O(0)         1.490e-015
        O2             7.449e-016  7.510e-016  -15.128  -15.124    0.004
Si           1.722e-006
        SiH3O4-         1.450e-006  1.220e-006   -5.839   -5.914   -0.075
        SiH2O4-2        1.922e-007  9.629e-008   -6.716   -7.016   -0.300
        CaSiH3O4+       7.771e-008  6.538e-008   -7.110   -7.185   -0.075
        H4SiO4          2.520e-009  2.540e-009   -8.599   -8.595    0.004

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT
```

```
        a-Cristobalite   -5.16   -8.59   -3.43  SiO2
        b-Cristobalite   -5.61   -8.59   -2.98  SiO2
        Ca(OH)2         -0.35   22.35   22.70  Ca(OH)2
        Chalcedony       -4.86   -8.59   -3.74  SiO2
        CSH(0.1)         -5.23   -6.36   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -4.64   -4.12    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -4.07   -1.89    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.52    0.35    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -2.99    2.58    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.47    4.82    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.98    7.05    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.52    9.29   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.41   10.02   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -1.25   12.80   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.75   13.76   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.44   14.54   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.24   15.19   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.12   15.74   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.05   16.21   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.02   16.62   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.00   16.98   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.00   17.30   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.02   17.57   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2              -35.44  -35.44   -0.00  H2
        Lime             -10.21   22.35   32.56  CaO
        O2              -12.24   70.89   83.13  O2
        Quartz           -4.57   -8.59   -4.03  SiO2
        SiO2(am)         -5.89   -8.59   -2.71  Si1.000O2.000
        Wollastonite      -0.03   13.76   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 18.
------------------------------------

        Title 18 CSH(1.8)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  1
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 19
-----
TITLE
-----

 18 CSH(1.8)

----------------------------------------
Beginning of batch-reaction calculations.
```

```
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -0.02   22.68   22.70 0.000e+000          0.000e+000
        CSH(0.1)       -5.76   -6.89   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -5.13   -4.62    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -4.53   -2.35    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -3.95   -0.08    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -3.39    2.18    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -2.84    4.45    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -2.31    6.72    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -1.82    8.99   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -1.69    9.74   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -1.54   12.51   14.05 0.000e+000          0.000e+000
        CSH(1.0)       -0.98   13.52   14.50 0.000e+000          0.000e+000
        CSH(1.1)       -0.62   14.36   14.97 0.000e+000          0.000e+000
        CSH(1.2)       -0.38   15.05   15.43 0.000e+000          0.000e+000
        CSH(1.3)       -0.22   15.64   15.86 0.000e+000          0.000e+000
        CSH(1.4)       -0.12   16.14   16.26 0.000e+000          0.000e+000
        CSH(1.5)       -0.06   16.57   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.02   16.96   16.98 0.000e+000          0.000e+000
        CSH(1.7)        0.00   17.30   17.30 0.000e+000 3.109e-001 3.109e-001
        CSH(1.8)        0.00   17.59   17.59 1.000e+000 6.712e-001-3.288e-001
        SiO2(am)       -6.45   -9.16   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Ca             1.789e-002  1.789e-002
        Si             6.706e-007  6.706e-007

----------------------------Description of solution----------------------------

                                pH  =  12.417     Charge balance
                                pe  =   5.435     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  4.717e-002
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  3.579e-002
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.726e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  66
                             Total H  = 1.110487e+002
                             Total O  = 5.554222e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            3.253e-002  2.653e-002   -1.488   -1.576   -0.089
        H+             4.473e-013  3.830e-013  -12.349  -12.417   -0.067
        H2O            5.551e+001  9.991e-001    1.744   -0.000    0.000
Ca           1.789e-002
        Ca+2           1.464e-002  7.032e-003   -1.835   -2.153   -0.318
        CaHO+          3.255e-003  2.684e-003   -2.487   -2.571   -0.084
        CaSiH3O4+      3.525e-008  2.908e-008   -7.453   -7.536   -0.084
H(0)         3.070e-039
```

```
        H2            1.535e-039  1.552e-039   -38.814   -38.809    0.005
O(0)          4.879e-015
        O2            2.440e-015  2.466e-015   -14.613   -14.608    0.005
Si            6.706e-007
        SiH3O4-        5.353e-007  4.415e-007    -6.271    -6.355    -0.084
        SiH2O4-2       9.940e-008  4.600e-008    -7.003    -7.337    -0.335
        CaSiH3O4+      3.525e-008  2.908e-008    -7.453    -7.536    -0.084
        H4SiO4         6.891e-010  6.967e-010    -9.162    -9.157     0.005

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -5.72   -9.16   -3.43  SiO2
        b-Cristobalite   -6.17   -9.16   -2.98  SiO2
        Ca(OH)2         -0.02   22.68   22.70  Ca(OH)2
        Chalcedony       -5.42   -9.16   -3.74  SiO2
        CSH(0.1)         -5.76   -6.89   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -5.13   -4.62    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -4.53   -2.35    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.95   -0.08    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -3.39    2.18    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.84    4.45    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -2.31    6.72    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.82    8.99   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.69    9.74   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -1.54   12.51   14.05  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.98   13.52   14.50  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.62   14.36   14.97  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.38   15.05   15.43  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.22   15.64   15.86  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.12   16.14   16.26  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.06   16.57   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.02   16.96   16.98  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)          0.00   17.30   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)          0.00   17.59   17.59  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.70  -35.70   -0.00  H2
        Lime            -9.88   22.68   32.56  CaO
        O2             -11.72   71.40   83.13  O2
        Quartz          -5.13   -9.16   -4.03  SiO2
        SiO2(am)        -6.45   -9.16   -2.71  Si1.000O2.000
        Wollastonite    -0.26   13.52   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 19.
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End of run.
-----------
```

付録- 3　Atkinson モデルから導いた解離式及び log K を用いて C-S-H ゲルの溶解／沈殿反応を PHREEQC で計算した結果（アウトプット）　ケース：JNC-TDB (2)

```
Input file: Atkinson Model JNCtdb(2) Input.pqi
Output file: Atkinson Model JNCtdb(2) Input.pqo
Database file: spron_phc_kai.txt

------------------
Reading data base.
------------------

        SOLUTION_MASTER_SPECIES
        SOLUTION_SPECIES
        PHASES
        END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

        DATABASE: spron_phc_kai.txt
        Title C-S-H dissolution using data from Atkinson model - case:JNCtdb(2)
        PHASES
        CSH(0.1)
            Ca 0.100 Si 1.000 O 2.100 : 0.110 H2O = 0.100 Ca+2 + 1.000 H4SiO4 -1.790 H2O - 0.200 H+
            log_K -1.132
        CSH(0.2)
            Ca 0.200 Si 1.000 O 2.200 : 0.220 H2O = 0.200 Ca+2 + 1.000 H4SiO4 -1.580 H2O - 0.400 H+
            log_K 0.512
        CSH(0.3)
            Ca 0.300 Si 1.000 O 2.300 : 0.330 H2O = 0.300 Ca+2 + 1.000 H4SiO4 -1.370 H2O - 0.600 H+
            log_K 2.181
        CSH(0.4)
            Ca 0.400 Si 1.000 O 2.400 : 0.440 H2O = 0.400 Ca+2 + 1.000 H4SiO4 -1.160 H2O - 0.800 H+
            log_K 3.868
        CSH(0.5)
            Ca 0.500 Si 1.000 O 2.500 : 0.550 H2O = 0.500 Ca+2 + 1.000 H4SiO4 -0.950 H2O - 1.000 H+
            log_K 5.569
        CSH(0.6)
            Ca 0.600 Si 1.000 O 2.600 : 0.661 H2O = 0.600 Ca+2 + 1.000 H4SiO4 -0.739 H2O - 1.200 H+
            log_K 7.288
        CSH(0.7)
            Ca 0.700 Si 1.000 O 2.700 : 0.771 H2O = 0.700 Ca+2 + 1.000 H4SiO4 -0.529 H2O - 1.400 H+
            log_K 9.027
        CSH(0.8)
            Ca 0.800 Si 1.000 O 2.800 : 0.881 H2O = 0.800 Ca+2 + 1.000 H4SiO4 -0.319 H2O - 1.600 H+
            log_K 10.809
        CSH(0.9)
            Ca 1.000 Si 1.111 O 3.222 : 1.093 H2O = 1.000 Ca+2 + 1.111 H4SiO4 -0.129 H2O - 2.000 H+
            log_K 14.039
        CSH(1.0)
            Ca 1.000 Si 1.000 O 3.000 : 1.084 H2O = 1.000 Ca+2 + 1.000 H4SiO4 + 0.084 H2O - 2.000 H+
            log_K 14.477
        CSH(1.1)
            Ca 1.000 Si 0.909 O 2.818 : 1.076 H2O = 1.000 Ca+2 + 0.909 H4SiO4 + 0.258 H2O - 2.000 H+
            log_K 14.935
        CSH(1.2)
            Ca 1.000 Si 0.833 O 2.666 : 1.070 H2O = 1.000 Ca+2 + 0.833 H4SiO4 + 0.404 H2O - 2.000 H+
            log_K 15.381
        CSH(1.3)
            Ca 1.000 Si 0.769 O 2.538 : 1.065 H2O = 1.000 Ca+2 + 0.769 H4SiO4 + 0.527 H2O - 2.000 H+
            log_K 15.803
        CSH(1.4)
            Ca 1.000 Si 0.714 O 2.428 : 1.060 H2O = 1.000 Ca+2 + 0.714 H4SiO4 + 0.632 H2O - 2.000 H+
            log_K 16.197
        CSH(1.5)
            Ca 1.000 Si 0.667 O 2.334 : 1.056 H2O = 1.000 Ca+2 + 0.667 H4SiO4 + 0.722 H2O - 2.000 H+
            log_K 16.562
        CSH(1.6)
            Ca 1.000 Si 0.625 O 2.250 : 1.053 H2O = 1.000 Ca+2 + 0.625 H4SiO4 + 0.803 H2O - 2.000 H+
            log_K 16.900
        CSH(1.7)
            Ca 1.000 Si 0.588 O 2.176 : 1.049 H2O = 1.000 Ca+2 + 0.588 H4SiO4 + 0.873 H2O - 2.000 H+
            log_K 17.213
```

```
        CSH(1.8)
            Ca 1.000 Si 0.556 O 2.112 : 1.047 H2O = 1.000 Ca+2 + 0.556 H4SiO4 + 0.935 H2O - 2.000 H+
            log_K 17.502
        SiO2(am)
            Si 1.000 O 2.000 = 1.000 H4SiO4 - 2.000 H2O
            log_K -2.706
        CSH(0.833)
            Ca 0.833 Si 1.000 O 2.833 : 0.917 H2O = 0.833 Ca+2 + 1.000 H4SiO4 -0.250 H2O - 1.666 H+
           log_K 11.428
        Ca(OH)2
            Ca(OH)2 = Ca+2 + 2H2O - 2 H+
            log_k 22.540
        Title 1 CSH(0.1)
        SOLUTION 1 DW
        units mol/L
        pH 7
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  1
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 2
        END
-----
TITLE
-----

 1 CSH(0.1)

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.       DW

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Pure water

----------------------------Description of solution----------------------------

                                pH =   7.000
                                pe =   4.000
                  Activity of water =   1.000
                     Ionic strength =  1.009e-007
                 Mass of water (kg) =  1.000e+000
            Total alkalinity (eq/kg) =  1.715e-009
               Total carbon (mol/kg) =  0.000e+000
                  Total CO2 (mol/kg) =  0.000e+000
                Temperature (deg C) =  25.000
             Electrical balance (eq) = -1.715e-009
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.85
                         Iterations  =   0
                           Total H  = 1.110124e+002
                           Total O  = 5.550622e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            1.018e-007  1.017e-007   -6.992   -6.993   -0.000
        H+             1.001e-007  1.000e-007   -7.000   -7.000   -0.000
        H2O            5.551e+001  1.000e+000    1.744    0.000    0.000
H(0)          1.565e-025
        H2             7.823e-026  7.823e-026  -25.107  -25.107    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -42.012  -42.012    0.000

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        H2            -22.00  -22.00   -0.00  H2
        O2            -39.13   44.00   83.13  O2

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -6.80   15.74   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -0.00   -1.13   -1.13 1.000e+000 9.923e-001-7.707e-003
        CSH(0.2)       -0.07    0.44    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.17    2.02    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.28    3.59    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.41    5.16    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.55    6.74    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.72    8.31    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.92    9.89   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -1.02   10.41   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -1.31   12.73   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -1.44   13.03   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -1.65   13.28   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -1.90   13.49   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -2.14   13.66   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -2.39   13.81   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -2.63   13.94   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -2.85   14.05   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -3.06   14.15   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -3.27   14.24   17.50 0.000e+000          0.000e+000
        SiO2(am)        0.00   -2.71   -2.71 0.000e+000 4.232e-003 4.232e-003

-----------------------------Solution composition-----------------------------

        Elements         Molality     Moles

        Ca             7.708e-004  7.707e-004
        Si             3.476e-003  3.475e-003

----------------------------Description of solution---------------------------

                                pH  =   9.474     Charge balance
```

```
                                pe  =   8.422     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  2.295e-003
                    Mass of water (kg)  =  9.999e-001
               Total alkalinity (eq/kg)  =  1.542e-003
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  =  15
                            Total H  = 1.110141e+002
                            Total O  = 5.551479e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            3.196e-005  3.030e-005   -4.495    -4.518   -0.023
         H+             3.525e-010  3.356e-010   -9.453    -9.474   -0.021
         H2O            5.551e+001  9.999e-001    1.744    -0.000    0.000
Ca            7.708e-004
         Ca+2           7.618e-004  6.191e-004   -3.118    -3.208   -0.090
         CaSiH3O4+       8.698e-006  8.251e-006   -5.061    -5.083   -0.023
         CaHO+          2.846e-007  2.699e-007   -6.546    -6.569   -0.023
H(0)          2.522e-039
         H2             1.261e-039  1.261e-039  -38.899   -38.899    0.000
O(0)          7.470e-015
         O2             3.735e-015  3.737e-015  -14.428   -14.427    0.000
Si            3.476e-003
         H4SiO4          1.967e-003  1.968e-003   -2.706    -2.706    0.000
         SiH3O4-         1.500e-003  1.423e-003   -2.824    -2.847   -0.023
         CaSiH3O4+       8.698e-006  8.251e-006   -5.061    -5.083   -0.023
         SiH2O4-2        2.090e-007  1.692e-007   -6.680    -6.772   -0.092

------------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite    0.73  -2.71  -3.43  SiO2
         b-Cristobalite    0.28  -2.71  -2.98  SiO2
         Ca(OH)2         -6.80   15.74   22.54  Ca(OH)2
         Chalcedony       1.03  -2.71  -3.74  SiO2
         CSH(0.1)        -0.00  -1.13  -1.13  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)        -0.07   0.44   0.51  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)        -0.17   2.02   2.18  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)        -0.28   3.59   3.87  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)        -0.41   5.16   5.57  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)        -0.55   6.74   7.29  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)        -0.72   8.31   9.03  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)        -0.92   9.89  10.81  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)      -1.02  10.41  11.43  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)        -1.31  12.73  14.04  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)        -1.44  13.03  14.48  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)        -1.65  13.28  14.94  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)        -1.90  13.49  15.38  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)        -2.14  13.66  15.80  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)        -2.39  13.81  16.20  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)        -2.63  13.94  16.56  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)        -2.85  14.05  16.90  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)        -3.06  14.15  17.21  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)        -3.27  14.24  17.50  Ca1.000Si0.556O2.112:1.047H2O
         H2            -35.79 -35.79  -0.00  H2
         Lime          -16.82  15.74  32.56  CaO
         O2            -11.54  71.58  83.13  O2
         Quartz          1.32  -2.71  -4.03  SiO2
         SiO2(am)        0.00  -2.71  -2.71  Si1.000O2.000
         Wollastonite   -0.75  13.03  13.78  CaSiO3

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```

```
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 2.
-----------------------------------

        Title 2 CSH(0.2)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  1
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 3
        END
-----
TITLE
-----

 2 CSH(0.2)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -6.10  16.44   22.54 0.000e+000          0.000e+000
        CSH(0.1)        0.00  -1.13   -1.13 0.000e+000 4.105e-003 4.105e-003
        CSH(0.2)        0.00   0.51    0.51 1.000e+000 9.918e-001-8.161e-003
        CSH(0.3)       -0.03   2.16    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.07   3.80    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.13   5.44    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.20   7.09    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.30   8.73    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.43  10.38   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.51  10.92   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.68  13.36   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.81  13.66   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -1.02  13.92   14.94 0.000e+000          0.000e+000
```

```
        CSH(1.2)       -1.25   14.13   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -1.50   14.31   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -1.74   14.46   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -1.97   14.59   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -2.19   14.71   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -2.41   14.81   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -2.61   14.90   17.50 0.000e+000          0.000e+000
        SiO2(am)       -0.07   -2.78   -2.71 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.222e-003  1.222e-003
        Si             4.056e-003  4.056e-003

----------------------------Description of solution---------------------------

                                pH  =   9.736     Charge balance
                                pe  =   8.044     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.623e-003
                   Mass of water (kg)  =  9.999e-001
               Total alkalinity (eq/kg)  =  2.444e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  = 162
                            Total H  = 1.110151e+002
                            Total O  = 5.551689e+001

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            5.914e-005  5.536e-005   -4.228   -4.257   -0.029
        H+             1.951e-010  1.837e-010   -9.710   -9.736   -0.026
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.222e-003
        Ca+2           1.200e-003  9.297e-004   -2.921   -3.032   -0.111
        CaSiH3O4+       2.057e-005  1.927e-005   -4.687   -4.715   -0.028
        CaHO+          7.905e-007  7.405e-007   -6.102   -6.130   -0.028
H(0)         4.317e-039
        H2             2.158e-039  2.160e-039  -38.666  -38.666    0.000
O(0)         2.547e-015
        O2             1.273e-015  1.274e-015  -14.895  -14.895    0.000
Si           4.056e-003
        SiH3O4-         2.362e-003  2.213e-003   -2.627   -2.655   -0.028
        H4SiO4         1.673e-003  1.675e-003   -2.776   -2.776    0.000
        CaSiH3O4+       2.057e-005  1.927e-005   -4.687   -4.715   -0.028
        SiH2O4-2        6.241e-007  4.806e-007   -6.205   -6.318   -0.113

----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.66  -2.78  -3.43  SiO2
        b-Cristobalite    0.21  -2.78  -2.98  SiO2
        Ca(OH)2         -6.10   16.44   22.54  Ca(OH)2
        Chalcedony       0.96  -2.78  -3.74  SiO2
        CSH(0.1)         0.00  -1.13  -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         0.00   0.51   0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.03   2.16   2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.07   3.80   3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.13   5.44   5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.20   7.09   7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.30   8.73   9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.43  10.38  10.81  Ca0.800Si1.000O2.800:0.881H2O
```

```
        CSH(0.833)      -0.51   10.92   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.68   13.36   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.81   13.66   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -1.02   13.92   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -1.25   14.13   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -1.50   14.31   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -1.74   14.46   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -1.97   14.59   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -2.19   14.71   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -2.41   14.81   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -2.61   14.90   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.56  -35.56   -0.00  H2
        Lime           -16.12   16.44   32.56  CaO
        O2             -12.01   71.12   83.13  O2
        Quartz           1.25   -2.78   -4.03  SiO2
        SiO2(am)        -0.07   -2.78   -2.71  Si1.000O2.000
        Wollastonite     -0.12   13.66   13.78  CaSiO3

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End of simulation.
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Reading input data for simulation 3.
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        Title 3 CSH(0.3)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  1
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1) 0.0 0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 4
        END
-----
TITLE
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 3 CSH(0.3)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

WARNING: Maximum iterations exceeded, 200
```

```
Numerical method failed with this set of convergence parameters.
WARNING: Trying diagonal scaling ...

WARNING: Maximum iterations exceeded, 200

Numerical method failed with this set of convergence parameters.
WARNING: Trying reduced tolerance 1e-016 ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -5.85   16.69   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -0.03   -1.16   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        0.00    0.51    0.51 0.000e+000 1.302e-003 1.302e-003
        CSH(0.3)       -0.00    2.18    2.18 1.000e+000 9.945e-001-5.487e-003
        CSH(0.4)       -0.02    3.85    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.05    5.52    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.10    7.19    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.17    8.86    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.28   10.53   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.35   11.08   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.49   13.55   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.61   13.86   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.81   14.12   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -1.05   14.34   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -1.29   14.52   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -1.52   14.67   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -1.76   14.81   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -1.98   14.92   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -2.18   15.03   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -2.38   15.12   17.50 0.000e+000          0.000e+000
        SiO2(am)       -0.12   -2.83   -2.71 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.386e-003  1.386e-003
        Si             4.186e-003  4.186e-003

-----------------------------Description of solution-----------------------------

                                pH =   9.837     Charge balance
                                pe =   8.039     Adjusted to redox equilibrium
                    Activity of water =   1.000
                       Ionic strength =  4.105e-003
                   Mass of water (kg) =  9.999e-001
              Total alkalinity (eq/kg) =  2.772e-003
                 Total carbon (mol/kg) =  0.000e+000
                    Total CO2 (mol/kg) =  0.000e+000
                  Temperature (deg C) =  25.000
               Electrical balance (eq) = -1.699e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.00
                          Iterations =  61
                            Total H  = 1.110155e+002
                            Total O  = 5.551750e+001

----------------------------Distribution of species-----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            7.497e-005  6.990e-005   -4.125   -4.156   -0.030
        H+             1.550e-010  1.455e-010   -9.810   -9.837   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.386e-003
```

```
        Ca+2          1.359e-003  1.037e-003   -2.867   -2.984   -0.117
        CaSiH3O4+      2.592e-005  2.418e-005   -4.586   -4.616   -0.030
        CaHO+         1.118e-006  1.043e-006   -5.952   -5.982   -0.030
H(0)         2.759e-039
        H2            1.380e-039  1.381e-039  -38.860  -38.860    0.000
O(0)         6.232e-015
        O2            3.116e-015  3.119e-015  -14.506  -14.506    0.000
Si           4.186e-003
        SiH3O4-        2.668e-003  2.490e-003   -2.574   -2.604   -0.030
        H4SiO4         1.491e-003  1.493e-003   -2.826   -2.826    0.000
        CaSiH3O4+      2.592e-005  2.418e-005   -4.586   -4.616   -0.030
        SiH2O4-2       9.006e-007  6.830e-007   -6.045   -6.166   -0.120

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   0.61  -2.83  -3.43  SiO2
        b-Cristobalite   0.16  -2.83  -2.98  SiO2
        Ca(OH)2        -5.85  16.69  22.54  Ca(OH)2
        Chalcedony      0.91  -2.83  -3.74  SiO2
        CSH(0.1)       -0.03  -1.16  -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        0.00   0.51   0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)       -0.00   2.18   2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)       -0.02   3.85   3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)       -0.05   5.52   5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)       -0.10   7.19   7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)       -0.17   8.86   9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)       -0.28  10.53  10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)     -0.35  11.08  11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)       -0.49  13.55  14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)       -0.61  13.86  14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)       -0.81  14.12  14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)       -1.05  14.34  15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)       -1.29  14.52  15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)       -1.52  14.67  16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)       -1.76  14.81  16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)       -1.98  14.92  16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)       -2.18  15.03  17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)       -2.38  15.12  17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.75 -35.75  -0.00  H2
        Lime          -15.87  16.69  32.56  CaO
        O2            -11.62  71.51  83.13  O2
        Quartz          1.20  -2.83  -4.03  SiO2
        SiO2(am)       -0.12  -2.83  -2.71  Si1.000O2.000
        Wollastonite    0.08  13.86  13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 4.
------------------------------------

        Title 4 CSH(0.4)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  1
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
```

```
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 5
        END
-----
TITLE
-----

 4 CSH(0.4)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -5.53   17.01   22.54 0.000e+000          0.000e+000
        CSH(0.1)        -0.10   -1.24   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        -0.05    0.47    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -0.01    2.17    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -0.00    3.87    3.87 1.000e+000 9.948e-001-5.248e-003
        CSH(0.5)        -0.00    5.57    5.57 0.000e+000 1.169e-003 1.169e-003
        CSH(0.6)        -0.02    7.27    7.29 0.000e+000          0.000e+000
        CSH(0.7)        -0.06    8.97    9.03 0.000e+000          0.000e+000
        CSH(0.8)        -0.14   10.67   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -0.19   11.23   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.29   13.75   14.04 0.000e+000          0.000e+000
        CSH(1.0)        -0.40   14.07   14.48 0.000e+000          0.000e+000
        CSH(1.1)        -0.59   14.34   14.94 0.000e+000          0.000e+000
        CSH(1.2)        -0.82   14.56   15.38 0.000e+000          0.000e+000
        CSH(1.3)        -1.05   14.75   15.80 0.000e+000          0.000e+000
        CSH(1.4)        -1.28   14.91   16.20 0.000e+000          0.000e+000
        CSH(1.5)        -1.51   15.05   16.56 0.000e+000          0.000e+000
        CSH(1.6)        -1.72   15.18   16.90 0.000e+000          0.000e+000
        CSH(1.7)        -1.93   15.28   17.21 0.000e+000          0.000e+000
        CSH(1.8)        -2.12   15.38   17.50 0.000e+000          0.000e+000
        SiO2(am)        -0.23   -2.94   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.515e-003  1.515e-003
        Si             4.079e-003  4.079e-003

----------------------------Description of solution----------------------------

                                pH  =   9.981     Charge balance
                                pe  =   7.947     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.481e-003
                    Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  3.029e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.715e-009
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  15
                           Total H  = 1.110158e+002
                           Total O  = 5.551755e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.046e-004  9.726e-005    -3.980    -4.012    -0.032
        H+             1.117e-010  1.046e-010    -9.952    -9.981    -0.028
        H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
Ca           1.515e-003
        Ca+2           1.483e-003  1.119e-003    -2.829    -2.951    -0.122
        CaSiH3O4+       3.029e-005  2.819e-005    -4.519    -4.550    -0.031
        CaHO+          1.683e-006  1.566e-006    -5.774    -5.805    -0.031
H(0)         2.182e-039
        H2             1.091e-039  1.092e-039   -38.962   -38.962     0.000
O(0)         9.963e-015
        O2             4.981e-015  4.987e-015   -14.303   -14.302     0.000
Si           4.079e-003
        SiH3O4-         2.890e-003  2.689e-003    -2.539    -2.570    -0.031
        H4SiO4         1.157e-003  1.159e-003    -2.937    -2.936     0.000
        CaSiH3O4+       3.029e-005  2.819e-005    -4.519    -4.550    -0.031
        SiH2O4-2        1.369e-006  1.026e-006    -5.864    -5.989    -0.125

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.50   -2.94   -3.43  SiO2
        b-Cristobalite    0.05   -2.94   -2.98  SiO2
        Ca(OH)2         -5.53   17.01   22.54  Ca(OH)2
        Chalcedony       0.80   -2.94   -3.74  SiO2
        CSH(0.1)        -0.10   -1.24   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.05    0.47    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.01    2.17    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.00    3.87    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.00    5.57    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.02    7.27    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.06    8.97    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.14   10.67   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.19   11.23   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.29   13.75   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.40   14.07   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.59   14.34   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.82   14.56   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -1.05   14.75   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -1.28   14.91   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -1.51   15.05   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -1.72   15.18   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.93   15.28   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -2.12   15.38   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.85  -35.86   -0.00  H2
        Lime           -15.55   17.01   32.56  CaO
        O2             -11.42   71.71   83.13  O2
        Quartz           1.09   -2.94   -4.03  SiO2
        SiO2(am)        -0.23   -2.94   -2.71  Si1.000O2.000
        Wollastonite     0.29   14.07   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 5.
-----------------------------------

        Title 5 CSH(0.5)
        USE SOLUTION 1 DW
```

```
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  1
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 6
        END
-----
TITLE
-----

 5 CSH(0.5)

-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -5.35  17.19  22.54 0.000e+000          0.000e+000
        CSH(0.1)       -0.18  -1.31  -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.10   0.41   0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.05   2.13   2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.02   3.85   3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.00   5.57   5.57 1.000e+000 9.921e-001-7.898e-003
        CSH(0.6)        0.00   7.29   7.29 0.000e+000 4.043e-003 4.043e-003
        CSH(0.7)       -0.02   9.01   9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.08  10.73  10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.13  11.29  11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.21  13.83  14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.31  14.16  14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.50  14.44  14.94 0.000e+000          0.000e+000
        CSH(1.2)       -0.71  14.67  15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.94  14.86  15.80 0.000e+000          0.000e+000
        CSH(1.4)       -1.17  15.03  16.20 0.000e+000          0.000e+000
        CSH(1.5)       -1.39  15.17  16.56 0.000e+000          0.000e+000
        CSH(1.6)       -1.60  15.30  16.90 0.000e+000          0.000e+000
        CSH(1.7)       -1.80  15.41  17.21 0.000e+000          0.000e+000
        CSH(1.8)       -1.99  15.51  17.50 0.000e+000          0.000e+000
        SiO2(am)       -0.32  -3.03  -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca            1.524e-003  1.524e-003
```

```
        Si            3.856e-003  3.856e-003

----------------------------Description of solution----------------------------

                                pH  =  10.069     Charge balance
                                pe  =   7.810     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.508e-003
                    Mass of water (kg)  =  9.999e-001
               Total alkalinity (eq/kg)  =  3.047e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.713e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  =  53
                            Total H  = 1.110158e+002
                            Total O  = 5.551712e+001

----------------------------Distribution of species----------------------------

                                                 Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.284e-004  1.194e-004   -3.891   -3.923   -0.032
        H+             9.100e-011  8.521e-011  -10.041  -10.069   -0.029
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.524e-003
        Ca+2           1.491e-003  1.125e-003   -2.826   -2.949   -0.122
        CaSiH3O4+       3.038e-005  2.826e-005   -4.517   -4.549   -0.031
        CaHO+          2.076e-006  1.932e-006   -5.683   -5.714   -0.031
H(0)         2.725e-039
        H2             1.362e-039  1.364e-039  -38.866  -38.865    0.000
O(0)         6.389e-015
        O2             3.194e-015  3.198e-015  -14.496  -14.495    0.000
Si           3.856e-003
        SiH3O4-         2.883e-003  2.682e-003   -2.540   -2.571   -0.031
        H4SiO4          9.407e-004  9.417e-004   -3.027   -3.026    0.000
        CaSiH3O4+       3.038e-005  2.826e-005   -4.517   -4.549   -0.031
        SiH2O4-2        1.677e-006  1.256e-006   -5.776   -5.901   -0.125

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.41   -3.03   -3.43  SiO2
        b-Cristobalite   -0.04   -3.03   -2.98  SiO2
        Ca(OH)2         -5.35   17.19   22.54  Ca(OH)2
        Chalcedony       0.71   -3.03   -3.74  SiO2
        CSH(0.1)        -0.18   -1.31   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.10    0.41    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.05    2.13    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.02    3.85    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.00    5.57    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         0.00    7.29    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.02    9.01    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.08   10.73   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.13   11.29   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.21   13.83   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.31   14.16   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.50   14.44   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.71   14.67   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.94   14.86   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -1.17   15.03   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -1.39   15.17   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -1.60   15.30   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.80   15.41   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.99   15.51   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.76  -35.76   -0.00  H2
        Lime          -15.37   17.19   32.56  CaO
        O2            -11.61   71.52   83.13  O2
```

```
        Quartz          1.00   -3.03   -4.03  SiO2
        SiO2(am)       -0.32   -3.03   -2.71  Si1.000O2.000
        Wollastonite    0.38   14.16   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 6.
-----------------------------------

        Title 6 CSH(0.6)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  1
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 7
        END
-----
TITLE
-----

 6 CSH(0.6)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase              SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -5.15   17.39   22.54 0.000e+000          0.000e+000
        CSH(0.1)        -0.27   -1.41   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        -0.18    0.33    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -0.11    2.07    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -0.06    3.81    3.87 0.000e+000          0.000e+000
        CSH(0.5)        -0.02    5.55    5.57 0.000e+000          0.000e+000
        CSH(0.6)        -0.00    7.29    7.29 1.000e+000 9.902e-001-9.776e-003
        CSH(0.7)        -0.00    9.03    9.03 0.000e+000 6.252e-003 6.252e-003
        CSH(0.8)        -0.04   10.77   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -0.09   11.34   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.14   13.89   14.04 0.000e+000          0.000e+000
        CSH(1.0)        -0.23   14.24   14.48 0.000e+000          0.000e+000
        CSH(1.1)        -0.40   14.53   14.94 0.000e+000          0.000e+000
```

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        CSH(1.2)       -0.61   14.77   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.83   14.97   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -1.05   15.14   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -1.27   15.29   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -1.48   15.42   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -1.67   15.54   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -1.86   15.64   17.50 0.000e+000          0.000e+000
        SiO2(am)       -0.44   -3.15   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.489e-003  1.489e-003
        Si             3.524e-003  3.523e-003

----------------------------Description of solution----------------------------

                                pH  =  10.174     Charge balance
                                pe  =   7.624     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.406e-003
                     Mass of water (kg)  =  9.999e-001
                Total alkalinity (eq/kg)  =  2.978e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.716e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  49
                             Total H  = 1.110157e+002
                             Total O  = 5.551639e+001

----------------------------Distribution of species----------------------------

                                                Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.631e-004  1.518e-004   -3.787   -3.819   -0.031
        H+             7.152e-011  6.701e-011  -10.146  -10.174   -0.028
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.489e-003
        Ca+2           1.458e-003  1.103e-003   -2.836   -2.958   -0.121
        CaSiH3O4+       2.870e-005  2.672e-005   -4.542   -4.573   -0.031
        CaHO+          2.586e-006  2.408e-006   -5.587   -5.618   -0.031
H(0)         3.964e-039
        H2             1.982e-039  1.984e-039  -38.703  -38.702    0.000
O(0)         3.018e-015
        O2             1.509e-015  1.511e-015  -14.821  -14.821    0.000
Si           3.524e-003
        SiH3O4-         2.779e-003  2.588e-003   -2.556   -2.587   -0.031
        H4SiO4         7.136e-004  7.144e-004   -3.147   -3.146    0.000
        CaSiH3O4+       2.870e-005  2.672e-005   -4.542   -4.573   -0.031
        SiH2O4-2        2.051e-006  1.541e-006   -5.688   -5.812   -0.124

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite    0.29  -3.15  -3.43  SiO2
        b-Cristobalite   -0.16  -3.15  -2.98  SiO2
        Ca(OH)2         -5.15  17.39  22.54  Ca(OH)2
        Chalcedony       0.59  -3.15  -3.74  SiO2
        CSH(0.1)        -0.27  -1.41  -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.18   0.33   0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.11   2.07   2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.06   3.81   3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.02   5.55   5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.00   7.29   7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.00   9.03   9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.04  10.77  10.81  Ca0.800Si1.000O2.800:0.881H2O
```

```
        CSH(0.833)      -0.09   11.34   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.14   13.89   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.23   14.24   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.40   14.53   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.61   14.77   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.83   14.97   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -1.05   15.14   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -1.27   15.29   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -1.48   15.42   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.67   15.54   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.86   15.64   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.59  -35.60   -0.00  H2
        Lime           -15.17   17.39   32.56  CaO
        O2             -11.93   71.19   83.13  O2
        Quartz           0.88   -3.15   -4.03  SiO2
        SiO2(am)        -0.44   -3.15   -2.71  Si1.000O2.000
        Wollastonite     0.46   14.24   13.78  CaSiO3

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End of simulation.
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Reading input data for simulation 7.
-----------------------------------

        Title 7 CSH(0.7)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  1
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 8
        END
-----
TITLE
-----

 7 CSH(0.7)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1.DW
Using pure phase assemblage 1.
```

```
-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.72   17.82   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -0.53   -1.66   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.39    0.12    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.28    1.90    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.19    3.68    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.11    5.46    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.04    7.24    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.00    9.03    9.03 1.000e+000 9.914e-001-8.629e-003
        CSH(0.8)       -0.00   10.81   10.81 0.000e+000 5.871e-003 5.871e-003
        CSH(0.833)     -0.03   11.40   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.05   13.99   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.10   14.37   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.25   14.69   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -0.43   14.95   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.63   15.17   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -0.84   15.36   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -1.04   15.52   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -1.23   15.67   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -1.42   15.79   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -1.60   15.90   17.50 0.000e+000          0.000e+000
        SiO2(am)       -0.74   -3.45   -2.71 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.344e-003  1.344e-003
        Si             2.758e-003  2.758e-003

-----------------------------Description of solution-----------------------------

                                pH  =  10.408     Charge balance
                                pe  =   7.502     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.981e-003
                   Mass of water (kg)  =  9.999e-001
               Total alkalinity (eq/kg)  =  2.687e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                 Temperature (deg C)  =  25.000
              Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  94
                              Total H  = 1.110154e+002
                              Total O  = 5.551456e+001

----------------------------Distribution of species-----------------------------

                                                Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            2.789e-004  2.603e-004   -3.555   -3.585   -0.030
        H+             4.159e-011  3.907e-011  -10.381  -10.408   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.344e-003
        Ca+2           1.317e-003  1.009e-003   -2.880   -2.996   -0.116
        CaSiH3O4+       2.245e-005  2.097e-005   -4.649   -4.678   -0.030
        CaHO+          4.045e-006  3.778e-006   -5.393   -5.423   -0.030
H(0)         2.360e-039
        H2             1.180e-039  1.181e-039  -38.928  -38.928    0.000
O(0)         8.520e-015
        O2             4.260e-015  4.264e-015  -14.371  -14.370    0.000
Si           2.758e-003
        SiH3O4-         2.376e-003  2.219e-003   -2.624   -2.654   -0.030
        H4SiO4          3.569e-004  3.572e-004   -3.447   -3.447    0.000
```

```
        CaSiH3O4+       2.245e-005  2.097e-005   -4.649   -4.678   -0.030
        SiH2O4-2        2.978e-006  2.267e-006   -5.526   -5.645   -0.118

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.01   -3.45   -3.43  SiO2
        b-Cristobalite   -0.47   -3.45   -2.98  SiO2
        Ca(OH)2         -4.72   17.82   22.54  Ca(OH)2
        Chalcedony       0.29   -3.45   -3.74  SiO2
        CSH(0.1)        -0.53   -1.66   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.39    0.12    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.28    1.90    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.19    3.68    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.11    5.46    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.04    7.24    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.00    9.03    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.00   10.81   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.03   11.40   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.05   13.99   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.10   14.37   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.25   14.69   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.43   14.95   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.63   15.17   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.84   15.36   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -1.04   15.52   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -1.23   15.67   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.42   15.79   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.60   15.90   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.82  -35.82   -0.00  H2
        Lime           -14.74   17.82   32.56  CaO
        O2             -11.48   71.64   83.13  O2
        Quartz           0.58   -3.45   -4.03  SiO2
        SiO2(am)        -0.74   -3.45   -2.71  Si1.000O2.000
        Wollastonite     0.59   14.37   13.78  CaSiO3

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End of simulation.
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-----------------------------------
Reading input data for simulation 8.
-----------------------------------

        Title 8 CSH(0.8)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  1
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 9
        END
```

```
-----
TITLE
-----

 8 CSH(0.8)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -4.28   18.26   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -0.84   -1.97   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.66   -0.15    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.50    1.68    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.36    3.51    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.24    5.33    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.13    7.16    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.04    8.98    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.00   10.81   10.81 1.000e+000 9.936e-001-6.429e-003
        CSH(0.833)     -0.02   11.41   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.00   14.04   14.04 0.000e+000 3.961e-003 3.961e-003
        CSH(1.0)       -0.02   14.46   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.13   14.81   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -0.29   15.09   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.47   15.34   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -0.65   15.55   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -0.84   15.72   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -1.02   15.88   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -1.19   16.02   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -1.36   16.15   17.50 0.000e+000          0.000e+000
        SiO2(am)       -1.09   -3.80   -2.71 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.183e-003  1.183e-003
        Si             2.029e-003  2.029e-003

----------------------------Description of solution----------------------------

                                pH  =  10.651     Charge balance
                                pe  =   7.169     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.509e-003
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.366e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  56
                             Total H  = 1.110151e+002
                             Total O  = 5.551279e+001

----------------------------Distribution of species----------------------------

                                            Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma
```

```
          HO-            4.859e-004  4.553e-004   -3.313   -3.342   -0.028
          H+             2.370e-011  2.234e-011  -10.625  -10.651   -0.026
          H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca             1.183e-003
          Ca+2           1.161e-003  9.024e-004   -2.935   -3.045   -0.109
          CaSiH3O4+       1.564e-005  1.466e-005   -4.806   -4.834   -0.028
          CaHO+          6.304e-006  5.911e-006   -5.200   -5.228   -0.028
H(0)           3.579e-039
          H2             1.790e-039  1.791e-039  -38.747  -38.747    0.000
O(0)           3.705e-015
          O2             1.853e-015  1.854e-015  -14.732  -14.732    0.000
Si             2.029e-003
          SiH3O4-         1.850e-003  1.735e-003   -2.733   -2.761   -0.028
          H4SiO4         1.595e-004  1.597e-004   -3.797   -3.797    0.000
          CaSiH3O4+       1.564e-005  1.466e-005   -4.806   -4.834   -0.028
          SiH2O4-2        4.009e-006  3.099e-006   -5.397   -5.509   -0.112

-----------------------------Saturation indices-------------------------------

          Phase            SI log IAP  log KT

          a-Cristobalite   -0.36   -3.80   -3.43  SiO2
          b-Cristobalite   -0.82   -3.80   -2.98  SiO2
          Ca(OH)2         -4.28   18.26   22.54  Ca(OH)2
          Chalcedony       -0.06   -3.80   -3.74  SiO2
          CSH(0.1)         -0.84   -1.97   -1.13  Ca0.100Si1.000O2.100:0.110H2O
          CSH(0.2)         -0.66   -0.15    0.51  Ca0.200Si1.000O2.200:0.220H2O
          CSH(0.3)         -0.50    1.68    2.18  Ca0.300Si1.000O2.300:0.330H2O
          CSH(0.4)         -0.36    3.51    3.87  Ca0.400Si1.000O2.400:0.440H2O
          CSH(0.5)         -0.24    5.33    5.57  Ca0.500Si1.000O2.500:0.550H2O
          CSH(0.6)         -0.13    7.16    7.29  Ca0.600Si1.000O2.600:0.661H2O
          CSH(0.7)         -0.04    8.98    9.03  Ca0.700Si1.000O2.700:0.771H2O
          CSH(0.8)         -0.00   10.81   10.81  Ca0.800Si1.000O2.800:0.881H2O
          CSH(0.833)       -0.02   11.41   11.43  Ca0.833Si1.000O2.833:0.917H2O
          CSH(0.9)         -0.00   14.04   14.04  Ca1.000Si1.111O3.222:1.093H2O
          CSH(1.0)         -0.02   14.46   14.48  Ca1.000Si1.000O3.000:1.084H2O
          CSH(1.1)         -0.13   14.81   14.94  Ca1.000Si0.909O2.818:1.076H2O
          CSH(1.2)         -0.29   15.09   15.38  Ca1.000Si0.833O2.666:1.070H2O
          CSH(1.3)         -0.47   15.34   15.80  Ca1.000Si0.769O2.538:1.065H2O
          CSH(1.4)         -0.65   15.55   16.20  Ca1.000Si0.714O2.428:1.060H2O
          CSH(1.5)         -0.84   15.72   16.56  Ca1.000Si0.667O2.334:1.056H2O
          CSH(1.6)         -1.02   15.88   16.90  Ca1.000Si0.625O2.250:1.053H2O
          CSH(1.7)         -1.19   16.02   17.21  Ca1.000Si0.588O2.176:1.049H2O
          CSH(1.8)         -1.36   16.15   17.50  Ca1.000Si0.556O2.112:1.047H2O
          H2             -35.64  -35.64   -0.00  H2
          Lime           -14.30   18.26   32.56  CaO
          O2             -11.85   71.28   83.13  O2
          Quartz           0.23   -3.80   -4.03  SiO2
          SiO2(am)         -1.09   -3.80   -2.71  Si1.000O2.000
          Wollastonite      0.68   14.46   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 9.
------------------------------------

          Title 9 CSH(0.9)
          USE SOLUTION 1 DW
          EQUILIBRIUM_PHASES
          CSH(0.1)  0.0  0.0
          CSH(0.2)  0.0  0.0
          CSH(0.3)  0.0  0.0
          CSH(0.4)  0.0  0.0
          CSH(0.5)  0.0  0.0
          CSH(0.6)  0.0  0.0
          CSH(0.7)  0.0  0.0
          CSH(0.8)  0.0  0.0
          CSH(0.9)  0.0  1
```

```
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 10
        END
-----
TITLE
-----

 9 CSH(0.9)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -4.12   18.42   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -0.97   -2.10   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -0.77   -0.26    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.60    1.58    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.44    3.42    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.30    5.27    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.18    7.11    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.08    8.95    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.02   10.79   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.03   11.40   11.43 0.000e+000          0.000e+000
        CSH(0.9)        0.00   14.04   14.04 1.000e+000 9.944e-001-5.643e-003
        CSH(1.0)        0.00   14.48   14.48 0.000e+000 4.518e-003 4.518e-003
        CSH(1.1)       -0.10   14.84   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -0.25   15.14   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.41   15.39   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -0.59   15.61   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -0.77   15.79   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -0.94   15.96   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -1.11   16.10   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -1.27   16.23   17.50 0.000e+000          0.000e+000
        SiO2(am)       -1.24   -3.95   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca            1.125e-003  1.125e-003
        Si            1.752e-003  1.752e-003

----------------------------Description of solution----------------------------

                                pH  =  10.743     Charge balance
                                pe  =   6.743     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.339e-003
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.251e-003
```

```
                Total carbon (mol/kg)  =  0.000e+000
                   Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
               Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  17
                           Total H  = 1.110150e+002
                           Total O  = 5.551212e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
         Species          Molality    Activity Molality Activity    Gamma

         HO-            6.002e-004  5.633e-004   -3.222   -3.249   -0.028
         H+             1.913e-011  1.806e-011  -10.718  -10.743   -0.025
         H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca            1.125e-003
         Ca+2           1.105e-003  8.635e-004   -2.957   -3.064   -0.107
         CaSiH3O4+       1.311e-005  1.231e-005   -4.882   -4.910   -0.027
         CaHO+          7.452e-006  6.998e-006   -5.128   -5.155   -0.027
H(0)          1.668e-038
         H2             8.339e-039  8.346e-039  -38.079  -38.079    0.000
O(0)          1.706e-016
         O2             8.532e-017  8.538e-017  -16.069  -16.069    0.000
Si            1.752e-003
         SiH3O4-         1.621e-003  1.522e-003   -2.790   -2.818   -0.027
         H4SiO4         1.132e-004  1.132e-004   -3.946   -3.946    0.000
         CaSiH3O4+       1.311e-005  1.231e-005   -4.882   -4.910   -0.027
         SiH2O4-2        4.327e-006  3.364e-006   -5.364   -5.473   -0.109

-----------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -0.51   -3.95   -3.43  SiO2
         b-Cristobalite   -0.96   -3.95   -2.98  SiO2
         Ca(OH)2         -4.12   18.42   22.54  Ca(OH)2
         Chalcedony       -0.21   -3.95   -3.74  SiO2
         CSH(0.1)         -0.97   -2.10   -1.13  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -0.77   -0.26    0.51  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -0.60    1.58    2.18  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -0.44    3.42    3.87  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -0.30    5.27    5.57  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -0.18    7.11    7.29  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -0.08    8.95    9.03  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -0.02   10.79   10.81  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -0.03   11.40   11.43  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)          0.00   14.04   14.04  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)          0.00   14.48   14.48  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)         -0.10   14.84   14.94  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.25   15.14   15.38  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.41   15.39   15.80  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)         -0.59   15.61   16.20  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.77   15.79   16.56  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -0.94   15.96   16.90  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)         -1.11   16.10   17.21  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)         -1.27   16.23   17.50  Ca1.000Si0.556O2.112:1.047H2O
         H2             -34.97  -34.97   -0.00  H2
         Lime           -14.14   18.42   32.56  CaO
         O2             -13.18   69.94   83.13  O2
         Quartz           0.08   -3.95   -4.03  SiO2
         SiO2(am)        -1.24   -3.95   -2.71  Si1.000O2.000
         Wollastonite     0.69   14.48   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 10.
```

```
------------------------------------

        Title 10 CSH(1.0)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  1
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 11
        END
-----
TITLE
-----

 10 CSH(1.0)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -3.65   18.89   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -1.39   -2.52   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -1.14   -0.63    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -0.92    1.26    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -0.72    3.15    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.53    5.03    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.37    6.92    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.22    8.81    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.11   10.70   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.10   11.32   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.05   13.99   14.04 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.48   14.48 1.000e+000 9.990e-001-1.036e-003
        CSH(1.1)       -0.06   14.88   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -0.17   15.21   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.31   15.50   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -0.46   15.74   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -0.62   15.95   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -0.77   16.13   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -0.92   16.29   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -1.07   16.43   17.50 0.000e+000          0.000e+000
        SiO2(am)       -1.70   -4.41   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------
```

```
        Elements         Molality     Moles

        Ca            1.036e-003  1.036e-003
        Si            1.036e-003  1.036e-003

----------------------------Description of solution----------------------------

                                pH  =  10.991     Charge balance
                                pe  =   6.800     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.074e-003
                   Mass of water (kg)  =  1.000e+000
              Total alkalinity (eq/kg)  =  2.072e-003
                 Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
               Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  15
                            Total H  = 1.110147e+002
                            Total O  = 5.551045e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-           1.058e-003  9.956e-004   -2.975   -3.002   -0.027
        H+            1.080e-011  1.022e-011  -10.966  -10.991   -0.024
        H2O           5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.036e-003
        Ca+2          1.017e-003  8.019e-004   -2.993   -3.096   -0.103
        CaHO+         1.220e-005  1.149e-005   -4.913   -4.940   -0.026
        CaSiH3O4+      7.399e-006  6.965e-006   -5.131   -5.157   -0.026
H(0)         4.106e-039
        H2            2.053e-039  2.055e-039  -38.688  -38.687    0.000
O(0)         2.816e-015
        O2            1.408e-015  1.409e-015  -14.851  -14.851    0.000
Si           1.036e-003
        SiH3O4-        9.852e-004  9.273e-004   -3.006   -3.033   -0.026
        H4SiO4         3.900e-005  3.903e-005   -4.409   -4.409    0.000
        CaSiH3O4+      7.399e-006  6.965e-006   -5.131   -5.157   -0.026
        SiH2O4-2       4.615e-006  3.623e-006   -5.336   -5.441   -0.105

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.97   -4.41   -3.43  SiO2
        b-Cristobalite   -1.43   -4.41   -2.98  SiO2
        Ca(OH)2         -3.65   18.89   22.54  Ca(OH)2
        Chalcedony       -0.67   -4.41   -3.74  SiO2
        CSH(0.1)         -1.39   -2.52   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -1.14   -0.63    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.92    1.26    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.72    3.15    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.53    5.03    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.37    6.92    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.22    8.81    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.11   10.70   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.10   11.32   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.05   13.99   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)          0.00   14.48   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.06   14.88   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.17   15.21   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.31   15.50   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.46   15.74   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.62   15.95   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.77   16.13   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.92   16.29   17.21  Ca1.000Si0.588O2.176:1.049H2O
```

```
        CSH(1.8)        -1.07   16.43   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.58  -35.58   -0.00  H2
        Lime           -13.68   18.89   32.56  CaO
        O2             -11.96   71.16   83.13  O2
        Quartz          -0.38   -4.41   -4.03  SiO2
        SiO2(am)        -1.70   -4.41   -2.71  Si1.000O2.000
        Wollastonite     0.69   14.48   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 11.
------------------------------------

        Title 11 CSH(1.1)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  1
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 12
        END
-----
TITLE
-----

 11 CSH(1.1)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -3.03   19.51   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -1.95   -3.08   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -1.64   -1.13    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -1.36    0.82    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -1.10    2.77    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -0.85    4.72    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.61    6.67    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.40    8.62    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.23   10.58   10.81 0.000e+000          0.000e+000
```

```
        CSH(0.833)      -0.21   11.22   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.12   13.92   14.04 0.000e+000          0.000e+000
        CSH(1.0)         0.00   14.48   14.48 0.000e+000 7.402e-003 7.402e-003
        CSH(1.1)        -0.00   14.93   14.94 1.000e+000 9.913e-001-8.652e-003
        CSH(1.2)        -0.06   15.32   15.38 0.000e+000          0.000e+000
        CSH(1.3)        -0.16   15.64   15.80 0.000e+000          0.000e+000
        CSH(1.4)        -0.28   15.92   16.20 0.000e+000          0.000e+000
        CSH(1.5)        -0.41   16.15   16.56 0.000e+000          0.000e+000
        CSH(1.6)        -0.54   16.36   16.90 0.000e+000          0.000e+000
        CSH(1.7)        -0.66   16.55   17.21 0.000e+000          0.000e+000
        CSH(1.8)        -0.79   16.71   17.50 0.000e+000          0.000e+000
        SiO2(am)        -2.33   -5.03   -2.71 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.250e-003  1.250e-003
        Si             4.626e-004  4.626e-004

----------------------------Description of solution---------------------------

                                pH  =  11.268     Charge balance
                                pe  =   6.674     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.691e-003
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  2.500e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.725e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  16
                             Total H  = 1.110150e+002
                             Total O  = 5.550968e+001

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            2.015e-003  1.885e-003    -2.696    -2.725    -0.029
        H+             5.731e-012  5.395e-012   -11.242   -11.268    -0.026
        H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
Ca           1.250e-003
        Ca+2           1.219e-003  9.418e-004    -2.914    -3.026    -0.112
        CaHO+          2.729e-005  2.555e-005    -4.564    -4.593    -0.029
        CaSiH3O4+      3.929e-006  3.678e-006    -5.406    -5.434    -0.029
H(0)         2.037e-039
        H2             1.018e-039  1.019e-039   -38.992   -38.992     0.000
O(0)         1.144e-014
        O2             5.719e-015  5.724e-015   -14.243   -14.242     0.000
Si           4.626e-004
        SiH3O4-        4.454e-004  4.170e-004    -3.351    -3.380    -0.029
        H4SiO4         9.260e-006  9.268e-006    -5.033    -5.033     0.000
        SiH2O4-2       4.015e-006  3.085e-006    -5.396    -5.511    -0.114
        CaSiH3O4+      3.929e-006  3.678e-006    -5.406    -5.434    -0.029

----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -1.60   -5.03   -3.43  SiO2
        b-Cristobalite   -2.05   -5.03   -2.98  SiO2
        Ca(OH)2         -3.03   19.51   22.54  Ca(OH)2
        Chalcedony       -1.29   -5.03   -3.74  SiO2
        CSH(0.1)        -1.95   -3.08   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -1.64   -1.13    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -1.36    0.82    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -1.10    2.77    3.87  Ca0.400Si1.000O2.400:0.440H2O
```

```
        CSH(0.5)        -0.85    4.72    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.61    6.67    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.40    8.62    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.23   10.58   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.21   11.22   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.12   13.92   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00   14.48   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.00   14.93   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.06   15.32   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.16   15.64   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.28   15.92   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.41   16.15   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.54   16.36   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.66   16.55   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.79   16.71   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2            -35.88  -35.89   -0.00  H2
        Lime          -13.05   19.51   32.56  CaO
        O2            -11.36   71.77   83.13  O2
        Quartz         -1.00   -5.03   -4.03  SiO2
        SiO2(am)       -2.33   -5.03   -2.71  Si1.000O2.000
        Wollastonite    0.69   14.48   13.78  CaSiO3

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End of simulation.
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------------------------------------
Reading input data for simulation 12.
------------------------------------

        Title 12 CSH(1.2)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  1
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 13
        END
-----
TITLE
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 12 CSH(1.2)

----------------------------------------
Beginning of batch-reaction calculations.
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Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.
```

```
-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -2.27   20.27   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -2.71   -3.84   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -2.33   -1.81    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -1.97    0.21    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -1.63    2.24    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -1.30    4.27    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -0.99    6.29    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -0.71    8.32    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.46   10.35   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.41   11.02   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.29   13.75   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.08   14.40   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.00   14.93   14.94 0.000e+000 2.113e-002 2.113e-002
        CSH(1.2)        0.00   15.38   15.38 1.000e+000 9.768e-001-2.322e-002
        CSH(1.3)       -0.05   15.76   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -0.12   16.08   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -0.21   16.36   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -0.30   16.60   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -0.39   16.82   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -0.50   17.01   17.50 0.000e+000          0.000e+000
        SiO2(am)       -3.16   -5.87   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             2.088e-003  2.088e-003
        Si             1.332e-004  1.332e-004

----------------------------Description of solution-----------------------------

                                pH  =  11.554     Charge balance
                                pe  =   6.324     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  6.098e-003
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  4.176e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  51
                             Total H  = 1.110166e+002
                             Total O  = 5.551068e+001

---------------------------Distribution of species-----------------------------

                                              Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            3.960e-003  3.640e-003   -2.402   -2.439   -0.036
        H+             3.010e-012  2.794e-012   -11.521  -11.554   -0.032
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           2.088e-003
        Ca+2           2.004e-003  1.452e-003   -2.698   -2.838   -0.140
        CaHO+          8.259e-005  7.603e-005   -4.083   -4.119   -0.036
        CaSiH3O4+       1.737e-006  1.599e-006   -5.760   -5.796   -0.036
H(0)         2.738e-039
        H2             1.369e-039  1.371e-039  -38.864  -38.863    0.001
O(0)         6.320e-015
        O2             3.160e-015  3.164e-015  -14.500  -14.500    0.001
Si           1.332e-004
        SiH3O4-         1.278e-004  1.176e-004   -3.894   -3.930   -0.036
        SiH2O4-2        2.340e-006  1.680e-006   -5.631   -5.775   -0.144
        CaSiH3O4+       1.737e-006  1.599e-006   -5.760   -5.796   -0.036
```

```
        H4SiO4         1.352e-006  1.354e-006   -5.869   -5.869    0.001

-----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -2.43   -5.87   -3.43  SiO2
        b-Cristobalite   -2.89   -5.87   -2.98  SiO2
        Ca(OH)2          -2.27   20.27   22.54  Ca(OH)2
        Chalcedony       -2.13   -5.87   -3.74  SiO2
        CSH(0.1)         -2.71   -3.84   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -2.33   -1.81    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -1.97    0.21    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -1.63    2.24    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -1.30    4.27    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.99    6.29    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.71    8.32    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.46   10.35   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.41   11.02   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.29   13.75   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.08   14.40   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.00   14.93   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)          0.00   15.38   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.05   15.76   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.12   16.08   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.21   16.36   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.30   16.60   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.39   16.82   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.50   17.01   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.75  -35.76   -0.00  H2
        Lime           -12.29   20.27   32.56  CaO
        O2             -11.61   71.51   83.13  O2
        Quartz          -1.84   -5.87   -4.03  SiO2
        SiO2(am)        -3.16   -5.87   -2.71  Si1.000O2.000
        Wollastonite     0.62   14.40   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 13.
------------------------------------

        Title 13 CSH(1.3)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  1
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 14
        END
-----
```

```
TITLE
-----

 13 CSH(1.3)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

WARNING: Maximum iterations exceeded, 200

Numerical method failed with this set of convergence parameters.
WARNING: Trying diagonal scaling ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -1.67   20.87   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -3.37   -4.51   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -2.93   -2.42    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -2.51   -0.33    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -2.11    1.76    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -1.73    3.84    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -1.36    5.93    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -1.01    8.02    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -0.70   10.11   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -0.63   10.79   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -0.49   13.55   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.20   14.28   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.06   14.88   14.94 0.000e+000          0.000e+000
        CSH(1.2)        0.00   15.38   15.38 0.000e+000 4.065e-002 4.065e-002
        CSH(1.3)        0.00   15.80   15.80 1.000e+000 9.559e-001-4.409e-002
        CSH(1.4)       -0.03   16.17   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -0.09   16.48   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -0.15   16.75   16.90 0.000e+000          0.000e+000
        CSH(1.7)       -0.22   17.00   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -0.29   17.21   17.50 0.000e+000          0.000e+000
        SiO2(am)       -3.89   -6.59   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             3.438e-003  3.438e-003
        Si             4.256e-005  4.256e-005

----------------------------Description of solution----------------------------

                                pH  =  11.769     Charge balance
                                pe  =   6.110     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  9.902e-003
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  6.877e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.718e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
```

```
                          Iterations  =  89
                            Total H  = 1.110194e+002
                            Total O  = 5.551320e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            6.627e-003  5.968e-003   -2.179   -2.224   -0.045
        H+             1.865e-012  1.704e-012  -11.729  -11.769   -0.039
        H2O            5.551e+001  9.998e-001    1.744   -0.000    0.000
Ca           3.438e-003
        Ca+2           3.231e-003  2.171e-003   -2.491   -2.663   -0.173
        CaHO+          2.066e-004  1.864e-004   -3.685   -3.729   -0.045
        CaSiH3O4+      8.177e-007  7.379e-007   -6.087   -6.132   -0.045
H(0)         2.728e-039
        H2             1.364e-039  1.367e-039  -38.865  -38.864    0.001
O(0)         6.346e-015
        O2             3.173e-015  3.180e-015  -14.499  -14.498    0.001
Si           4.256e-005
        SiH3O4-        4.021e-005  3.629e-005   -4.396   -4.440   -0.045
        SiH2O4-2       1.281e-006  8.498e-007   -5.892   -6.071   -0.178
        CaSiH3O4+      8.177e-007  7.379e-007   -6.087   -6.132   -0.045
        H4SiO4         2.542e-007  2.547e-007   -6.595   -6.594    0.001

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -3.16  -6.59  -3.43  SiO2
        b-Cristobalite  -3.61  -6.59  -2.98  SiO2
        Ca(OH)2        -1.67  20.87  22.54  Ca(OH)2
        Chalcedony      -2.86  -6.59  -3.74  SiO2
        CSH(0.1)        -3.37  -4.51  -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -2.93  -2.42   0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -2.51  -0.33   2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -2.11   1.76   3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -1.73   3.84   5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -1.36   5.93   7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -1.01   8.02   9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.70  10.11  10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.63  10.79  11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.49  13.55  14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.20  14.28  14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.06  14.88  14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         0.00  15.38  15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         0.00  15.80  15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.03  16.17  16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.09  16.48  16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.15  16.75  16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.22  17.00  17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.29  17.21  17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.75 -35.76  -0.00  H2
        Lime           -11.69  20.87  32.56  CaO
        O2             -11.61  71.51  83.13  O2
        Quartz          -2.57  -6.59  -4.03  SiO2
        SiO2(am)        -3.89  -6.59  -2.71  Si1.000O2.000
        Wollastonite     0.50  14.28  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 14.
------------------------------------

        Title 14 CSH(1.4)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
```

```
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  1
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 15
        END
-----
TITLE
-----

 14 CSH(1.4)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase              SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2         -1.23   21.31   22.54 0.000e+000          0.000e+000
        CSH(0.1)        -3.90   -5.03   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        -3.41   -2.90    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -2.95   -0.77    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -2.51    1.36    3.87 0.000e+000          0.000e+000
        CSH(0.5)        -2.08    3.49    5.57 0.000e+000          0.000e+000
        CSH(0.6)        -1.66    5.62    7.29 0.000e+000          0.000e+000
        CSH(0.7)        -1.27    7.75    9.03 0.000e+000          0.000e+000
        CSH(0.8)        -0.92    9.89   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -0.84   10.59   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.69   13.35   14.04 0.000e+000          0.000e+000
        CSH(1.0)        -0.33   14.15   14.48 0.000e+000          0.000e+000
        CSH(1.1)        -0.13   14.80   14.94 0.000e+000          0.000e+000
        CSH(1.2)        -0.04   15.34   15.38 0.000e+000          0.000e+000
        CSH(1.3)         0.00   15.80   15.80 0.000e+000 6.507e-002 6.507e-002
        CSH(1.4)        -0.00   16.20   16.20 1.000e+000 9.299e-001-7.011e-002
        CSH(1.5)        -0.03   16.53   16.56 0.000e+000          0.000e+000
        CSH(1.6)        -0.07   16.83   16.90 0.000e+000          0.000e+000
        CSH(1.7)        -0.11   17.10   17.21 0.000e+000          0.000e+000
        CSH(1.8)        -0.17   17.33   17.50 0.000e+000          0.000e+000
        SiO2(am)        -4.46   -7.16   -2.71 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------
```

```
        Elements         Molality     Moles

        Ca             5.036e-003  5.036e-003
        Si             1.700e-005  1.700e-005

----------------------------Description of solution----------------------------

                                pH  =  11.924     Charge balance
                                pe  =  -5.600     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.430e-002
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  1.007e-002
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.730e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  84
                              Total H  = 1.110225e+002
                              Total O  = 5.551630e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            9.651e-003  8.532e-003   -2.015   -2.069   -0.054
        H+             1.322e-012  1.192e-012  -11.879  -11.924   -0.045
        H2O            5.551e+001  9.998e-001    1.744   -0.000    0.000
Ca           5.036e-003
        Ca+2           4.632e-003  2.914e-003   -2.334   -2.535   -0.201
        CaHO+          4.034e-004  3.577e-004   -3.394   -3.446   -0.052
        CaSiH3O4+      4.298e-007  3.812e-007   -6.367   -6.419   -0.052
H(0)         3.507e-016
        H2             1.753e-016  1.759e-016  -15.756  -15.755    0.001
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -60.718  -60.717    0.001
Si           1.700e-005
        SiH3O4-        1.575e-005  1.397e-005   -4.803   -4.855   -0.052
        SiH2O4-2       7.564e-007  4.676e-007   -6.121   -6.330   -0.209
        CaSiH3O4+      4.298e-007  3.812e-007   -6.367   -6.419   -0.052
        H4SiO4         6.835e-008  6.857e-008   -7.165   -7.164    0.001

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -3.73  -7.16  -3.43  SiO2
        b-Cristobalite  -4.18  -7.16  -2.98  SiO2
        Ca(OH)2         -1.23  21.31  22.54  Ca(OH)2
        Chalcedony      -3.43  -7.16  -3.74  SiO2
        CSH(0.1)        -3.90  -5.03  -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -3.41  -2.90   0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -2.95  -0.77   2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -2.51   1.36   3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -2.08   3.49   5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -1.66   5.62   7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -1.27   7.75   9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.92   9.89  10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.84  10.59  11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.69  13.35  14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.33  14.15  14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.13  14.80  14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.04  15.34  15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         0.00  15.80  15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.00  16.20  16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.03  16.53  16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.07  16.83  16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.11  17.10  17.21  Ca1.000Si0.588O2.176:1.049H2O
```

```
        CSH(1.8)        -0.17   17.33   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -12.64  -12.65   -0.00  H2
        Lime           -11.25   21.31   32.56  CaO
        O2             -57.83   25.30   83.13  O2
        Quartz          -3.14   -7.16   -4.03  SiO2
        SiO2(am)        -4.46   -7.16   -2.71  Si1.000O2.000
        Wollastonite     0.37   14.15   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 15.
------------------------------------

        Title 15 CSH(1.5)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  1
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 16
        END
-----
TITLE
-----

 15 CSH(1.5)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase              SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -0.80   21.74   22.54 0.000e+000          0.000e+000
        CSH(0.1)        -4.46   -5.59   -1.13 0.000e+000          0.000e+000
        CSH(0.2)        -3.93   -3.42    0.51 0.000e+000          0.000e+000
        CSH(0.3)        -3.42   -1.24    2.18 0.000e+000          0.000e+000
        CSH(0.4)        -2.94    0.93    3.87 0.000e+000          0.000e+000
        CSH(0.5)        -2.46    3.10    5.57 0.000e+000          0.000e+000
        CSH(0.6)        -2.01    5.28    7.29 0.000e+000          0.000e+000
        CSH(0.7)        -1.57    7.45    9.03 0.000e+000          0.000e+000
        CSH(0.8)        -1.18    9.63   10.81 0.000e+000          0.000e+000
```

```
        CSH(0.833)      -1.08   10.35   11.43 0.000e+000          0.000e+000
        CSH(0.9)        -0.93   13.11   14.04 0.000e+000          0.000e+000
        CSH(1.0)        -0.50   13.98   14.48 0.000e+000          0.000e+000
        CSH(1.1)        -0.25   14.68   14.94 0.000e+000          0.000e+000
        CSH(1.2)        -0.11   15.27   15.38 0.000e+000          0.000e+000
        CSH(1.3)        -0.03   15.77   15.80 0.000e+000          0.000e+000
        CSH(1.4)        -0.00   16.20   16.20 0.000e+000 1.050e-001 1.050e-001
        CSH(1.5)        -0.00   16.56   16.56 1.000e+000 8.876e-001-1.124e-001
        CSH(1.6)        -0.01   16.89   16.90 0.000e+000          0.000e+000
        CSH(1.7)        -0.04   17.18   17.21 0.000e+000          0.000e+000
        CSH(1.8)        -0.08   17.42   17.50 0.000e+000          0.000e+000
        SiO2(am)        -5.06   -7.77   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             7.409e-003  7.409e-003
        Si             6.351e-006  6.351e-006

----------------------------Description of solution----------------------------

                                pH  =  12.077     Charge balance
                                pe  =   5.572     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  2.067e-002
                   Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  1.482e-002
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                 Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  89
                              Total H  = 1.110272e+002
                              Total O  = 5.552104e+001

----------------------------Distribution of species----------------------------

                                                Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.403e-002  1.214e-002   -1.853   -1.916   -0.063
        H+             9.425e-013  8.373e-013  -12.026  -12.077   -0.051
        H2O            5.551e+001  9.996e-001    1.744   -0.000    0.000
Ca           7.409e-003
        Ca+2           6.631e-003  3.873e-003   -2.178   -2.412   -0.234
        CaHO+          7.784e-004  6.766e-004   -3.109   -3.170   -0.061
        CaSiH3O4+       2.072e-007  1.801e-007   -6.684   -6.744   -0.061
H(0)         7.828e-039
        H2             3.914e-039  3.932e-039  -38.407  -38.405    0.002
O(0)         7.650e-016
        O2             3.825e-016  3.843e-016  -15.417  -15.415    0.002
Si           6.351e-006
        SiH3O4-         5.713e-006  4.966e-006   -5.243   -5.304   -0.061
        SiH2O4-2        4.145e-007  2.367e-007   -6.382   -6.626   -0.243
        CaSiH3O4+       2.072e-007  1.801e-007   -6.684   -6.744   -0.061
        H4SiO4         1.705e-008  1.713e-008   -7.768   -7.766    0.002

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -4.33   -7.77   -3.43  SiO2
        b-Cristobalite   -4.78   -7.77   -2.98  SiO2
        Ca(OH)2         -0.80   21.74   22.54  Ca(OH)2
        Chalcedony       -4.03   -7.77   -3.74  SiO2
        CSH(0.1)        -4.46   -5.59   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -3.93   -3.42    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -3.42   -1.24    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -2.94    0.93    3.87  Ca0.400Si1.000O2.400:0.440H2O
```

```
          CSH(0.5)        -2.46    3.10    5.57  Ca0.500Si1.000O2.500:0.550H2O
          CSH(0.6)        -2.01    5.28    7.29  Ca0.600Si1.000O2.600:0.661H2O
          CSH(0.7)        -1.57    7.45    9.03  Ca0.700Si1.000O2.700:0.771H2O
          CSH(0.8)        -1.18    9.63   10.81  Ca0.800Si1.000O2.800:0.881H2O
          CSH(0.833)       -1.08   10.35   11.43  Ca0.833Si1.000O2.833:0.917H2O
          CSH(0.9)        -0.93   13.11   14.04  Ca1.000Si1.111O3.222:1.093H2O
          CSH(1.0)        -0.50   13.98   14.48  Ca1.000Si1.000O3.000:1.084H2O
          CSH(1.1)        -0.25   14.68   14.94  Ca1.000Si0.909O2.818:1.076H2O
          CSH(1.2)        -0.11   15.27   15.38  Ca1.000Si0.833O2.666:1.070H2O
          CSH(1.3)        -0.03   15.77   15.80  Ca1.000Si0.769O2.538:1.065H2O
          CSH(1.4)        -0.00   16.20   16.20  Ca1.000Si0.714O2.428:1.060H2O
          CSH(1.5)        -0.00   16.56   16.56  Ca1.000Si0.667O2.334:1.056H2O
          CSH(1.6)        -0.01   16.89   16.90  Ca1.000Si0.625O2.250:1.053H2O
          CSH(1.7)        -0.04   17.18   17.21  Ca1.000Si0.588O2.176:1.049H2O
          CSH(1.8)        -0.08   17.42   17.50  Ca1.000Si0.556O2.112:1.047H2O
          H2             -35.30  -35.30   -0.00  H2
          Lime           -10.82   21.74   32.56  CaO
          O2             -12.53   70.60   83.13  O2
          Quartz          -3.74   -7.77   -4.03  SiO2
          SiO2(am)        -5.06   -7.77   -2.71  Si1.000O2.000
          Wollastonite     0.19   13.98   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 16.
------------------------------------

          Title 16 CSH(1.6)
          USE SOLUTION 1 DW
          EQUILIBRIUM_PHASES
          CSH(0.1)  0.0  0.0
          CSH(0.2)  0.0  0.0
          CSH(0.3)  0.0  0.0
          CSH(0.4)  0.0  0.0
          CSH(0.5)  0.0  0.0
          CSH(0.6)  0.0  0.0
          CSH(0.7)  0.0  0.0
          CSH(0.8)  0.0  0.0
          CSH(0.9)  0.0  0.0
          CSH(1.0)  0.0  0.0
          CSH(1.1)  0.0  0.0
          CSH(1.2)  0.0  0.0
          CSH(1.3)  0.0  0.0
          CSH(1.4)  0.0  0.0
          CSH(1.5)  0.0  0.0
          CSH(1.6)  0.0  1
          CSH(1.7)  0.0  0.0
          CSH(1.8)  0.0  0.0
          SiO2(am)  0.0  0.0
          CSH(0.833) 0.0 0.0
          Ca(OH)2   0.0  0.0
          Save Solution 17
          END
-----
TITLE
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 16 CSH(1.6)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.
```

```
-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -0.61   21.93   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -4.72   -5.85   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -4.17   -3.66    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -3.65   -1.47    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -3.14    0.72    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -2.65    2.92    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -2.18    5.11    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -1.72    7.30    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -1.31    9.50   10.81 0.000e+000          0.000e+000
        CSH(0.833)     -1.21   10.22   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -1.05   12.99   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.59   13.88   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.32   14.61   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -0.15   15.23   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.06   15.74   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -0.01   16.18   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -0.00   16.56   16.56 0.000e+000 1.309e-001 1.309e-001
        CSH(1.6)       -0.00   16.90   16.90 1.000e+000 8.603e-001-1.397e-001
        CSH(1.7)       -0.02   17.20   17.21 0.000e+000          0.000e+000
        CSH(1.8)       -0.05   17.46   17.50 0.000e+000          0.000e+000
        SiO2(am)       -5.34   -8.05   -2.71 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             8.801e-003  8.801e-003
        Si             3.981e-006  3.981e-006

-----------------------------Description of solution-----------------------------

                                pH  =  12.145     Charge balance
                                pe  =   5.762     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  2.433e-002
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  1.760e-002
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  95
                             Total H  = 1.110302e+002
                             Total O  = 5.552390e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            1.656e-002  1.418e-002   -1.781   -1.848   -0.067
        H+             8.126e-013  7.169e-013  -12.090  -12.145   -0.054
        H2O            5.551e+001  9.996e-001    1.744   -0.000    0.000
Ca           8.801e-003
        Ca+2           7.764e-003  4.376e-003   -2.110   -2.359   -0.249
        CaHO+          1.037e-003  8.929e-004   -2.984   -3.049   -0.065
        CaSiH3O4+       1.443e-007  1.243e-007   -6.841   -6.906   -0.065
H(0)         2.392e-039
        H2             1.196e-039  1.202e-039  -38.922  -38.920    0.002
O(0)         8.173e-015
        O2             4.087e-015  4.110e-015  -14.389  -14.386    0.002
Si           3.981e-006
        SiH3O4-         3.521e-006  3.032e-006   -5.453   -5.518   -0.065
        SiH2O4-2        3.071e-007  1.687e-007   -6.513   -6.773   -0.260
        CaSiH3O4+       1.443e-007  1.243e-007   -6.841   -6.906   -0.065
```

```
        H4SiO4          8.904e-009  8.954e-009    -8.050    -8.048     0.002

-----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -4.61   -8.05   -3.43  SiO2
        b-Cristobalite   -5.07   -8.05   -2.98  SiO2
        Ca(OH)2          -0.61   21.93   22.54  Ca(OH)2
        Chalcedony       -4.31   -8.05   -3.74  SiO2
        CSH(0.1)         -4.72   -5.85   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -4.17   -3.66    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -3.65   -1.47    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.14    0.72    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -2.65    2.92    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.18    5.11    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.72    7.30    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.31    9.50   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.21   10.22   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -1.05   12.99   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.59   13.88   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.32   14.61   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.15   15.23   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.06   15.74   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.01   16.18   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.00   16.56   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.00   16.90   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.02   17.20   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.05   17.46   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.81  -35.81   -0.00  H2
        Lime           -10.63   21.93   32.56  CaO
        O2             -11.50   71.63   83.13  O2
        Quartz          -4.02   -8.05   -4.03  SiO2
        SiO2(am)        -5.34   -8.05   -2.71  Si1.000O2.000
        Wollastonite     0.10   13.88   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 17.
------------------------------------

        Title 17 CSH(1.7)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  1
        CSH(1.8)  0.0  0.0
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 18
        END
-----
```

```
TITLE
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 17 CSH(1.7)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -0.35   22.19   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -5.11   -6.24   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -4.53   -4.02    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -3.98   -1.80    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -3.45    0.42    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -2.93    2.63    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -2.44    4.85    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -1.96    7.07    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -1.52    9.29   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -1.41   10.02   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -1.25   12.79   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.75   13.73   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.44   14.50   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -0.24   15.14   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.12   15.68   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -0.05   16.15   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -0.02   16.54   16.56 0.000e+000          0.000e+000
        CSH(1.6)        0.00   16.90   16.90 0.000e+000 1.776e-001 1.776e-001
        CSH(1.7)        0.00   17.21   17.21 1.000e+000 8.112e-001-1.888e-001
        CSH(1.8)       -0.02   17.48   17.50 0.000e+000          0.000e+000
        SiO2(am)       -5.75   -8.46   -2.71 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.118e-002  1.118e-002
        Si             1.991e-006  1.991e-006

-----------------------------Description of solution-----------------------------

                                pH  =  12.237     Charge balance
                                pe  =   5.480     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  3.047e-002
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.236e-002
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.757e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  18
                             Total H  = 1.110345e+002
                             Total O  = 5.552842e+001

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            2.082e-002  1.756e-002   -1.681   -1.755   -0.074
```

```
        H+            6.627e-013  5.789e-013   -12.179   -12.237    -0.059
        H2O           5.551e+001  9.995e-001    1.744    -0.000     0.000
Ca           1.118e-002
        Ca+2          9.645e-003  5.163e-003    -2.016    -2.287    -0.271
        CaHO+         1.536e-003  1.304e-003    -2.814    -2.885    -0.071
        CaSiH3O4+      8.280e-008  7.031e-008    -7.082    -7.153    -0.071
H(0)         5.702e-039
        H2            2.851e-039  2.871e-039   -38.545   -38.542     0.003
O(0)         1.431e-015
        O2            7.157e-016  7.207e-016   -15.145   -15.142     0.003
Si           1.991e-006
        SiH3O4-        1.712e-006  1.454e-006    -5.766    -5.837    -0.071
        SiH2O4-2       1.928e-007  1.002e-007    -6.715    -6.999    -0.284
        CaSiH3O4+      8.280e-008  7.031e-008    -7.082    -7.153    -0.071
        H4SiO4         3.444e-009  3.468e-009    -8.463    -8.460     0.003

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -5.03   -8.46   -3.43  SiO2
        b-Cristobalite   -5.48   -8.46   -2.98  SiO2
        Ca(OH)2         -0.35   22.19   22.54  Ca(OH)2
        Chalcedony       -4.72   -8.46   -3.74  SiO2
        CSH(0.1)         -5.11   -6.24   -1.13  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -4.53   -4.02    0.51  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -3.98   -1.80    2.18  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.45    0.42    3.87  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -2.93    2.63    5.57  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.44    4.85    7.29  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.96    7.07    9.03  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.52    9.29   10.81  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.41   10.02   11.43  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -1.25   12.79   14.04  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.75   13.73   14.48  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.44   14.50   14.94  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.24   15.14   15.38  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.12   15.68   15.80  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.05   16.15   16.20  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.02   16.54   16.56  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)          0.00   16.90   16.90  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)          0.00   17.21   17.21  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.02   17.48   17.50  Ca1.000Si0.556O2.112:1.047H2O
        H2             -35.43  -35.44   -0.00  H2
        Lime           -10.37   22.19   32.56  CaO
        O2             -12.26   70.87   83.13  O2
        Quartz           -4.43   -8.46   -4.03  SiO2
        SiO2(am)         -5.75   -8.46   -2.71  Si1.000O2.000
        Wollastonite     -0.06   13.73   13.78  CaSiO3

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End of simulation.
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--------------------------------------
Reading input data for simulation 18.
--------------------------------------

        Title 18 CSH(1.8)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(0.1)  0.0  0.0
        CSH(0.2)  0.0  0.0
        CSH(0.3)  0.0  0.0
        CSH(0.4)  0.0  0.0
        CSH(0.5)  0.0  0.0
        CSH(0.6)  0.0  0.0
        CSH(0.7)  0.0  0.0
        CSH(0.8)  0.0  0.0
        CSH(0.9)  0.0  0.0
        CSH(1.0)  0.0  0.0
```

```
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  1
        SiO2(am)  0.0  0.0
        CSH(0.833) 0.0 0.0
        Ca(OH)2   0.0  0.0
        Save Solution 19
-----
TITLE
-----

 18 CSH(1.8)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -0.02   22.52   22.54 0.000e+000          0.000e+000
        CSH(0.1)       -5.65   -6.78   -1.13 0.000e+000          0.000e+000
        CSH(0.2)       -5.04   -4.53    0.51 0.000e+000          0.000e+000
        CSH(0.3)       -4.46   -2.27    2.18 0.000e+000          0.000e+000
        CSH(0.4)       -3.89   -0.02    3.87 0.000e+000          0.000e+000
        CSH(0.5)       -3.34    2.23    5.57 0.000e+000          0.000e+000
        CSH(0.6)       -2.81    4.48    7.29 0.000e+000          0.000e+000
        CSH(0.7)       -2.29    6.74    9.03 0.000e+000          0.000e+000
        CSH(0.8)       -1.82    8.99   10.81 0.000e+000          0.000e+000
        CSH(0.833)      -1.70    9.73   11.43 0.000e+000          0.000e+000
        CSH(0.9)       -1.55   12.49   14.04 0.000e+000          0.000e+000
        CSH(1.0)       -0.98   13.49   14.48 0.000e+000          0.000e+000
        CSH(1.1)       -0.62   14.31   14.94 0.000e+000          0.000e+000
        CSH(1.2)       -0.38   15.00   15.38 0.000e+000          0.000e+000
        CSH(1.3)       -0.22   15.58   15.80 0.000e+000          0.000e+000
        CSH(1.4)       -0.12   16.08   16.20 0.000e+000          0.000e+000
        CSH(1.5)       -0.06   16.50   16.56 0.000e+000          0.000e+000
        CSH(1.6)       -0.02   16.88   16.90 0.000e+000          0.000e+000
        CSH(1.7)        0.00   17.21   17.21 0.000e+000 2.673e-001 2.673e-001
        CSH(1.8)        0.00   17.50   17.50 1.000e+000 7.174e-001-2.826e-001
        SiO2(am)       -6.33   -9.03   -2.71 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca            1.538e-002  1.538e-002
        Si            7.559e-007  7.559e-007

----------------------------Description of solution----------------------------

                                pH  =  12.360     Charge balance
                                pe  =   5.485     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  4.102e-002
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  3.077e-002
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
```

```
                  Temperature (deg C)  =  25.000
               Electrical balance (eq)  = -1.714e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  25
                           Total H  = 1.110436e+002
                           Total O  = 5.553717e+001

----------------------------Distribution of species----------------------------

                                                Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            2.820e-002  2.326e-002   -1.550   -1.633   -0.084
         H+             5.070e-013  4.370e-013  -12.295  -12.360   -0.065
         H2O            5.551e+001  9.993e-001    1.744   -0.000    0.000
Ca            1.538e-002
         Ca+2           1.282e-002  6.382e-003   -1.892   -2.195   -0.303
         CaHO+          2.565e-003  2.136e-003   -2.591   -2.670   -0.080
         CaSiH3O4+       3.705e-008  3.085e-008   -7.431   -7.511   -0.080
H(0)          3.178e-039
         H2             1.589e-039  1.604e-039  -38.799  -38.795    0.004
O(0)          4.573e-015
         O2             2.286e-015  2.308e-015  -14.641  -14.637    0.004
Si            7.559e-007
         SiH3O4-         6.199e-007  5.162e-007   -6.208   -6.287   -0.080
         SiH2O4-2        9.804e-008  4.714e-008   -7.009   -7.327   -0.318
         CaSiH3O4+       3.705e-008  3.085e-008   -7.431   -7.511   -0.080
         H4SiO4          9.205e-010  9.292e-010   -9.036   -9.032    0.004

------------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -5.60   -9.03   -3.43  SiO2
         b-Cristobalite   -6.05   -9.03   -2.98  SiO2
         Ca(OH)2         -0.02   22.52   22.54  Ca(OH)2
         Chalcedony       -5.29   -9.03   -3.74  SiO2
         CSH(0.1)         -5.65   -6.78   -1.13  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -5.04   -4.53    0.51  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -4.46   -2.27    2.18  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -3.89   -0.02    3.87  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -3.34    2.23    5.57  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -2.81    4.48    7.29  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -2.29    6.74    9.03  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -1.82    8.99   10.81  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -1.70    9.73   11.43  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)         -1.55   12.49   14.04  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)         -0.98   13.49   14.48  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)         -0.62   14.31   14.94  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.38   15.00   15.38  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.22   15.58   15.80  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)         -0.12   16.08   16.20  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.06   16.50   16.56  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -0.02   16.88   16.90  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)          0.00   17.21   17.21  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)          0.00   17.50   17.50  Ca1.000Si0.556O2.112:1.047H2O
         H2             -35.68  -35.69   -0.00  H2
         Lime           -10.04   22.52   32.56  CaO
         O2             -11.75   71.38   83.13  O2
         Quartz          -5.00   -9.03   -4.03  SiO2
         SiO2(am)        -6.33   -9.03   -2.71  Si1.000O2.000
         Wollastonite     -0.29   13.49   13.78  CaSiO3

------------------
End of simulation.
------------------

-------------------------------------
Reading input data for simulation 19.
-------------------------------------
```

```
-----------
End of run.
-----------
```

付録- 4　Reardonモデルから導いた解離式及びlog Kを用いてC-S-Hゲルの溶解／沈殿反応をPHREEQCで計算した結果（アウトプット）

```
Input file: Reardon Model Input.pqi
Output file: Reardon Model Input.pqo
Database file: spron_phc_kai.txt

------------------
Reading data base.
------------------

        SOLUTION_MASTER_SPECIES
        SOLUTION_SPECIES
        PHASES
        END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

        DATABASE: spron_phc_kai.txt
        Title C-S-H Dissolution using data from Reardon model
        PHASES
        CSH(1.0)
          Ca 1.0 Si 1.0 O 3.0 : 1.0 H2O + 1.0 H2O = 1.0 Ca+2 + 1.0 SiH3O4- + 1.0 HO-
          log_K -8.918
        CSH(1.1)
          Ca 1.1 Si 1.0 O 3.1 : 1.1 H2O + 1.0 H2O = 1.1 Ca+2 + 1.0 SiH3O4- + 1.2 HO-
          log_K -9.749
        CSH(1.2)
          Ca 1.2 Si 1.0 O 3.2 : 1.2 H2O + 1.0 H2O= 1.2 Ca+2 + 1.0 SiH3O4- + 1.4 HO-
          log_k -10.532
        CSH(1.3)
          Ca 1.3 Si 1.0 O 3.3 : 1.3 H2O + 1.0 H2O = 1.3 Ca+2 + 1.0 SiH3O4- + 1.6 HO-
          log_k -11.23
        CSH(1.4)
          Ca 1.4 Si 1.0 O 3.4 : 1.4 H2O + 1.0 H2O = 1.4 Ca+2 + 1.0 SiH3O4- + 1.8 HO-
          log_k -11.853
        CSH(1.5)
          Ca 1.5 Si 1.0 O 3.5 : 1.5 H2O + 1.0 H2O = 1.5 Ca+2 + 1.0 SiH3O4- + 2.0 HO-
          log_k -12.417
        CSH(1.6)
          Ca 1.6 Si 1.0 O 3.6 : 1.6 H2O + 1.0 H2O = 1.6 Ca+2 + 1.0 SiH3O4- + 2.2 HO-
          log_k -12.932
        CSH(1.7)
          Ca 1.7 Si 1.0 O 3.7 : 1.7 H2O + 1.0 H2O = 1.7 Ca+2 + 1.0 SiH3O4- + 2.4 HO-
          log_K -13.407
        CSH(1.8)
          Ca 1.8 Si 1.0 O 3.8 : 1.8 H2O + 1.0 H2O = 1.8 Ca+2 + 1.0 SiH3O4- + 2.6 HO-
          log_K -13.848
        Ca(OH)2
          Ca(OH)2 = Ca+2 + 2 HO-
          log_k -5.19
        SOLUTION 1 DW
        units mol/L
        pH 7
        Title 2 CSH(1.0)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(1.0)  0.0  1.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 3
        END
-----
TITLE
-----
```

```
 2 CSH(1.0)

-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.       DW

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Pure water

---------------------------Description of solution----------------------------

                                pH  =   7.000
                                pe  =   4.000
                    Activity of water  =   1.000
                       Ionic strength  =  1.009e-007
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  1.715e-009
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.85
                          Iterations  =  0
                            Total H  = 1.110124e+002
                            Total O  = 5.550622e+001

----------------------------Distribution of species----------------------------

                                                Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.018e-007  1.017e-007   -6.992   -6.993   -0.000
        H+             1.001e-007  1.000e-007   -7.000   -7.000   -0.000
        H2O            5.551e+001  1.000e+000    1.744    0.000    0.000
H(0)          1.565e-025
        H2             7.823e-026  7.823e-026  -25.107  -25.107    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -42.012  -42.012    0.000

-------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        H2            -22.00  -22.00   -0.00  H2
        O2            -39.13   44.00   83.13  O2

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage-------------------------------

                                                 Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -3.70   19.09   22.80 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.69   14.69 1.000e+000 9.988e-001-1.235e-003
        CSH(1.1)       -0.06   16.60   16.66 0.000e+000          0.000e+000
        CSH(1.2)       -0.16   18.51   18.67 0.000e+000          0.000e+000
        CSH(1.3)       -0.36   20.42   20.77 0.000e+000          0.000e+000
```

```
        CSH(1.4)       -0.62   22.33   22.95 0.000e+000          0.000e+000
        CSH(1.5)       -0.95   24.24   25.18 0.000e+000          0.000e+000
        CSH(1.6)       -1.32   26.15   27.47 0.000e+000          0.000e+000
        CSH(1.7)       -1.74   28.05   29.79 0.000e+000          0.000e+000
        CSH(1.8)       -2.18   29.96   32.15 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca            1.235e-003  1.235e-003
        Si            1.235e-003  1.235e-003

----------------------------Description of solution----------------------------

                                pH  =  11.061     Charge balance
                                pe  =   6.729     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.657e-003
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  2.470e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.716e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  15
                              Total H  = 1.110149e+002
                              Total O  = 5.551116e+001

----------------------------Distribution of species----------------------------

                                                Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.251e-003  1.171e-003    -2.903    -2.932    -0.029
        H+             9.225e-012  8.687e-012   -11.035   -11.061    -0.026
        H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
Ca           1.235e-003
        Ca+2           1.208e-003  9.345e-004    -2.918    -3.029    -0.111
        CaHO+          1.681e-005  1.574e-005    -4.774    -4.803    -0.028
        CaSiH3O4+      1.032e-005  9.661e-006    -4.987    -5.015    -0.028
H(0)         4.105e-039
        H2             2.052e-039  2.054e-039   -38.688   -38.687     0.000
O(0)         2.816e-015
        O2             1.408e-015  1.409e-015   -14.851   -14.851     0.000
Si           1.235e-003
        SiH3O4-        1.179e-003  1.104e-003    -2.929    -2.957    -0.028
        H4SiO4         3.947e-005  3.950e-005    -4.404    -4.403     0.000
        CaSiH3O4+      1.032e-005  9.661e-006    -4.987    -5.015    -0.028
        SiH2O4-2       6.593e-006  5.071e-006    -5.181    -5.295    -0.114

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.97   -4.40   -3.43  SiO2
        b-Cristobalite   -1.42   -4.40   -2.98  SiO2
        Ca(OH)2          -3.70   19.09   22.80  Ca(OH)2
        Chalcedony       -0.67   -4.40   -3.74  SiO2
        CSH(1.0)          0.00   14.69   14.69  Ca1.0Si1.0O3.0:1.0H2O
        CSH(1.1)         -0.06   16.60   16.66  Ca1.1Si1.0O3.1:1.1H2O
        CSH(1.2)         -0.16   18.51   18.67  Ca1.2Si1.0O3.2:1.2H2O
        CSH(1.3)         -0.36   20.42   20.77  Ca1.3Si1.0O3.3:1.3H2O
        CSH(1.4)         -0.62   22.33   22.95  Ca1.4Si1.0O3.4:1.4H2O
        CSH(1.5)         -0.95   24.24   25.18  Ca1.5Si1.0O3.5:1.5H2O
        CSH(1.6)         -1.32   26.15   27.47  Ca1.6Si1.0O3.6:1.6H2O
        CSH(1.7)         -1.74   28.05   29.79  Ca1.7Si1.0O3.7:1.7H2O
        CSH(1.8)         -2.18   29.96   32.15  Ca1.8Si1.0O3.8:1.8H2O
        H2             -35.58  -35.58   -0.00  H2
        Lime           -13.47   19.09   32.56  CaO
```

```
        O2           -11.96   71.16   83.13  O2
        Quartz         -0.37   -4.40   -4.03  SiO2
        Wollastonite    0.91   14.69   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 2.
-----------------------------------

        Title 3 CSH(1.1)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  1.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 4
        END
-----
TITLE
-----

 3 CSH(1.1)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -3.12   19.68   22.80 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.69   14.69 0.000e+000 8.102e-003 8.102e-003
        CSH(1.1)       -0.00   16.66   16.66 1.000e+000 9.913e-001-8.689e-003
        CSH(1.2)       -0.05   18.62   18.67 0.000e+000          0.000e+000
        CSH(1.3)       -0.18   20.59   20.77 0.000e+000          0.000e+000
        CSH(1.4)       -0.39   22.56   22.95 0.000e+000          0.000e+000
        CSH(1.5)       -0.66   24.53   25.18 0.000e+000          0.000e+000
        CSH(1.6)       -0.97   26.49   27.47 0.000e+000          0.000e+000
        CSH(1.7)       -1.33   28.46   29.79 0.000e+000          0.000e+000
        CSH(1.8)       -1.72   30.43   32.15 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca            1.456e-003  1.456e-003
        Si            5.870e-004  5.870e-004

----------------------------Description of solution----------------------------

                                pH  =  11.322     Charge balance
                                pe  =   6.571     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.291e-003
```

```
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  2.912e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.718e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  16
                             Total H  = 1.110153e+002
                             Total O  = 5.551030e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
         Species          Molality   Activity  Molality  Activity    Gamma

         HO-            2.294e-003  2.136e-003   -2.639   -2.670   -0.031
         H+             5.079e-012  4.762e-012  -11.294  -11.322   -0.028
         H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.456e-003
         Ca+2           1.415e-003  1.074e-003   -2.849   -2.969   -0.120
         CaHO+          3.541e-005  3.299e-005   -4.451   -4.482   -0.031
         CaSiH3O4+      5.683e-006  5.296e-006   -5.245   -5.276   -0.031
H(0)         2.556e-039
         H2             1.278e-039  1.279e-039  -38.893  -38.893    0.000
O(0)         7.258e-015
         O2             3.629e-015  3.633e-015  -14.440  -14.440    0.000
Si           5.870e-004
         SiH3O4-        5.652e-004  5.266e-004   -3.248   -3.278   -0.031
         H4SiO4         1.032e-005  1.033e-005   -4.986   -4.986    0.000
         SiH2O4-2       5.853e-006  4.413e-006   -5.233   -5.355   -0.123
         CaSiH3O4+      5.683e-006  5.296e-006   -5.245   -5.276   -0.031

------------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -1.55   -4.99   -3.43  SiO2
         b-Cristobalite   -2.00   -4.99   -2.98  SiO2
         Ca(OH)2          -3.12   19.68   22.80  Ca(OH)2
         Chalcedony       -1.25   -4.99   -3.74  SiO2
         CSH(1.0)          0.00   14.69   14.69  Ca1.0Si1.0O3.0:1.0H2O
         CSH(1.1)         -0.00   16.66   16.66  Ca1.1Si1.0O3.1:1.1H2O
         CSH(1.2)         -0.05   18.62   18.67  Ca1.2Si1.0O3.2:1.2H2O
         CSH(1.3)         -0.18   20.59   20.77  Ca1.3Si1.0O3.3:1.3H2O
         CSH(1.4)         -0.39   22.56   22.95  Ca1.4Si1.0O3.4:1.4H2O
         CSH(1.5)         -0.66   24.53   25.18  Ca1.5Si1.0O3.5:1.5H2O
         CSH(1.6)         -0.97   26.49   27.47  Ca1.6Si1.0O3.6:1.6H2O
         CSH(1.7)         -1.33   28.46   29.79  Ca1.7Si1.0O3.7:1.7H2O
         CSH(1.8)         -1.72   30.43   32.15  Ca1.8Si1.0O3.8:1.8H2O
         H2              -35.78  -35.79   -0.00  H2
         Lime            -12.89   19.68   32.56  CaO
         O2              -11.55   71.57   83.13  O2
         Quartz           -0.96   -4.99   -4.03  SiO2
         Wollastonite      0.91   14.69   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 3.
------------------------------------

         Title 4 CSH(1.2)
         USE SOLUTION 1 DW
         EQUILIBRIUM_PHASES
         CSH(1.0)  0.0  0.0
         CSH(1.1)  0.0  0.0
         CSH(1.2)  0.0  1.0
         CSH(1.3)  0.0  0.0
```

```
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 5
        END
-----
TITLE
-----

 4 CSH(1.2)

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -2.64   20.16   22.80 0.000e+000          0.000e+000
        CSH(1.0)        -0.05   14.64   14.69 0.000e+000          0.000e+000
        CSH(1.1)         0.00   16.66   16.66 0.000e+000 1.627e-002 1.627e-002
        CSH(1.2)        -0.00   18.67   18.67 1.000e+000 9.835e-001-1.654e-002
        CSH(1.3)        -0.08   20.69   20.77 0.000e+000          0.000e+000
        CSH(1.4)        -0.24   22.70   22.95 0.000e+000          0.000e+000
        CSH(1.5)        -0.46   24.72   25.18 0.000e+000          0.000e+000
        CSH(1.6)        -0.73   26.73   27.47 0.000e+000          0.000e+000
        CSH(1.7)        -1.04   28.75   29.79 0.000e+000          0.000e+000
        CSH(1.8)        -1.38   30.77   32.15 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.952e-003  1.952e-003
        Si             2.707e-004  2.707e-004

----------------------------Description of solution----------------------------

                                pH  =  11.509     Charge balance
                                pe  =   6.335     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  5.712e-003
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  3.903e-003
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.722e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  17
                              Total H  = 1.110163e+002
                              Total O  = 5.551066e+001

---------------------------Distribution of species----------------------------

                                           Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            3.561e-003  3.282e-003   -2.448   -2.484   -0.035
        H+             3.331e-012  3.099e-012  -11.477  -11.509   -0.031
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
```

```
Ca            1.952e-003
        Ca+2           1.878e-003  1.373e-003   -2.726   -2.862   -0.136
        CaHO+          7.026e-005  6.484e-005   -4.153   -4.188   -0.035
        CaSiH3O4+       3.344e-006  3.085e-006   -5.476   -5.511   -0.035
H(0)          3.211e-039
        H2             1.606e-039  1.608e-039  -38.794  -38.794    0.001
O(0)          4.595e-015
        O2             2.298e-015  2.301e-015  -14.639  -14.638    0.001
Si            2.707e-004
        SiH3O4-         2.600e-004  2.400e-004   -3.585   -3.620   -0.035
        SiH2O4-2        4.262e-006  3.090e-006   -5.370   -5.510   -0.140
        CaSiH3O4+       3.344e-006  3.085e-006   -5.476   -5.511   -0.035
        H4SiO4          3.059e-006  3.063e-006   -5.514   -5.514    0.001

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -2.08   -5.51   -3.43  SiO2
        b-Cristobalite   -2.53   -5.51   -2.98  SiO2
        Ca(OH)2         -2.64   20.16   22.80  Ca(OH)2
        Chalcedony       -1.78   -5.51   -3.74  SiO2
        CSH(1.0)        -0.05   14.64   14.69  Ca1.0Si1.0O3.0:1.0H2O
        CSH(1.1)         0.00   16.66   16.66  Ca1.1Si1.0O3.1:1.1H2O
        CSH(1.2)        -0.00   18.67   18.67  Ca1.2Si1.0O3.2:1.2H2O
        CSH(1.3)        -0.08   20.69   20.77  Ca1.3Si1.0O3.3:1.3H2O
        CSH(1.4)        -0.24   22.70   22.95  Ca1.4Si1.0O3.4:1.4H2O
        CSH(1.5)        -0.46   24.72   25.18  Ca1.5Si1.0O3.5:1.5H2O
        CSH(1.6)        -0.73   26.73   27.47  Ca1.6Si1.0O3.6:1.6H2O
        CSH(1.7)        -1.04   28.75   29.79  Ca1.7Si1.0O3.7:1.7H2O
        CSH(1.8)        -1.38   30.77   32.15  Ca1.8Si1.0O3.8:1.8H2O
        H2             -35.68  -35.69   -0.00  H2
        Lime           -12.41   20.16   32.56  CaO
        O2             -11.75   71.37   83.13  O2
        Quartz          -1.49   -5.51   -4.03  SiO2
        Wollastonite     0.86   14.64   13.78  CaSiO3

------------------
End of simulation.
------------------

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Reading input data for simulation 4.
-----------------------------------

        Title 5 CSH(1.3)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  1.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 6
        END
-----
TITLE
-----

 5 CSH(1.3)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.
```

```
Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -1.79   21.01   22.80 0.000e+000          0.000e+000
        CSH(1.0)       -0.22   14.47   14.69 0.000e+000          0.000e+000
        CSH(1.1)       -0.08   16.57   16.66 0.000e+000          0.000e+000
        CSH(1.2)        0.00   18.67   18.67 0.000e+000 3.788e-002 3.788e-002
        CSH(1.3)        0.00   20.77   20.77 1.000e+000 9.621e-001-3.794e-002
        CSH(1.4)       -0.08   22.87   22.95 0.000e+000          0.000e+000
        CSH(1.5)       -0.21   24.97   25.18 0.000e+000          0.000e+000
        CSH(1.6)       -0.39   27.07   27.47 0.000e+000          0.000e+000
        CSH(1.7)       -0.62   29.18   29.79 0.000e+000          0.000e+000
        CSH(1.8)       -0.87   31.28   32.15 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             3.860e-003  3.860e-003
        Si             5.490e-005  5.490e-005

----------------------------Description of solution----------------------------

                                pH  =  11.815     Charge balance
                                pe  =   5.979     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.107e-002
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  7.719e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.704e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                            Iterations  =  53
                              Total H  = 1.110202e+002
                              Total O  = 5.551405e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            7.410e-003  6.637e-003   -2.130   -2.178   -0.048
        H+             1.683e-012  1.532e-012   -11.774  -11.815   -0.041
        H2O            5.551e+001  9.998e-001    1.744   -0.000    0.000
Ca           3.860e-003
        Ca+2           3.606e-003  2.377e-003   -2.443   -2.624   -0.181
        CaHO+          2.528e-004  2.270e-004   -3.597   -3.644   -0.047
        CaSiH3O4+       1.149e-006  1.031e-006   -5.940   -5.987   -0.047
H(0)         4.028e-039
        H2             2.014e-039  2.019e-039   -38.696  -38.695    0.001
O(0)         2.909e-015
        O2             1.454e-015  1.458e-015   -14.837  -14.836    0.001
Si           5.490e-005
        SiH3O4-         5.161e-005  4.634e-005    -4.287   -4.334   -0.047
        SiH2O4-2        1.857e-006  1.207e-006    -5.731   -5.918   -0.187
        CaSiH3O4+       1.149e-006  1.031e-006    -5.940   -5.987   -0.047
        H4SiO4          2.917e-007  2.925e-007    -6.535   -6.534    0.001

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -3.10   -6.53   -3.43  SiO2
```

```
        b-Cristobalite   -3.55   -6.53   -2.98  SiO2
        Ca(OH)2         -1.79   21.01   22.80  Ca(OH)2
        Chalcedony       -2.80   -6.53   -3.74  SiO2
        CSH(1.0)         -0.22   14.47   14.69  Ca1.0Si1.0O3.0:1.0H2O
        CSH(1.1)         -0.08   16.57   16.66  Ca1.1Si1.0O3.1:1.1H2O
        CSH(1.2)          0.00   18.67   18.67  Ca1.2Si1.0O3.2:1.2H2O
        CSH(1.3)          0.00   20.77   20.77  Ca1.3Si1.0O3.3:1.3H2O
        CSH(1.4)         -0.08   22.87   22.95  Ca1.4Si1.0O3.4:1.4H2O
        CSH(1.5)         -0.21   24.97   25.18  Ca1.5Si1.0O3.5:1.5H2O
        CSH(1.6)         -0.39   27.07   27.47  Ca1.6Si1.0O3.6:1.6H2O
        CSH(1.7)         -0.62   29.18   29.79  Ca1.7Si1.0O3.7:1.7H2O
        CSH(1.8)         -0.87   31.28   32.15  Ca1.8Si1.0O3.8:1.8H2O
        H2              -35.58  -35.59   -0.00  H2
        Lime            -11.56   21.01   32.56  CaO
        O2              -11.95   71.18   83.13  O2
        Quartz           -2.51   -6.53   -4.03  SiO2
        Wollastonite      0.69   14.47   13.78  CaSiO3

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End of simulation.
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------------------------------------
Reading input data for simulation 5.
------------------------------------

        Title 6 CSH(1.4)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  1.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 7
        END
-----
TITLE
-----

 6 CSH(1.4)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase              SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2         -1.04   21.76   22.80 0.000e+000          0.000e+000
        CSH(1.0)        -0.44   14.25   14.69 0.000e+000          0.000e+000
        CSH(1.1)        -0.24   16.42   16.66 0.000e+000          0.000e+000
        CSH(1.2)        -0.08   18.60   18.67 0.000e+000          0.000e+000
        CSH(1.3)        -0.00   20.77   20.77 0.000e+000 7.486e-002 7.486e-002
        CSH(1.4)         0.00   22.95   22.95 1.000e+000 9.251e-001-7.487e-002
        CSH(1.5)        -0.06   25.12   25.18 0.000e+000          0.000e+000
        CSH(1.6)        -0.17   27.30   27.47 0.000e+000          0.000e+000
        CSH(1.7)        -0.31   29.48   29.79 0.000e+000          0.000e+000
        CSH(1.8)        -0.50   31.65   32.15 0.000e+000          0.000e+000
```

```
-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Ca             7.502e-003  7.502e-003
        Si             1.163e-005  1.163e-005

----------------------------Description of solution----------------------------

                                pH  =  12.082     Charge balance
                                pe  =   5.798     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  2.092e-002
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  1.500e-002
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  19
                             Total H  = 1.110274e+002
                             Total O  = 5.552124e+001

---------------------------Distribution of species---------------------------

                                            Log      Log        Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.420e-002  1.228e-002    -1.848    -1.911    -0.063
        H+             9.328e-013  8.283e-013   -12.030   -12.082    -0.052
        H2O            5.551e+001  9.996e-001     1.744    -0.000     0.000
Ca           7.502e-003
        Ca+2           6.707e-003  3.907e-003    -2.173    -2.408    -0.235
        CaHO+          7.945e-004  6.901e-004    -3.100    -3.161    -0.061
        CaSiH3O4+      3.824e-007  3.321e-007    -6.418    -6.479    -0.061
H(0)         2.710e-039
        H2             1.355e-039  1.362e-039   -38.868   -38.866     0.002
O(0)         6.379e-015
        O2             3.190e-015  3.205e-015   -14.496   -14.494     0.002
Si           1.163e-005
        SiH3O4-        1.045e-005  9.076e-006    -4.981    -5.042    -0.061
        SiH2O4-2       7.681e-007  4.373e-007    -6.115    -6.359    -0.245
        CaSiH3O4+      3.824e-007  3.321e-007    -6.418    -6.479    -0.061
        H4SiO4         3.082e-008  3.097e-008    -7.511    -7.509     0.002

-----------------------------Saturation indices------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -4.07   -7.51   -3.43  SiO2
        b-Cristobalite   -4.53   -7.51   -2.98  SiO2
        Ca(OH)2          -1.04   21.76   22.80  Ca(OH)2
        Chalcedony       -3.77   -7.51   -3.74  SiO2
        CSH(1.0)         -0.44   14.25   14.69  Ca1.0Si1.0O3.0:1.0H2O
        CSH(1.1)         -0.24   16.42   16.66  Ca1.1Si1.0O3.1:1.1H2O
        CSH(1.2)         -0.08   18.60   18.67  Ca1.2Si1.0O3.2:1.2H2O
        CSH(1.3)         -0.00   20.77   20.77  Ca1.3Si1.0O3.3:1.3H2O
        CSH(1.4)          0.00   22.95   22.95  Ca1.4Si1.0O3.4:1.4H2O
        CSH(1.5)         -0.06   25.12   25.18  Ca1.5Si1.0O3.5:1.5H2O
        CSH(1.6)         -0.17   27.30   27.47  Ca1.6Si1.0O3.6:1.6H2O
        CSH(1.7)         -0.31   29.48   29.79  Ca1.7Si1.0O3.7:1.7H2O
        CSH(1.8)         -0.50   31.65   32.15  Ca1.8Si1.0O3.8:1.8H2O
        H2             -35.76  -35.76   -0.00  H2
        Lime           -10.81   21.76   32.56  CaO
        O2             -11.61   71.52   83.13  O2
        Quartz          -3.48   -7.51   -4.03  SiO2
        Wollastonite     0.46   14.25   13.78  CaSiO3

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```

```
End of simulation.
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-----------------------------------
Reading input data for simulation 6.
-----------------------------------

        Title 7 CSH(1.5)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  1.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 8
        END
-----
TITLE
-----

 7 CSH(1.5)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -0.45   22.35   22.80 0.000e+000          0.000e+000
        CSH(1.0)       -0.68   14.01   14.69 0.000e+000          0.000e+000
        CSH(1.1)       -0.41   16.25   16.66 0.000e+000          0.000e+000
        CSH(1.2)       -0.19   18.48   18.67 0.000e+000          0.000e+000
        CSH(1.3)       -0.06   20.71   20.77 0.000e+000          0.000e+000
        CSH(1.4)        0.00   22.95   22.95 0.000e+000 1.297e-001 1.297e-001
        CSH(1.5)       -0.00   25.18   25.18 1.000e+000 8.702e-001-1.298e-001
        CSH(1.6)       -0.05   27.42   27.47 0.000e+000          0.000e+000
        CSH(1.7)       -0.14   29.65   29.79 0.000e+000          0.000e+000
        CSH(1.8)       -0.26   31.89   32.15 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality      Moles

        Ca             1.298e-002  1.298e-002
        Si             3.119e-006  3.119e-006

----------------------------Description of solution----------------------------

                                pH  =  12.295     Charge balance
                                pe  =   5.526     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  3.503e-002
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  2.596e-002
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
```

```
              Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  42
                           Total H  = 1.110384e+002
                           Total O  = 5.553218e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
         Species          Molality    Activity Molality Activity    Gamma

         HO-            2.400e-002  2.003e-002   -1.620   -1.698   -0.078
         H+             5.844e-013  5.074e-013  -12.233  -12.295   -0.061
         H2O            5.551e+001  9.994e-001    1.744   -0.000    0.000
Ca            1.298e-002
         Ca+2           1.102e-002  5.708e-003   -1.958   -2.244   -0.286
         CaHO+          1.955e-003  1.645e-003   -2.709   -2.784   -0.075
         CaSiH3O4+       1.404e-007  1.182e-007   -6.853   -6.928   -0.075
H(0)          3.552e-039
         H2             1.776e-039  1.791e-039  -38.751  -38.747    0.004
O(0)          3.676e-015
         O2             1.838e-015  1.853e-015  -14.736  -14.732    0.004
Si            3.119e-006
         SiH3O4-         2.627e-006  2.211e-006   -5.581   -5.656   -0.075
         SiH2O4-2        3.467e-007  1.739e-007   -6.460   -6.760   -0.300
         CaSiH3O4+       1.404e-007  1.182e-007   -6.853   -6.928   -0.075
         H4SiO4          4.584e-009  4.621e-009   -8.339   -8.335    0.004

------------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -4.90   -8.33   -3.43  SiO2
         b-Cristobalite   -5.35   -8.33   -2.98  SiO2
         Ca(OH)2         -0.45   22.35   22.80  Ca(OH)2
         Chalcedony       -4.60   -8.33   -3.74  SiO2
         CSH(1.0)         -0.68   14.01   14.69  Ca1.0Si1.0O3.0:1.0H2O
         CSH(1.1)         -0.41   16.25   16.66  Ca1.1Si1.0O3.1:1.1H2O
         CSH(1.2)         -0.19   18.48   18.67  Ca1.2Si1.0O3.2:1.2H2O
         CSH(1.3)         -0.06   20.71   20.77  Ca1.3Si1.0O3.3:1.3H2O
         CSH(1.4)          0.00   22.95   22.95  Ca1.4Si1.0O3.4:1.4H2O
         CSH(1.5)         -0.00   25.18   25.18  Ca1.5Si1.0O3.5:1.5H2O
         CSH(1.6)         -0.05   27.42   27.47  Ca1.6Si1.0O3.6:1.6H2O
         CSH(1.7)         -0.14   29.65   29.79  Ca1.7Si1.0O3.7:1.7H2O
         CSH(1.8)         -0.26   31.89   32.15  Ca1.8Si1.0O3.8:1.8H2O
         H2             -35.64  -35.64   -0.00  H2
         Lime           -10.22   22.35   32.56  CaO
         O2             -11.85   71.28   83.13  O2
         Quartz          -4.31   -8.33   -4.03  SiO2
         Wollastonite     0.23   14.01   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 7.
------------------------------------

         Title 8 CSH(1.6)
         USE SOLUTION 1 DW
         EQUILIBRIUM_PHASES
         CSH(1.0)  0.0  0.0
         CSH(1.1)  0.0  0.0
         CSH(1.2)  0.0  0.0
         CSH(1.3)  0.0  0.0
         CSH(1.4)  0.0  0.0
         CSH(1.5)  0.0  0.0
         CSH(1.6)  0.0  1.0
         CSH(1.7)  0.0  0.0
         CSH(1.8)  0.0  0.0
```

```
        Ca(OH)2   0.0  0.0
        Save Solution 9
        END
-----
TITLE
-----

 8 CSH(1.6)

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -0.00   22.80   22.80 0.000e+000 7.998e-002 7.998e-002
        CSH(1.0)       -0.90   13.79   14.69 0.000e+000          0.000e+000
        CSH(1.1)       -0.59   16.07   16.66 0.000e+000          0.000e+000
        CSH(1.2)       -0.33   18.34   18.67 0.000e+000          0.000e+000
        CSH(1.3)       -0.15   20.62   20.77 0.000e+000          0.000e+000
        CSH(1.4)       -0.05   22.90   22.95 0.000e+000          0.000e+000
        CSH(1.5)        0.00   25.18   25.18 0.000e+000 1.000e+000 1.000e+000
        CSH(1.6)       -0.00   27.46   27.47 1.000e+000         -1.000e+000
        CSH(1.7)       -0.05   29.74   29.79 0.000e+000          0.000e+000
        CSH(1.8)       -0.13   32.02   32.15 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             2.002e-002  2.002e-002
        Si             1.067e-006  1.067e-006

----------------------------Description of solution----------------------------

                                pH  =  12.459     Charge balance
                                pe  =   5.172     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  5.231e-002
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  4.005e-002
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -2.224e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                            Iterations  =  48
                              Total H  = 1.110525e+002
                              Total O  = 5.554627e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            3.617e-002  2.925e-002   -1.442   -1.534   -0.092
        H+             4.078e-013  3.475e-013  -12.390  -12.459   -0.070
        H2O            5.551e+001  9.990e-001    1.744   -0.000    0.000
Ca           2.002e-002
        Ca+2           1.614e-002  7.549e-003   -1.792   -2.122   -0.330
        CaHO+          3.879e-003  3.176e-003   -2.411   -2.498   -0.087
        CaSiH3O4+      5.887e-008  4.820e-008   -7.230   -7.317   -0.087
H(0)         8.446e-039
```

```
        H2             4.223e-039  4.274e-039   -38.374   -38.369    0.005
O(0)          6.422e-016
        O2             3.211e-016  3.250e-016   -15.493   -15.488    0.005
Si           1.067e-006
        SiH3O4-         8.326e-007  6.818e-007    -6.080    -6.166    -0.087
        SiH2O4-2        1.742e-007  7.831e-008    -6.759    -7.106    -0.347
        CaSiH3O4+       5.887e-008  4.820e-008    -7.230    -7.317    -0.087
        H4SiO4          9.643e-010  9.759e-010    -9.016    -9.011     0.005

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -5.58   -9.01   -3.43  SiO2
        b-Cristobalite   -6.03   -9.01   -2.98  SiO2
        Ca(OH)2         -0.00   22.80   22.80  Ca(OH)2
        Chalcedony       -5.27   -9.01   -3.74  SiO2
        CSH(1.0)         -0.90   13.79   14.69  Ca1.0Si1.0O3.0:1.0H2O
        CSH(1.1)         -0.59   16.07   16.66  Ca1.1Si1.0O3.1:1.1H2O
        CSH(1.2)         -0.33   18.34   18.67  Ca1.2Si1.0O3.2:1.2H2O
        CSH(1.3)         -0.15   20.62   20.77  Ca1.3Si1.0O3.3:1.3H2O
        CSH(1.4)         -0.05   22.90   22.95  Ca1.4Si1.0O3.4:1.4H2O
        CSH(1.5)          0.00   25.18   25.18  Ca1.5Si1.0O3.5:1.5H2O
        CSH(1.6)         -0.00   27.46   27.47  Ca1.6Si1.0O3.6:1.6H2O
        CSH(1.7)         -0.05   29.74   29.79  Ca1.7Si1.0O3.7:1.7H2O
        CSH(1.8)         -0.13   32.02   32.15  Ca1.8Si1.0O3.8:1.8H2O
        H2             -35.26  -35.26   -0.00  H2
        Lime            -9.77   22.80   32.56  CaO
        O2             -12.60   70.52   83.13  O2
        Quartz          -4.98   -9.01   -4.03  SiO2
        Wollastonite     0.00   13.79   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 8.
------------------------------------

        Title 9 CSH(1.7)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  1.0
        CSH(1.8)  0.0  0.0
        Ca(OH)2   0.0  0.0
        Save Solution 10
        END
-----
TITLE
-----

 9 CSH(1.7)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------
```

```
                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2          0.00   22.80   22.80 0.000e+000 1.800e-001 1.800e-001
        CSH(1.0)        -0.90   13.79   14.69 0.000e+000          0.000e+000
        CSH(1.1)        -0.59   16.07   16.66 0.000e+000          0.000e+000
        CSH(1.2)        -0.33   18.34   18.67 0.000e+000          0.000e+000
        CSH(1.3)        -0.15   20.62   20.77 0.000e+000          0.000e+000
        CSH(1.4)        -0.05   22.90   22.95 0.000e+000          0.000e+000
        CSH(1.5)         0.00   25.18   25.18 0.000e+000 1.000e+000 1.000e+000
        CSH(1.6)        -0.00   27.46   27.47 0.000e+000          0.000e+000
        CSH(1.7)        -0.05   29.74   29.79 1.000e+000         -1.000e+000
        CSH(1.8)        -0.13   32.02   32.15 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             2.002e-002  2.002e-002
        Si             1.067e-006  1.067e-006

----------------------------Description of solution---------------------------

                                pH  =  12.459     Charge balance
                                pe  =   5.401     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  5.231e-002
                    Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  4.005e-002
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  19
                             Total H  = 1.110525e+002
                             Total O  = 5.554627e+001

----------------------------Distribution of species---------------------------

                                          Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            3.617e-002  2.925e-002   -1.442   -1.534   -0.092
        H+             4.078e-013  3.475e-013  -12.390  -12.459   -0.070
        H2O            5.551e+001  9.990e-001    1.744   -0.000    0.000
Ca           2.002e-002
        Ca+2           1.614e-002  7.549e-003   -1.792   -2.122   -0.330
        CaHO+          3.879e-003  3.176e-003   -2.411   -2.498   -0.087
        CaSiH3O4+      5.887e-008  4.820e-008   -7.230   -7.317   -0.087
H(0)         2.941e-039
        H2             1.470e-039  1.488e-039  -38.833  -38.827    0.005
O(0)         5.297e-015
        O2             2.649e-015  2.681e-015  -14.577  -14.572    0.005
Si           1.067e-006
        SiH3O4-        8.326e-007  6.818e-007   -6.080   -6.166   -0.087
        SiH2O4-2       1.742e-007  7.831e-008   -6.759   -7.106   -0.347
        CaSiH3O4+      5.887e-008  4.820e-008   -7.230   -7.317   -0.087
        H4SiO4         9.643e-010  9.759e-010   -9.016   -9.011    0.005

----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -5.58   -9.01   -3.43  SiO2
        b-Cristobalite  -6.03   -9.01   -2.98  SiO2
        Ca(OH)2          0.00   22.80   22.80  Ca(OH)2
        Chalcedony      -5.27   -9.01   -3.74  SiO2
        CSH(1.0)        -0.90   13.79   14.69  Ca1.0Si1.0O3.0:1.0H2O
        CSH(1.1)        -0.59   16.07   16.66  Ca1.1Si1.0O3.1:1.1H2O
```

```
        CSH(1.2)        -0.33   18.34   18.67  Ca1.2Si1.0O3.2:1.2H2O
        CSH(1.3)        -0.15   20.62   20.77  Ca1.3Si1.0O3.3:1.3H2O
        CSH(1.4)        -0.05   22.90   22.95  Ca1.4Si1.0O3.4:1.4H2O
        CSH(1.5)         0.00   25.18   25.18  Ca1.5Si1.0O3.5:1.5H2O
        CSH(1.6)        -0.00   27.46   27.47  Ca1.6Si1.0O3.6:1.6H2O
        CSH(1.7)        -0.05   29.74   29.79  Ca1.7Si1.0O3.7:1.7H2O
        CSH(1.8)        -0.13   32.02   32.15  Ca1.8Si1.0O3.8:1.8H2O
        H2            -35.72  -35.72   -0.00  H2
        Lime           -9.77   22.80   32.56  CaO
        O2            -11.69   71.44   83.13  O2
        Quartz         -4.98   -9.01   -4.03  SiO2
        Wollastonite    0.00   13.79   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 9.
-----------------------------------

        Title 10 CSH(1.8)
        USE SOLUTION 1 DW
        EQUILIBRIUM_PHASES
        CSH(1.0)  0.0  0.0
        CSH(1.1)  0.0  0.0
        CSH(1.2)  0.0  0.0
        CSH(1.3)  0.0  0.0
        CSH(1.4)  0.0  0.0
        CSH(1.5)  0.0  0.0
        CSH(1.6)  0.0  0.0
        CSH(1.7)  0.0  0.0
        CSH(1.8)  0.0  1.0
        Ca(OH)2   0.0  0.0
        Save Solution 11
        END
-----
TITLE
-----

 10 CSH(1.8)

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW
Using pure phase assemblage 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2          0.00   22.80   22.80 0.000e+000 2.800e-001 2.800e-001
        CSH(1.0)        -0.90   13.79   14.69 0.000e+000          0.000e+000
        CSH(1.1)        -0.59   16.07   16.66 0.000e+000          0.000e+000
        CSH(1.2)        -0.33   18.34   18.67 0.000e+000          0.000e+000
        CSH(1.3)        -0.15   20.62   20.77 0.000e+000          0.000e+000
        CSH(1.4)        -0.05   22.90   22.95 0.000e+000          0.000e+000
        CSH(1.5)        -0.00   25.18   25.18 0.000e+000 1.000e+000 1.000e+000
        CSH(1.6)        -0.00   27.46   27.47 0.000e+000          0.000e+000
        CSH(1.7)        -0.05   29.74   29.79 0.000e+000          0.000e+000
        CSH(1.8)        -0.13   32.02   32.15 1.000e+000         -1.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality      Moles
```

```
        Ca            2.002e-002  2.002e-002
        Si            1.067e-006  1.067e-006

----------------------------Description of solution----------------------------

                                pH  =  12.459     Charge balance
                                pe  =   5.359     Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  5.231e-002
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  4.005e-002
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.715e-009
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  50
                             Total H  = 1.110525e+002
                             Total O  = 5.554627e+001

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            3.617e-002  2.925e-002   -1.442   -1.534   -0.092
        H+             4.078e-013  3.475e-013  -12.390  -12.459   -0.070
        H2O            5.551e+001  9.990e-001    1.744   -0.000    0.000
Ca           2.002e-002
        Ca+2           1.614e-002  7.549e-003   -1.792   -2.122   -0.330
        CaHO+          3.879e-003  3.176e-003   -2.411   -2.498   -0.087
        CaSiH3O4+      5.887e-008  4.820e-008   -7.230   -7.317   -0.087
H(0)         3.569e-039
        H2             1.784e-039  1.806e-039  -38.749  -38.743    0.005
O(0)         3.597e-015
        O2             1.798e-015  1.820e-015  -14.745  -14.740    0.005
Si           1.067e-006
        SiH3O4-        8.326e-007  6.818e-007   -6.080   -6.166   -0.087
        SiH2O4-2       1.742e-007  7.831e-008   -6.759   -7.106   -0.347
        CaSiH3O4+      5.887e-008  4.820e-008   -7.230   -7.317   -0.087
        H4SiO4         9.643e-010  9.759e-010   -9.016   -9.011    0.005

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -5.58   -9.01   -3.43  SiO2
        b-Cristobalite   -6.03   -9.01   -2.98  SiO2
        Ca(OH)2           0.00   22.80   22.80  Ca(OH)2
        Chalcedony       -5.27   -9.01   -3.74  SiO2
        CSH(1.0)         -0.90   13.79   14.69  Ca1.0Si1.0O3.0:1.0H2O
        CSH(1.1)         -0.59   16.07   16.66  Ca1.1Si1.0O3.1:1.1H2O
        CSH(1.2)         -0.33   18.34   18.67  Ca1.2Si1.0O3.2:1.2H2O
        CSH(1.3)         -0.15   20.62   20.77  Ca1.3Si1.0O3.3:1.3H2O
        CSH(1.4)         -0.05   22.90   22.95  Ca1.4Si1.0O3.4:1.4H2O
        CSH(1.5)         -0.00   25.18   25.18  Ca1.5Si1.0O3.5:1.5H2O
        CSH(1.6)         -0.00   27.46   27.47  Ca1.6Si1.0O3.6:1.6H2O
        CSH(1.7)         -0.05   29.74   29.79  Ca1.7Si1.0O3.7:1.7H2O
        CSH(1.8)         -0.13   32.02   32.15  Ca1.8Si1.0O3.8:1.8H2O
        H2             -35.63  -35.64   -0.00  H2
        Lime            -9.77   22.80   32.56  CaO
        O2             -11.85   71.27   83.13  O2
        Quartz          -4.98   -9.01   -4.03  SiO2
        Wollastonite     0.00   13.79   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 10.
```

```
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-----------
End of run.
-----------
```

付録- 5　回分方式で液相を交換したときの純水中での C-S-H ゲルの溶解／沈殿反応を PHREEQC で計算した結果（アウトプット）

```
Input file: Atkinson Model Input water exchange (purewater).pqi
Output file: Atkinson Model Input water exchange (purewater).pqo
Database file: spron_phc_kai.txt

------------------
Reading data base.
------------------

        SOLUTION_MASTER_SPECIES
        SOLUTION_SPECIES
        PHASES
        END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

        DATABASE: spron_phc_kai.txt
        TITLE C-S-H dissolution in water exchange system (Purewater), data: Atkinson case
        PHASES
        CSH(0.1)
            Ca 0.100 Si 1.000 O 2.100 : 0.110 H2O = 0.100 Ca+2 + 1.000 H4SiO4 -1.790 H2O - 0.200 H+
            log_K -1.071
        CSH(0.2)
            Ca 0.200 Si 1.000 O 2.200 : 0.220 H2O = 0.200 Ca+2 + 1.000 H4SiO4 -1.580 H2O - 0.400 H+
            log_K 0.565
        CSH(0.3)
            Ca 0.300 Si 1.000 O 2.300 : 0.330 H2O = 0.300 Ca+2 + 1.000 H4SiO4 -1.370 H2O - 0.600 H+
            log_K 2.227
        CSH(0.4)
            Ca 0.400 Si 1.000 O 2.400 : 0.440 H2O = 0.400 Ca+2 + 1.000 H4SiO4 -1.160 H2O - 0.800 H+
            log_K 3.907
        CSH(0.5)
            Ca 0.500 Si 1.000 O 2.500 : 0.550 H2O = 0.500 Ca+2 + 1.000 H4SiO4 -0.950 H2O - 1.000 H+
            log_K 5.601
        CSH(0.6)
            Ca 0.600 Si 1.000 O 2.600 : 0.661 H2O = 0.600 Ca+2 + 1.000 H4SiO4 -0.739 H2O - 1.200 H+
            log_K 7.312
        CSH(0.7)
            Ca 0.700 Si 1.000 O 2.700 : 0.771 H2O = 0.700 Ca+2 + 1.000 H4SiO4 -0.529 H2O - 1.400 H+
            log_K 9.045
        CSH(0.8)
            Ca 0.800 Si 1.000 O 2.800 : 0.881 H2O = 0.800 Ca+2 + 1.000 H4SiO4 -0.319 H2O - 1.600 H+
            log_K 10.819
        CSH(0.9)
            Ca 1.000 Si 1.111 O 3.222 : 1.093 H2O = 1.000 Ca+2 + 1.111 H4SiO4 -0.129 H2O - 2.000 H+
            log_K 14.061
        CSH(1.0)
            Ca 1.000 Si 1.000 O 3.000 : 1.084 H2O = 1.000 Ca+2 + 1.000 H4SiO4 + 0.084 H2O - 2.000 H+
            log_K 14.514
        CSH(1.1)
            Ca 1.000 Si 0.909 O 2.818 : 1.076 H2O = 1.000 Ca+2 + 0.909 H4SiO4 + 0.258 H2O - 2.000 H+
            log_K 14.983
        CSH(1.2)
            Ca 1.000 Si 0.833 O 2.666 : 1.070 H2O = 1.000 Ca+2 + 0.833 H4SiO4 + 0.404 H2O - 2.000 H+
            log_K 15.439
        CSH(1.3)
            Ca 1.000 Si 0.769 O 2.538 : 1.065 H2O = 1.000 Ca+2 + 0.769 H4SiO4 + 0.527 H2O - 2.000 H+
            log_K 15.870
        CSH(1.4)
            Ca 1.000 Si 0.714 O 2.428 : 1.060 H2O = 1.000 Ca+2 + 0.714 H4SiO4 + 0.632 H2O - 2.000 H+
            log_K 16.272
        CSH(1.5)
            Ca 1.000 Si 0.667 O 2.334 : 1.056 H2O = 1.000 Ca+2 + 0.667 H4SiO4 + 0.722 H2O - 2.000 H+
            log_K 16.643
        CSH(1.6)
            Ca 1.000 Si 0.625 O 2.250 : 1.053 H2O = 1.000 Ca+2 + 0.625 H4SiO4 + 0.803 H2O - 2.000 H+
            log_K 16.987
        CSH(1.7)
            Ca 1.000 Si 0.588 O 2.176 : 1.049 H2O = 1.000 Ca+2 + 0.588 H4SiO4 + 0.873 H2O - 2.000 H+
            log_K 17.304
```

```
        CSH(1.8)
            Ca 1.000 Si 0.556 O 2.112 : 1.047 H2O = 1.000 Ca+2 + 0.556 H4SiO4 + 0.935 H2O - 2.000 H+
            log_K 17.597
        Ca(OH)2
            Ca(OH)2 = Ca+2 + 2H2O - 2 H+
            log_k 22.710
        SiO2(am)
            Si 1.000 O 2.000 = 1.000 H4SiO4 - 2.000 H2O
            log_K -2.639
        CSH(0.833)
            Ca 0.833 Si 1.000 O 2.833 : 0.917 H2O = 0.833 Ca+2 + 1.000 H4SiO4 -0.250 H2O - 1.666 H+
           log_K 11.436
        TITLE 1 Liquid solid ratio 100
        SOLUTION 1 DW 100g
           temp     25
           pH       7
           pe       4
           redox    pe
           units    mol/l
           density  1
           water   0.1 # kg
        USE solution 1
        EQUILIBRIUM_PHASES 1 C-S-H(1.8) 1g
           Ca(OH)2  0 0
           CSH(0.1)  0 0
           CSH(0.2)  0 0
           CSH(0.3)  0 0
           CSH(0.4)  0 0
           CSH(0.5)  0 0
           CSH(0.6)  0 0
           CSH(0.7)  0 0
           CSH(0.8)  0 0
           CSH(0.833) 0 0
           CSH(0.9)  0 0
           CSH(1.0)  0 0
           CSH(1.1)  0 0
           CSH(1.2)  0 0
           CSH(1.3)  0 0
           CSH(1.4)  0 0
           CSH(1.5)  0 0
           CSH(1.6)  0 0
           CSH(1.7)  0 0
           CSH(1.8)  0 0.00932
           SiO2(am)  0 0
        SAVE equilibrium_phases 2
        END
-----
TITLE
-----

 1 Liquid solid ratio 100

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.       DW 100g

-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        Pure water

----------------------------Description of solution----------------------------

                                pH =   7.000
                                pe =   4.000
                  Activity of water =   1.000
                     Ionic strength =  1.009e-007
                 Mass of water (kg) =  1.000e-001
```

```
              Total alkalinity (eq/kg)  =  1.714e-009
                 Total carbon (mol/kg)  =  0.000e+000
                   Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
               Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.85
                         Iterations  =  2
                           Total H  = 1.110124e+001
                           Total O  = 5.550622e+000

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            1.018e-007  1.017e-007   -6.992   -6.993   -0.000
        H+             1.000e-007  1.000e-007   -7.000   -7.000   -0.000
        H2O            5.551e+001  1.000e+000    1.744   -0.000    0.000
H(0)          1.565e-025
        H2             7.823e-026  7.823e-026  -25.107  -25.107    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -42.012  -42.012    0.000

-----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        H2            -22.00  -22.00   -0.00  H2
        O2            -39.13   44.00   83.13  O2

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 1.    C-S-H(1.8) 1g

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -0.60   22.11   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -4.91   -5.98   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -4.33   -3.77    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -3.79   -1.56    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -3.26    0.65    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -2.74    2.86    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -2.24    5.07    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -1.76    7.28    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -1.32    9.49   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -1.21   10.22   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -1.05   13.01   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.60   13.92   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.32   14.66   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.16   15.28   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.06   15.81   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.01   16.26   16.27 0.000e+000          0.000e+000
        CSH(1.5)        0.00   16.64   16.64 0.000e+000 1.037e-004 1.037e-004
        CSH(1.6)        0.00   16.99   16.99 0.000e+000 8.180e-003 8.180e-003
        CSH(1.7)       -0.01   17.29   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.04   17.55   17.60 9.320e-003         -9.320e-003
        SiO2(am)       -5.55   -8.19   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.036e-002  1.036e-003
```

```
        Si            3.410e-006  3.410e-007

----------------------------Description of solution----------------------------

                                pH  =  12.208     Charge balance
                                pe  =  -6.629     Adjusted to redox equilibrium
                    Activity of water  =   0.999
                       Ionic strength  =  2.838e-002
                   Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  2.073e-002
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  =  56
                            Total H  = 1.110331e+001
                            Total O  = 5.552694e+000

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.937e-002  1.641e-002   -1.713   -1.785   -0.072
        H+             7.067e-013  6.194e-013  -12.151  -12.208   -0.057
        H2O            5.551e+001  9.995e-001    1.744   -0.000    0.000
Ca           1.036e-002
        Ca+2           9.007e-003  4.902e-003   -2.045   -2.310   -0.264
        CaHO+          1.357e-003  1.158e-003   -2.867   -2.936   -0.069
        CaSiH3O4+      1.359e-007  1.159e-007   -6.867   -6.936   -0.069
H(0)         1.078e-014
        H2             5.392e-015  5.428e-015  -14.268  -14.265    0.003
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -63.698  -63.695    0.003
Si           3.410e-006
        SiH3O4-        2.960e-006  2.525e-006   -5.529   -5.598   -0.069
        SiH2O4-2       3.074e-007  1.627e-007   -6.512   -6.789   -0.276
        CaSiH3O4+      1.359e-007  1.159e-007   -6.867   -6.936   -0.069
        H4SiO4         6.401e-009  6.443e-009   -8.194   -8.191    0.003

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -4.76   -8.19   -3.43  SiO2
        b-Cristobalite   -5.21   -8.19   -2.98  SiO2
        Ca(OH)2          -0.60   22.11   22.71  Ca(OH)2
        Chalcedony       -4.45   -8.19   -3.74  SiO2
        CSH(0.1)         -4.91   -5.98   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -4.33   -3.77    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -3.79   -1.56    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.26    0.65    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -2.74    2.86    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.24    5.07    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.76    7.28    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.32    9.49   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.21   10.22   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -1.05   13.01   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.60   13.92   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.32   14.66   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.16   15.28   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.06   15.81   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.01   16.26   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)          0.00   16.64   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)          0.00   16.99   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.01   17.29   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.04   17.55   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -11.16  -11.16   -0.00  H2
        Lime           -10.46   22.11   32.56  CaO
        O2             -60.81   22.32   83.13  O2
```

```
        Quartz         -4.16   -8.19   -4.03  SiO2
        SiO2(am)       -5.55   -8.19   -2.64  Si1.000O2.000
        Wollastonite    0.13   13.92   13.78  CaSiO3

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 2.
-----------------------------------

        TITLE 2 Total liquid solid ratio 200
        USE solution 1
        USE equilibrium_phases 2
        SAVE equilibrium_phases 3
        END
-----
TITLE
-----

 2 Total liquid solid ratio 200

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 2.    Pure-phase assemblage after simulation 1.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -0.80   21.91   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -4.63   -5.70   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -4.08   -3.51    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -3.55   -1.32    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -3.04    0.87    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -2.54    3.06    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -2.06    5.25    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -1.60    7.44    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -1.19    9.63   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -1.08   10.36   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.92   13.14   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.50   14.01   14.51 0.000e+000          0.000e+000
        CSH(1.1)        -0.25   14.73   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.11   15.33   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.03   15.84   15.87 0.000e+000          0.000e+000
        CSH(1.4)         0.00   16.27   16.27 0.000e+000 4.922e-003 4.922e-003
        CSH(1.5)         0.00   16.64   16.64 1.037e-004 2.499e-003 2.395e-003
        CSH(1.6)        -0.01   16.97   16.99 8.180e-003         -8.180e-003
        CSH(1.7)        -0.04   17.27   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.08   17.52   17.60 0.000e+000          0.000e+000
        SiO2(am)        -5.25   -7.89   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             8.627e-003  8.627e-004
        Si             5.557e-006  5.557e-007

----------------------------Description of solution----------------------------

                                pH  =  12.137     Charge balance
                                pe  =  -6.315     Adjusted to redox equilibrium
                    Activity of water  =   1.000
```

```
                    Ionic strength  =  2.388e-002
                Mass of water (kg)  =  1.000e-001
             Total alkalinity (eq/kg)  =  1.725e-002
               Total carbon (mol/kg)  =  0.000e+000
                  Total CO2 (mol/kg)  =  0.000e+000
                Temperature (deg C)  =  25.000
             Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                       Iterations  =  34
                         Total H  = 1.110298e+001
                         Total O  = 5.552352e+000

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
         Species          Molality   Activity Molality Activity    Gamma

         HO-            1.625e-002  1.393e-002   -1.789   -1.856   -0.067
         H+             8.267e-013  7.300e-013  -12.083  -12.137   -0.054
         H2O            5.551e+001  9.996e-001    1.744   -0.000    0.000
Ca            8.627e-003
         Ca+2           7.624e-003  4.315e-003   -2.118   -2.365   -0.247
         CaHO+          1.003e-003  8.648e-004   -2.999   -3.063   -0.065
         CaSiH3O4+      1.990e-007  1.716e-007   -6.701   -6.766   -0.065
H(0)          3.537e-015
         H2             1.768e-015  1.778e-015  -14.752  -14.750    0.002
O(0)          0.000e+000
         O2             0.000e+000  0.000e+000  -62.728  -62.726    0.002
Si            5.557e-006
         SiH3O4-        4.925e-006  4.245e-006   -5.308   -5.372   -0.065
         SiH2O4-2       4.204e-007  2.321e-007   -6.376   -6.634   -0.258
         CaSiH3O4+      1.990e-007  1.716e-007   -6.701   -6.766   -0.065
         H4SiO4         1.270e-008  1.277e-008   -7.896   -7.894    0.002

-----------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -4.46   -7.89   -3.43  SiO2
         b-Cristobalite   -4.91   -7.89   -2.98  SiO2
         Ca(OH)2          -0.80   21.91   22.71  Ca(OH)2
         Chalcedony       -4.16   -7.89   -3.74  SiO2
         CSH(0.1)         -4.63   -5.70   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -4.08   -3.51    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -3.55   -1.32    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -3.04    0.87    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -2.54    3.06    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -2.06    5.25    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -1.60    7.44    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -1.19    9.63   10.82  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -1.08   10.36   11.44  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)         -0.92   13.14   14.06  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)         -0.50   14.01   14.51  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)         -0.25   14.73   14.98  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.11   15.33   15.44  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.03   15.84   15.87  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)          0.00   16.27   16.27  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)          0.00   16.64   16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -0.01   16.97   16.99  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)         -0.04   17.27   17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)         -0.08   17.52   17.60  Ca1.000Si0.556O2.112:1.047H2O
         H2             -11.64  -11.64   -0.00  H2
         Lime           -10.65   21.91   32.56  CaO
         O2             -59.84   23.29   83.13  O2
         Quartz          -3.87   -7.89   -4.03  SiO2
         SiO2(am)        -5.25   -7.89   -2.64  Si1.000O2.000
         Wollastonite     0.23   14.01   13.78  CaSiO3

------------------
End of simulation.
------------------
```

```
-----------------------------------
Reading input data for simulation 3.
-----------------------------------

        TITLE 3 Total liquid solid ratio 300
        USE solution 1
        USE equilibrium_phases 3
        SAVE equilibrium_phases 4
        END
-----
TITLE
-----

 3 Total liquid solid ratio 300

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 3.    Pure-phase assemblage after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -1.22   21.49   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -4.09   -5.16   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -3.58   -3.01    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -3.09   -0.86    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -2.62    1.29    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -2.16    3.44    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.73    5.59    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -1.31    7.73    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.94    9.88   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.84   10.59   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.69   13.37   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.33   14.18   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.14   14.85   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.04   15.40   15.44 0.000e+000          0.000e+000
        CSH(1.3)        0.00   15.87   15.87 0.000e+000 5.506e-003 5.506e-003
        CSH(1.4)        0.00   16.27   16.27 4.922e-003 1.324e-003-3.598e-003
        CSH(1.5)       -0.03   16.62   16.64 2.499e-003         -2.499e-003
        CSH(1.6)       -0.06   16.92   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.11   17.19   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.17   17.43   17.60 0.000e+000          0.000e+000
        SiO2(am)       -4.67   -7.31   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             5.907e-003  5.907e-004
        Si             1.435e-005  1.435e-006

----------------------------Description of solution----------------------------

                                pH  =  11.987     Charge balance
                                pe  =  -6.431     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.666e-002
                    Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  1.181e-002
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.714e-010
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  60
                           Total H  = 1.110242e+001
                           Total O  = 5.551804e+000

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.127e-002  9.877e-003    -1.948    -2.005    -0.057
        H+             1.149e-012  1.030e-012   -11.940   -11.987    -0.048
        H2O            5.551e+001  9.997e-001     1.744    -0.000     0.000
Ca           5.907e-003
        Ca+2           5.376e-003  3.283e-003    -2.270    -2.484    -0.214
        CaHO+          5.303e-004  4.665e-004    -3.275    -3.331    -0.056
        CaSiH3O4+       4.042e-007  3.556e-007    -6.393    -6.449    -0.056
H(0)         1.201e-014
        H2             6.003e-015  6.026e-015   -14.222   -14.220     0.002
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000   -63.788   -63.786     0.002
Si           1.435e-005
        SiH3O4-         1.315e-005  1.156e-005    -4.881    -4.937    -0.056
        SiH2O4-2        7.486e-007  4.483e-007    -6.126    -6.348    -0.223
        CaSiH3O4+       4.042e-007  3.556e-007    -6.393    -6.449    -0.056
        H4SiO4          4.887e-008  4.905e-008    -7.311    -7.309     0.002

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -3.88   -7.31   -3.43  SiO2
        b-Cristobalite   -4.33   -7.31   -2.98  SiO2
        Ca(OH)2         -1.22   21.49   22.71  Ca(OH)2
        Chalcedony       -3.57   -7.31   -3.74  SiO2
        CSH(0.1)         -4.09   -5.16   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -3.58   -3.01    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -3.09   -0.86    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -2.62    1.29    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -2.16    3.44    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -1.73    5.59    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.31    7.73    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.94    9.88   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.84   10.59   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.69   13.37   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.33   14.18   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.14   14.85   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.04   15.40   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)          0.00   15.87   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)          0.00   16.27   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.03   16.62   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.06   16.92   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.11   17.19   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.17   17.43   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -11.11  -11.11   -0.00  H2
        Lime           -11.07   21.49   32.56  CaO
        O2             -60.90   22.23   83.13  O2
        Quartz          -3.28   -7.31   -4.03  SiO2
        SiO2(am)        -4.67   -7.31   -2.64  Si1.000O2.000
        Wollastonite     0.40   14.18   13.78  CaSiO3

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End of simulation.
------------------

-----------------------------------
Reading input data for simulation 4.
-----------------------------------

        TITLE 4 Total liquid solid ratio 400
        USE solution 1
```

```
        USE equilibrium_phases 4
        SAVE equilibrium_phases 5
        END
-----
TITLE
-----

 4 Total liquid solid ratio 400

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 4.    Pure-phase assemblage after simulation 3.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -1.66   21.05   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -3.56   -4.63   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -3.09   -2.52    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -2.65   -0.42    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -2.22    1.69    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -1.81    3.79    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.42    5.89    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -1.05    8.00    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.71   10.10   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.64   10.80   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.49   13.57   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.20   14.31   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.06   14.93   14.98 0.000e+000          0.000e+000
        CSH(1.2)        0.00   15.44   15.44 0.000e+000 3.614e-003 3.614e-003
        CSH(1.3)        0.00   15.87   15.87 5.506e-003 2.816e-003-2.690e-003
        CSH(1.4)       -0.03   16.24   16.27 1.324e-003         -1.324e-003
        CSH(1.5)       -0.09   16.56   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.15   16.84   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.22   17.09   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.29   17.30   17.60 0.000e+000          0.000e+000
        SiO2(am)       -4.10   -6.73   -2.64 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             4.001e-003  4.001e-004
        Si             3.599e-005  3.599e-006

----------------------------Description of solution----------------------------

                                pH  =  11.830     Charge balance
                                pe  =  -6.219     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  1.146e-002
                    Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  8.002e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.752e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  =  36
                            Total H  = 1.110205e+001
                            Total O  = 5.551430e+000

---------------------------Distribution of species---------------------------
```

```
                                                  Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            7.695e-003  6.881e-003   -2.114    -2.162    -0.049
        H+             1.626e-012  1.478e-012  -11.789   -11.830    -0.041
        H2O            5.551e+001  9.998e-001    1.744    -0.000     0.000
Ca           4.001e-003
        Ca+2           3.730e-003  2.444e-003   -2.428    -2.612    -0.184
        CaHO+          2.700e-004  2.420e-004   -3.569    -3.616    -0.048
        CaSiH3O4+      7.729e-007  6.929e-007   -6.112    -6.159    -0.048
H(0)         9.331e-015
        H2             4.665e-015  4.678e-015  -14.331   -14.330     0.001
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -63.567   -63.566     0.001
Si           3.599e-005
        SiH3O4-        3.377e-005  3.027e-005   -4.472    -4.519    -0.048
        SiH2O4-2       1.266e-006  8.173e-007   -5.898    -6.088    -0.190
        CaSiH3O4+      7.729e-007  6.929e-007   -6.112    -6.159    -0.048
        H4SiO4         1.838e-007  1.843e-007   -6.736    -6.735     0.001

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -3.30   -6.73   -3.43  SiO2
        b-Cristobalite   -3.75   -6.73   -2.98  SiO2
        Ca(OH)2          -1.66   21.05   22.71  Ca(OH)2
        Chalcedony       -3.00   -6.73   -3.74  SiO2
        CSH(0.1)         -3.56   -4.63   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -3.09   -2.52    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -2.65   -0.42    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -2.22    1.69    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -1.81    3.79    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -1.42    5.89    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.05    8.00    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.71   10.10   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.64   10.80   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.49   13.57   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.20   14.31   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.06   14.93   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)          0.00   15.44   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)          0.00   15.87   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.03   16.24   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.09   16.56   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.15   16.84   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.22   17.09   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.29   17.30   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -11.22  -11.22   -0.00  H2
        Lime           -11.51   21.05   32.56  CaO
        O2             -60.68   22.45   83.13  O2
        Quartz          -2.71   -6.73   -4.03  SiO2
        SiO2(am)        -4.10   -6.73   -2.64  Si1.000O2.000
        Wollastonite     0.53   14.31   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 5.
------------------------------------

        TITLE 5 Total liquid solid ratio 500
        USE solution 1
        USE equilibrium_phases 5
        SAVE equilibrium_phases 6
        END
-----
TITLE
-----
```

```
 5 Total liquid solid ratio 500

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 5.    Pure-phase assemblage after simulation 4.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase             SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2         -2.27   20.44   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -2.89   -3.96   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -2.48   -1.91    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -2.10    0.13    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -1.73    2.17    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -1.38    4.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -1.05    6.26    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.74    8.31    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.47   10.35   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.41   11.02   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.29   13.77   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.08   14.44   14.51 0.000e+000          0.000e+000
        CSH(1.1)         0.00   14.98   14.98 0.000e+000 1.018e-004 1.018e-004
        CSH(1.2)         0.00   15.44   15.44 3.614e-003 6.089e-003 2.475e-003
        CSH(1.3)        -0.05   15.82   15.87 2.816e-003         -2.816e-003
        CSH(1.4)        -0.12   16.15   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.21   16.44   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.30   16.69   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -0.39   16.91   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.50   17.10   17.60 0.000e+000          0.000e+000
        SiO2(am)        -3.36   -6.00   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             2.393e-003  2.393e-004
        Si             1.137e-004  1.137e-005

----------------------------Description of solution----------------------------

                                pH  =  11.613     Charge balance
                                pe  =  -6.053     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  6.965e-003
                   Mass of water (kg)  =  1.000e-001
              Total alkalinity (eq/kg)  =  4.786e-003
                 Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
               Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  17
                              Total H  = 1.110173e+001
                              Total O  = 5.551125e+000

---------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            4.565e-003  4.175e-003   -2.341   -2.379   -0.039
        H+             2.635e-012  2.436e-012   -11.579  -11.613   -0.034
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           2.393e-003
```

```
        Ca+2          2.285e-003  1.624e-003   -2.641   -2.790   -0.148
        CaHO+         1.065e-004  9.753e-005   -3.973   -4.011   -0.038
        CaSiH3O4+      1.654e-006  1.515e-006   -5.781   -5.820   -0.038
H(0)         1.186e-014
        H2            5.929e-015  5.938e-015  -14.227  -14.226    0.001
O(0)         0.000e+000
        O2            0.000e+000  0.000e+000  -63.774  -63.773    0.001
Si           1.137e-004
        SiH3O4-       1.088e-004  9.962e-005   -3.964   -4.002   -0.038
        SiH2O4-2       2.319e-006  1.632e-006   -5.635   -5.787   -0.153
        CaSiH3O4+      1.654e-006  1.515e-006   -5.781   -5.820   -0.038
        H4SiO4        9.982e-007  9.998e-007   -6.001   -6.000    0.001

------------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -2.57   -6.00   -3.43  SiO2
        b-Cristobalite   -3.02   -6.00   -2.98  SiO2
        Ca(OH)2        -2.27   20.44   22.71  Ca(OH)2
        Chalcedony      -2.26   -6.00   -3.74  SiO2
        CSH(0.1)       -2.89   -3.96   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)       -2.48   -1.91    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)       -2.10    0.13    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)       -1.73    2.17    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)       -1.38    4.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)       -1.05    6.26    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)       -0.74    8.31    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)       -0.47   10.35   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.41   11.02   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)       -0.29   13.77   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)       -0.08   14.44   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        0.00   15.44   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)       -0.05   15.82   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)       -0.12   16.15   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)       -0.21   16.44   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)       -0.30   16.69   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)       -0.39   16.91   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)       -0.50   17.10   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2           -11.12  -11.12   -0.00  H2
        Lime          -12.12   20.44   32.56  CaO
        O2           -60.89   22.24   83.13  O2
        Quartz         -1.97   -6.00   -4.03  SiO2
        SiO2(am)       -3.36   -6.00   -2.64  Si1.000O2.000
        Wollastonite     0.65   14.44   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 6.
------------------------------------

        TITLE 6 Total liquid solid ratio 600
        USE solution 1
        USE equilibrium_phases 6
        SAVE equilibrium_phases 7
        END
-----
TITLE
-----

 6 Total liquid solid ratio 600

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.
```

```
Using solution 1.DW 100g
Using pure phase assemblage 6.    Pure-phase assemblage after simulation 5.

-------------------------------Phase assemblage--------------------------------

                                                    Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -2.27   20.44   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -2.89   -3.96   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -2.48   -1.91    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -2.10    0.13    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -1.73    2.17    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -1.38    4.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.05    6.26    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.74    8.31    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.47   10.35   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.41   11.02   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.29   13.77   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.08   14.44   14.51 0.000e+000          0.000e+000
        CSH(1.1)        0.00   14.98   14.98 1.018e-004 2.575e-003 2.473e-003
        CSH(1.2)        0.00   15.44   15.44 6.089e-003 3.376e-003-2.713e-003
        CSH(1.3)       -0.05   15.82   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.12   16.15   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.21   16.44   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.30   16.69   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.39   16.91   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.50   17.10   17.60 0.000e+000          0.000e+000
        SiO2(am)       -3.36   -6.00   -2.64 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality      Moles

        Ca             2.393e-003  2.393e-004
        Si             1.137e-004  1.137e-005

-----------------------------Description of solution-----------------------------

                                pH  =  11.613     Charge balance
                                pe  =  -6.139     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  6.965e-003
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  4.786e-003
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  16
                             Total H  = 1.110173e+001
                             Total O  = 5.551125e+000

----------------------------Distribution of species----------------------------

                                            Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            4.565e-003  4.175e-003   -2.341   -2.379   -0.039
        H+             2.635e-012  2.436e-012   -11.579  -11.613   -0.034
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           2.393e-003
        Ca+2           2.285e-003  1.624e-003   -2.641   -2.790   -0.148
        CaHO+          1.065e-004  9.753e-005   -3.973   -4.011   -0.038
        CaSiH3O4+      1.654e-006  1.515e-006   -5.781   -5.820   -0.038
H(0)         1.761e-014
        H2             8.805e-015  8.819e-015  -14.055  -14.055    0.001
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -64.117  -64.117    0.001
```

```
Si            1.137e-004
        SiH3O4-         1.088e-004  9.962e-005   -3.964   -4.002   -0.038
        SiH2O4-2        2.319e-006  1.632e-006   -5.635   -5.787   -0.153
        CaSiH3O4+       1.654e-006  1.515e-006   -5.781   -5.820   -0.038
        H4SiO4          9.982e-007  9.998e-007   -6.001   -6.000    0.001

-----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -2.57  -6.00  -3.43  SiO2
        b-Cristobalite  -3.02  -6.00  -2.98  SiO2
        Ca(OH)2         -2.27  20.44  22.71  Ca(OH)2
        Chalcedony      -2.26  -6.00  -3.74  SiO2
        CSH(0.1)        -2.89  -3.96  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -2.48  -1.91   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -2.10   0.13   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -1.73   2.17   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -1.38   4.22   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -1.05   6.26   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.74   8.31   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.47  10.35  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.41  11.02  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.29  13.77  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.08  14.44  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         0.00  14.98  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         0.00  15.44  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.05  15.82  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.12  16.15  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.21  16.44  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.30  16.69  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.39  16.91  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.50  17.10  17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -10.94 -10.95  -0.00  H2
        Lime           -12.12  20.44  32.56  CaO
        O2             -61.23  21.90  83.13  O2
        Quartz          -1.97  -6.00  -4.03  SiO2
        SiO2(am)        -3.36  -6.00  -2.64  Si1.000O2.000
        Wollastonite     0.65  14.44  13.78  CaSiO3

------------------
End of simulation.
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-----------------------------------
Reading input data for simulation 7.
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        TITLE 7 Total liquid solid ratio 700
        USE solution 1
        USE equilibrium_phases 7
        SAVE equilibrium_phases 8
        END
-----
TITLE
-----

 7 Total liquid solid ratio 700

----------------------------------------
Beginning of batch-reaction calculations.
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Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 7.    Pure-phase assemblage after simulation 6.

-------------------------------Phase assemblage---------------------------------

                                          Moles in assemblage
```

Phase	SI	log IAP	log KT	Initial	Final	Delta
Ca(OH)2	-2.27	20.44	22.71	0.000e+000	0.000e+000	
CSH(0.1)	-2.89	-3.96	-1.07	0.000e+000	0.000e+000	
CSH(0.2)	-2.48	-1.91	0.56	0.000e+000	0.000e+000	
CSH(0.3)	-2.10	0.13	2.23	0.000e+000	0.000e+000	
CSH(0.4)	-1.73	2.17	3.91	0.000e+000	0.000e+000	
CSH(0.5)	-1.38	4.22	5.60	0.000e+000	0.000e+000	
CSH(0.6)	-1.05	6.26	7.31	0.000e+000	0.000e+000	
CSH(0.7)	-0.74	8.31	9.04	0.000e+000	0.000e+000	
CSH(0.8)	-0.47	10.35	10.82	0.000e+000	0.000e+000	
CSH(0.833)	-0.41	11.02	11.44	0.000e+000	0.000e+000	
CSH(0.9)	-0.29	13.77	14.06	0.000e+000	0.000e+000	
CSH(1.0)	-0.08	14.44	14.51	0.000e+000	0.000e+000	
CSH(1.1)	0.00	14.98	14.98	2.575e-003	5.049e-003	2.473e-003
CSH(1.2)	0.00	15.44	15.44	3.376e-003	6.636e-004	-2.713e-003
CSH(1.3)	-0.05	15.82	15.87	0.000e+000	0.000e+000	
CSH(1.4)	-0.12	16.15	16.27	0.000e+000	0.000e+000	
CSH(1.5)	-0.21	16.44	16.64	0.000e+000	0.000e+000	
CSH(1.6)	-0.30	16.69	16.99	0.000e+000	0.000e+000	
CSH(1.7)	-0.39	16.91	17.30	0.000e+000	0.000e+000	
CSH(1.8)	-0.50	17.10	17.60	0.000e+000	0.000e+000	
SiO2(am)	-3.36	-6.00	-2.64	0.000e+000	0.000e+000	

----------Solution composition----------

Elements	Molality	Moles
Ca	2.393e-003	2.393e-004
Si	1.137e-004	1.137e-005

----------Description of solution----------

pH = 11.613 Charge balance
pe = -6.139 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 6.965e-003
Mass of water (kg) = 1.000e-001
Total alkalinity (eq/kg) = 4.786e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.714e-010
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 16
Total H = 1.110173e+001
Total O = 5.551125e+000

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	4.565e-003	4.175e-003	-2.341	-2.379	-0.039
H+	2.635e-012	2.436e-012	-11.579	-11.613	-0.034
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
Ca	2.393e-003				
Ca+2	2.285e-003	1.624e-003	-2.641	-2.790	-0.148
CaHO+	1.065e-004	9.753e-005	-3.973	-4.011	-0.038
CaSiH3O4+	1.654e-006	1.515e-006	-5.781	-5.820	-0.038
H(0)	1.762e-014				
H2	8.809e-015	8.824e-015	-14.055	-14.054	0.001
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-64.118	-64.117	0.001
Si	1.137e-004				
SiH3O4-	1.088e-004	9.962e-005	-3.964	-4.002	-0.038
SiH2O4-2	2.319e-006	1.632e-006	-5.635	-5.787	-0.153
CaSiH3O4+	1.654e-006	1.515e-006	-5.781	-5.820	-0.038
H4SiO4	9.982e-007	9.998e-007	-6.001	-6.000	0.001

----------Saturation indices----------

```
        Phase            SI log IAP  log KT

        a-Cristobalite   -2.57   -6.00   -3.43  SiO2
        b-Cristobalite   -3.02   -6.00   -2.98  SiO2
        Ca(OH)2         -2.27   20.44   22.71  Ca(OH)2
        Chalcedony       -2.26   -6.00   -3.74  SiO2
        CSH(0.1)         -2.89   -3.96   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -2.48   -1.91    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -2.10    0.13    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -1.73    2.17    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -1.38    4.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -1.05    6.26    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.74    8.31    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.47   10.35   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.41   11.02   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.29   13.77   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.08   14.44   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)          0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)          0.00   15.44   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.05   15.82   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.12   16.15   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.21   16.44   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.30   16.69   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.39   16.91   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.50   17.10   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -10.94  -10.95   -0.00  H2
        Lime           -12.12   20.44   32.56  CaO
        O2             -61.23   21.90   83.13  O2
        Quartz          -1.97   -6.00   -4.03  SiO2
        SiO2(am)        -3.36   -6.00   -2.64  Si1.000O2.000
        Wollastonite     0.65   14.44   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 8.
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        TITLE 8 Total liquid solid ratio 800
        USE solution 1
        USE equilibrium_phases 8
        SAVE equilibrium_phases 9
        END
-----
TITLE
-----

 8 Total liquid solid ratio 800

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 8.    Pure-phase assemblage after simulation 7.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -3.04   19.67   22.71 0.000e+000          0.000e+000
        CSH(0.1)         -2.12   -3.19   -1.07 0.000e+000          0.000e+000
        CSH(0.2)         -1.79   -1.22    0.56 0.000e+000          0.000e+000
        CSH(0.3)         -1.48    0.75    2.23 0.000e+000          0.000e+000
        CSH(0.4)         -1.19    2.71    3.91 0.000e+000          0.000e+000
```

```
        CSH(0.5)        -0.92    4.68    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.67    6.65    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.43    8.61    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.24   10.58   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.21   11.23   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.12   13.94   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.00   14.51   14.51 0.000e+000 3.802e-004 3.802e-004
        CSH(1.1)        -0.00   14.98   14.98 5.049e-003 5.194e-003 1.455e-004
        CSH(1.2)        -0.06   15.37   15.44 6.636e-004         -6.636e-004
        CSH(1.3)        -0.17   15.70   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.28   15.99   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.41   16.23   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.54   16.45   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -0.67   16.64   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.79   16.80   17.60 0.000e+000          0.000e+000
        SiO2(am)        -2.51   -5.15   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.379e-003  1.379e-004
        Si             4.036e-004  4.036e-005

----------------------------Description of solution----------------------------

                                pH  =  11.329     Charge balance
                                pe  =  -5.854     Adjusted to redox equilibrium
                     Activity of water  =  1.000
                        Ionic strength  =  4.067e-003
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  2.759e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  19
                             Total H  = 1.110153e+001
                             Total O  = 5.550982e+000

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            2.324e-003  2.168e-003   -2.634   -2.664   -0.030
        H+             4.997e-012  4.692e-012   -11.301  -11.329   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.379e-003
        Ca+2           1.341e-003  1.025e-003   -2.872   -2.989   -0.117
        CaHO+          3.424e-005  3.196e-005   -4.465   -4.495   -0.030
        CaSiH3O4+      3.732e-006  3.484e-006   -5.428   -5.458   -0.030
H(0)         1.758e-014
        H2             8.790e-015  8.798e-015  -14.056  -14.056    0.000
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -64.115  -64.114    0.000
Si           4.036e-004
        SiH3O4-        3.888e-004  3.629e-004   -3.410   -3.440   -0.030
        H4SiO4         7.010e-006  7.016e-006   -5.154   -5.154    0.000
        SiH2O4-2       4.066e-006  3.087e-006   -5.391   -5.510   -0.120
        CaSiH3O4+      3.732e-006  3.484e-006   -5.428   -5.458   -0.030

----------------------------Saturation indices---------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -1.72   -5.15   -3.43  SiO2
        b-Cristobalite   -2.17   -5.15   -2.98  SiO2
        Ca(OH)2         -3.04   19.67   22.71  Ca(OH)2
        Chalcedony       -1.42   -5.15   -3.74  SiO2
```

```
        CSH(0.1)        -2.12   -3.19   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -1.79   -1.22    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -1.48    0.75    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -1.19    2.71    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.92    4.68    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.67    6.65    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.43    8.61    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.24   10.58   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.21   11.23   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.12   13.94   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.06   15.37   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.17   15.70   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.28   15.99   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.41   16.23   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.54   16.45   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.67   16.64   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.79   16.80   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -10.95  -10.95   -0.00  H2
        Lime          -12.89   19.67   32.56  CaO
        O2            -61.23   21.90   83.13  O2
        Quartz         -1.13   -5.15   -4.03  SiO2
        SiO2(am)       -2.51   -5.15   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 9.
------------------------------------

        TITLE 9 Total liquid solid ratio 900
        USE solution 1
        USE equilibrium_phases 9
        SAVE equilibrium_phases 10
        END
-----
TITLE
-----

 9 Total liquid solid ratio 900

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 9.    Pure-phase assemblage after simulation 8.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -3.04   19.67   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -2.12   -3.19   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -1.79   -1.22    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -1.48    0.75    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -1.19    2.71    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.92    4.68    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.67    6.65    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.43    8.61    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.24   10.58   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.21   11.23   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.12   13.94   14.06 0.000e+000          0.000e+000
        CSH(1.0)         0.00   14.51   14.51 3.802e-004 1.315e-003 9.344e-004
```

```
        CSH(1.1)        0.00   14.98   14.98 5.194e-003 4.122e-003-1.072e-003
        CSH(1.2)       -0.06   15.37   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.17   15.70   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.28   15.99   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.41   16.23   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.54   16.45   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.67   16.64   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.79   16.80   17.60 0.000e+000          0.000e+000
        SiO2(am)       -2.51   -5.15   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.379e-003  1.379e-004
        Si             4.036e-004  4.036e-005

----------------------------Description of solution----------------------------

                                pH  =  11.329     Charge balance
                                pe  =  -5.747     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.067e-003
                     Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  2.759e-003
                   Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.729e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  15
                             Total H  = 1.110153e+001
                             Total O  = 5.550981e+000

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            2.324e-003  2.168e-003   -2.634   -2.664   -0.030
        H+             4.997e-012  4.692e-012  -11.301  -11.329   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.379e-003
        Ca+2           1.341e-003  1.025e-003   -2.872   -2.989   -0.117
        CaHO+          3.424e-005  3.196e-005   -4.465   -4.495   -0.030
        CaSiH3O4+      3.732e-006  3.484e-006   -5.428   -5.458   -0.030
H(0)         1.074e-014
        H2             5.372e-015  5.377e-015  -14.270  -14.269    0.000
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -63.687  -63.687    0.000
Si           4.036e-004
        SiH3O4-        3.888e-004  3.629e-004   -3.410   -3.440   -0.030
        H4SiO4         7.010e-006  7.016e-006   -5.154   -5.154    0.000
        SiH2O4-2       4.066e-006  3.087e-006   -5.391   -5.510   -0.120
        CaSiH3O4+      3.732e-006  3.484e-006   -5.428   -5.458   -0.030

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -1.72   -5.15   -3.43  SiO2
        b-Cristobalite   -2.17   -5.15   -2.98  SiO2
        Ca(OH)2          -3.04   19.67   22.71  Ca(OH)2
        Chalcedony       -1.42   -5.15   -3.74  SiO2
        CSH(0.1)         -2.12   -3.19   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -1.79   -1.22    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -1.48    0.75    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -1.19    2.71    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.92    4.68    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.67    6.65    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.43    8.61    9.04  Ca0.700Si1.000O2.700:0.771H2O
```

```
        CSH(0.8)        -0.24   10.58   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.21   11.23   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.12   13.94   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.06   15.37   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.17   15.70   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.28   15.99   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.41   16.23   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.54   16.45   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.67   16.64   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.79   16.80   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -11.16  -11.16   -0.00  H2
        Lime          -12.89   19.67   32.56  CaO
        O2            -60.80   22.33   83.13  O2
        Quartz         -1.13   -5.15   -4.03  SiO2
        SiO2(am)       -2.51   -5.15   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 10.
------------------------------------

        TITLE 10 Total liquid solid ratio 1000
        USE solution 1
        USE equilibrium_phases 10
        SAVE equilibrium_phases 11
        END
-----
TITLE
-----

 10 Total liquid solid ratio 1000

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 10.   Pure-phase assemblage after simulation 9.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -3.04   19.67   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -2.12   -3.19   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -1.79   -1.22    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -1.48    0.75    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -1.19    2.71    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.92    4.68    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.67    6.65    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.43    8.61    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.24   10.58   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.21   11.23   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.12   13.94   14.06 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.51   14.51 1.315e-003 2.249e-003 9.344e-004
        CSH(1.1)        0.00   14.98   14.98 4.122e-003 3.049e-003-1.072e-003
        CSH(1.2)       -0.06   15.37   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.17   15.70   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.28   15.99   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.41   16.23   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.54   16.45   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.67   16.64   17.30 0.000e+000          0.000e+000
```

```
        CSH(1.8)        -0.79   16.80   17.60 0.000e+000          0.000e+000
        SiO2(am)        -2.51   -5.15   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.379e-003  1.379e-004
        Si             4.036e-004  4.036e-005

----------------------------Description of solution---------------------------

                                pH  =  11.329     Charge balance
                                pe  =  -5.747     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.067e-003
                   Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  2.759e-003
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.729e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  =  15
                            Total H  = 1.110153e+001
                            Total O  = 5.550981e+000

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            2.324e-003  2.168e-003   -2.634   -2.664   -0.030
        H+             4.997e-012  4.692e-012  -11.301  -11.329   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.379e-003
        Ca+2           1.341e-003  1.025e-003   -2.872   -2.989   -0.117
        CaHO+          3.424e-005  3.196e-005   -4.465   -4.495   -0.030
        CaSiH3O4+      3.732e-006  3.484e-006   -5.428   -5.458   -0.030
H(0)         1.074e-014
        H2             5.372e-015  5.377e-015  -14.270  -14.269    0.000
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -63.687  -63.687    0.000
Si           4.036e-004
        SiH3O4-        3.888e-004  3.629e-004   -3.410   -3.440   -0.030
        H4SiO4         7.010e-006  7.016e-006   -5.154   -5.154    0.000
        SiH2O4-2       4.066e-006  3.087e-006   -5.391   -5.510   -0.120
        CaSiH3O4+      3.732e-006  3.484e-006   -5.428   -5.458   -0.030

----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -1.72   -5.15   -3.43  SiO2
        b-Cristobalite  -2.17   -5.15   -2.98  SiO2
        Ca(OH)2        -3.04   19.67   22.71  Ca(OH)2
        Chalcedony      -1.42   -5.15   -3.74  SiO2
        CSH(0.1)       -2.12   -3.19   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)       -1.79   -1.22    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)       -1.48    0.75    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)       -1.19    2.71    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)       -0.92    4.68    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)       -0.67    6.65    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)       -0.43    8.61    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)       -0.24   10.58   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)     -0.21   11.23   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)       -0.12   13.94   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)       -0.06   15.37   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)       -0.17   15.70   15.87  Ca1.000Si0.769O2.538:1.065H2O
```

```
        CSH(1.4)        -0.28   15.99   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.41   16.23   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.54   16.45   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.67   16.64   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.79   16.80   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -11.16  -11.16   -0.00  H2
        Lime          -12.89   19.67   32.56  CaO
        O2            -60.80   22.33   83.13  O2
        Quartz         -1.13   -5.15   -4.03  SiO2
        SiO2(am)       -2.51   -5.15   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 11.
------------------------------------

        TITLE 11 Total liquid solid ratio 1100
        USE solution 1
        USE equilibrium_phases 11
        SAVE equilibrium_phases 12
        END
-----
TITLE
-----

 11 Total liquid solid ratio 1100

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 11.   Pure-phase assemblage after simulation 10.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -3.04   19.67   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -2.12   -3.19   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -1.79   -1.22    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -1.48    0.75    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -1.19    2.71    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.92    4.68    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.67    6.65    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.43    8.61    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.24   10.58   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.21   11.23   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.12   13.94   14.06 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.51   14.51 2.249e-003 3.183e-003 9.344e-004
        CSH(1.1)        0.00   14.98   14.98 3.049e-003 1.977e-003-1.072e-003
        CSH(1.2)       -0.06   15.37   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.17   15.70   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.28   15.99   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.41   16.23   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.54   16.45   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.67   16.64   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.79   16.80   17.60 0.000e+000          0.000e+000
        SiO2(am)       -2.51   -5.15   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles
```

```
         Ca            1.379e-003  1.379e-004
         Si            4.036e-004  4.036e-005

----------------------------Description of solution----------------------------

                                pH  =  11.329     Charge balance
                                pe  =  -5.747     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.067e-003
                     Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  2.759e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.729e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  15
                             Total H  = 1.110153e+001
                             Total O  = 5.550981e+000

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            2.324e-003  2.168e-003   -2.634   -2.664   -0.030
         H+             4.997e-012  4.692e-012   -11.301  -11.329   -0.027
         H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca            1.379e-003
         Ca+2           1.341e-003  1.025e-003   -2.872   -2.989   -0.117
         CaHO+          3.424e-005  3.196e-005   -4.465   -4.495   -0.030
         CaSiH3O4+       3.732e-006  3.484e-006   -5.428   -5.458   -0.030
H(0)          1.075e-014
         H2             5.373e-015  5.378e-015   -14.270  -14.269    0.000
O(0)          0.000e+000
         O2             0.000e+000  0.000e+000   -63.687  -63.687    0.000
Si            4.036e-004
         SiH3O4-         3.888e-004  3.629e-004   -3.410   -3.440   -0.030
         H4SiO4          7.010e-006  7.016e-006   -5.154   -5.154    0.000
         SiH2O4-2        4.066e-006  3.087e-006   -5.391   -5.510   -0.120
         CaSiH3O4+       3.732e-006  3.484e-006   -5.428   -5.458   -0.030

-----------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -1.72   -5.15   -3.43  SiO2
         b-Cristobalite   -2.17   -5.15   -2.98  SiO2
         Ca(OH)2         -3.04   19.67   22.71  Ca(OH)2
         Chalcedony       -1.42   -5.15   -3.74  SiO2
         CSH(0.1)         -2.12   -3.19   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -1.79   -1.22    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -1.48    0.75    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -1.19    2.71    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -0.92    4.68    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -0.67    6.65    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -0.43    8.61    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -0.24   10.58   10.82  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -0.21   11.23   11.44  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)         -0.12   13.94   14.06  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)          0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)          0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.06   15.37   15.44  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.17   15.70   15.87  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)         -0.28   15.99   16.27  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.41   16.23   16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -0.54   16.45   16.99  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)         -0.67   16.64   17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)         -0.79   16.80   17.60  Ca1.000Si0.556O2.112:1.047H2O
         H2             -11.16  -11.16   -0.00  H2
         Lime           -12.89   19.67   32.56  CaO
```

```
        O2           -60.80   22.33   83.13  O2
        Quartz         -1.13   -5.15   -4.03  SiO2
        SiO2(am)       -2.51   -5.15   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 12.
------------------------------------

        TITLE 12 Total liquid solid ratio 1200
        USE solution 1
        USE equilibrium_phases 12
        SAVE equilibrium_phases 13
        END
-----
TITLE
-----

 12 Total liquid solid ratio 1200

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 12.   Pure-phase assemblage after simulation 11.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -3.04   19.67   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -2.12   -3.19   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -1.79   -1.22    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -1.48    0.75    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -1.19    2.71    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.92    4.68    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.67    6.65    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.43    8.61    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.24   10.58   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.21   11.23   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.12   13.94   14.06 0.000e+000          0.000e+000
        CSH(1.0)         0.00   14.51   14.51 3.183e-003 4.118e-003 9.344e-004
        CSH(1.1)         0.00   14.98   14.98 1.977e-003 9.047e-004-1.072e-003
        CSH(1.2)        -0.06   15.37   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.17   15.70   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.28   15.99   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.41   16.23   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.54   16.45   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -0.67   16.64   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.79   16.80   17.60 0.000e+000          0.000e+000
        SiO2(am)        -2.51   -5.15   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.379e-003  1.379e-004
        Si             4.036e-004  4.036e-005

---------------------------Description of solution----------------------------

                                pH  =  11.329     Charge balance
                                pe  =  -5.747     Adjusted to redox equilibrium
```

```
                    Activity of water =  1.000
                      Ionic strength =  4.067e-003
                   Mass of water (kg) =  1.000e-001
               Total alkalinity (eq/kg) =  2.759e-003
                  Total carbon (mol/kg) =  0.000e+000
                    Total CO2 (mol/kg) =  0.000e+000
                  Temperature (deg C) =  25.000
              Electrical balance (eq) = -1.729e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.00
                         Iterations =  15
                           Total H  = 1.110153e+001
                           Total O  = 5.550981e+000

----------------------------Distribution of species-----------------------------

                                                 Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            2.324e-003  2.168e-003    -2.634    -2.664    -0.030
         H+             4.997e-012  4.692e-012   -11.301   -11.329    -0.027
         H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
Ca            1.379e-003
         Ca+2           1.341e-003  1.025e-003    -2.872    -2.989    -0.117
         CaHO+          3.424e-005  3.196e-005    -4.465    -4.495    -0.030
         CaSiH3O4+       3.732e-006  3.484e-006    -5.428    -5.458    -0.030
H(0)          1.075e-014
         H2             5.373e-015  5.378e-015   -14.270   -14.269     0.000
O(0)          0.000e+000
         O2             0.000e+000  0.000e+000   -63.687   -63.687     0.000
Si            4.036e-004
         SiH3O4-         3.888e-004  3.629e-004    -3.410    -3.440    -0.030
         H4SiO4          7.010e-006  7.016e-006    -5.154    -5.154     0.000
         SiH2O4-2        4.066e-006  3.087e-006    -5.391    -5.510    -0.120
         CaSiH3O4+       3.732e-006  3.484e-006    -5.428    -5.458    -0.030

-----------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -1.72   -5.15   -3.43  SiO2
         b-Cristobalite   -2.17   -5.15   -2.98  SiO2
         Ca(OH)2         -3.04   19.67   22.71  Ca(OH)2
         Chalcedony       -1.42   -5.15   -3.74  SiO2
         CSH(0.1)         -2.12   -3.19   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -1.79   -1.22    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -1.48    0.75    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -1.19    2.71    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -0.92    4.68    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -0.67    6.65    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -0.43    8.61    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -0.24   10.58   10.82  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -0.21   11.23   11.44  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)         -0.12   13.94   14.06  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)          0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)          0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.06   15.37   15.44  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.17   15.70   15.87  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)         -0.28   15.99   16.27  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.41   16.23   16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -0.54   16.45   16.99  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)         -0.67   16.64   17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)         -0.79   16.80   17.60  Ca1.000Si0.556O2.112:1.047H2O
         H2             -11.16  -11.16   -0.00  H2
         Lime           -12.89   19.67   32.56  CaO
         O2             -60.80   22.33   83.13  O2
         Quartz          -1.13   -5.15   -4.03  SiO2
         SiO2(am)        -2.51   -5.15   -2.64  Si1.000O2.000
         Wollastonite     0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
```

```
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------------------------------------
Reading input data for simulation 13.
------------------------------------

        TITLE 13 Total liquid solid ratio 1300
        USE solution 1
        USE equilibrium_phases 13
        SAVE equilibrium_phases 14
        END
-----
TITLE
-----

 13 Total liquid solid ratio 1300

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 13.   Pure-phase assemblage after simulation 12.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2         -3.15   19.56   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -2.01   -3.09   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -1.70   -1.13    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -1.40    0.83    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -1.13    2.78    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.86    4.74    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.62    6.69    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.40    8.65    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.22   10.60   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.19   11.25   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.11   13.95   14.06 0.000e+000          0.000e+000
        CSH(1.0)         0.00   14.51   14.51 4.118e-003 4.893e-003 7.752e-004
        CSH(1.1)        -0.01   14.97   14.98 9.047e-004         -9.047e-004
        CSH(1.2)        -0.08   15.36   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.19   15.68   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.32   15.96   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.45   16.19   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.58   16.40   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -0.71   16.59   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.84   16.75   17.60 0.000e+000          0.000e+000
        SiO2(am)        -2.40   -5.04   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.295e-003  1.295e-004
        Si             4.714e-004  4.714e-005

----------------------------Description of solution----------------------------

                                pH  =  11.284     Charge balance
                                pe  =  -5.703     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.821e-003
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  2.589e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                 Temperature (deg C)  =  25.000
```

```
              Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  16
                           Total H  = 1.110151e+001
                           Total O  = 5.550979e+000

----------------------------Distribution of species----------------------------

                                                Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            2.093e-003  1.956e-003   -2.679   -2.709   -0.029
         H+             5.527e-012  5.198e-012  -11.258  -11.284   -0.027
         H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca            1.295e-003
         Ca+2           1.261e-003  9.708e-004   -2.899   -3.013   -0.114
         CaHO+          2.922e-005  2.733e-005   -4.534   -4.563   -0.029
         CaSiH3O4+       4.127e-006  3.860e-006   -5.384   -5.413   -0.029
H(0)          1.075e-014
         H2             5.374e-015  5.378e-015  -14.270  -14.269    0.000
O(0)          0.000e+000
         O2             0.000e+000  0.000e+000  -63.687  -63.687    0.000
Si            4.714e-004
         SiH3O4-         4.539e-004  4.245e-004   -3.343   -3.372   -0.029
         H4SiO4          9.084e-006  9.092e-006   -5.042   -5.041    0.000
         SiH2O4-2        4.259e-006  3.259e-006   -5.371   -5.487   -0.116
         CaSiH3O4+       4.127e-006  3.860e-006   -5.384   -5.413   -0.029

-----------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -1.61   -5.04   -3.43  SiO2
         b-Cristobalite   -2.06   -5.04   -2.98  SiO2
         Ca(OH)2         -3.15   19.56   22.71  Ca(OH)2
         Chalcedony       -1.30   -5.04   -3.74  SiO2
         CSH(0.1)         -2.01   -3.09   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -1.70   -1.13    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -1.40    0.83    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -1.13    2.78    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -0.86    4.74    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -0.62    6.69    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -0.40    8.65    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -0.22   10.60   10.82  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -0.19   11.25   11.44  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)         -0.11   13.95   14.06  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)          0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)         -0.01   14.97   14.98  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.08   15.36   15.44  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.19   15.68   15.87  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)         -0.32   15.96   16.27  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.45   16.19   16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -0.58   16.40   16.99  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)         -0.71   16.59   17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)         -0.84   16.75   17.60  Ca1.000Si0.556O2.112:1.047H2O
         H2             -11.16  -11.16   -0.00  H2
         Lime           -13.01   19.56   32.56  CaO
         O2             -60.80   22.33   83.13  O2
         Quartz          -1.01   -5.04   -4.03  SiO2
         SiO2(am)        -2.40   -5.04   -2.64  Si1.000O2.000
         Wollastonite     0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 14.
------------------------------------

         TITLE 14 Total liquid solid ratio 1400
```

```
        USE solution 1
        USE equilibrium_phases 14
        SAVE equilibrium_phases 15
        END
-----
TITLE
-----

 14 Total liquid solid ratio 1400

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 14.   Pure-phase assemblage after simulation 13.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -3.79   18.92   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -1.44   -2.52   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -1.19   -0.62    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.96    1.27    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.75    3.16    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.55    5.05    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.37    6.95    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.21    8.84    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.09   10.73   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.08   11.35   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.04   14.02   14.06 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.51   14.51 4.893e-003 4.786e-003-1.068e-004
        CSH(1.1)       -0.07   14.92   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.19   15.25   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.34   15.53   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.50   15.77   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.66   15.98   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.82   16.17   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.97   16.33   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.13   16.47   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.77   -4.41   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.068e-003  1.068e-004
        Si             1.068e-003  1.068e-004

----------------------------Description of solution----------------------------

                                pH  =  11.003     Charge balance
                                pe  =  -5.422     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.168e-003
                   Mass of water (kg)  =  1.000e-001
              Total alkalinity (eq/kg)  =  2.137e-003
                 Total carbon (mol/kg)  =  0.000e+000
                   Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
               Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                         Iterations  =  15
                           Total H  = 1.110147e+001
                           Total O  = 5.551058e+000

---------------------------Distribution of species----------------------------
```

```
                                        Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            1.090e-003  1.024e-003   -2.963   -2.990   -0.027
        H+             1.051e-011  9.932e-012  -10.978  -11.003   -0.025
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.068e-003
        Ca+2           1.048e-003  8.236e-004   -2.980   -3.084   -0.104
        CaHO+          1.290e-005  1.213e-005   -4.889   -4.916   -0.027
        CaSiH3O4+      7.841e-006  7.374e-006   -5.106   -5.132   -0.027
H(0)         1.075e-014
        H2             5.377e-015  5.381e-015  -14.269  -14.269    0.000
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -63.688  -63.687    0.000
Si           1.068e-003
        SiH3O4-        1.016e-003  9.559e-004   -2.993   -3.020   -0.027
        H4SiO4         3.909e-005  3.911e-005   -4.408   -4.408    0.000
        CaSiH3O4+      7.841e-006  7.374e-006   -5.106   -5.132   -0.027
        SiH2O4-2       4.910e-006  3.841e-006   -5.309   -5.416   -0.107

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.97   -4.41   -3.43  SiO2
        b-Cristobalite   -1.43   -4.41   -2.98  SiO2
        Ca(OH)2          -3.79   18.92   22.71  Ca(OH)2
        Chalcedony       -0.67   -4.41   -3.74  SiO2
        CSH(0.1)         -1.44   -2.52   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -1.19   -0.62    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.96    1.27    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.75    3.16    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.55    5.05    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.37    6.95    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.21    8.84    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.09   10.73   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.08   11.35   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.04   14.02   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)          0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.07   14.92   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.19   15.25   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.34   15.53   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.50   15.77   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.66   15.98   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.82   16.17   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.97   16.33   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -1.13   16.47   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -11.16  -11.16   -0.00  H2
        Lime           -13.64   18.92   32.56  CaO
        O2             -60.80   22.32   83.13  O2
        Quartz          -0.38   -4.41   -4.03  SiO2
        SiO2(am)        -1.77   -4.41   -2.64  Si1.000O2.000
        Wollastonite     0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 15.
------------------------------------

        TITLE 15 Total liquid solid ratio 1500
        USE solution 1
        USE equilibrium_phases 15
        SAVE equilibrium_phases 16
        END
-----
TITLE
-----
```

```
 15 Total liquid solid ratio 1500

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 15.   Pure-phase assemblage after simulation 14.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -3.79   18.92   22.71 0.000e+000          0.000e+000
        CSH(0.1)       -1.44   -2.52   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -1.19   -0.62    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.96    1.27    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.75    3.16    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.55    5.05    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.37    6.95    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.21    8.84    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.09   10.73   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.08   11.35   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.04   14.02   14.06 0.000e+000          0.000e+000
        CSH(1.0)        0.00   14.51   14.51 4.786e-003 4.679e-003-1.068e-004
        CSH(1.1)       -0.07   14.92   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.19   15.25   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.34   15.53   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.50   15.77   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.66   15.98   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.82   16.17   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.97   16.33   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.13   16.47   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.77   -4.41   -2.64 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        Ca             1.068e-003  1.068e-004
        Si             1.068e-003  1.068e-004

----------------------------Description of solution----------------------------

                                pH  =  11.003     Charge balance
                                pe  =  -5.422     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.168e-003
                   Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  2.137e-003
                  Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  15
                              Total H  = 1.110147e+001
                              Total O  = 5.551058e+000

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity Molality Activity    Gamma

        HO-            1.090e-003  1.024e-003   -2.963   -2.990   -0.027
        H+             1.051e-011  9.932e-012  -10.978  -11.003   -0.025
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
```

```
Ca            1.068e-003
        Ca+2           1.048e-003  8.236e-004   -2.980   -3.084   -0.104
        CaHO+          1.290e-005  1.213e-005   -4.889   -4.916   -0.027
        CaSiH3O4+      7.841e-006  7.374e-006   -5.106   -5.132   -0.027
H(0)          1.075e-014
        H2             5.377e-015  5.381e-015  -14.269  -14.269    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -63.688  -63.687    0.000
Si            1.068e-003
        SiH3O4-        1.016e-003  9.559e-004   -2.993   -3.020   -0.027
        H4SiO4         3.909e-005  3.911e-005   -4.408   -4.408    0.000
        CaSiH3O4+      7.841e-006  7.374e-006   -5.106   -5.132   -0.027
        SiH2O4-2       4.910e-006  3.841e-006   -5.309   -5.416   -0.107

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -0.97  -4.41  -3.43  SiO2
        b-Cristobalite  -1.43  -4.41  -2.98  SiO2
        Ca(OH)2         -3.79  18.92  22.71  Ca(OH)2
        Chalcedony      -0.67  -4.41  -3.74  SiO2
        CSH(0.1)        -1.44  -2.52  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -1.19  -0.62   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.96   1.27   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.75   3.16   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.55   5.05   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.37   6.95   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.21   8.84   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.09  10.73  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.08  11.35  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.04  14.02  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00  14.51  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.07  14.92  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.19  15.25  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.34  15.53  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.50  15.77  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.66  15.98  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.82  16.17  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.97  16.33  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.13  16.47  17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -11.16 -11.16  -0.00  H2
        Lime           -13.64  18.92  32.56  CaO
        O2             -60.80  22.32  83.13  O2
        Quartz          -0.38  -4.41  -4.03  SiO2
        SiO2(am)        -1.77  -4.41  -2.64  Si1.000O2.000
        Wollastonite     0.73  14.51  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 16.
------------------------------------

        TITLE 16 Total liquid solid ratio 1600
        USE solution 1
        USE equilibrium_phases 16
        SAVE equilibrium_phases 17
        END
-----
TITLE
-----

 16 Total liquid solid ratio 1600

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------
```

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 16. Pure-phase assemblage after simulation 15.

-------------------------------Phase assemblage--------------------------------

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca(OH)2	-3.79	18.92	22.71	0.000e+000	0.000e+000	
CSH(0.1)	-1.44	-2.52	-1.07	0.000e+000	0.000e+000	
CSH(0.2)	-1.19	-0.62	0.56	0.000e+000	0.000e+000	
CSH(0.3)	-0.96	1.27	2.23	0.000e+000	0.000e+000	
CSH(0.4)	-0.75	3.16	3.91	0.000e+000	0.000e+000	
CSH(0.5)	-0.55	5.05	5.60	0.000e+000	0.000e+000	
CSH(0.6)	-0.37	6.95	7.31	0.000e+000	0.000e+000	
CSH(0.7)	-0.21	8.84	9.04	0.000e+000	0.000e+000	
CSH(0.8)	-0.09	10.73	10.82	0.000e+000	0.000e+000	
CSH(0.833)	-0.08	11.35	11.44	0.000e+000	0.000e+000	
CSH(0.9)	-0.04	14.02	14.06	0.000e+000	0.000e+000	
CSH(1.0)	0.00	14.51	14.51	4.679e-003	4.572e-003	-1.068e-004
CSH(1.1)	-0.07	14.92	14.98	0.000e+000	0.000e+000	
CSH(1.2)	-0.19	15.25	15.44	0.000e+000	0.000e+000	
CSH(1.3)	-0.34	15.53	15.87	0.000e+000	0.000e+000	
CSH(1.4)	-0.50	15.77	16.27	0.000e+000	0.000e+000	
CSH(1.5)	-0.66	15.98	16.64	0.000e+000	0.000e+000	
CSH(1.6)	-0.82	16.17	16.99	0.000e+000	0.000e+000	
CSH(1.7)	-0.97	16.33	17.30	0.000e+000	0.000e+000	
CSH(1.8)	-1.13	16.47	17.60	0.000e+000	0.000e+000	
SiO2(am)	-1.77	-4.41	-2.64	0.000e+000	0.000e+000	

------------------------------Solution composition-------------------------------

Elements	Molality	Moles
Ca	1.068e-003	1.068e-004
Si	1.068e-003	1.068e-004

----------------------------Description of solution----------------------------

pH = 11.003 Charge balance
pe = -5.422 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 3.168e-003
Mass of water (kg) = 1.000e-001
Total alkalinity (eq/kg) = 2.137e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.714e-010
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 15
Total H = 1.110147e+001
Total O = 5.551058e+000

---------------------------Distribution of species---------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	1.090e-003	1.024e-003	-2.963	-2.990	-0.027
H+	1.051e-011	9.932e-012	-10.978	-11.003	-0.025
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
Ca	1.068e-003				
Ca+2	1.048e-003	8.236e-004	-2.980	-3.084	-0.104
CaHO+	1.290e-005	1.213e-005	-4.889	-4.916	-0.027
CaSiH3O4+	7.841e-006	7.374e-006	-5.106	-5.132	-0.027
H(0)	1.075e-014				
H2	5.377e-015	5.381e-015	-14.269	-14.269	0.000
O(0)	0.000e+000				

```
        O2            0.000e+000  0.000e+000   -63.688   -63.687    0.000
Si           1.068e-003
        SiH3O4-        1.016e-003  9.559e-004    -2.993    -3.020   -0.027
        H4SiO4         3.909e-005  3.911e-005    -4.408    -4.408    0.000
        CaSiH3O4+      7.841e-006  7.374e-006    -5.106    -5.132   -0.027
        SiH2O4-2       4.910e-006  3.841e-006    -5.309    -5.416   -0.107

------------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.97   -4.41   -3.43  SiO2
        b-Cristobalite   -1.43   -4.41   -2.98  SiO2
        Ca(OH)2         -3.79   18.92   22.71  Ca(OH)2
        Chalcedony       -0.67   -4.41   -3.74  SiO2
        CSH(0.1)         -1.44   -2.52   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -1.19   -0.62    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.96    1.27    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.75    3.16    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.55    5.05    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.37    6.95    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.21    8.84    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.09   10.73   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.08   11.35   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.04   14.02   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)          0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.07   14.92   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.19   15.25   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.34   15.53   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.50   15.77   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.66   15.98   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.82   16.17   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.97   16.33   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -1.13   16.47   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2              -11.16  -11.16   -0.00  H2
        Lime            -13.64   18.92   32.56  CaO
        O2              -60.80   22.32   83.13  O2
        Quartz           -0.38   -4.41   -4.03  SiO2
        SiO2(am)         -1.77   -4.41   -2.64  Si1.000O2.000
        Wollastonite      0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 17.
------------------------------------

        TITLE 17 Total liquid solid ratio 1700
        USE solution 1
        USE equilibrium_phases 17
        SAVE equilibrium_phases 18
        END
-----
TITLE
-----

 17 Total liquid solid ratio 1700

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 17.   Pure-phase assemblage after simulation 16.

-------------------------------Phase assemblage---------------------------------
```

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca(OH)2	-3.79	18.92	22.71	0.000e+000	0.000e+000	0.000e+000
CSH(0.1)	-1.44	-2.52	-1.07	0.000e+000	0.000e+000	0.000e+000
CSH(0.2)	-1.19	-0.62	0.56	0.000e+000	0.000e+000	0.000e+000
CSH(0.3)	-0.96	1.27	2.23	0.000e+000	0.000e+000	0.000e+000
CSH(0.4)	-0.75	3.16	3.91	0.000e+000	0.000e+000	0.000e+000
CSH(0.5)	-0.55	5.05	5.60	0.000e+000	0.000e+000	0.000e+000
CSH(0.6)	-0.37	6.95	7.31	0.000e+000	0.000e+000	0.000e+000
CSH(0.7)	-0.21	8.84	9.04	0.000e+000	0.000e+000	0.000e+000
CSH(0.8)	-0.09	10.73	10.82	0.000e+000	0.000e+000	0.000e+000
CSH(0.833)	-0.08	11.35	11.44	0.000e+000	0.000e+000	0.000e+000
CSH(0.9)	-0.04	14.02	14.06	0.000e+000	0.000e+000	0.000e+000
CSH(1.0)	0.00	14.51	14.51	4.572e-003	4.466e-003	-1.068e-004
CSH(1.1)	-0.07	14.92	14.98	0.000e+000	0.000e+000	0.000e+000
CSH(1.2)	-0.19	15.25	15.44	0.000e+000	0.000e+000	0.000e+000
CSH(1.3)	-0.34	15.53	15.87	0.000e+000	0.000e+000	0.000e+000
CSH(1.4)	-0.50	15.77	16.27	0.000e+000	0.000e+000	0.000e+000
CSH(1.5)	-0.66	15.98	16.64	0.000e+000	0.000e+000	0.000e+000
CSH(1.6)	-0.82	16.17	16.99	0.000e+000	0.000e+000	0.000e+000
CSH(1.7)	-0.97	16.33	17.30	0.000e+000	0.000e+000	0.000e+000
CSH(1.8)	-1.13	16.47	17.60	0.000e+000	0.000e+000	0.000e+000
SiO2(am)	-1.77	-4.41	-2.64	0.000e+000	0.000e+000	0.000e+000

----------Solution composition----------

Elements	Molality	Moles
Ca	1.068e-003	1.068e-004
Si	1.068e-003	1.068e-004

----------Description of solution----------

pH = 11.003 Charge balance
pe = -5.422 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 3.168e-003
Mass of water (kg) = 1.000e-001
Total alkalinity (eq/kg) = 2.137e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.714e-010
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 15
Total H = 1.110147e+001
Total O = 5.551058e+000

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	1.090e-003	1.024e-003	-2.963	-2.990	-0.027
H+	1.051e-011	9.932e-012	-10.978	-11.003	-0.025
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
Ca	1.068e-003				
Ca+2	1.048e-003	8.236e-004	-2.980	-3.084	-0.104
CaHO+	1.290e-005	1.213e-005	-4.889	-4.916	-0.027
CaSiH3O4+	7.841e-006	7.374e-006	-5.106	-5.132	-0.027
H(0)	1.075e-014				
H2	5.377e-015	5.381e-015	-14.269	-14.269	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-63.688	-63.687	0.000
Si	1.068e-003				
SiH3O4-	1.016e-003	9.559e-004	-2.993	-3.020	-0.027
H4SiO4	3.909e-005	3.911e-005	-4.408	-4.408	0.000
CaSiH3O4+	7.841e-006	7.374e-006	-5.106	-5.132	-0.027
SiH2O4-2	4.910e-006	3.841e-006	-5.309	-5.416	-0.107

```
-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.97  -4.41  -3.43  SiO2
        b-Cristobalite   -1.43  -4.41  -2.98  SiO2
        Ca(OH)2         -3.79  18.92  22.71  Ca(OH)2
        Chalcedony       -0.67  -4.41  -3.74  SiO2
        CSH(0.1)         -1.44  -2.52  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -1.19  -0.62   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.96   1.27   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.75   3.16   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.55   5.05   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.37   6.95   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.21   8.84   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.09  10.73  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.08  11.35  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.04  14.02  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)          0.00  14.51  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.07  14.92  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.19  15.25  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.34  15.53  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.50  15.77  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.66  15.98  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.82  16.17  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.97  16.33  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -1.13  16.47  17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2              -11.16 -11.16  -0.00  H2
        Lime            -13.64  18.92  32.56  CaO
        O2              -60.80  22.32  83.13  O2
        Quartz           -0.38  -4.41  -4.03  SiO2
        SiO2(am)         -1.77  -4.41  -2.64  Si1.000O2.000
        Wollastonite      0.73  14.51  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 18.
------------------------------------

        TITLE 18 Total liquid solid ratio 1800
        USE solution 1
        USE equilibrium_phases 18
        SAVE equilibrium_phases 19
        END
-----
TITLE
-----

 18 Total liquid solid ratio 1800

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 18.    Pure-phase assemblage after simulation 17.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -3.79  18.92  22.71 0.000e+000          0.000e+000
        CSH(0.1)         -1.44  -2.52  -1.07 0.000e+000          0.000e+000
        CSH(0.2)         -1.19  -0.62   0.56 0.000e+000          0.000e+000
        CSH(0.3)         -0.96   1.27   2.23 0.000e+000          0.000e+000
```

```
        CSH(0.4)        -0.75    3.16    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.55    5.05    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.37    6.95    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.21    8.84    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.09   10.73   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.08   11.35   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.04   14.02   14.06 0.000e+000          0.000e+000
        CSH(1.0)         0.00   14.51   14.51 4.466e-003 4.359e-003-1.068e-004
        CSH(1.1)        -0.07   14.92   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.19   15.25   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.34   15.53   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.50   15.77   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.66   15.98   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.82   16.17   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -0.97   16.33   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.13   16.47   17.60 0.000e+000          0.000e+000
        SiO2(am)        -1.77   -4.41   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.068e-003  1.068e-004
        Si             1.068e-003  1.068e-004

----------------------------Description of solution---------------------------

                                pH  =  11.003     Charge balance
                                pe  =  -5.422     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.168e-003
                     Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  2.137e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  15
                              Total H  = 1.110147e+001
                              Total O  = 5.551058e+000

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.090e-003  1.024e-003   -2.963   -2.990   -0.027
        H+             1.051e-011  9.932e-012  -10.978  -11.003   -0.025
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.068e-003
        Ca+2           1.048e-003  8.236e-004   -2.980   -3.084   -0.104
        CaHO+          1.290e-005  1.213e-005   -4.889   -4.916   -0.027
        CaSiH3O4+      7.841e-006  7.374e-006   -5.106   -5.132   -0.027
H(0)         1.075e-014
        H2             5.377e-015  5.381e-015  -14.269  -14.269    0.000
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -63.688  -63.687    0.000
Si           1.068e-003
        SiH3O4-        1.016e-003  9.559e-004   -2.993   -3.020   -0.027
        H4SiO4         3.909e-005  3.911e-005   -4.408   -4.408    0.000
        CaSiH3O4+      7.841e-006  7.374e-006   -5.106   -5.132   -0.027
        SiH2O4-2       4.910e-006  3.841e-006   -5.309   -5.416   -0.107

----------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -0.97  -4.41  -3.43  SiO2
        b-Cristobalite  -1.43  -4.41  -2.98  SiO2
        Ca(OH)2        -3.79  18.92  22.71  Ca(OH)2
```

```
        Chalcedony      -0.67   -4.41   -3.74  SiO2
        CSH(0.1)        -1.44   -2.52   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -1.19   -0.62    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.96    1.27    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.75    3.16    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.55    5.05    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.37    6.95    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.21    8.84    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.09   10.73   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.08   11.35   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.04   14.02   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.07   14.92   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.19   15.25   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.34   15.53   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.50   15.77   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.66   15.98   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.82   16.17   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.97   16.33   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.13   16.47   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -11.16  -11.16   -0.00  H2
        Lime           -13.64   18.92   32.56  CaO
        O2             -60.80   22.32   83.13  O2
        Quartz          -0.38   -4.41   -4.03  SiO2
        SiO2(am)        -1.77   -4.41   -2.64  Si1.000O2.000
        Wollastonite     0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

-------------------------------------
Reading input data for simulation 19.
-------------------------------------

        TITLE 19 Total liquid solid ratio 1900
        USE solution 1
        USE equilibrium_phases 19
        SAVE equilibrium_phases 20
        END
-----
TITLE
-----

 19 Total liquid solid ratio 1900

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 19.   Pure-phase assemblage after simulation 18.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase              SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -3.79   18.92   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -1.44   -2.52   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -1.19   -0.62    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -0.96    1.27    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -0.75    3.16    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.55    5.05    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.37    6.95    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.21    8.84    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.09   10.73   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.08   11.35   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.04   14.02   14.06 0.000e+000          0.000e+000
```

```
        CSH(1.0)        0.00   14.51   14.51 4.359e-003 4.252e-003-1.068e-004
        CSH(1.1)       -0.07   14.92   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.19   15.25   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.34   15.53   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.50   15.77   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.66   15.98   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.82   16.17   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.97   16.33   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.13   16.47   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.77   -4.41   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca            1.068e-003  1.068e-004
        Si            1.068e-003  1.068e-004

----------------------------Description of solution----------------------------

                                pH  =  11.003     Charge balance
                                pe  =  -5.422     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.168e-003
                   Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  2.137e-003
                  Total carbon (mol/kg)  =  0.000e+000
                     Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  15
                              Total H  = 1.110147e+001
                              Total O  = 5.551058e+000

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-           1.090e-003  1.024e-003   -2.963   -2.990   -0.027
        H+            1.051e-011  9.932e-012  -10.978  -11.003   -0.025
        H2O           5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.068e-003
        Ca+2          1.048e-003  8.236e-004   -2.980   -3.084   -0.104
        CaHO+         1.290e-005  1.213e-005   -4.889   -4.916   -0.027
        CaSiH3O4+      7.841e-006  7.374e-006   -5.106   -5.132   -0.027
H(0)         1.075e-014
        H2            5.377e-015  5.381e-015  -14.269  -14.269    0.000
O(0)         0.000e+000
        O2            0.000e+000  0.000e+000  -63.688  -63.687    0.000
Si           1.068e-003
        SiH3O4-        1.016e-003  9.559e-004   -2.993   -3.020   -0.027
        H4SiO4         3.909e-005  3.911e-005   -4.408   -4.408    0.000
        CaSiH3O4+      7.841e-006  7.374e-006   -5.106   -5.132   -0.027
        SiH2O4-2       4.910e-006  3.841e-006   -5.309   -5.416   -0.107

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.97   -4.41   -3.43  SiO2
        b-Cristobalite   -1.43   -4.41   -2.98  SiO2
        Ca(OH)2         -3.79   18.92   22.71  Ca(OH)2
        Chalcedony       -0.67   -4.41   -3.74  SiO2
        CSH(0.1)        -1.44   -2.52   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -1.19   -0.62    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.96    1.27    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.75    3.16    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.55    5.05    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.37    6.95    7.31  Ca0.600Si1.000O2.600:0.661H2O
```

```
        CSH(0.7)        -0.21    8.84    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.09   10.73   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.08   11.35   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.04   14.02   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.07   14.92   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.19   15.25   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.34   15.53   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.50   15.77   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.66   15.98   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.82   16.17   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.97   16.33   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.13   16.47   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2             -11.16  -11.16   -0.00  H2
        Lime           -13.64   18.92   32.56  CaO
        O2             -60.80   22.32   83.13  O2
        Quartz          -0.38   -4.41   -4.03  SiO2
        SiO2(am)        -1.77   -4.41   -2.64  Si1.000O2.000
        Wollastonite     0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

--------------------------------------
Reading input data for simulation 20.
--------------------------------------

        TITLE 20 Total liquid solid ratio 2000
        USE solution 1
        USE equilibrium_phases 20
        SAVE equilibrium_phases 21
        END
-----
TITLE
-----

 20 Total liquid solid ratio 2000

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.DW 100g
Using pure phase assemblage 20.   Pure-phase assemblage after simulation 19.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase              SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2         -3.79   18.92   22.71 0.000e+000          0.000e+000
        CSH(0.1)        -1.44   -2.52   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -1.19   -0.62    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -0.96    1.27    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -0.75    3.16    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.55    5.05    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.37    6.95    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.21    8.84    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.09   10.73   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.08   11.35   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.04   14.02   14.06 0.000e+000          0.000e+000
        CSH(1.0)         0.00   14.51   14.51 4.252e-003 4.145e-003-1.068e-004
        CSH(1.1)        -0.07   14.92   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.19   15.25   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.34   15.53   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.50   15.77   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.66   15.98   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.82   16.17   16.99 0.000e+000          0.000e+000
```

```
        CSH(1.7)        -0.97   16.33   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.13   16.47   17.60 0.000e+000          0.000e+000
        SiO2(am)        -1.77   -4.41   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        Ca             1.068e-003  1.068e-004
        Si             1.068e-003  1.068e-004

----------------------------Description of solution----------------------------

                                pH  =  11.003     Charge balance
                                pe  =  -5.422     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.168e-003
                      Mass of water (kg)  =  1.000e-001
                 Total alkalinity (eq/kg)  =  2.137e-003
                    Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  25.000
                  Electrical balance (eq)  = -1.714e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  15
                              Total H  = 1.110147e+001
                              Total O  = 5.551058e+000

----------------------------Distribution of species----------------------------

                                                Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            1.090e-003  1.024e-003   -2.963   -2.990   -0.027
        H+             1.051e-011  9.932e-012  -10.978  -11.003   -0.025
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
Ca           1.068e-003
        Ca+2           1.048e-003  8.236e-004   -2.980   -3.084   -0.104
        CaHO+          1.290e-005  1.213e-005   -4.889   -4.916   -0.027
        CaSiH3O4+       7.841e-006  7.374e-006   -5.106   -5.132   -0.027
H(0)         1.075e-014
        H2             5.377e-015  5.381e-015  -14.269  -14.269    0.000
O(0)         0.000e+000
        O2             0.000e+000  0.000e+000  -63.688  -63.687    0.000
Si           1.068e-003
        SiH3O4-         1.016e-003  9.559e-004   -2.993   -3.020   -0.027
        H4SiO4         3.909e-005  3.911e-005   -4.408   -4.408    0.000
        CaSiH3O4+       7.841e-006  7.374e-006   -5.106   -5.132   -0.027
        SiH2O4-2        4.910e-006  3.841e-006   -5.309   -5.416   -0.107

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.97   -4.41   -3.43  SiO2
        b-Cristobalite   -1.43   -4.41   -2.98  SiO2
        Ca(OH)2         -3.79   18.92   22.71  Ca(OH)2
        Chalcedony       -0.67   -4.41   -3.74  SiO2
        CSH(0.1)        -1.44   -2.52   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -1.19   -0.62    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.96    1.27    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.75    3.16    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.55    5.05    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.37    6.95    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.21    8.84    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.09   10.73   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.08   11.35   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.04   14.02   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.07   14.92   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.19   15.25   15.44  Ca1.000Si0.833O2.666:1.070H2O
```

```
        CSH(1.3)        -0.34   15.53   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.50   15.77   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.66   15.98   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.82   16.17   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.97   16.33   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.13   16.47   17.60  Ca1.000Si0.556O2.112:1.047H2O
        H2            -11.16  -11.16   -0.00  H2
        Lime          -13.64   18.92   32.56  CaO
        O2            -60.80   22.32   83.13  O2
        Quartz         -0.38   -4.41   -4.03  SiO2
        SiO2(am)       -1.77   -4.41   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 21.
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-----------
End of run.
-----------
```

付録- 6　回分方式で液相を交換したときの炭酸イオン共存下での C-S-H ゲルの溶解／沈殿反応を PHREEQC で計算した結果（アウトプット）

```
Input file: Atkinson Model Input water exchange (carbonate).pqi
Output file: Atkinson Model Input water exchange (carbonate).pqo
Database file: spron_phc_kai.txt

------------------
Reading data base.
------------------

         SOLUTION_MASTER_SPECIES
        SOLUTION_SPECIES
        PHASES
         END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

        DATABASE: spron_phc_kai.txt
        TITLE C-S-H dissolution in water exchange system (NaHCO3 2E-3M), data: Atkinson case
        PHASES
        CSH(0.1)
            Ca 0.100 Si 1.000 O 2.100 : 0.110 H2O = 0.100 Ca+2 + 1.000 H4SiO4 -1.790 H2O - 0.200 H+
            log_K -1.071
        CSH(0.2)
            Ca 0.200 Si 1.000 O 2.200 : 0.220 H2O = 0.200 Ca+2 + 1.000 H4SiO4 -1.580 H2O - 0.400 H+
            log_K 0.565
        CSH(0.3)
            Ca 0.300 Si 1.000 O 2.300 : 0.330 H2O = 0.300 Ca+2 + 1.000 H4SiO4 -1.370 H2O - 0.600 H+
            log_K 2.227
        CSH(0.4)
            Ca 0.400 Si 1.000 O 2.400 : 0.440 H2O = 0.400 Ca+2 + 1.000 H4SiO4 -1.160 H2O - 0.800 H+
            log_K 3.907
        CSH(0.5)
            Ca 0.500 Si 1.000 O 2.500 : 0.550 H2O = 0.500 Ca+2 + 1.000 H4SiO4 -0.950 H2O - 1.000 H+
            log_K 5.601
        CSH(0.6)
            Ca 0.600 Si 1.000 O 2.600 : 0.661 H2O = 0.600 Ca+2 + 1.000 H4SiO4 -0.739 H2O - 1.200 H+
            log_K 7.312
        CSH(0.7)
            Ca 0.700 Si 1.000 O 2.700 : 0.771 H2O = 0.700 Ca+2 + 1.000 H4SiO4 -0.529 H2O - 1.400 H+
            log_K 9.045
        CSH(0.8)
            Ca 0.800 Si 1.000 O 2.800 : 0.881 H2O = 0.800 Ca+2 + 1.000 H4SiO4 -0.319 H2O - 1.600 H+
            log_K 10.819
        CSH(0.9)
            Ca 1.000 Si 1.111 O 3.222 : 1.093 H2O = 1.000 Ca+2 + 1.111 H4SiO4 -0.129 H2O - 2.000 H+
            log_K 14.061
        CSH(1.0)
            Ca 1.000 Si 1.000 O 3.000 : 1.084 H2O = 1.000 Ca+2 + 1.000 H4SiO4 + 0.084 H2O - 2.000 H+
            log_K 14.514
        CSH(1.1)
            Ca 1.000 Si 0.909 O 2.818 : 1.076 H2O = 1.000 Ca+2 + 0.909 H4SiO4 + 0.258 H2O - 2.000 H+
            log_K 14.983
        CSH(1.2)
            Ca 1.000 Si 0.833 O 2.666 : 1.070 H2O = 1.000 Ca+2 + 0.833 H4SiO4 + 0.404 H2O - 2.000 H+
            log_K 15.439
        CSH(1.3)
            Ca 1.000 Si 0.769 O 2.538 : 1.065 H2O = 1.000 Ca+2 + 0.769 H4SiO4 + 0.527 H2O - 2.000 H+
            log_K 15.870
        CSH(1.4)
            Ca 1.000 Si 0.714 O 2.428 : 1.060 H2O = 1.000 Ca+2 + 0.714 H4SiO4 + 0.632 H2O - 2.000 H+
            log_K 16.272
        CSH(1.5)
            Ca 1.000 Si 0.667 O 2.334 : 1.056 H2O = 1.000 Ca+2 + 0.667 H4SiO4 + 0.722 H2O - 2.000 H+
            log_K 16.643
        CSH(1.6)
            Ca 1.000 Si 0.625 O 2.250 : 1.053 H2O = 1.000 Ca+2 + 0.625 H4SiO4 + 0.803 H2O - 2.000 H+
            log_K 16.987
        CSH(1.7)
            Ca 1.000 Si 0.588 O 2.176 : 1.049 H2O = 1.000 Ca+2 + 0.588 H4SiO4 + 0.873 H2O - 2.000 H+
            log_K 17.304
```

```
        CSH(1.8)
            Ca 1.000 Si 0.556 O 2.112 : 1.047 H2O = 1.000 Ca+2 + 0.556 H4SiO4 + 0.935 H2O - 2.000 H+
            log_K 17.597
        Ca(OH)2
            Ca(OH)2 = Ca+2 + 2H2O - 2 H+
            log_k 22.710
        SiO2(am)
            Si 1.000 O 2.000 = 1.000 H4SiO4 - 2.000 H2O
            log_K -2.639
        CSH(0.833)
            Ca 0.833 Si 1.000 O 2.833 : 0.917 H2O = 0.833 Ca+2 + 1.000 H4SiO4 -0.250 H2O - 1.666 H+
           log_K 11.436
        TITLE 1 Liquid solid ratio 100
        SOLUTION 1 NaHCO3 100g
           temp     25
           pH       7 charge
           pe       4
           redox    pe
           units    mol/l
           density  1
           Na       0.002
           C(4)     0.002
           water    0.1 # kg
        USE solution 1
        EQUILIBRIUM_PHASES 1 C-S-H(1.8) 1g
           Ca(OH)2   0 0
           Calcite   0 0
           CSH(0.1)  0 0
           CSH(0.2)  0 0
           CSH(0.3)  0 0
           CSH(0.4)  0 0
           CSH(0.5)  0 0
           CSH(0.6)  0 0
           CSH(0.7)  0 0
           CSH(0.8)  0 0
           CSH(0.833) 0 0
           CSH(0.9)  0 0
           CSH(1.0)  0 0
           CSH(1.1)  0 0
           CSH(1.2)  0 0
           CSH(1.3)  0 0
           CSH(1.4)  0 0
           CSH(1.5)  0 0
           CSH(1.6)  0 0
           CSH(1.7)  0 0
           CSH(1.8)  0 0.00932
           SiO2(am)  0 0
        SAVE equilibrium_phases 2
        END
-----
TITLE
-----

 1 Liquid solid ratio 100

------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 1.       NaHCO3 100g

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C(4)           2.000e-003  2.000e-004
        Na             2.000e-003  2.000e-004

----------------------------Description of solution----------------------------

                                pH  =   8.255     Charge balance
```

```
                                pe =  4.000
                    Activity of water =  1.000
                      Ionic strength =  2.020e-003
                   Mass of water (kg) =  1.000e-001
              Total alkalinity (eq/kg) = -2.000e-003
                   Total CO2 (mol/kg) =  2.000e-003
                  Temperature (deg C) =  25.000
               Electrical balance (eq) =  3.957e-018
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =  0.00
                         Iterations =  6
                           Total H  = 1.110144e+001
                           Total O  = 5.551220e+000

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
         Species          Molality    Activity Molality Activity    Gamma

         HO-            1.923e-006  1.829e-006   -5.716   -5.738   -0.022
         H+             5.825e-009  5.560e-009   -8.235   -8.255   -0.020
         H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
C(4)          2.000e-003
         CHO3-           1.960e-003  1.867e-003   -2.708   -2.729   -0.021
         CO2            2.115e-005  2.116e-005   -4.675   -4.675    0.000
         CO3-2           1.923e-005  1.582e-005   -4.716   -4.801   -0.085
H(0)          4.834e-028
         H2             2.417e-028  2.418e-028  -27.617  -27.617    0.000
Na           2.000e-003
         Na+            2.000e-003  1.904e-003   -2.699   -2.720   -0.021
         NaHO           5.620e-010  5.623e-010   -9.250   -9.250    0.000
O(0)          2.033e-037
         O2             1.016e-037  1.017e-037  -36.993  -36.993    0.000

------------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         Graphite       -38.14  -70.33  -32.19  C
         H2            -24.51  -24.51   -0.00  H2
         O2            -34.11   49.02   83.13  O2
         PCO2           -3.20  -21.31  -18.11  CO2

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 1.    C-S-H(1.8) 1g

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
         Phase            SI log IAP  log KT   Initial     Final     Delta

         Ca(OH)2         -0.60   22.11   22.71 0.000e+000          0.000e+000
         Calcite          0.00   -8.47   -8.47 0.000e+000 1.992e-004 1.992e-004
         CSH(0.1)        -4.91   -5.98   -1.07 0.000e+000          0.000e+000
         CSH(0.2)        -4.33   -3.77    0.56 0.000e+000          0.000e+000
         CSH(0.3)        -3.79   -1.56    2.23 0.000e+000          0.000e+000
         CSH(0.4)        -3.26    0.65    3.91 0.000e+000          0.000e+000
         CSH(0.5)        -2.74    2.86    5.60 0.000e+000          0.000e+000
         CSH(0.6)        -2.24    5.07    7.31 0.000e+000          0.000e+000
         CSH(0.7)        -1.76    7.28    9.04 0.000e+000          0.000e+000
         CSH(0.8)        -1.32    9.49   10.82 0.000e+000          0.000e+000
         CSH(0.833)      -1.21   10.22   11.44 0.000e+000          0.000e+000
         CSH(0.9)        -1.05   13.01   14.06 0.000e+000          0.000e+000
         CSH(1.0)        -0.60   13.92   14.51 0.000e+000          0.000e+000
         CSH(1.1)        -0.32   14.66   14.98 0.000e+000          0.000e+000
         CSH(1.2)        -0.16   15.28   15.44 0.000e+000          0.000e+000
```

```
        CSH(1.3)        -0.06   15.81   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.01   16.26   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.00   16.64   16.64 0.000e+000 2.090e-003 2.090e-003
        CSH(1.6)        -0.00   16.99   16.99 0.000e+000 6.060e-003 6.060e-003
        CSH(1.7)        -0.01   17.29   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.04   17.55   17.60 9.320e-003         -9.320e-003
        SiO2(am)        -5.55   -8.19   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              8.289e-006  8.290e-007
        Ca             9.707e-003  9.708e-004
        Na             2.000e-003  2.000e-004
        Si             3.842e-006  3.842e-007

----------------------------Description of solution---------------------------

                                pH  =  12.224     Charge balance
                                pe  =  -6.816     Adjusted to redox equilibrium
                    Activity of water  =   0.999
                       Ionic strength  =  2.848e-002
                   Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  2.140e-002
                    Total CO2 (mol/kg)  =  8.289e-006
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.023e-015
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                          Iterations  =  32
                             Total H  = 1.110378e+001
                             Total O  = 5.552963e+000

----------------------------Distribution of species---------------------------

                                                 Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            2.008e-002  1.701e-002   -1.697   -1.769   -0.072
        H+             6.819e-013  5.976e-013  -12.166  -12.224   -0.057
        H2O            5.551e+001  9.995e-001    1.744   -0.000    0.000
C(-4)         2.203e-036
        CH4            2.203e-036  2.217e-036  -35.657  -35.654    0.003
C(4)          8.289e-006
        CaCO3           6.914e-006  6.959e-006   -5.160   -5.157    0.003
        CO3-2          1.364e-006  7.417e-007   -5.865   -6.130   -0.265
        CHO3-          1.095e-008  9.404e-009   -7.961   -8.027   -0.066
        CaCHO3+         5.764e-010  4.949e-010   -9.239   -9.305   -0.066
        CO2            1.139e-014  1.146e-014  -13.944  -13.941    0.003
Ca            9.707e-003
        Ca+2           8.390e-003  4.563e-003   -2.076   -2.341   -0.265
        CaHO+          1.310e-003  1.117e-003   -2.883   -2.952   -0.069
        CaCO3          6.914e-006  6.959e-006   -5.160   -5.157    0.003
        CaSiH3O4+       1.312e-007  1.118e-007   -6.882   -6.951   -0.069
        CaCHO3+         5.764e-010  4.949e-010   -9.239   -9.305   -0.066
H(0)          2.383e-014
        H2             1.192e-014  1.199e-014  -13.924  -13.921    0.003
Na            2.000e-003
        Na+            1.995e-003  1.705e-003   -2.700   -2.768   -0.068
        NaHO           4.653e-006  4.684e-006   -5.332   -5.329    0.003
        NaSiH3O4        3.044e-007  3.064e-007   -6.517   -6.514    0.003
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -64.387  -64.384    0.003
Si            3.842e-006
        SiH3O4-         3.069e-006  2.617e-006   -5.513   -5.582   -0.069
        SiH2O4-2        3.306e-007  1.748e-007   -6.481   -6.758   -0.277
        NaSiH3O4        3.044e-007  3.064e-007   -6.517   -6.514    0.003
        CaSiH3O4+       1.312e-007  1.118e-007   -6.882   -6.951   -0.069
        H4SiO4          6.401e-009  6.443e-009   -8.194   -8.191    0.003

----------------------------Saturation indices--------------------------------
```

```
        Phase            SI log IAP  log KT

        a-Cristobalite   -4.76   -8.19   -3.43  SiO2
        Aragonite        -0.16   -8.47   -8.31  CaCO3
        b-Cristobalite   -5.21   -8.19   -2.98  SiO2
        Ca(OH)2          -0.60   22.11   22.71  Ca(OH)2
        Calcite           0.00   -8.47   -8.47  CaCO3
        CH4             -32.81  -73.83  -41.02  CH4
        Chalcedony       -4.45   -8.19   -3.74  SiO2
        CSH(0.1)         -4.91   -5.98   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -4.33   -3.77    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -3.79   -1.56    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -3.26    0.65    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -2.74    2.86    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -2.24    5.07    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.76    7.28    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.32    9.49   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.21   10.22   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -1.05   13.01   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.60   13.92   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.32   14.66   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.16   15.28   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.06   15.81   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.01   16.26   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.00   16.64   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.00   16.99   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.01   17.29   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.04   17.55   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite        -20.01  -52.21  -32.19  C
        H2              -10.81  -10.81   -0.00  H2
        Lime            -10.46   22.11   32.56  CaO
        O2              -61.50   21.63   83.13  O2
        PCO2            -12.47  -30.58  -18.11  CO2
        Quartz           -4.16   -8.19   -4.03  SiO2
        SiO2(am)         -5.55   -8.19   -2.64  Si1.000O2.000
        Wollastonite      0.13   13.92   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

        TITLE 2 Liquid solid ration 200
        USE solution 1
        USE equilibrium_phases 2
        SAVE equilibrium_phases 3
        END
-----
TITLE
-----

 2 Liquid solid ration 200

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 2.    Pure-phase assemblage after simulation 1.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta
```

```
        Ca(OH)2        -0.94   21.77   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 1.992e-004 3.984e-004 1.992e-004
        CSH(0.1)       -4.45   -5.52   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -3.91   -3.35    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -3.40   -1.17    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -2.90    1.01    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -2.42    3.19    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.95    5.36    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -1.51    7.54    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -1.10    9.72   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -1.00   10.43   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.85   13.22   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.44   14.07   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.21   14.77   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.08   15.36   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.02   15.85   15.87 0.000e+000          0.000e+000
        CSH(1.4)        0.00   16.27   16.27 0.000e+000 7.256e-003 7.256e-003
        CSH(1.5)       -0.01   16.63   16.64 2.090e-003         -2.090e-003
        CSH(1.6)       -0.03   16.96   16.99 6.060e-003         -6.060e-003
        CSH(1.7)       -0.06   17.24   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.11   17.49   17.60 0.000e+000          0.000e+000
        SiO2(am)       -5.06   -7.70   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              8.572e-006  8.572e-007
        Ca             6.950e-003  6.950e-004
        Na             2.000e-003  2.000e-004
        Si             8.711e-006  8.711e-007

----------------------------Description of solution---------------------------

                                pH  =  12.108     Charge balance
                                pe  =  -6.618     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  2.128e-002
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  1.588e-002
                    Total CO2 (mol/kg)  =  8.572e-006
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -7.967e-016
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  26
                             Total H  = 1.110323e+001
                             Total O  = 5.552415e+000

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            1.510e-002  1.304e-002   -1.821   -1.885   -0.064
        H+             8.788e-013  7.798e-013  -12.056  -12.108   -0.052
        H2O            5.551e+001  9.996e-001    1.744   -0.000    0.000
C(-4)         1.032e-036
        CH4            1.032e-036  1.037e-036  -35.987  -35.984    0.002
C(4)          8.572e-006
        CaCO3           6.925e-006  6.959e-006   -5.160   -5.157    0.002
        CO3-2          1.628e-006  9.452e-007   -5.788   -6.024   -0.236
        CHO3-          1.792e-008  1.564e-008   -7.747   -7.806   -0.059
        CaCHO3+         7.399e-010  6.459e-010   -9.131   -9.190   -0.059
        CO2            2.475e-014  2.487e-014  -13.606  -13.604    0.002
Ca            6.950e-003
        Ca+2           6.169e-003  3.581e-003   -2.210   -2.446   -0.236
        CaHO+          7.740e-004  6.717e-004   -3.111   -3.173   -0.062
        CaCO3          6.925e-006  6.959e-006   -5.160   -5.157    0.002
        CaSiH3O4+       2.399e-007  2.082e-007   -6.620   -6.682   -0.062
        CaCHO3+         7.399e-010  6.459e-010   -9.131   -9.190   -0.059
H(0)          1.627e-014
```

```
        H2            8.133e-015  8.173e-015   -14.090   -14.088    0.002
Na           2.000e-003
        Na+           1.996e-003  1.735e-003    -2.700    -2.761   -0.061
        NaHO          3.635e-006  3.653e-006    -5.439    -5.437    0.002
        NaSiH3O4       7.360e-007  7.396e-007    -6.133    -6.131    0.002
O(0)         0.000e+000
        O2            0.000e+000  0.000e+000   -64.053   -64.051    0.002
Si           8.711e-006
        SiH3O4-        7.155e-006  6.209e-006    -5.145    -5.207   -0.062
        NaSiH3O4       7.360e-007  7.396e-007    -6.133    -6.131    0.002
        SiH2O4-2       5.603e-007  3.178e-007    -6.252    -6.498   -0.246
        CaSiH3O4+      2.399e-007  2.082e-007    -6.620    -6.682   -0.062
        H4SiO4         1.985e-008  1.995e-008    -7.702    -7.700    0.002

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -4.27   -7.70   -3.43  SiO2
        Aragonite        -0.16   -8.47   -8.31  CaCO3
        b-Cristobalite   -4.72   -7.70   -2.98  SiO2
        Ca(OH)2          -0.94   21.77   22.71  Ca(OH)2
        Calcite           0.00   -8.47   -8.47  CaCO3
        CH4             -33.14  -74.16  -41.02  CH4
        Chalcedony       -3.96   -7.70   -3.74  SiO2
        CSH(0.1)         -4.45   -5.52   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -3.91   -3.35    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -3.40   -1.17    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -2.90    1.01    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -2.42    3.19    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -1.95    5.36    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.51    7.54    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -1.10    9.72   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -1.00   10.43   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.85   13.22   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.44   14.07   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.21   14.77   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.08   15.36   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.02   15.85   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)          0.00   16.27   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.01   16.63   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.03   16.96   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.06   17.24   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.11   17.49   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite        -20.01  -52.20  -32.19  C
        H2              -10.98  -10.98   -0.00  H2
        Lime            -10.79   21.77   32.56  CaO
        O2              -61.16   21.96   83.13  O2
        PCO2            -12.13  -30.24  -18.11  CO2
        Quartz           -3.67   -7.70   -4.03  SiO2
        SiO2(am)         -5.06   -7.70   -2.64  Si1.000O2.000
        Wollastonite      0.29   14.07   13.78  CaSiO3

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End of simulation.
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------------------------------------
Reading input data for simulation 3.
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        TITLE 3 Liquid solid ration 300
        USE solution 1
        USE equilibrium_phases 3
        SAVE equilibrium_phases 4
        END
-----
TITLE
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 3 Liquid solid ration 300
```

```
----------------------------------------
Beginning of batch-reaction calculations.
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Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 3.    Pure-phase assemblage after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -1.66   21.05   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 3.984e-004 5.975e-004 1.991e-004
        CSH(0.1)       -3.56   -4.63   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -3.09   -2.52    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -2.65   -0.42    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -2.22    1.69    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -1.81    3.79    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.42    5.89    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -1.05    8.00    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.71   10.10   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.64   10.80   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.49   13.57   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.20   14.31   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.06   14.93   14.98 0.000e+000          0.000e+000
        CSH(1.2)        0.00   15.44   15.44 0.000e+000 1.404e-004 1.404e-004
        CSH(1.3)        0.00   15.87   15.87 0.000e+000 6.579e-003 6.579e-003
        CSH(1.4)       -0.03   16.24   16.27 7.256e-003         -7.256e-003
        CSH(1.5)       -0.09   16.56   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.15   16.84   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.22   17.09   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.29   17.30   17.60 0.000e+000          0.000e+000
        SiO2(am)       -4.10   -6.73   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              9.532e-006  9.533e-007
        Ca             3.372e-003  3.372e-004
        Na             2.000e-003  2.000e-004
        Si             4.346e-005  4.346e-006

----------------------------Description of solution----------------------------

                                pH  =  11.870     Charge balance
                                pe  =  -6.469     Adjusted to redox equilibrium
                     Activity of water  =  1.000
                        Ionic strength  =  1.160e-002
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  8.725e-003
                    Total CO2 (mol/kg)  =  9.532e-006
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.378e-013
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  25
                              Total H  = 1.110251e+001
                              Total O  = 5.551702e+000

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            8.432e-003  7.535e-003   -2.074    -2.123    -0.049
        H+             1.485e-012  1.350e-012  -11.828   -11.870    -0.042
        H2O            5.551e+001  9.998e-001    1.744    -0.000     0.000
```

```
C(-4)          2.858e-035
        CH4            2.858e-035  2.866e-035   -34.544   -34.543    0.001
C(4)           9.532e-006
        CaCO3           6.941e-006  6.959e-006    -5.159    -5.157    0.001
        CO3-2           2.537e-006  1.660e-006    -5.596    -5.780   -0.184
        CHO3-           5.286e-008  4.755e-008    -7.277    -7.323   -0.046
        CaCHO3+         1.243e-009  1.118e-009    -8.906    -8.952   -0.046
        CO2            1.305e-013  1.308e-013   -12.884   -12.883    0.001
Ca             3.372e-003
        Ca+2            3.118e-003  2.038e-003    -2.506    -2.691   -0.185
        CaHO+           2.467e-004  2.210e-004    -3.608    -3.656   -0.048
        CaCO3           6.941e-006  6.959e-006    -5.159    -5.157    0.001
        CaSiH3O4+       7.062e-007  6.327e-007    -6.151    -6.199   -0.048
        CaCHO3+         1.243e-009  1.118e-009    -8.906    -8.952   -0.046
H(0)           2.468e-014
        H2             1.234e-014  1.238e-014   -13.909   -13.907    0.001
Na             2.000e-003
        Na+            1.994e-003  1.789e-003    -2.700    -2.747   -0.047
        NaSiH3O4        4.059e-006  4.070e-006    -5.392    -5.390    0.001
        NaHO           2.170e-006  2.176e-006    -5.663    -5.662    0.001
O(0)           0.000e+000
        O2             0.000e+000  0.000e+000   -64.412   -64.411    0.001
Si             4.346e-005
        SiH3O4-         3.699e-005  3.314e-005    -4.432    -4.480   -0.048
        NaSiH3O4        4.059e-006  4.070e-006    -5.392    -5.390    0.001
        SiH2O4-2        1.521e-006  9.800e-007    -5.818    -6.009   -0.191
        CaSiH3O4+       7.062e-007  6.327e-007    -6.151    -6.199   -0.048
        H4SiO4          1.838e-007  1.843e-007    -6.736    -6.735    0.001

-----------------------------Saturation indices-------------------------------

        Phase              SI log IAP  log KT

        a-Cristobalite   -3.30   -6.73   -3.43  SiO2
        Aragonite        -0.16   -8.47   -8.31  CaCO3
        b-Cristobalite   -3.75   -6.73   -2.98  SiO2
        Ca(OH)2          -1.66   21.05   22.71  Ca(OH)2
        Calcite           0.00   -8.47   -8.47  CaCO3
        CH4            -31.70  -72.72  -41.02  CH4
        Chalcedony       -3.00   -6.73   -3.74  SiO2
        CSH(0.1)         -3.56   -4.63   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -3.09   -2.52    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -2.65   -0.42    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -2.22    1.69    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -1.81    3.79    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -1.42    5.89    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -1.05    8.00    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.71   10.10   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.64   10.80   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.49   13.57   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         -0.20   14.31   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         -0.06   14.93   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)          0.00   15.44   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)          0.00   15.87   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.03   16.24   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.09   16.56   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.15   16.84   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.22   17.09   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.29   17.30   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite        -18.93  -51.12  -32.19  C
        H2             -10.80  -10.80   -0.00  H2
        Lime           -11.51   21.05   32.56  CaO
        O2             -61.52   21.60   83.13  O2
        PCO2           -11.41  -29.52  -18.11  CO2
        Quartz          -2.71   -6.73   -4.03  SiO2
        SiO2(am)        -4.10   -6.73   -2.64  Si1.000O2.000
        Wollastonite     0.53   14.31   13.78  CaSiO3

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End of simulation.
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```
-----------------------------------
Reading input data for simulation 4.
-----------------------------------

        TITLE 4 Liquid solid ration 400
        USE solution 1
        USE equilibrium_phases 4
        SAVE equilibrium_phases 5
        END
-----
TITLE
-----

 4 Liquid solid ration 400

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 4.    Pure-phase assemblage after simulation 3.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -1.74   20.97   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 5.975e-004 7.965e-004 1.991e-004
        CSH(0.1)       -3.48   -4.55   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -3.01   -2.45    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -2.58   -0.35    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -2.16    1.74    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -1.76    3.84    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.37    5.94    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -1.01    8.04    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.68   10.13   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.61   10.83   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.47   13.59   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.18   14.33   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.05   14.93   14.98 0.000e+000          0.000e+000
        CSH(1.2)        0.00   15.44   15.44 1.404e-004 6.208e-003 6.068e-003
        CSH(1.3)       -0.01   15.86   15.87 6.579e-003         -6.579e-003
        CSH(1.4)       -0.04   16.23   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.10   16.54   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.17   16.82   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.24   17.07   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.32   17.28   17.60 0.000e+000          0.000e+000
        SiO2(am)       -4.01   -6.64   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              9.674e-006  9.674e-007
        Ca             3.124e-003  3.125e-004
        Na             2.000e-003  2.000e-004
        Si             5.032e-005  5.032e-006

----------------------------Description of solution----------------------------

                                pH  =  11.846     Charge balance
                                pe  =  -6.444     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.091e-002
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  8.230e-003
                    Total CO2 (mol/kg)  =  9.674e-006
```

```
                Temperature (deg C)  =  25.000
             Electrical balance (eq)  =  2.457e-015
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                       Iterations  =  18
                         Total H  = 1.110247e+001
                         Total O  = 5.551659e+000

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
         Species          Molality   Activity Molality Activity    Gamma

         HO-            7.957e-003  7.133e-003   -2.099   -2.147   -0.047
         H+             1.566e-012  1.426e-012  -11.805  -11.846   -0.041
         H2O            5.551e+001  9.998e-001    1.744   -0.000    0.000
C(-4)         3.319e-035
         CH4            3.319e-035  3.328e-035  -34.479  -34.478    0.001
C(4)          9.674e-006
         CaCO3          6.942e-006  6.959e-006   -5.159   -5.157    0.001
         CO3-2          2.672e-006  1.767e-006   -5.573   -5.753   -0.180
         CHO3-          5.928e-008  5.346e-008   -7.227   -7.272   -0.045
         CaCHO3+        1.309e-009  1.181e-009   -8.883   -8.928   -0.045
         CO2            1.550e-013  1.554e-013  -12.810  -12.809    0.001
Ca            3.124e-003
         Ca+2           2.898e-003  1.915e-003   -2.538   -2.718   -0.180
         CaHO+          2.188e-004  1.966e-004   -3.660   -3.707   -0.047
         CaCO3          6.942e-006  6.959e-006   -5.159   -5.157    0.001
         CaSiH3O4+      7.701e-007  6.919e-007   -6.113   -6.160   -0.047
         CaCHO3+        1.309e-009  1.181e-009   -8.883   -8.928   -0.045
H(0)          2.455e-014
         H2             1.227e-014  1.231e-014  -13.911  -13.910    0.001
Na            2.000e-003
         Na+            1.993e-003  1.793e-003   -2.700   -2.746   -0.046
         NaSiH3O4       4.736e-006  4.748e-006   -5.325   -5.323    0.001
         NaHO           2.060e-006  2.065e-006   -5.686   -5.685    0.001
O(0)          0.000e+000
         O2             0.000e+000  0.000e+000  -64.407  -64.406    0.001
Si            5.032e-005
         SiH3O4-        4.293e-005  3.857e-005   -4.367   -4.414   -0.047
         NaSiH3O4       4.736e-006  4.748e-006   -5.325   -5.323    0.001
         SiH2O4-2       1.657e-006  1.080e-006   -5.781   -5.967   -0.186
         CaSiH3O4+      7.701e-007  6.919e-007   -6.113   -6.160   -0.047
         H4SiO4         2.260e-007  2.265e-007   -6.646   -6.645    0.001

-----------------------------Saturation indices------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -3.21   -6.64   -3.43  SiO2
         Aragonite        -0.16   -8.47   -8.31  CaCO3
         b-Cristobalite   -3.66   -6.64   -2.98  SiO2
         Ca(OH)2          -1.74   20.97   22.71  Ca(OH)2
         Calcite           0.00   -8.47   -8.47  CaCO3
         CH4             -31.63  -72.66  -41.02  CH4
         Chalcedony       -2.91   -6.64   -3.74  SiO2
         CSH(0.1)         -3.48   -4.55   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -3.01   -2.45    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -2.58   -0.35    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -2.16    1.74    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -1.76    3.84    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -1.37    5.94    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -1.01    8.04    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -0.68   10.13   10.82  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -0.61   10.83   11.44  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)         -0.47   13.59   14.06  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)         -0.18   14.33   14.51  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)         -0.05   14.93   14.98  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)          0.00   15.44   15.44  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.01   15.86   15.87  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)         -0.04   16.23   16.27  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.10   16.54   16.64  Ca1.000Si0.667O2.334:1.056H2O
```

```
        CSH(1.6)       -0.17   16.82   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)       -0.24   17.07   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)       -0.32   17.28   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite      -18.86  -51.05  -32.19  C
        H2            -10.80  -10.80   -0.00  H2
        Lime          -11.59   20.97   32.56  CaO
        O2            -61.52   21.61   83.13  O2
        PCO2          -11.34  -29.44  -18.11  CO2
        Quartz         -2.62   -6.64   -4.03  SiO2
        SiO2(am)       -4.01   -6.64   -2.64  Si1.000O2.000
        Wollastonite    0.55   14.33   13.78  CaSiO3

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End of simulation.
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-----------------------------------
Reading input data for simulation 5.
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        TITLE 5 Liquid solid ration 500
        USE solution 1
        USE equilibrium_phases 5
        SAVE equilibrium_phases 6
        END
-----
TITLE
-----

 5 Liquid solid ration 500

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 5.    Pure-phase assemblage after simulation 4.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -2.27   20.44   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 7.965e-004 9.955e-004 1.989e-004
        CSH(0.1)       -2.89   -3.96   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -2.48   -1.91    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -2.10    0.13    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -1.73    2.17    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -1.38    4.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -1.05    6.26    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.74    8.31    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.47   10.35   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.41   11.02   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.29   13.77   14.06 0.000e+000          0.000e+000
        CSH(1.0)       -0.08   14.44   14.51 0.000e+000          0.000e+000
        CSH(1.1)        0.00   14.98   14.98 0.000e+000 3.952e-003 3.952e-003
        CSH(1.2)        0.00   15.44   15.44 6.208e-003 1.878e-003-4.330e-003
        CSH(1.3)       -0.05   15.82   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.12   16.15   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.21   16.44   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.30   16.69   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -0.39   16.91   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -0.50   17.10   17.60 0.000e+000          0.000e+000
        SiO2(am)       -3.36   -6.00   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles
```

```
        C             1.108e-005  1.108e-006
        Ca            1.792e-003  1.792e-004
        Na            2.000e-003  2.000e-004
        Si            1.468e-004  1.468e-005

----------------------------Description of solution----------------------------

                                pH  =  11.679     Charge balance
                                pe  =  -6.278     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  7.162e-003
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  5.563e-003
                    Total CO2 (mol/kg)  =  1.108e-005
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  =  3.026e-017
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                          Iterations  =  21
                             Total H  = 1.110220e+001
                             Total O  = 5.551412e+000

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            5.321e-003  4.861e-003   -2.274   -2.313   -0.039
        H+             2.265e-012  2.092e-012  -11.645  -11.679   -0.034
        H2O            5.551e+001  9.998e-001    1.744   -0.000    0.000
C(-4)         1.151e-034
        CH4            1.151e-034  1.153e-034  -33.939  -33.938    0.001
C(4)          1.108e-005
        CaCO3           6.948e-006  6.959e-006   -5.158   -5.157    0.001
        CO3-2           3.991e-006  2.826e-006   -5.399   -5.549   -0.150
        CHO3-           1.368e-007  1.255e-007   -6.864   -6.902   -0.037
        CaCHO3+         1.889e-009  1.733e-009   -8.724   -8.761   -0.037
        CO2            5.343e-013  5.352e-013  -12.272  -12.271    0.001
Ca            1.792e-003
        Ca+2           1.692e-003  1.198e-003   -2.771   -2.922   -0.150
        CaHO+           9.155e-005  8.376e-005   -4.038   -4.077   -0.039
        CaCO3           6.948e-006  6.959e-006   -5.158   -5.157    0.001
        CaSiH3O4+       1.422e-006  1.301e-006   -5.847   -5.886   -0.039
        CaCHO3+         1.889e-009  1.733e-009   -8.724   -8.761   -0.037
H(0)          2.461e-014
        H2             1.230e-014  1.232e-014  -13.910  -13.909    0.001
Na            2.000e-003
        Na+            1.984e-003  1.817e-003   -2.702   -2.741   -0.038
        NaSiH3O4        1.444e-005  1.447e-005   -4.840   -4.840    0.001
        NaHO           1.424e-006  1.426e-006   -5.847   -5.846    0.001
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -64.408  -64.407    0.001
Si            1.468e-004
        SiH3O4-         1.268e-004  1.160e-004   -3.897   -3.936   -0.039
        NaSiH3O4        1.444e-005  1.447e-005   -4.840   -4.840    0.001
        SiH2O4-2        3.158e-006  2.212e-006   -5.501   -5.655   -0.155
        CaSiH3O4+       1.422e-006  1.301e-006   -5.847   -5.886   -0.039
        H4SiO4          9.981e-007  9.997e-007   -6.001   -6.000    0.001

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -2.57   -6.00   -3.43  SiO2
        Aragonite        -0.16   -8.47   -8.31  CaCO3
        b-Cristobalite   -3.02   -6.00   -2.98  SiO2
        Ca(OH)2          -2.27   20.44   22.71  Ca(OH)2
        Calcite           0.00   -8.47   -8.47  CaCO3
        CH4             -31.09  -72.12  -41.02  CH4
        Chalcedony       -2.26   -6.00   -3.74  SiO2
        CSH(0.1)         -2.89   -3.96   -1.07  Ca0.100Si1.000O2.100:0.110H2O
```

```
        CSH(0.2)        -2.48   -1.91    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -2.10    0.13    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -1.73    2.17    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -1.38    4.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -1.05    6.26    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.74    8.31    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.47   10.35   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.41   11.02   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.29   13.77   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.08   14.44   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)         0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         0.00   15.44   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.05   15.82   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.12   16.15   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.21   16.44   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.30   16.69   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.39   16.91   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.50   17.10   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -18.32  -50.51  -32.19  C
        H2             -10.80  -10.80   -0.00  H2
        Lime           -12.12   20.44   32.56  CaO
        O2             -61.52   21.61   83.13  O2
        PCO2           -10.80  -28.91  -18.11  CO2
        Quartz          -1.97   -6.00   -4.03  SiO2
        SiO2(am)        -3.36   -6.00   -2.64  Si1.000O2.000
        Wollastonite     0.65   14.44   13.78  CaSiO3

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End of simulation.
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Reading input data for simulation 6.
-----------------------------------

        TITLE 6 Liquid solid ration 600
        USE solution 1
        USE equilibrium_phases 6
        SAVE equilibrium_phases 7
        END
-----
TITLE
-----

 6 Liquid solid ration 600

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 6.    Pure-phase assemblage after simulation 5.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -3.04   19.67   22.71 0.000e+000          0.000e+000
        Calcite          0.00   -8.47   -8.47 9.955e-004 1.194e-003 1.986e-004
        CSH(0.1)        -2.12   -3.19   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -1.79   -1.22    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -1.48    0.75    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -1.19    2.71    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.92    4.68    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.67    6.65    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.43    8.61    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.24   10.58   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.21   11.23   11.44 0.000e+000          0.000e+000
```

CSH(0.9)	-0.12	13.94	14.06	0.000e+000	0.000e+000	
CSH(1.0)	-0.00	14.51	14.51	0.000e+000	6.091e-004	6.091e-004
CSH(1.1)	-0.00	14.98	14.98	3.952e-003	4.939e-003	9.869e-004
CSH(1.2)	-0.06	15.37	15.44	1.878e-003	-1.878e-003	
CSH(1.3)	-0.17	15.70	15.87	0.000e+000	0.000e+000	
CSH(1.4)	-0.28	15.99	16.27	0.000e+000	0.000e+000	
CSH(1.5)	-0.41	16.23	16.64	0.000e+000	0.000e+000	
CSH(1.6)	-0.54	16.45	16.99	0.000e+000	0.000e+000	
CSH(1.7)	-0.67	16.64	17.30	0.000e+000	0.000e+000	
CSH(1.8)	-0.79	16.80	17.60	0.000e+000	0.000e+000	
SiO2(am)	-2.51	-5.15	-2.64	0.000e+000	0.000e+000	

----------Solution composition----------

Elements	Molality	Moles
C	1.480e-005	1.480e-006
Ca	8.354e-004	8.355e-005
Na	2.000e-003	2.000e-004
Si	5.827e-004	5.827e-005

----------Description of solution----------

pH = 11.443 Charge balance
pe = -6.087 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 4.382e-003
Mass of water (kg) = 1.000e-001
Total alkalinity (eq/kg) = 3.642e-003
Total CO2 (mol/kg) = 1.480e-005
Temperature (deg C) = 25.000
Electrical balance (eq) = 4.113e-015
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 17
Total H = 1.110201e+001
Total O = 5.551310e+000

----------Distribution of species----------

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	HO-	3.032e-003	2.821e-003	-2.518	-2.550	-0.031
	H+	3.847e-012	3.605e-012	-11.415	-11.443	-0.028
	H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
C(-4)	1.553e-033					
	CH4	1.553e-033	1.555e-033	-32.809	-32.808	0.000
C(4)	1.480e-005					
	CO3-2	7.386e-006	5.594e-006	-5.132	-5.252	-0.121
	CaCO3	6.952e-006	6.959e-006	-5.158	-5.157	0.000
	CHO3-	4.587e-007	4.279e-007	-6.338	-6.369	-0.030
	CaCHO3+	3.201e-009	2.986e-009	-8.495	-8.525	-0.030
	CO2	3.142e-012	3.145e-012	-11.503	-11.502	0.000
Ca	8.354e-004					
	Ca+2	7.992e-004	6.050e-004	-3.097	-3.218	-0.121
	CaHO+	2.637e-005	2.456e-005	-4.579	-4.610	-0.031
	CaCO3	6.952e-006	6.959e-006	-5.158	-5.157	0.000
	CaSiH3O4+	2.874e-006	2.677e-006	-5.541	-5.572	-0.031
	CaCHO3+	3.201e-009	2.986e-009	-8.495	-8.525	-0.030
H(0)	3.031e-014					
	H2	1.515e-014	1.517e-014	-13.819	-13.819	0.000
Na	2.000e-003					
	Na+	1.941e-003	1.808e-003	-2.712	-2.743	-0.031
	NaSiH3O4	5.858e-005	5.864e-005	-4.232	-4.232	0.000
	NaHO	8.229e-007	8.237e-007	-6.085	-6.084	0.000
O(0)	0.000e+000					
	O2	0.000e+000	0.000e+000	-64.588	-64.588	0.000
Si	5.827e-004					
	SiH3O4-	5.073e-004	4.724e-004	-3.295	-3.326	-0.031
	NaSiH3O4	5.858e-005	5.864e-005	-4.232	-4.232	0.000
	H4SiO4	7.009e-006	7.016e-006	-5.154	-5.154	0.000

```
        SiH2O4-2       6.954e-006  5.229e-006   -5.158   -5.282   -0.124
        CaSiH3O4+      2.874e-006  2.677e-006   -5.541   -5.572   -0.031

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -1.72  -5.15  -3.43  SiO2
        Aragonite       -0.16  -8.47  -8.31  CaCO3
        b-Cristobalite  -2.17  -5.15  -2.98  SiO2
        Ca(OH)2         -3.04  19.67  22.71  Ca(OH)2
        Calcite          0.00  -8.47  -8.47  CaCO3
        CH4            -29.96 -70.99 -41.02  CH4
        Chalcedony      -1.42  -5.15  -3.74  SiO2
        CSH(0.1)        -2.12  -3.19  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -1.79  -1.22   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -1.48   0.75   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -1.19   2.71   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.92   4.68   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.67   6.65   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.43   8.61   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.24  10.58  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.21  11.23  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.12  13.94  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.00  14.51  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.00  14.98  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.06  15.37  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.17  15.70  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.28  15.99  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.41  16.23  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.54  16.45  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -0.67  16.64  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -0.79  16.80  17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -17.37 -49.56 -32.19  C
        H2             -10.71 -10.71  -0.00  H2
        Lime           -12.89  19.67  32.56  CaO
        O2             -61.70  21.42  83.13  O2
        PCO2           -10.03 -28.14 -18.11  CO2
        Quartz          -1.13  -5.15  -4.03  SiO2
        SiO2(am)        -2.51  -5.15  -2.64  Si1.000O2.000
        Wollastonite     0.73  14.51  13.78  CaSiO3

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End of simulation.
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Reading input data for simulation 7.
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        TITLE 7 Liquid solid ration 700
        USE solution 1
        USE equilibrium_phases 7
        SAVE equilibrium_phases 8
        END
-----
TITLE
-----

 7 Liquid solid ration 700

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 7.    Pure-phase assemblage after simulation 6.

-------------------------------Phase assemblage--------------------------------
```

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca(OH)2	-3.04	19.67	22.71	0.000e+000	0.000e+000	
Calcite	0.00	-8.47	-8.47	1.194e-003	1.393e-003	1.986e-004
CSH(0.1)	-2.12	-3.19	-1.07	0.000e+000	0.000e+000	
CSH(0.2)	-1.79	-1.22	0.56	0.000e+000	0.000e+000	
CSH(0.3)	-1.48	0.75	2.23	0.000e+000	0.000e+000	
CSH(0.4)	-1.19	2.71	3.91	0.000e+000	0.000e+000	
CSH(0.5)	-0.92	4.68	5.60	0.000e+000	0.000e+000	
CSH(0.6)	-0.67	6.65	7.31	0.000e+000	0.000e+000	
CSH(0.7)	-0.43	8.61	9.04	0.000e+000	0.000e+000	
CSH(0.8)	-0.24	10.58	10.82	0.000e+000	0.000e+000	
CSH(0.833)	-0.21	11.23	11.44	0.000e+000	0.000e+000	
CSH(0.9)	-0.12	13.94	14.06	0.000e+000	0.000e+000	
CSH(1.0)	0.00	14.51	14.51	6.091e-004	2.787e-003	2.178e-003
CSH(1.1)	0.00	14.98	14.98	4.939e-003	2.479e-003	-2.460e-003
CSH(1.2)	-0.06	15.37	15.44	0.000e+000	0.000e+000	
CSH(1.3)	-0.17	15.70	15.87	0.000e+000	0.000e+000	
CSH(1.4)	-0.28	15.99	16.27	0.000e+000	0.000e+000	
CSH(1.5)	-0.41	16.23	16.64	0.000e+000	0.000e+000	
CSH(1.6)	-0.54	16.45	16.99	0.000e+000	0.000e+000	
CSH(1.7)	-0.67	16.64	17.30	0.000e+000	0.000e+000	
CSH(1.8)	-0.79	16.80	17.60	0.000e+000	0.000e+000	
SiO2(am)	-2.51	-5.15	-2.64	0.000e+000	0.000e+000	

----------Solution composition----------

Elements	Molality	Moles
C	1.480e-005	1.480e-006
Ca	8.354e-004	8.355e-005
Na	2.000e-003	2.000e-004
Si	5.827e-004	5.827e-005

----------Description of solution----------

pH = 11.443 Charge balance
pe = -6.031 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 4.382e-003
Mass of water (kg) = 1.000e-001
Total alkalinity (eq/kg) = 3.642e-003
Total CO2 (mol/kg) = 1.480e-005
Temperature (deg C) = 25.000
Electrical balance (eq) = 8.784e-016
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 17
Total H = 1.110201e+001
Total O = 5.551309e+000

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	3.032e-003	2.821e-003	-2.518	-2.550	-0.031
H+	3.847e-012	3.605e-012	-11.415	-11.443	-0.028
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
C(-4) 5.572e-034					
CH4	5.572e-034	5.577e-034	-33.254	-33.254	0.000
C(4) 1.480e-005					
CO3-2	7.386e-006	5.594e-006	-5.132	-5.252	-0.121
CaCO3	6.952e-006	6.959e-006	-5.158	-5.157	0.000
CHO3-	4.587e-007	4.279e-007	-6.338	-6.369	-0.030
CaCHO3+	3.201e-009	2.986e-009	-8.495	-8.525	-0.030
CO2	3.142e-012	3.145e-012	-11.503	-11.502	0.000
Ca 8.354e-004					
Ca+2	7.992e-004	6.050e-004	-3.097	-3.218	-0.121
CaHO+	2.637e-005	2.456e-005	-4.579	-4.610	-0.031

```
        CaCO3          6.952e-006  6.959e-006   -5.158   -5.157    0.000
        CaSiH3O4+       2.874e-006  2.677e-006   -5.541   -5.572   -0.031
        CaCHO3+        3.201e-009  2.986e-009   -8.495   -8.525   -0.030
H(0)          2.345e-014
        H2             1.173e-014  1.174e-014  -13.931  -13.930    0.000
Na            2.000e-003
        Na+            1.941e-003  1.808e-003   -2.712   -2.743   -0.031
        NaSiH3O4        5.858e-005  5.864e-005   -4.232   -4.232    0.000
        NaHO           8.229e-007  8.237e-007   -6.085   -6.084    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -64.365  -64.365    0.000
Si            5.827e-004
        SiH3O4-         5.073e-004  4.724e-004   -3.295   -3.326   -0.031
        NaSiH3O4        5.858e-005  5.864e-005   -4.232   -4.232    0.000
        H4SiO4          7.009e-006  7.016e-006   -5.154   -5.154    0.000
        SiH2O4-2        6.954e-006  5.229e-006   -5.158   -5.282   -0.124
        CaSiH3O4+       2.874e-006  2.677e-006   -5.541   -5.572   -0.031

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -1.72   -5.15   -3.43  SiO2
        Aragonite        -0.16   -8.47   -8.31  CaCO3
        b-Cristobalite   -2.17   -5.15   -2.98  SiO2
        Ca(OH)2          -3.04   19.67   22.71  Ca(OH)2
        Calcite           0.00   -8.47   -8.47  CaCO3
        CH4            -30.41  -71.43  -41.02  CH4
        Chalcedony       -1.42   -5.15   -3.74  SiO2
        CSH(0.1)         -2.12   -3.19   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -1.79   -1.22    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -1.48    0.75    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -1.19    2.71    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)         -0.92    4.68    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)         -0.67    6.65    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)         -0.43    8.61    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         -0.24   10.58   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)       -0.21   11.23   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         -0.12   13.94   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)          0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)          0.00   14.98   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)         -0.06   15.37   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)         -0.17   15.70   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)         -0.28   15.99   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)         -0.41   16.23   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)         -0.54   16.45   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)         -0.67   16.64   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)         -0.79   16.80   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite        -17.59  -49.79  -32.19  C
        H2              -10.82  -10.82   -0.00  H2
        Lime            -12.89   19.67   32.56  CaO
        O2              -61.48   21.65   83.13  O2
        PCO2            -10.03  -28.14  -18.11  CO2
        Quartz           -1.13   -5.15   -4.03  SiO2
        SiO2(am)         -2.51   -5.15   -2.64  Si1.000O2.000
        Wollastonite      0.73   14.51   13.78  CaSiO3

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End of simulation.
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Reading input data for simulation 8.
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        TITLE 8 Liquid solid ration 800
        USE solution 1
        USE equilibrium_phases 8
        SAVE equilibrium_phases 9
        END
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```

```
TITLE
-----

 8 Liquid solid ration 800

-----------------------------------------
Beginning of batch-reaction calculations.
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Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 8.     Pure-phase assemblage after simulation 7.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase             SI log IAP  log KT    Initial      Final      Delta

        Ca(OH)2         -3.04   19.67   22.71 0.000e+000          0.000e+000
        Calcite          0.00   -8.47   -8.47 1.393e-003 1.591e-003 1.986e-004
        CSH(0.1)        -2.12   -3.19   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -1.79   -1.22    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -1.48    0.75    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -1.19    2.71    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.92    4.68    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.67    6.65    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.43    8.61    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.24   10.58   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.21   11.23   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.12   13.94   14.06 0.000e+000          0.000e+000
        CSH(1.0)        -0.00   14.51   14.51 2.787e-003 4.964e-003 2.178e-003
        CSH(1.1)        -0.00   14.98   14.98 2.479e-003 1.939e-005-2.460e-003
        CSH(1.2)        -0.06   15.37   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.17   15.70   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.28   15.99   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.41   16.23   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.54   16.45   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -0.67   16.64   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -0.79   16.80   17.60 0.000e+000          0.000e+000
        SiO2(am)        -2.51   -5.15   -2.64 0.000e+000          0.000e+000

------------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        C              1.480e-005  1.480e-006
        Ca             8.354e-004  8.355e-005
        Na             2.000e-003  2.000e-004
        Si             5.827e-004  5.827e-005

----------------------------Description of solution----------------------------

                                pH  =  11.443     Charge balance
                                pe  =  -6.031     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  4.382e-003
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  3.642e-003
                    Total CO2 (mol/kg)  =  1.480e-005
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  =  1.616e-015
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                           Iterations  =  17
                             Total H  = 1.110201e+001
                             Total O  = 5.551309e+000

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma
```

```
          HO-            3.032e-003  2.821e-003   -2.518   -2.550   -0.031
          H+             3.847e-012  3.605e-012  -11.415  -11.443   -0.028
          H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
C(-4)          5.557e-034
          CH4            5.557e-034  5.562e-034  -33.255  -33.255    0.000
C(4)           1.480e-005
          CO3-2          7.386e-006  5.594e-006   -5.132   -5.252   -0.121
          CaCO3          6.952e-006  6.959e-006   -5.158   -5.157    0.000
          CHO3-          4.587e-007  4.279e-007   -6.338   -6.369   -0.030
          CaCHO3+        3.201e-009  2.986e-009   -8.495   -8.525   -0.030
          CO2            3.142e-012  3.145e-012  -11.503  -11.502    0.000
Ca             8.354e-004
          Ca+2           7.992e-004  6.050e-004   -3.097   -3.218   -0.121
          CaHO+          2.637e-005  2.456e-005   -4.579   -4.610   -0.031
          CaCO3          6.952e-006  6.959e-006   -5.158   -5.157    0.000
          CaSiH3O4+      2.874e-006  2.677e-006   -5.541   -5.572   -0.031
          CaCHO3+        3.201e-009  2.986e-009   -8.495   -8.525   -0.030
H(0)           2.344e-014
          H2             1.172e-014  1.173e-014  -13.931  -13.931    0.000
Na             2.000e-003
          Na+            1.941e-003  1.808e-003   -2.712   -2.743   -0.031
          NaSiH3O4       5.858e-005  5.864e-005   -4.232   -4.232    0.000
          NaHO           8.229e-007  8.237e-007   -6.085   -6.084    0.000
O(0)           0.000e+000
          O2             0.000e+000  0.000e+000  -64.365  -64.364    0.000
Si             5.827e-004
          SiH3O4-        5.073e-004  4.724e-004   -3.295   -3.326   -0.031
          NaSiH3O4       5.858e-005  5.864e-005   -4.232   -4.232    0.000
          H4SiO4         7.009e-006  7.016e-006   -5.154   -5.154    0.000
          SiH2O4-2       6.954e-006  5.229e-006   -5.158   -5.282   -0.124
          CaSiH3O4+      2.874e-006  2.677e-006   -5.541   -5.572   -0.031

-----------------------------Saturation indices-------------------------------

          Phase            SI log IAP  log KT

          a-Cristobalite  -1.72  -5.15  -3.43  SiO2
          Aragonite       -0.16  -8.47  -8.31  CaCO3
          b-Cristobalite  -2.17  -5.15  -2.98  SiO2
          Ca(OH)2         -3.04  19.67  22.71  Ca(OH)2
          Calcite          0.00  -8.47  -8.47  CaCO3
          CH4            -30.41 -71.43 -41.02  CH4
          Chalcedony      -1.42  -5.15  -3.74  SiO2
          CSH(0.1)        -2.12  -3.19  -1.07  Ca0.100Si1.000O2.100:0.110H2O
          CSH(0.2)        -1.79  -1.22   0.56  Ca0.200Si1.000O2.200:0.220H2O
          CSH(0.3)        -1.48   0.75   2.23  Ca0.300Si1.000O2.300:0.330H2O
          CSH(0.4)        -1.19   2.71   3.91  Ca0.400Si1.000O2.400:0.440H2O
          CSH(0.5)        -0.92   4.68   5.60  Ca0.500Si1.000O2.500:0.550H2O
          CSH(0.6)        -0.67   6.65   7.31  Ca0.600Si1.000O2.600:0.661H2O
          CSH(0.7)        -0.43   8.61   9.04  Ca0.700Si1.000O2.700:0.771H2O
          CSH(0.8)        -0.24  10.58  10.82  Ca0.800Si1.000O2.800:0.881H2O
          CSH(0.833)      -0.21  11.23  11.44  Ca0.833Si1.000O2.833:0.917H2O
          CSH(0.9)        -0.12  13.94  14.06  Ca1.000Si1.111O3.222:1.093H2O
          CSH(1.0)        -0.00  14.51  14.51  Ca1.000Si1.000O3.000:1.084H2O
          CSH(1.1)        -0.00  14.98  14.98  Ca1.000Si0.909O2.818:1.076H2O
          CSH(1.2)        -0.06  15.37  15.44  Ca1.000Si0.833O2.666:1.070H2O
          CSH(1.3)        -0.17  15.70  15.87  Ca1.000Si0.769O2.538:1.065H2O
          CSH(1.4)        -0.28  15.99  16.27  Ca1.000Si0.714O2.428:1.060H2O
          CSH(1.5)        -0.41  16.23  16.64  Ca1.000Si0.667O2.334:1.056H2O
          CSH(1.6)        -0.54  16.45  16.99  Ca1.000Si0.625O2.250:1.053H2O
          CSH(1.7)        -0.67  16.64  17.30  Ca1.000Si0.588O2.176:1.049H2O
          CSH(1.8)        -0.79  16.80  17.60  Ca1.000Si0.556O2.112:1.047H2O
          Graphite       -17.59 -49.79 -32.19  C
          H2             -10.82 -10.82  -0.00  H2
          Lime           -12.89  19.67  32.56  CaO
          O2             -61.48  21.65  83.13  O2
          PCO2           -10.03 -28.14 -18.11  CO2
          Quartz          -1.13  -5.15  -4.03  SiO2
          SiO2(am)        -2.51  -5.15  -2.64  Si1.000O2.000
          Wollastonite     0.73  14.51  13.78  CaSiO3
```

```
------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 9.
------------------------------------

        TITLE 9 Liquid solid ration 900
        USE solution 1
        USE equilibrium_phases 9
        SAVE equilibrium_phases 10
        END
-----
TITLE
-----

 9 Liquid solid ration 900

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 9.    Pure-phase assemblage after simulation 8.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.11   18.60   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 1.591e-003 1.789e-003 1.982e-004
        CSH(0.1)       -1.15   -2.22   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.93   -0.36    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.73    1.50    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.55    3.36    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.38    5.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.24    7.08    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.11    8.94    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.02   10.79   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.03   11.41   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.00   14.06   14.06 0.000e+000 2.736e-004 2.736e-004
        CSH(1.0)        0.00   14.51   14.51 4.964e-003 4.449e-003-5.150e-004
        CSH(1.1)       -0.10   14.89   14.98 1.939e-005         -1.939e-005
        CSH(1.2)       -0.24   15.20   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.41   15.46   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.59   15.68   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.77   15.87   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.94   16.04   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.11   16.20   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.27   16.33   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.44   -4.08   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              1.810e-005  1.810e-006
        Ca             6.255e-004  6.255e-005
        Na             2.000e-003  2.000e-004
        Si             2.286e-003  2.286e-004

----------------------------Description of solution----------------------------

                                pH  =  10.963     Charge balance
                                pe  =  -5.551     Adjusted to redox equilibrium
                    Activity of water  =   1.000
```

```
                    Ionic strength  =  3.631e-003
                Mass of water (kg)  =  1.000e-001
            Total alkalinity (eq/kg)  =  3.215e-003
                 Total CO2 (mol/kg)  =  1.810e-005
                Temperature (deg C)  =  25.000
             Electrical balance (eq)  =  1.008e-017
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                      Iterations  =  18
                        Total H  = 1.110200e+001
                        Total O  = 5.551623e+000

----------------------------Distribution of species----------------------------

                                          Log      Log       Log
        Species          Molality   Activity  Molality  Activity    Gamma

        HO-            9.976e-004  9.338e-004   -3.001   -3.030   -0.029
        H+             1.156e-011  1.089e-011  -10.937  -10.963   -0.026
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
C(-4)         6.594e-033
        CH4            6.594e-033  6.599e-033  -32.181  -32.181    0.000
C(4)          1.810e-005
        CO3-2           9.355e-006  7.247e-006   -5.029   -5.140   -0.111
        CaCO3           6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CHO3-           1.785e-006  1.675e-006   -5.748   -5.776   -0.028
        CaCHO3+         9.616e-009  9.021e-009   -8.017   -8.045   -0.028
        CO2            3.716e-011  3.719e-011  -10.430  -10.430    0.000
Ca            6.255e-004
        Ca+2           6.032e-004  4.670e-004   -3.220   -3.331   -0.111
        CaSiH3O4+       8.632e-006  8.086e-006   -5.064   -5.092   -0.028
        CaCO3           6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CaHO+           6.698e-006  6.274e-006   -5.174   -5.202   -0.028
        CaCHO3+         9.616e-009  9.021e-009   -8.017   -8.045   -0.028
H(0)          2.346e-014
        H2             1.173e-014  1.174e-014  -13.931  -13.930    0.000
Na            2.000e-003
        Na+            1.788e-003  1.675e-003   -2.748   -2.776   -0.028
        NaSiH3O4        2.124e-004  2.126e-004   -3.673   -3.672    0.000
        NaHO           2.524e-007  2.526e-007   -6.598   -6.598    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -64.366  -64.365    0.000
Si            2.286e-003
        SiH3O4-         1.974e-003  1.849e-003   -2.705   -2.733   -0.028
        NaSiH3O4        2.124e-004  2.126e-004   -3.673   -3.672    0.000
        H4SiO4          8.288e-005  8.295e-005   -4.082   -4.081    0.000
        SiH2O4-2        8.798e-006  6.774e-006   -5.056   -5.169   -0.114
        CaSiH3O4+       8.632e-006  8.086e-006   -5.064   -5.092   -0.028

-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.65   -4.08   -3.43  SiO2
        Aragonite        -0.16   -8.47   -8.31  CaCO3
        b-Cristobalite   -1.10   -4.08   -2.98  SiO2
        Ca(OH)2          -4.11   18.60   22.71  Ca(OH)2
        Calcite           0.00   -8.47   -8.47  CaCO3
        CH4             -29.34  -70.36  -41.02  CH4
        Chalcedony        -0.34   -4.08   -3.74  SiO2
        CSH(0.1)          -1.15   -2.22   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)          -0.93   -0.36    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)          -0.73    1.50    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)          -0.55    3.36    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)          -0.38    5.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)          -0.24    7.08    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)          -0.11    8.94    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)          -0.02   10.79   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)        -0.03   11.41   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)          -0.00   14.06   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)           0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)          -0.10   14.89   14.98  Ca1.000Si0.909O2.818:1.076H2O
```

```
        CSH(1.2)        -0.24   15.20   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.41   15.46   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.59   15.68   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.77   15.87   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.94   16.04   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.11   16.20   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.27   16.33   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -16.52  -48.71  -32.19  C
        H2             -10.82  -10.82   -0.00  H2
        Lime           -13.97   18.60   32.56  CaO
        O2             -61.48   21.65   83.13  O2
        PCO2            -8.96  -27.07  -18.11  CO2
        Quartz          -0.05   -4.08   -4.03  SiO2
        SiO2(am)        -1.44   -4.08   -2.64  Si1.000O2.000
        Wollastonite     0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 10.
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        TITLE 10 Liquid solid ration 1000
        USE solution 1
        USE equilibrium_phases 10
        SAVE equilibrium_phases 11
        END
-----
TITLE
-----

 10 Liquid solid ration 1000

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 10.   Pure-phase assemblage after simulation 9.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase             SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2         -4.11   18.60   22.71 0.000e+000          0.000e+000
        Calcite          0.00   -8.47   -8.47 1.789e-003 1.988e-003 1.982e-004
        CSH(0.1)        -1.15   -2.22   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -0.93   -0.36    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -0.73    1.50    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -0.55    3.36    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.38    5.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.24    7.08    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.11    8.94    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.02   10.79   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.03   11.41   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.00   14.06   14.06 2.736e-004 5.630e-004 2.895e-004
        CSH(1.0)         0.00   14.51   14.51 4.449e-003 3.899e-003-5.502e-004
        CSH(1.1)        -0.10   14.89   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.24   15.20   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.41   15.46   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.59   15.68   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.77   15.87   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.94   16.04   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -1.11   16.20   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.27   16.33   17.60 0.000e+000          0.000e+000
        SiO2(am)        -1.44   -4.08   -2.64 0.000e+000          0.000e+000
```

```
-----------------------------Solution composition------------------------------

        Elements         Molality      Moles

        C              1.810e-005  1.810e-006
        Ca             6.255e-004  6.255e-005
        Na             2.000e-003  2.000e-004
        Si             2.286e-003  2.286e-004

----------------------------Description of solution----------------------------

                                pH  =  10.963     Charge balance
                                pe  =  -5.572     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.631e-003
                   Mass of water (kg)  =  1.000e-001
              Total alkalinity (eq/kg)  =  3.215e-003
                   Total CO2 (mol/kg)  =  1.810e-005
                  Temperature (deg C)  =  25.000
                Electrical balance (eq)  =  2.889e-014
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                          Iterations  =  16
                             Total H  = 1.110200e+001
                             Total O  = 5.551623e+000

----------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            9.976e-004  9.338e-004    -3.001    -3.030   -0.029
        H+             1.156e-011  1.089e-011   -10.937   -10.963   -0.026
        H2O            5.551e+001  9.999e-001     1.744    -0.000    0.000
C(-4)          9.713e-033
        CH4            9.713e-033  9.722e-033   -32.013   -32.012    0.000
C(4)           1.810e-005
        CO3-2           9.355e-006  7.247e-006    -5.029    -5.140   -0.111
        CaCO3           6.953e-006  6.959e-006    -5.158    -5.157    0.000
        CHO3-           1.785e-006  1.675e-006    -5.748    -5.776   -0.028
        CaCHO3+         9.616e-009  9.021e-009    -8.017    -8.045   -0.028
        CO2            3.716e-011  3.719e-011   -10.430   -10.430    0.000
Ca             6.255e-004
        Ca+2           6.032e-004  4.670e-004    -3.220    -3.331   -0.111
        CaSiH3O4+       8.632e-006  8.086e-006    -5.064    -5.092   -0.028
        CaCO3           6.953e-006  6.959e-006    -5.158    -5.157    0.000
        CaHO+           6.698e-006  6.274e-006    -5.174    -5.202   -0.028
        CaCHO3+         9.616e-009  9.021e-009    -8.017    -8.045   -0.028
H(0)           2.585e-014
        H2             1.292e-014  1.294e-014   -13.889   -13.888    0.000
Na             2.000e-003
        Na+            1.788e-003  1.675e-003    -2.748    -2.776   -0.028
        NaSiH3O4        2.124e-004  2.126e-004    -3.673    -3.672    0.000
        NaHO           2.524e-007  2.526e-007    -6.598    -6.598    0.000
O(0)           0.000e+000
        O2             0.000e+000  0.000e+000   -64.450   -64.449    0.000
Si             2.286e-003
        SiH3O4-         1.974e-003  1.849e-003    -2.705    -2.733   -0.028
        NaSiH3O4        2.124e-004  2.126e-004    -3.673    -3.672    0.000
        H4SiO4          8.288e-005  8.295e-005    -4.082    -4.081    0.000
        SiH2O4-2        8.798e-006  6.774e-006    -5.056    -5.169   -0.114
        CaSiH3O4+       8.632e-006  8.086e-006    -5.064    -5.092   -0.028

----------------------------Saturation indices---------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.65   -4.08   -3.43  SiO2
        Aragonite       -0.16   -8.47   -8.31  CaCO3
        b-Cristobalite   -1.10   -4.08   -2.98  SiO2
        Ca(OH)2         -4.11   18.60   22.71  Ca(OH)2
```

```
        Calcite         0.00   -8.47   -8.47  CaCO3
        CH4           -29.17  -70.19  -41.02  CH4
        Chalcedony     -0.34   -4.08   -3.74  SiO2
        CSH(0.1)       -1.15   -2.22   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)       -0.93   -0.36    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)       -0.73    1.50    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)       -0.55    3.36    3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)       -0.38    5.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)       -0.24    7.08    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)       -0.11    8.94    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)       -0.02   10.79   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)     -0.03   11.41   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)       -0.00   14.06   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)       -0.10   14.89   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)       -0.24   15.20   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)       -0.41   15.46   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)       -0.59   15.68   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)       -0.77   15.87   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)       -0.94   16.04   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)       -1.11   16.20   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)       -1.27   16.33   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite      -16.43  -48.63  -32.19  C
        H2            -10.78  -10.78   -0.00  H2
        Lime          -13.97   18.60   32.56  CaO
        O2            -61.56   21.56   83.13  O2
        PCO2           -8.96  -27.07  -18.11  CO2
        Quartz         -0.05   -4.08   -4.03  SiO2
        SiO2(am)       -1.44   -4.08   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

--------------------------------------
Reading input data for simulation 11.
--------------------------------------

        TITLE 11 Liquid solid ration 1100
        USE solution 1
        USE equilibrium_phases 11
        SAVE equilibrium_phases 12
        END
-----
TITLE
-----

 11 Liquid solid ration 1100

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 11.   Pure-phase assemblage after simulation 10.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.11   18.60   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 1.988e-003 2.186e-003 1.982e-004
        CSH(0.1)       -1.15   -2.22   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.93   -0.36    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.73    1.50    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.55    3.36    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.38    5.22    5.60 0.000e+000          0.000e+000
```

```
        CSH(0.6)        -0.24    7.08    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.11    8.94    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.02   10.79   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.03   11.41   11.44 0.000e+000          0.000e+000
        CSH(0.9)         0.00   14.06   14.06 5.630e-004 8.525e-004 2.895e-004
        CSH(1.0)         0.00   14.51   14.51 3.899e-003 3.349e-003-5.502e-004
        CSH(1.1)        -0.10   14.89   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.24   15.20   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.41   15.46   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.59   15.68   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.77   15.87   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.94   16.04   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -1.11   16.20   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.27   16.33   17.60 0.000e+000          0.000e+000
        SiO2(am)        -1.44   -4.08   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              1.810e-005  1.810e-006
        Ca             6.255e-004  6.255e-005
        Na             2.000e-003  2.000e-004
        Si             2.286e-003  2.286e-004

----------------------------Description of solution----------------------------

                                pH  =  10.963     Charge balance
                                pe  =  -5.572     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.631e-003
                     Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  3.215e-003
                     Total CO2 (mol/kg)  =  1.810e-005
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  =  2.889e-014
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                           Iterations  =  16
                              Total H  = 1.110200e+001
                              Total O  = 5.551623e+000

---------------------------Distribution of species----------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            9.976e-004  9.338e-004   -3.001   -3.030   -0.029
        H+             1.156e-011  1.089e-011  -10.937  -10.963   -0.026
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
C(-4)         9.694e-033
        CH4            9.694e-033  9.702e-033  -32.014  -32.013    0.000
C(4)          1.810e-005
        CO3-2          9.355e-006  7.247e-006   -5.029   -5.140   -0.111
        CaCO3          6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CHO3-          1.785e-006  1.675e-006   -5.748   -5.776   -0.028
        CaCHO3+        9.616e-009  9.021e-009   -8.017   -8.045   -0.028
        CO2            3.716e-011  3.719e-011  -10.430  -10.430    0.000
Ca            6.255e-004
        Ca+2           6.032e-004  4.670e-004   -3.220   -3.331   -0.111
        CaSiH3O4+      8.632e-006  8.086e-006   -5.064   -5.092   -0.028
        CaCO3          6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CaHO+          6.698e-006  6.274e-006   -5.174   -5.202   -0.028
        CaCHO3+        9.616e-009  9.021e-009   -8.017   -8.045   -0.028
H(0)          2.584e-014
        H2             1.292e-014  1.293e-014  -13.889  -13.888    0.000
Na            2.000e-003
        Na+            1.788e-003  1.675e-003   -2.748   -2.776   -0.028
        NaSiH3O4       2.124e-004  2.126e-004   -3.673   -3.672    0.000
        NaHO           2.524e-007  2.526e-007   -6.598   -6.598    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -64.449  -64.449    0.000
```

```
Si           2.286e-003
        SiH3O4-        1.974e-003  1.849e-003   -2.705   -2.733   -0.028
        NaSiH3O4       2.124e-004  2.126e-004   -3.673   -3.672    0.000
        H4SiO4         8.288e-005  8.295e-005   -4.082   -4.081    0.000
        SiH2O4-2       8.798e-006  6.774e-006   -5.056   -5.169   -0.114
        CaSiH3O4+      8.632e-006  8.086e-006   -5.064   -5.092   -0.028

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -0.65  -4.08  -3.43  SiO2
        Aragonite       -0.16  -8.47  -8.31  CaCO3
        b-Cristobalite  -1.10  -4.08  -2.98  SiO2
        Ca(OH)2         -4.11  18.60  22.71  Ca(OH)2
        Calcite          0.00  -8.47  -8.47  CaCO3
        CH4            -29.17 -70.19 -41.02  CH4
        Chalcedony      -0.34  -4.08  -3.74  SiO2
        CSH(0.1)        -1.15  -2.22  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.93  -0.36   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.73   1.50   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.55   3.36   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.38   5.22   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.24   7.08   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.11   8.94   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.02  10.79  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.03  11.41  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         0.00  14.06  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00  14.51  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.10  14.89  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.24  15.20  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.41  15.46  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.59  15.68  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.77  15.87  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.94  16.04  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.11  16.20  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.27  16.33  17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -16.43 -48.63 -32.19  C
        H2             -10.78 -10.78  -0.00  H2
        Lime           -13.97  18.60  32.56  CaO
        O2             -61.56  21.56  83.13  O2
        PCO2            -8.96 -27.07 -18.11  CO2
        Quartz          -0.05  -4.08  -4.03  SiO2
        SiO2(am)        -1.44  -4.08  -2.64  Si1.000O2.000
        Wollastonite     0.73  14.51  13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 12.
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        TITLE 12 Liquid solid ration 1200
        USE solution 1
        USE equilibrium_phases 12
        SAVE equilibrium_phases 13
        END
-----
TITLE
-----

 12 Liquid solid ration 1200

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.
```

Using solution 1.NaHCO3 100g
Using pure phase assemblage 12. Pure-phase assemblage after simulation 11.

-------------------------------Phase assemblage--------------------------------

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca(OH)2	-4.11	18.60	22.71	0.000e+000	0.000e+000	
Calcite	0.00	-8.47	-8.47	2.186e-003	2.384e-003	1.982e-004
CSH(0.1)	-1.15	-2.22	-1.07	0.000e+000	0.000e+000	
CSH(0.2)	-0.93	-0.36	0.56	0.000e+000	0.000e+000	
CSH(0.3)	-0.73	1.50	2.23	0.000e+000	0.000e+000	
CSH(0.4)	-0.55	3.36	3.91	0.000e+000	0.000e+000	
CSH(0.5)	-0.38	5.22	5.60	0.000e+000	0.000e+000	
CSH(0.6)	-0.24	7.08	7.31	0.000e+000	0.000e+000	
CSH(0.7)	-0.11	8.94	9.04	0.000e+000	0.000e+000	
CSH(0.8)	-0.02	10.79	10.82	0.000e+000	0.000e+000	
CSH(0.833)	-0.03	11.41	11.44	0.000e+000	0.000e+000	
CSH(0.9)	0.00	14.06	14.06	8.525e-004	1.142e-003	2.895e-004
CSH(1.0)	0.00	14.51	14.51	3.349e-003	2.799e-003	-5.502e-004
CSH(1.1)	-0.10	14.89	14.98	0.000e+000	0.000e+000	
CSH(1.2)	-0.24	15.20	15.44	0.000e+000	0.000e+000	
CSH(1.3)	-0.41	15.46	15.87	0.000e+000	0.000e+000	
CSH(1.4)	-0.59	15.68	16.27	0.000e+000	0.000e+000	
CSH(1.5)	-0.77	15.87	16.64	0.000e+000	0.000e+000	
CSH(1.6)	-0.94	16.04	16.99	0.000e+000	0.000e+000	
CSH(1.7)	-1.11	16.20	17.30	0.000e+000	0.000e+000	
CSH(1.8)	-1.27	16.33	17.60	0.000e+000	0.000e+000	
SiO2(am)	-1.44	-4.08	-2.64	0.000e+000	0.000e+000	

------------------------------Solution composition-------------------------------

Elements	Molality	Moles
C	1.810e-005	1.810e-006
Ca	6.255e-004	6.255e-005
Na	2.000e-003	2.000e-004
Si	2.286e-003	2.286e-004

------------------------------Description of solution------------------------------

pH = 10.963 Charge balance
pe = -5.572 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 3.631e-003
Mass of water (kg) = 1.000e-001
Total alkalinity (eq/kg) = 3.215e-003
Total CO2 (mol/kg) = 1.810e-005
Temperature (deg C) = 25.000
Electrical balance (eq) = 2.889e-014
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 16
Total H = 1.110200e+001
Total O = 5.551623e+000

-----------------------------Distribution of species-----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	9.976e-004	9.338e-004	-3.001	-3.030	-0.029
H+	1.156e-011	1.089e-011	-10.937	-10.963	-0.026
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
C(-4)	9.695e-033				
CH4	9.695e-033	9.703e-033	-32.013	-32.013	0.000
C(4)	1.810e-005				
CO3-2	9.355e-006	7.247e-006	-5.029	-5.140	-0.111
CaCO3	6.953e-006	6.959e-006	-5.158	-5.157	0.000
CHO3-	1.785e-006	1.675e-006	-5.748	-5.776	-0.028
CaCHO3+	9.616e-009	9.021e-009	-8.017	-8.045	-0.028

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        CO2           3.716e-011  3.719e-011   -10.430   -10.430    0.000
Ca           6.255e-004
        Ca+2          6.032e-004  4.670e-004    -3.220    -3.331   -0.111
        CaSiH3O4+      8.632e-006  8.086e-006    -5.064    -5.092   -0.028
        CaCO3         6.953e-006  6.959e-006    -5.158    -5.157    0.000
        CaHO+         6.698e-006  6.274e-006    -5.174    -5.202   -0.028
        CaCHO3+        9.616e-009  9.021e-009    -8.017    -8.045   -0.028
H(0)         2.584e-014
        H2            1.292e-014  1.293e-014   -13.889   -13.888    0.000
Na           2.000e-003
        Na+           1.788e-003  1.675e-003    -2.748    -2.776   -0.028
        NaSiH3O4       2.124e-004  2.126e-004    -3.673    -3.672    0.000
        NaHO          2.524e-007  2.526e-007    -6.598    -6.598    0.000
O(0)         0.000e+000
        O2            0.000e+000  0.000e+000   -64.449   -64.449    0.000
Si           2.286e-003
        SiH3O4-        1.974e-003  1.849e-003    -2.705    -2.733   -0.028
        NaSiH3O4       2.124e-004  2.126e-004    -3.673    -3.672    0.000
        H4SiO4         8.288e-005  8.295e-005    -4.082    -4.081    0.000
        SiH2O4-2       8.798e-006  6.774e-006    -5.056    -5.169   -0.114
        CaSiH3O4+      8.632e-006  8.086e-006    -5.064    -5.092   -0.028

------------------------------Saturation indices--------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -0.65  -4.08  -3.43  SiO2
        Aragonite       -0.16  -8.47  -8.31  CaCO3
        b-Cristobalite  -1.10  -4.08  -2.98  SiO2
        Ca(OH)2         -4.11  18.60  22.71  Ca(OH)2
        Calcite          0.00  -8.47  -8.47  CaCO3
        CH4           -29.17 -70.19 -41.02  CH4
        Chalcedony      -0.34  -4.08  -3.74  SiO2
        CSH(0.1)        -1.15  -2.22  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.93  -0.36   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.73   1.50   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.55   3.36   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.38   5.22   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.24   7.08   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.11   8.94   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.02  10.79  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.03  11.41  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         0.00  14.06  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00  14.51  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.10  14.89  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.24  15.20  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.41  15.46  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.59  15.68  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.77  15.87  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.94  16.04  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.11  16.20  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.27  16.33  17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -16.43 -48.63 -32.19  C
        H2             -10.78 -10.78  -0.00  H2
        Lime           -13.97  18.60  32.56  CaO
        O2             -61.56  21.56  83.13  O2
        PCO2            -8.96 -27.07 -18.11  CO2
        Quartz          -0.05  -4.08  -4.03  SiO2
        SiO2(am)        -1.44  -4.08  -2.64  Si1.000O2.000
        Wollastonite     0.73  14.51  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 13.
------------------------------------

        TITLE 13 Liquid solid ration 1300
        USE solution 1
```

```
        USE equilibrium_phases 13
        SAVE equilibrium_phases 14
        END
-----
TITLE
-----

 13 Liquid solid ration 1300

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 13.   Pure-phase assemblage after simulation 12.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.11   18.60   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 2.384e-003 2.582e-003 1.982e-004
        CSH(0.1)       -1.15   -2.22   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.93   -0.36    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.73    1.50    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.55    3.36    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.38    5.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.24    7.08    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.11    8.94    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.02   10.79   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.03   11.41   11.44 0.000e+000          0.000e+000
        CSH(0.9)        0.00   14.06   14.06 1.142e-003 1.431e-003 2.895e-004
        CSH(1.0)        0.00   14.51   14.51 2.799e-003 2.248e-003-5.502e-004
        CSH(1.1)       -0.10   14.89   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.24   15.20   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.41   15.46   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.59   15.68   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.77   15.87   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.94   16.04   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.11   16.20   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.27   16.33   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.44   -4.08   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              1.810e-005  1.810e-006
        Ca             6.255e-004  6.255e-005
        Na             2.000e-003  2.000e-004
        Si             2.286e-003  2.286e-004

----------------------------Description of solution----------------------------

                                pH  =  10.963     Charge balance
                                pe  =  -5.572     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.631e-003
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  3.215e-003
                    Total CO2 (mol/kg)  =  1.810e-005
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  =  2.889e-014
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                          Iterations  =  16
                             Total H  = 1.110200e+001
                             Total O  = 5.551623e+000
```

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	9.976e-004	9.338e-004	-3.001	-3.030	-0.029
H+	1.156e-011	1.089e-011	-10.937	-10.963	-0.026
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
C(-4)	9.717e-033				
CH4	9.717e-033	9.725e-033	-32.012	-32.012	0.000
C(4)	1.810e-005				
CO3-2	9.355e-006	7.247e-006	-5.029	-5.140	-0.111
CaCO3	6.953e-006	6.959e-006	-5.158	-5.157	0.000
CHO3-	1.785e-006	1.675e-006	-5.748	-5.776	-0.028
CaCHO3+	9.616e-009	9.021e-009	-8.017	-8.045	-0.028
CO2	3.716e-011	3.719e-011	-10.430	-10.430	0.000
Ca	6.255e-004				
Ca+2	6.032e-004	4.670e-004	-3.220	-3.331	-0.111
CaSiH3O4+	8.632e-006	8.086e-006	-5.064	-5.092	-0.028
CaCO3	6.953e-006	6.959e-006	-5.158	-5.157	0.000
CaHO+	6.698e-006	6.274e-006	-5.174	-5.202	-0.028
CaCHO3+	9.616e-009	9.021e-009	-8.017	-8.045	-0.028
H(0)	2.585e-014				
H2	1.293e-014	1.294e-014	-13.889	-13.888	0.000
Na	2.000e-003				
Na+	1.788e-003	1.675e-003	-2.748	-2.776	-0.028
NaSiH3O4	2.124e-004	2.126e-004	-3.673	-3.672	0.000
NaHO	2.524e-007	2.526e-007	-6.598	-6.598	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-64.450	-64.449	0.000
Si	2.286e-003				
SiH3O4-	1.974e-003	1.849e-003	-2.705	-2.733	-0.028
NaSiH3O4	2.124e-004	2.126e-004	-3.673	-3.672	0.000
H4SiO4	8.288e-005	8.295e-005	-4.082	-4.081	0.000
SiH2O4-2	8.798e-006	6.774e-006	-5.056	-5.169	-0.114
CaSiH3O4+	8.632e-006	8.086e-006	-5.064	-5.092	-0.028

----------Saturation indices----------

Phase	SI	log IAP	log KT	
a-Cristobalite	-0.65	-4.08	-3.43	SiO2
Aragonite	-0.16	-8.47	-8.31	CaCO3
b-Cristobalite	-1.10	-4.08	-2.98	SiO2
Ca(OH)2	-4.11	18.60	22.71	Ca(OH)2
Calcite	0.00	-8.47	-8.47	CaCO3
CH4	-29.17	-70.19	-41.02	CH4
Chalcedony	-0.34	-4.08	-3.74	SiO2
CSH(0.1)	-1.15	-2.22	-1.07	Ca0.100Si1.000O2.100:0.110H2O
CSH(0.2)	-0.93	-0.36	0.56	Ca0.200Si1.000O2.200:0.220H2O
CSH(0.3)	-0.73	1.50	2.23	Ca0.300Si1.000O2.300:0.330H2O
CSH(0.4)	-0.55	3.36	3.91	Ca0.400Si1.000O2.400:0.440H2O
CSH(0.5)	-0.38	5.22	5.60	Ca0.500Si1.000O2.500:0.550H2O
CSH(0.6)	-0.24	7.08	7.31	Ca0.600Si1.000O2.600:0.661H2O
CSH(0.7)	-0.11	8.94	9.04	Ca0.700Si1.000O2.700:0.771H2O
CSH(0.8)	-0.02	10.79	10.82	Ca0.800Si1.000O2.800:0.881H2O
CSH(0.833)	-0.03	11.41	11.44	Ca0.833Si1.000O2.833:0.917H2O
CSH(0.9)	0.00	14.06	14.06	Ca1.000Si1.111O3.222:1.093H2O
CSH(1.0)	0.00	14.51	14.51	Ca1.000Si1.000O3.000:1.084H2O
CSH(1.1)	-0.10	14.89	14.98	Ca1.000Si0.909O2.818:1.076H2O
CSH(1.2)	-0.24	15.20	15.44	Ca1.000Si0.833O2.666:1.070H2O
CSH(1.3)	-0.41	15.46	15.87	Ca1.000Si0.769O2.538:1.065H2O
CSH(1.4)	-0.59	15.68	16.27	Ca1.000Si0.714O2.428:1.060H2O
CSH(1.5)	-0.77	15.87	16.64	Ca1.000Si0.667O2.334:1.056H2O
CSH(1.6)	-0.94	16.04	16.99	Ca1.000Si0.625O2.250:1.053H2O
CSH(1.7)	-1.11	16.20	17.30	Ca1.000Si0.588O2.176:1.049H2O
CSH(1.8)	-1.27	16.33	17.60	Ca1.000Si0.556O2.112:1.047H2O
Graphite	-16.43	-48.63	-32.19	C
H2	-10.78	-10.78	-0.00	H2
Lime	-13.97	18.60	32.56	CaO
O2	-61.56	21.56	83.13	O2

```
        PCO2           -8.96  -27.07  -18.11  CO2
        Quartz         -0.05   -4.08   -4.03  SiO2
        SiO2(am)       -1.44   -4.08   -2.64  Si1.000O2.000
        Wollastonite    0.73   14.51   13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 14.
------------------------------------

        TITLE 14 Liquid solid ration 1400
        USE solution 1
        USE equilibrium_phases 14
        SAVE equilibrium_phases 15
        END
-----
TITLE
-----

 14 Liquid solid ration 1400

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 14.   Pure-phase assemblage after simulation 13.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.11   18.60   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 2.582e-003 2.780e-003 1.982e-004
        CSH(0.1)       -1.15   -2.22   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.93   -0.36    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.73    1.50    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.55    3.36    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.38    5.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.24    7.08    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.11    8.94    9.04 0.000e+000          0.000e+000
        CSH(0.8)       -0.02   10.79   10.82 0.000e+000          0.000e+000
        CSH(0.833)     -0.03   11.41   11.44 0.000e+000          0.000e+000
        CSH(0.9)       -0.00   14.06   14.06 1.431e-003 1.721e-003 2.895e-004
        CSH(1.0)       -0.00   14.51   14.51 2.248e-003 1.698e-003-5.502e-004
        CSH(1.1)       -0.10   14.89   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.24   15.20   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.41   15.46   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.59   15.68   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.77   15.87   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -0.94   16.04   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.11   16.20   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.27   16.33   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.44   -4.08   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        C              1.810e-005  1.810e-006
        Ca             6.255e-004  6.255e-005
        Na             2.000e-003  2.000e-004
        Si             2.286e-003  2.286e-004

----------------------------Description of solution-----------------------------
```

```
                                  pH  =  10.963     Charge balance
                                  pe  =  -5.572     Adjusted to redox equilibrium
                       Activity of water  =   1.000
                          Ionic strength  =  3.631e-003
                      Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  3.215e-003
                     Total CO2 (mol/kg)  =  1.810e-005
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -3.235e-014
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  21
                             Total H  = 1.110200e+001
                             Total O  = 5.551623e+000

----------------------------Distribution of species----------------------------

                                                 Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            9.976e-004  9.338e-004   -3.001   -3.030   -0.029
         H+             1.156e-011  1.089e-011   -10.937  -10.963   -0.026
         H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
C(-4)          9.739e-033
         CH4            9.739e-033  9.747e-033   -32.011  -32.011    0.000
C(4)           1.810e-005
         CO3-2           9.355e-006  7.247e-006   -5.029   -5.140   -0.111
         CaCO3           6.953e-006  6.959e-006   -5.158   -5.157    0.000
         CHO3-           1.785e-006  1.675e-006   -5.748   -5.776   -0.028
         CaCHO3+         9.616e-009  9.021e-009   -8.017   -8.045   -0.028
         CO2            3.716e-011  3.719e-011   -10.430  -10.430    0.000
Ca             6.255e-004
         Ca+2            6.032e-004  4.670e-004   -3.220   -3.331   -0.111
         CaSiH3O4+        8.632e-006  8.086e-006   -5.064   -5.092   -0.028
         CaCO3           6.953e-006  6.959e-006   -5.158   -5.157    0.000
         CaHO+           6.698e-006  6.274e-006   -5.174   -5.202   -0.028
         CaCHO3+         9.616e-009  9.021e-009   -8.017   -8.045   -0.028
H(0)           2.587e-014
         H2             1.293e-014  1.294e-014   -13.888  -13.888    0.000
Na             2.000e-003
         Na+            1.788e-003  1.675e-003   -2.748   -2.776   -0.028
         NaSiH3O4        2.124e-004  2.126e-004   -3.673   -3.672    0.000
         NaHO           2.524e-007  2.526e-007   -6.598   -6.598    0.000
O(0)           0.000e+000
         O2             0.000e+000  0.000e+000   -64.450  -64.450    0.000
Si             2.286e-003
         SiH3O4-         1.974e-003  1.849e-003   -2.705   -2.733   -0.028
         NaSiH3O4        2.124e-004  2.126e-004   -3.673   -3.672    0.000
         H4SiO4          8.288e-005  8.295e-005   -4.082   -4.081    0.000
         SiH2O4-2        8.798e-006  6.774e-006   -5.056   -5.169   -0.114
         CaSiH3O4+        8.632e-006  8.086e-006   -5.064   -5.092   -0.028

-----------------------------Saturation indices-------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -0.65   -4.08   -3.43  SiO2
         Aragonite        -0.16   -8.47   -8.31  CaCO3
         b-Cristobalite   -1.10   -4.08   -2.98  SiO2
         Ca(OH)2          -4.11   18.60   22.71  Ca(OH)2
         Calcite           0.00   -8.47   -8.47  CaCO3
         CH4             -29.17  -70.19  -41.02  CH4
         Chalcedony       -0.34   -4.08   -3.74  SiO2
         CSH(0.1)         -1.15   -2.22   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -0.93   -0.36    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -0.73    1.50    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -0.55    3.36    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -0.38    5.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -0.24    7.08    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -0.11    8.94    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)         -0.02   10.79   10.82  Ca0.800Si1.000O2.800:0.881H2O
```

```
        CSH(0.833)      -0.03   11.41   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.00   14.06   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.10   14.89   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.24   15.20   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.41   15.46   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.59   15.68   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.77   15.87   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.94   16.04   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.11   16.20   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.27   16.33   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -16.43  -48.63  -32.19  C
        H2             -10.78  -10.78   -0.00  H2
        Lime           -13.97   18.60   32.56  CaO
        O2             -61.56   21.56   83.13  O2
        PCO2            -8.96  -27.07  -18.11  CO2
        Quartz          -0.05   -4.08   -4.03  SiO2
        SiO2(am)        -1.44   -4.08   -2.64  Si1.000O2.000
        Wollastonite     0.73   14.51   13.78  CaSiO3

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End of simulation.
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--------------------------------------
Reading input data for simulation 15.
--------------------------------------

        TITLE 15 Liquid solid ration 1500
        USE solution 1
        USE equilibrium_phases 15
        SAVE equilibrium_phases 16
        END
-----
TITLE
-----

 15 Liquid solid ration 1500

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 15.   Pure-phase assemblage after simulation 14.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
        Phase             SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2         -4.11   18.60   22.71 0.000e+000          0.000e+000
        Calcite          0.00   -8.47   -8.47 2.780e-003 2.979e-003 1.982e-004
        CSH(0.1)        -1.15   -2.22   -1.07 0.000e+000          0.000e+000
        CSH(0.2)        -0.93   -0.36    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -0.73    1.50    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -0.55    3.36    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.38    5.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.24    7.08    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.11    8.94    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.02   10.79   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.03   11.41   11.44 0.000e+000          0.000e+000
        CSH(0.9)        -0.00   14.06   14.06 1.721e-003 2.010e-003 2.895e-004
        CSH(1.0)        -0.00   14.51   14.51 1.698e-003 1.148e-003-5.502e-004
        CSH(1.1)        -0.10   14.89   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.24   15.20   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.41   15.46   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.59   15.68   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.77   15.87   16.64 0.000e+000          0.000e+000
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```
        CSH(1.6)        -0.94   16.04   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -1.11   16.20   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.27   16.33   17.60 0.000e+000          0.000e+000
        SiO2(am)        -1.44   -4.08   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              1.810e-005  1.810e-006
        Ca             6.255e-004  6.255e-005
        Na             2.000e-003  2.000e-004
        Si             2.286e-003  2.286e-004

----------------------------Description of solution----------------------------

                                pH  =  10.963     Charge balance
                                pe  =  -5.572     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.631e-003
                     Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  3.215e-003
                     Total CO2 (mol/kg)  =  1.810e-005
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -6.196e-013
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  16
                              Total H  = 1.110200e+001
                              Total O  = 5.551623e+000

----------------------------Distribution of species----------------------------

                                                 Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            9.976e-004  9.338e-004    -3.001    -3.030    -0.029
        H+             1.156e-011  1.089e-011   -10.937   -10.963    -0.026
        H2O            5.551e+001  9.999e-001     1.744    -0.000     0.000
C(-4)          9.741e-033
        CH4            9.741e-033  9.749e-033   -32.011   -32.011     0.000
C(4)           1.810e-005
        CO3-2           9.355e-006  7.247e-006    -5.029    -5.140    -0.111
        CaCO3           6.953e-006  6.959e-006    -5.158    -5.157     0.000
        CHO3-           1.785e-006  1.675e-006    -5.748    -5.776    -0.028
        CaCHO3+         9.616e-009  9.021e-009    -8.017    -8.045    -0.028
        CO2            3.716e-011  3.719e-011   -10.430   -10.430     0.000
Ca             6.255e-004
        Ca+2           6.032e-004  4.670e-004    -3.220    -3.331    -0.111
        CaSiH3O4+       8.632e-006  8.086e-006    -5.064    -5.092    -0.028
        CaCO3           6.953e-006  6.959e-006    -5.158    -5.157     0.000
        CaHO+           6.698e-006  6.274e-006    -5.174    -5.202    -0.028
        CaCHO3+         9.616e-009  9.021e-009    -8.017    -8.045    -0.028
H(0)           2.587e-014
        H2             1.293e-014  1.294e-014   -13.888   -13.888     0.000
Na             2.000e-003
        Na+            1.788e-003  1.675e-003    -2.748    -2.776    -0.028
        NaSiH3O4        2.124e-004  2.126e-004    -3.673    -3.672     0.000
        NaHO           2.524e-007  2.526e-007    -6.598    -6.598     0.000
O(0)           0.000e+000
        O2             0.000e+000  0.000e+000   -64.450   -64.450     0.000
Si             2.286e-003
        SiH3O4-         1.974e-003  1.849e-003    -2.705    -2.733    -0.028
        NaSiH3O4        2.124e-004  2.126e-004    -3.673    -3.672     0.000
        H4SiO4          8.288e-005  8.295e-005    -4.082    -4.081     0.000
        SiH2O4-2        8.798e-006  6.774e-006    -5.056    -5.169    -0.114
        CaSiH3O4+       8.632e-006  8.086e-006    -5.064    -5.092    -0.028

----------------------------Saturation indices---------------------------------

        Phase            SI log IAP  log KT
```

```
        a-Cristobalite  -0.65  -4.08  -3.43  SiO2
        Aragonite       -0.16  -8.47  -8.31  CaCO3
        b-Cristobalite  -1.10  -4.08  -2.98  SiO2
        Ca(OH)2        -4.11  18.60  22.71  Ca(OH)2
        Calcite         0.00  -8.47  -8.47  CaCO3
        CH4           -29.17 -70.19 -41.02  CH4
        Chalcedony      -0.34  -4.08  -3.74  SiO2
        CSH(0.1)        -1.15  -2.22  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.93  -0.36   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.73   1.50   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.55   3.36   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.38   5.22   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.24   7.08   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.11   8.94   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.02  10.79  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.03  11.41  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)        -0.00  14.06  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.00  14.51  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.10  14.89  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.24  15.20  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.41  15.46  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.59  15.68  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.77  15.87  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.94  16.04  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.11  16.20  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.27  16.33  17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -16.43 -48.63 -32.19  C
        H2             -10.78 -10.78  -0.00  H2
        Lime           -13.97  18.60  32.56  CaO
        O2             -61.56  21.56  83.13  O2
        PCO2            -8.96 -27.07 -18.11  CO2
        Quartz          -0.05  -4.08  -4.03  SiO2
        SiO2(am)        -1.44  -4.08  -2.64  Si1.000O2.000
        Wollastonite     0.73  14.51  13.78  CaSiO3

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 16.
------------------------------------

        TITLE 16 Liquid solid ration 1600
        USE solution 1
        USE equilibrium_phases 16
        SAVE equilibrium_phases 17
        END
-----
TITLE
-----

 16 Liquid solid ration 1600

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 16.   Pure-phase assemblage after simulation 15.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.11  18.60  22.71 0.000e+000          0.000e+000
        Calcite         0.00  -8.47  -8.47 2.979e-003 3.177e-003 1.982e-004
        CSH(0.1)       -1.15  -2.22  -1.07 0.000e+000          0.000e+000
```

```
        CSH(0.2)        -0.93   -0.36    0.56 0.000e+000          0.000e+000
        CSH(0.3)        -0.73    1.50    2.23 0.000e+000          0.000e+000
        CSH(0.4)        -0.55    3.36    3.91 0.000e+000          0.000e+000
        CSH(0.5)        -0.38    5.22    5.60 0.000e+000          0.000e+000
        CSH(0.6)        -0.24    7.08    7.31 0.000e+000          0.000e+000
        CSH(0.7)        -0.11    8.94    9.04 0.000e+000          0.000e+000
        CSH(0.8)        -0.02   10.79   10.82 0.000e+000          0.000e+000
        CSH(0.833)      -0.03   11.41   11.44 0.000e+000          0.000e+000
        CSH(0.9)         0.00   14.06   14.06 2.010e-003 2.300e-003 2.895e-004
        CSH(1.0)         0.00   14.51   14.51 1.148e-003 5.976e-004-5.502e-004
        CSH(1.1)        -0.10   14.89   14.98 0.000e+000          0.000e+000
        CSH(1.2)        -0.24   15.20   15.44 0.000e+000          0.000e+000
        CSH(1.3)        -0.41   15.46   15.87 0.000e+000          0.000e+000
        CSH(1.4)        -0.59   15.68   16.27 0.000e+000          0.000e+000
        CSH(1.5)        -0.77   15.87   16.64 0.000e+000          0.000e+000
        CSH(1.6)        -0.94   16.04   16.99 0.000e+000          0.000e+000
        CSH(1.7)        -1.11   16.20   17.30 0.000e+000          0.000e+000
        CSH(1.8)        -1.27   16.33   17.60 0.000e+000          0.000e+000
        SiO2(am)        -1.44   -4.08   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition------------------------------

        Elements         Molality     Moles

        C              1.810e-005  1.810e-006
        Ca             6.255e-004  6.255e-005
        Na             2.000e-003  2.000e-004
        Si             2.286e-003  2.286e-004

----------------------------Description of solution---------------------------

                                pH  =  10.963     Charge balance
                                pe  =  -5.572     Adjusted to redox equilibrium
                     Activity of water  =  1.000
                        Ionic strength  =  3.631e-003
                    Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  3.215e-003
                    Total CO2 (mol/kg)  =  1.810e-005
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.546e-016
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  17
                              Total H  = 1.110200e+001
                              Total O  = 5.551623e+000

----------------------------Distribution of species---------------------------

                                              Log      Log       Log
        Species          Molality    Activity Molality Activity    Gamma

        HO-            9.976e-004  9.338e-004   -3.001   -3.030   -0.029
        H+             1.156e-011  1.089e-011  -10.937  -10.963   -0.026
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
C(-4)          9.744e-033
        CH4            9.744e-033  9.752e-033  -32.011  -32.011    0.000
C(4)           1.810e-005
        CO3-2          9.355e-006  7.247e-006   -5.029   -5.140   -0.111
        CaCO3          6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CHO3-          1.785e-006  1.675e-006   -5.748   -5.776   -0.028
        CaCHO3+        9.616e-009  9.021e-009   -8.017   -8.045   -0.028
        CO2            3.716e-011  3.719e-011  -10.430  -10.430    0.000
Ca             6.255e-004
        Ca+2           6.032e-004  4.670e-004   -3.220   -3.331   -0.111
        CaSiH3O4+      8.632e-006  8.086e-006   -5.064   -5.092   -0.028
        CaCO3          6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CaHO+          6.698e-006  6.274e-006   -5.174   -5.202   -0.028
        CaCHO3+        9.616e-009  9.021e-009   -8.017   -8.045   -0.028
H(0)           2.587e-014
        H2             1.293e-014  1.295e-014  -13.888  -13.888    0.000
Na             2.000e-003
        Na+            1.788e-003  1.675e-003   -2.748   -2.776   -0.028
```

```
        NaSiH3O4       2.124e-004  2.126e-004   -3.673   -3.672    0.000
        NaHO           2.524e-007  2.526e-007   -6.598   -6.598    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -64.450  -64.450    0.000
Si           2.286e-003
        SiH3O4-        1.974e-003  1.849e-003   -2.705   -2.733   -0.028
        NaSiH3O4       2.124e-004  2.126e-004   -3.673   -3.672    0.000
        H4SiO4         8.288e-005  8.295e-005   -4.082   -4.081    0.000
        SiH2O4-2       8.798e-006  6.774e-006   -5.056   -5.169   -0.114
        CaSiH3O4+      8.632e-006  8.086e-006   -5.064   -5.092   -0.028

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -0.65  -4.08  -3.43  SiO2
        Aragonite       -0.16  -8.47  -8.31  CaCO3
        b-Cristobalite  -1.10  -4.08  -2.98  SiO2
        Ca(OH)2         -4.11  18.60  22.71  Ca(OH)2
        Calcite          0.00  -8.47  -8.47  CaCO3
        CH4            -29.17 -70.19 -41.02  CH4
        Chalcedony      -0.34  -4.08  -3.74  SiO2
        CSH(0.1)        -1.15  -2.22  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.93  -0.36   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.73   1.50   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.55   3.36   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.38   5.22   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.24   7.08   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.11   8.94   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)        -0.02  10.79  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.03  11.41  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         0.00  14.06  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)         0.00  14.51  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.10  14.89  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.24  15.20  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.41  15.46  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.59  15.68  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.77  15.87  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -0.94  16.04  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.11  16.20  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.27  16.33  17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -16.43 -48.63 -32.19  C
        H2             -10.78 -10.78  -0.00  H2
        Lime           -13.97  18.60  32.56  CaO
        O2             -61.56  21.56  83.13  O2
        PCO2            -8.96 -27.07 -18.11  CO2
        Quartz          -0.05  -4.08  -4.03  SiO2
        SiO2(am)        -1.44  -4.08  -2.64  Si1.000O2.000
        Wollastonite     0.73  14.51  13.78  CaSiO3

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End of simulation.
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Reading input data for simulation 17.
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        TITLE 17 Liquid solid ration 1700
        USE solution 1
        USE equilibrium_phases 17
        SAVE equilibrium_phases 18
        END
-----
TITLE
-----

 17 Liquid solid ration 1700

----------------------------------------
Beginning of batch-reaction calculations.
```

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 17. Pure-phase assemblage after simulation 16.

-------------------------------Phase assemblage--------------------------------

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca(OH)2	-4.11	18.60	22.71	0.000e+000	0.000e+000	
Calcite	0.00	-8.47	-8.47	3.177e-003	3.375e-003	1.982e-004
CSH(0.1)	-1.15	-2.22	-1.07	0.000e+000	0.000e+000	
CSH(0.2)	-0.93	-0.36	0.56	0.000e+000	0.000e+000	
CSH(0.3)	-0.73	1.50	2.23	0.000e+000	0.000e+000	
CSH(0.4)	-0.55	3.36	3.91	0.000e+000	0.000e+000	
CSH(0.5)	-0.38	5.22	5.60	0.000e+000	0.000e+000	
CSH(0.6)	-0.24	7.08	7.31	0.000e+000	0.000e+000	
CSH(0.7)	-0.11	8.94	9.04	0.000e+000	0.000e+000	
CSH(0.8)	-0.02	10.79	10.82	0.000e+000	0.000e+000	
CSH(0.833)	-0.03	11.41	11.44	0.000e+000	0.000e+000	
CSH(0.9)	-0.00	14.06	14.06	2.300e-003	2.589e-003	2.895e-004
CSH(1.0)	0.00	14.51	14.51	5.976e-004	4.739e-005	-5.502e-004
CSH(1.1)	-0.10	14.89	14.98	0.000e+000	0.000e+000	
CSH(1.2)	-0.24	15.20	15.44	0.000e+000	0.000e+000	
CSH(1.3)	-0.41	15.46	15.87	0.000e+000	0.000e+000	
CSH(1.4)	-0.59	15.68	16.27	0.000e+000	0.000e+000	
CSH(1.5)	-0.77	15.87	16.64	0.000e+000	0.000e+000	
CSH(1.6)	-0.94	16.04	16.99	0.000e+000	0.000e+000	
CSH(1.7)	-1.11	16.20	17.30	0.000e+000	0.000e+000	
CSH(1.8)	-1.27	16.33	17.60	0.000e+000	0.000e+000	
SiO2(am)	-1.44	-4.08	-2.64	0.000e+000	0.000e+000	

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
C	1.810e-005	1.810e-006
Ca	6.255e-004	6.255e-005
Na	2.000e-003	2.000e-004
Si	2.286e-003	2.286e-004

----------------------------Description of solution----------------------------

pH = 10.963 Charge balance
pe = -5.572 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 3.631e-003
Mass of water (kg) = 1.000e-001
Total alkalinity (eq/kg) = 3.215e-003
Total CO2 (mol/kg) = 1.810e-005
Temperature (deg C) = 25.000
Electrical balance (eq) = -6.687e-016
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 18
Total H = 1.110200e+001
Total O = 5.551623e+000

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
HO-	9.976e-004	9.338e-004	-3.001	-3.030	-0.029
H+	1.156e-011	1.089e-011	-10.937	-10.963	-0.026
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
C(-4)	9.728e-033				
CH4	9.728e-033	9.736e-033	-32.012	-32.012	0.000
C(4)	1.810e-005				

```
          CO3-2          9.355e-006  7.247e-006   -5.029   -5.140   -0.111
          CaCO3          6.953e-006  6.959e-006   -5.158   -5.157    0.000
          CHO3-          1.785e-006  1.675e-006   -5.748   -5.776   -0.028
          CaCHO3+         9.616e-009  9.021e-009   -8.017   -8.045   -0.028
          CO2            3.716e-011  3.719e-011  -10.430  -10.430    0.000
Ca             6.255e-004
          Ca+2           6.032e-004  4.670e-004   -3.220   -3.331   -0.111
          CaSiH3O4+       8.632e-006  8.086e-006   -5.064   -5.092   -0.028
          CaCO3          6.953e-006  6.959e-006   -5.158   -5.157    0.000
          CaHO+          6.698e-006  6.274e-006   -5.174   -5.202   -0.028
          CaCHO3+         9.616e-009  9.021e-009   -8.017   -8.045   -0.028
H(0)           2.586e-014
          H2             1.293e-014  1.294e-014  -13.888  -13.888    0.000
Na             2.000e-003
          Na+            1.788e-003  1.675e-003   -2.748   -2.776   -0.028
          NaSiH3O4        2.124e-004  2.126e-004   -3.673   -3.672    0.000
          NaHO           2.524e-007  2.526e-007   -6.598   -6.598    0.000
O(0)           0.000e+000
          O2             0.000e+000  0.000e+000  -64.450  -64.450    0.000
Si             2.286e-003
          SiH3O4-         1.974e-003  1.849e-003   -2.705   -2.733   -0.028
          NaSiH3O4        2.124e-004  2.126e-004   -3.673   -3.672    0.000
          H4SiO4         8.288e-005  8.295e-005   -4.082   -4.081    0.000
          SiH2O4-2        8.798e-006  6.774e-006   -5.056   -5.169   -0.114
          CaSiH3O4+       8.632e-006  8.086e-006   -5.064   -5.092   -0.028

-----------------------------Saturation indices--------------------------------

          Phase              SI log IAP  log KT

          a-Cristobalite   -0.65   -4.08   -3.43  SiO2
          Aragonite        -0.16   -8.47   -8.31  CaCO3
          b-Cristobalite   -1.10   -4.08   -2.98  SiO2
          Ca(OH)2          -4.11   18.60   22.71  Ca(OH)2
          Calcite           0.00   -8.47   -8.47  CaCO3
          CH4            -29.17  -70.19  -41.02  CH4
          Chalcedony       -0.34   -4.08   -3.74  SiO2
          CSH(0.1)         -1.15   -2.22   -1.07  Ca0.100Si1.000O2.100:0.110H2O
          CSH(0.2)         -0.93   -0.36    0.56  Ca0.200Si1.000O2.200:0.220H2O
          CSH(0.3)         -0.73    1.50    2.23  Ca0.300Si1.000O2.300:0.330H2O
          CSH(0.4)         -0.55    3.36    3.91  Ca0.400Si1.000O2.400:0.440H2O
          CSH(0.5)         -0.38    5.22    5.60  Ca0.500Si1.000O2.500:0.550H2O
          CSH(0.6)         -0.24    7.08    7.31  Ca0.600Si1.000O2.600:0.661H2O
          CSH(0.7)         -0.11    8.94    9.04  Ca0.700Si1.000O2.700:0.771H2O
          CSH(0.8)         -0.02   10.79   10.82  Ca0.800Si1.000O2.800:0.881H2O
          CSH(0.833)       -0.03   11.41   11.44  Ca0.833Si1.000O2.833:0.917H2O
          CSH(0.9)         -0.00   14.06   14.06  Ca1.000Si1.111O3.222:1.093H2O
          CSH(1.0)          0.00   14.51   14.51  Ca1.000Si1.000O3.000:1.084H2O
          CSH(1.1)         -0.10   14.89   14.98  Ca1.000Si0.909O2.818:1.076H2O
          CSH(1.2)         -0.24   15.20   15.44  Ca1.000Si0.833O2.666:1.070H2O
          CSH(1.3)         -0.41   15.46   15.87  Ca1.000Si0.769O2.538:1.065H2O
          CSH(1.4)         -0.59   15.68   16.27  Ca1.000Si0.714O2.428:1.060H2O
          CSH(1.5)         -0.77   15.87   16.64  Ca1.000Si0.667O2.334:1.056H2O
          CSH(1.6)         -0.94   16.04   16.99  Ca1.000Si0.625O2.250:1.053H2O
          CSH(1.7)         -1.11   16.20   17.30  Ca1.000Si0.588O2.176:1.049H2O
          CSH(1.8)         -1.27   16.33   17.60  Ca1.000Si0.556O2.112:1.047H2O
          Graphite        -16.43  -48.63  -32.19  C
          H2              -10.78  -10.78   -0.00  H2
          Lime            -13.97   18.60   32.56  CaO
          O2              -61.56   21.56   83.13  O2
          PCO2             -8.96  -27.07  -18.11  CO2
          Quartz           -0.05   -4.08   -4.03  SiO2
          SiO2(am)         -1.44   -4.08   -2.64  Si1.000O2.000
          Wollastonite      0.73   14.51   13.78  CaSiO3

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End of simulation.
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------------------------------------
Reading input data for simulation 18.
```

```
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        TITLE 18 Liquid solid ration 1800
        USE solution 1
        USE equilibrium_phases 18
        SAVE equilibrium_phases 19
        END
-----
TITLE
-----

 18 Liquid solid ration 1800

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 18.   Pure-phase assemblage after simulation 17.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -4.35   18.36   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 3.375e-003 3.573e-003 1.983e-004
        CSH(0.1)       -0.96   -2.03   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.76   -0.19    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.59    1.64    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.43    3.48    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.29    5.31    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.16    7.15    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.06    8.98    9.04 0.000e+000          0.000e+000
        CSH(0.8)        0.00   10.82   10.82 0.000e+000 1.503e-004 1.503e-004
        CSH(0.833)     -0.01   11.42   11.44 0.000e+000          0.000e+000
        CSH(0.9)        0.00   14.06   14.06 2.589e-003 2.249e-003-3.403e-004
        CSH(1.0)       -0.02   14.49   14.51 4.739e-005         -4.739e-005
        CSH(1.1)       -0.14   14.84   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.30   15.14   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.49   15.38   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.68   15.60   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.87   15.78   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -1.05   15.94   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.22   16.08   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.39   16.21   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.23   -3.87   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        C             1.775e-005  1.775e-006
        Ca            6.914e-004  6.914e-005
        Na            2.000e-003  2.000e-004
        Si            2.751e-003  2.751e-004

----------------------------Description of solution-----------------------------

                                pH  =  10.822     Charge balance
                                pe  =  -5.431     Adjusted to redox equilibrium
                    Activity of water  =   1.000
                       Ionic strength  =  3.789e-003
                   Mass of water (kg)  =  1.000e-001
               Total alkalinity (eq/kg)  =  3.348e-003
                    Total CO2 (mol/kg)  =  1.775e-005
                   Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -3.650e-013
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
```

```
                          Iterations  =  17
                            Total H  = 1.110202e+001
                            Total O  = 5.551734e+000

----------------------------Distribution of species----------------------------

                                                 Log      Log       Log
         Species          Molality    Activity  Molality  Activity    Gamma

         HO-            7.220e-004  6.749e-004   -3.141   -3.171   -0.029
         H+             1.602e-011  1.507e-011   -10.795  -10.822   -0.027
         H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
C(-4)         1.691e-032
         CH4            1.691e-032  1.693e-032   -31.772  -31.771    0.000
C(4)          1.775e-005
         CO3-2           8.534e-006  6.578e-006   -5.069   -5.182   -0.113
         CaCO3           6.953e-006  6.959e-006   -5.158   -5.157    0.000
         CHO3-           2.245e-006  2.103e-006   -5.649   -5.677   -0.028
         CaCHO3+         1.332e-008  1.248e-008   -7.875   -7.904   -0.028
         CO2            6.457e-011  6.462e-011   -10.190  -10.190    0.000
Ca            6.914e-004
         Ca+2           6.678e-004  5.145e-004   -3.175   -3.289   -0.113
         CaSiH3O4+       1.132e-005  1.059e-005   -4.946   -4.975   -0.029
         CaCO3           6.953e-006  6.959e-006   -5.158   -5.157    0.000
         CaHO+           5.340e-006  4.996e-006   -5.272   -5.301   -0.029
         CaCHO3+         1.332e-008  1.248e-008   -7.875   -7.904   -0.028
H(0)          2.586e-014
         H2             1.293e-014  1.294e-014   -13.888  -13.888    0.000
Na            2.000e-003
         Na+            1.753e-003  1.641e-003   -2.756   -2.785   -0.029
         NaSiH3O4        2.473e-004  2.475e-004   -3.607   -3.606    0.000
         NaHO           1.786e-007  1.788e-007   -6.748   -6.748    0.000
O(0)          0.000e+000
         O2             0.000e+000  0.000e+000   -64.450  -64.450    0.000
Si            2.751e-003
         SiH3O4-         2.349e-003  2.197e-003   -2.629   -2.658   -0.029
         NaSiH3O4        2.473e-004  2.475e-004   -3.607   -3.606    0.000
         H4SiO4          1.363e-004  1.364e-004   -3.866   -3.865    0.000
         CaSiH3O4+       1.132e-005  1.059e-005   -4.946   -4.975   -0.029
         SiH2O4-2        7.597e-006  5.819e-006   -5.119   -5.235   -0.116

----------------------------Saturation indices---------------------------------

         Phase            SI log IAP  log KT

         a-Cristobalite   -0.43   -3.87   -3.43  SiO2
         Aragonite       -0.16   -8.47   -8.31  CaCO3
         b-Cristobalite   -0.88   -3.87   -2.98  SiO2
         Ca(OH)2         -4.35   18.36   22.71  Ca(OH)2
         Calcite          0.00   -8.47   -8.47  CaCO3
         CH4            -28.93  -69.95  -41.02  CH4
         Chalcedony       -0.13   -3.87   -3.74  SiO2
         CSH(0.1)         -0.96   -2.03   -1.07  Ca0.100Si1.000O2.100:0.110H2O
         CSH(0.2)         -0.76   -0.19    0.56  Ca0.200Si1.000O2.200:0.220H2O
         CSH(0.3)         -0.59    1.64    2.23  Ca0.300Si1.000O2.300:0.330H2O
         CSH(0.4)         -0.43    3.48    3.91  Ca0.400Si1.000O2.400:0.440H2O
         CSH(0.5)         -0.29    5.31    5.60  Ca0.500Si1.000O2.500:0.550H2O
         CSH(0.6)         -0.16    7.15    7.31  Ca0.600Si1.000O2.600:0.661H2O
         CSH(0.7)         -0.06    8.98    9.04  Ca0.700Si1.000O2.700:0.771H2O
         CSH(0.8)          0.00   10.82   10.82  Ca0.800Si1.000O2.800:0.881H2O
         CSH(0.833)       -0.01   11.42   11.44  Ca0.833Si1.000O2.833:0.917H2O
         CSH(0.9)          0.00   14.06   14.06  Ca1.000Si1.111O3.222:1.093H2O
         CSH(1.0)         -0.02   14.49   14.51  Ca1.000Si1.000O3.000:1.084H2O
         CSH(1.1)         -0.14   14.84   14.98  Ca1.000Si0.909O2.818:1.076H2O
         CSH(1.2)         -0.30   15.14   15.44  Ca1.000Si0.833O2.666:1.070H2O
         CSH(1.3)         -0.49   15.38   15.87  Ca1.000Si0.769O2.538:1.065H2O
         CSH(1.4)         -0.68   15.60   16.27  Ca1.000Si0.714O2.428:1.060H2O
         CSH(1.5)         -0.87   15.78   16.64  Ca1.000Si0.667O2.334:1.056H2O
         CSH(1.6)         -1.05   15.94   16.99  Ca1.000Si0.625O2.250:1.053H2O
         CSH(1.7)         -1.22   16.08   17.30  Ca1.000Si0.588O2.176:1.049H2O
         CSH(1.8)         -1.39   16.21   17.60  Ca1.000Si0.556O2.112:1.047H2O
```

```
        Graphite      -16.19  -48.39  -32.19  C
        H2            -10.78  -10.78   -0.00  H2
        Lime          -14.21   18.36   32.56  CaO
        O2            -61.56   21.56   83.13  O2
        PCO2           -8.72  -26.83  -18.11  CO2
        Quartz          0.16   -3.87   -4.03  SiO2
        SiO2(am)       -1.23   -3.87   -2.64  Si1.000O2.000
        Wollastonite    0.71   14.49   13.78  CaSiO3

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End of simulation.
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------------------------------------
Reading input data for simulation 19.
------------------------------------

        TITLE 19 Liquid solid ration 1900
        USE solution 1
        USE equilibrium_phases 19
        SAVE equilibrium_phases 20
        END
-----
TITLE
-----

 19 Liquid solid ration 1900

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 19.   Pure-phase assemblage after simulation 18.

-------------------------------Phase assemblage--------------------------------

                                                 Moles in assemblage
        Phase            SI log IAP  log KT    Initial     Final     Delta

        Ca(OH)2        -4.35   18.36   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 3.573e-003 3.772e-003 1.983e-004
        CSH(0.1)       -0.96   -2.03   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.76   -0.19    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.59    1.64    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.43    3.48    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.29    5.31    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.16    7.15    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.06    8.98    9.04 0.000e+000          0.000e+000
        CSH(0.8)        0.00   10.82   10.82 1.503e-004 3.479e-004 1.976e-004
        CSH(0.833)     -0.01   11.42   11.44 0.000e+000          0.000e+000
        CSH(0.9)        0.00   14.06   14.06 2.249e-003 1.823e-003-4.255e-004
        CSH(1.0)       -0.02   14.49   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.14   14.84   14.98 0.000e+000          0.000e+000
        CSH(1.2)       -0.30   15.14   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.49   15.38   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.68   15.60   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.87   15.78   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -1.05   15.94   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.22   16.08   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.39   16.21   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.23   -3.87   -2.64 0.000e+000          0.000e+000

-----------------------------Solution composition-------------------------------

        Elements         Molality     Moles

        C              1.775e-005  1.775e-006
        Ca             6.914e-004  6.914e-005
```

```
        Na            2.000e-003  2.000e-004
        Si            2.751e-003  2.751e-004

----------------------------Description of solution----------------------------

                                pH  =  10.822     Charge balance
                                pe  =  -5.410     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.789e-003
                     Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  3.348e-003
                     Total CO2 (mol/kg)  =  1.775e-005
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -2.410e-016
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  17
                             Total H  = 1.110202e+001
                             Total O  = 5.551734e+000

----------------------------Distribution of species----------------------------

                                                 Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-           7.220e-004  6.749e-004   -3.141   -3.171   -0.029
        H+            1.602e-011  1.507e-011  -10.795  -10.822   -0.027
        H2O           5.551e+001  9.999e-001    1.744   -0.000    0.000
C(-4)         1.151e-032
        CH4           1.151e-032  1.152e-032  -31.939  -31.938    0.000
C(4)          1.775e-005
        CO3-2          8.534e-006  6.578e-006   -5.069   -5.182   -0.113
        CaCO3          6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CHO3-          2.245e-006  2.103e-006   -5.649   -5.677   -0.028
        CaCHO3+        1.332e-008  1.248e-008   -7.875   -7.904   -0.028
        CO2           6.457e-011  6.462e-011  -10.190  -10.190    0.000
Ca            6.914e-004
        Ca+2           6.678e-004  5.145e-004   -3.175   -3.289   -0.113
        CaSiH3O4+       1.132e-005  1.059e-005   -4.946   -4.975   -0.029
        CaCO3          6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CaHO+          5.340e-006  4.996e-006   -5.272   -5.301   -0.029
        CaCHO3+        1.332e-008  1.248e-008   -7.875   -7.904   -0.028
H(0)          2.349e-014
        H2            1.175e-014  1.176e-014  -13.930  -13.930    0.000
Na            2.000e-003
        Na+           1.753e-003  1.641e-003   -2.756   -2.785   -0.029
        NaSiH3O4       2.473e-004  2.475e-004   -3.607   -3.606    0.000
        NaHO           1.786e-007  1.788e-007   -6.748   -6.748    0.000
O(0)          0.000e+000
        O2            0.000e+000  0.000e+000  -64.367  -64.366    0.000
Si            2.751e-003
        SiH3O4-        2.349e-003  2.197e-003   -2.629   -2.658   -0.029
        NaSiH3O4       2.473e-004  2.475e-004   -3.607   -3.606    0.000
        H4SiO4         1.363e-004  1.364e-004   -3.866   -3.865    0.000
        CaSiH3O4+       1.132e-005  1.059e-005   -4.946   -4.975   -0.029
        SiH2O4-2       7.597e-006  5.819e-006   -5.119   -5.235   -0.116

------------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite   -0.43   -3.87   -3.43  SiO2
        Aragonite       -0.16   -8.47   -8.31  CaCO3
        b-Cristobalite   -0.88   -3.87   -2.98  SiO2
        Ca(OH)2         -4.35   18.36   22.71  Ca(OH)2
        Calcite          0.00   -8.47   -8.47  CaCO3
        CH4           -29.09  -70.12  -41.02  CH4
        Chalcedony       -0.13   -3.87   -3.74  SiO2
        CSH(0.1)         -0.96   -2.03   -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)         -0.76   -0.19    0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)         -0.59    1.64    2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)         -0.43    3.48    3.91  Ca0.400Si1.000O2.400:0.440H2O
```

```
        CSH(0.5)        -0.29    5.31    5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.16    7.15    7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.06    8.98    9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         0.00   10.82   10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.01   11.42   11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         0.00   14.06   14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.02   14.49   14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.14   14.84   14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.30   15.14   15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.49   15.38   15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.68   15.60   16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.87   15.78   16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -1.05   15.94   16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.22   16.08   17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.39   16.21   17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -16.28  -48.47  -32.19  C
        H2             -10.82  -10.82   -0.00  H2
        Lime           -14.21   18.36   32.56  CaO
        O2             -61.48   21.65   83.13  O2
        PCO2            -8.72  -26.83  -18.11  CO2
        Quartz           0.16   -3.87   -4.03  SiO2
        SiO2(am)        -1.23   -3.87   -2.64  Si1.000O2.000
        Wollastonite     0.71   14.49   13.78  CaSiO3

------------------
End of simulation.
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------------------------------------
Reading input data for simulation 20.
------------------------------------

        TITLE 20 Liquid solid ration 2000
        USE solution 1
        USE equilibrium_phases 20
        SAVE equilibrium_phases 21
        END
-----
TITLE
-----

 20 Liquid solid ration 2000

----------------------------------------
Beginning of batch-reaction calculations.
----------------------------------------

Reaction step 1.

Using solution 1.NaHCO3 100g
Using pure phase assemblage 20.   Pure-phase assemblage after simulation 19.

-------------------------------Phase assemblage--------------------------------

                                          Moles in assemblage
        Phase            SI log IAP  log KT   Initial     Final     Delta

        Ca(OH)2        -4.35   18.36   22.71 0.000e+000          0.000e+000
        Calcite         0.00   -8.47   -8.47 3.772e-003 3.970e-003 1.983e-004
        CSH(0.1)       -0.96   -2.03   -1.07 0.000e+000          0.000e+000
        CSH(0.2)       -0.76   -0.19    0.56 0.000e+000          0.000e+000
        CSH(0.3)       -0.59    1.64    2.23 0.000e+000          0.000e+000
        CSH(0.4)       -0.43    3.48    3.91 0.000e+000          0.000e+000
        CSH(0.5)       -0.29    5.31    5.60 0.000e+000          0.000e+000
        CSH(0.6)       -0.16    7.15    7.31 0.000e+000          0.000e+000
        CSH(0.7)       -0.06    8.98    9.04 0.000e+000          0.000e+000
        CSH(0.8)        0.00   10.82   10.82 3.479e-004 5.455e-004 1.976e-004
        CSH(0.833)     -0.01   11.42   11.44 0.000e+000          0.000e+000
        CSH(0.9)        0.00   14.06   14.06 1.823e-003 1.398e-003-4.255e-004
        CSH(1.0)       -0.02   14.49   14.51 0.000e+000          0.000e+000
        CSH(1.1)       -0.14   14.84   14.98 0.000e+000          0.000e+000
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```
        CSH(1.2)       -0.30   15.14   15.44 0.000e+000          0.000e+000
        CSH(1.3)       -0.49   15.38   15.87 0.000e+000          0.000e+000
        CSH(1.4)       -0.68   15.60   16.27 0.000e+000          0.000e+000
        CSH(1.5)       -0.87   15.78   16.64 0.000e+000          0.000e+000
        CSH(1.6)       -1.05   15.94   16.99 0.000e+000          0.000e+000
        CSH(1.7)       -1.22   16.08   17.30 0.000e+000          0.000e+000
        CSH(1.8)       -1.39   16.21   17.60 0.000e+000          0.000e+000
        SiO2(am)       -1.23   -3.87   -2.64 0.000e+000          0.000e+000

----------------------------Solution composition--------------------------------

        Elements         Molality     Moles

        C              1.775e-005  1.775e-006
        Ca             6.914e-004  6.914e-005
        Na             2.000e-003  2.000e-004
        Si             2.751e-003  2.751e-004

----------------------------Description of solution-----------------------------

                                pH  =  10.822     Charge balance
                                pe  =  -5.410     Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  3.789e-003
                     Mass of water (kg)  =  1.000e-001
                Total alkalinity (eq/kg)  =  3.348e-003
                     Total CO2 (mol/kg)  =  1.775e-005
                    Temperature (deg C)  =  25.000
                 Electrical balance (eq)  = -3.743e-015
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  17
                              Total H  = 1.110202e+001
                              Total O  = 5.551734e+000

----------------------------Distribution of species-----------------------------

                                                Log      Log       Log
        Species          Molality    Activity  Molality  Activity    Gamma

        HO-            7.220e-004  6.749e-004   -3.141   -3.171   -0.029
        H+             1.602e-011  1.507e-011  -10.795  -10.822   -0.027
        H2O            5.551e+001  9.999e-001    1.744   -0.000    0.000
C(-4)         1.154e-032
        CH4            1.154e-032  1.155e-032  -31.938  -31.937    0.000
C(4)          1.775e-005
        CO3-2           8.534e-006  6.578e-006   -5.069   -5.182   -0.113
        CaCO3           6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CHO3-           2.245e-006  2.103e-006   -5.649   -5.677   -0.028
        CaCHO3+         1.332e-008  1.248e-008   -7.875   -7.904   -0.028
        CO2            6.457e-011  6.462e-011  -10.190  -10.190    0.000
Ca            6.914e-004
        Ca+2           6.678e-004  5.145e-004   -3.175   -3.289   -0.113
        CaSiH3O4+       1.132e-005  1.059e-005   -4.946   -4.975   -0.029
        CaCO3           6.953e-006  6.959e-006   -5.158   -5.157    0.000
        CaHO+           5.340e-006  4.996e-006   -5.272   -5.301   -0.029
        CaCHO3+         1.332e-008  1.248e-008   -7.875   -7.904   -0.028
H(0)          2.350e-014
        H2             1.175e-014  1.176e-014  -13.930  -13.930    0.000
Na            2.000e-003
        Na+            1.753e-003  1.641e-003   -2.756   -2.785   -0.029
        NaSiH3O4        2.473e-004  2.475e-004   -3.607   -3.606    0.000
        NaHO           1.786e-007  1.788e-007   -6.748   -6.748    0.000
O(0)          0.000e+000
        O2             0.000e+000  0.000e+000  -64.367  -64.367    0.000
Si            2.751e-003
        SiH3O4-         2.349e-003  2.197e-003   -2.629   -2.658   -0.029
        NaSiH3O4        2.473e-004  2.475e-004   -3.607   -3.606    0.000
        H4SiO4         1.363e-004  1.364e-004   -3.866   -3.865    0.000
        CaSiH3O4+       1.132e-005  1.059e-005   -4.946   -4.975   -0.029
        SiH2O4-2        7.597e-006  5.819e-006   -5.119   -5.235   -0.116
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-----------------------------Saturation indices-------------------------------

        Phase            SI log IAP  log KT

        a-Cristobalite  -0.43  -3.87  -3.43  SiO2
        Aragonite       -0.16  -8.47  -8.31  CaCO3
        b-Cristobalite  -0.88  -3.87  -2.98  SiO2
        Ca(OH)2         -4.35  18.36  22.71  Ca(OH)2
        Calcite          0.00  -8.47  -8.47  CaCO3
        CH4            -29.09 -70.12 -41.02  CH4
        Chalcedony      -0.13  -3.87  -3.74  SiO2
        CSH(0.1)        -0.96  -2.03  -1.07  Ca0.100Si1.000O2.100:0.110H2O
        CSH(0.2)        -0.76  -0.19   0.56  Ca0.200Si1.000O2.200:0.220H2O
        CSH(0.3)        -0.59   1.64   2.23  Ca0.300Si1.000O2.300:0.330H2O
        CSH(0.4)        -0.43   3.48   3.91  Ca0.400Si1.000O2.400:0.440H2O
        CSH(0.5)        -0.29   5.31   5.60  Ca0.500Si1.000O2.500:0.550H2O
        CSH(0.6)        -0.16   7.15   7.31  Ca0.600Si1.000O2.600:0.661H2O
        CSH(0.7)        -0.06   8.98   9.04  Ca0.700Si1.000O2.700:0.771H2O
        CSH(0.8)         0.00  10.82  10.82  Ca0.800Si1.000O2.800:0.881H2O
        CSH(0.833)      -0.01  11.42  11.44  Ca0.833Si1.000O2.833:0.917H2O
        CSH(0.9)         0.00  14.06  14.06  Ca1.000Si1.111O3.222:1.093H2O
        CSH(1.0)        -0.02  14.49  14.51  Ca1.000Si1.000O3.000:1.084H2O
        CSH(1.1)        -0.14  14.84  14.98  Ca1.000Si0.909O2.818:1.076H2O
        CSH(1.2)        -0.30  15.14  15.44  Ca1.000Si0.833O2.666:1.070H2O
        CSH(1.3)        -0.49  15.38  15.87  Ca1.000Si0.769O2.538:1.065H2O
        CSH(1.4)        -0.68  15.60  16.27  Ca1.000Si0.714O2.428:1.060H2O
        CSH(1.5)        -0.87  15.78  16.64  Ca1.000Si0.667O2.334:1.056H2O
        CSH(1.6)        -1.05  15.94  16.99  Ca1.000Si0.625O2.250:1.053H2O
        CSH(1.7)        -1.22  16.08  17.30  Ca1.000Si0.588O2.176:1.049H2O
        CSH(1.8)        -1.39  16.21  17.60  Ca1.000Si0.556O2.112:1.047H2O
        Graphite       -16.28 -48.47 -32.19  C
        H2             -10.82 -10.82  -0.00  H2
        Lime           -14.21  18.36  32.56  CaO
        O2             -61.48  21.65  83.13  O2
        PCO2            -8.72 -26.83 -18.11  CO2
        Quartz           0.16  -3.87  -4.03  SiO2
        SiO2(am)        -1.23  -3.87  -2.64  Si1.000O2.000
        Wollastonite     0.71  14.49  13.78  CaSiO3

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End of simulation.
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Reading input data for simulation 21.
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End of run.
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