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Japan Atomic Energy Agency (JAEA) has been developing a number of databases that formed an important basis for the H12 performance assessment (PA) of high-level radioactive waste disposal in Japan. These databases include extensive compilations of sorption K_d data (JNC-SDB). JAEA has been and is continuing to improve and update the JNC-SDB in view of potential future data needs. This on-going program has focused on testing the usefulness of the existing databases for possible applications to K_d-setting and keeping the databases up-to-date and assuring the desired quality level.

In the present report, a first test and illustration was performed regarding the applicability of the JNC-SDB to the derivation of K_d-values for Th, Np, Cs, and Se valid for Horonobe rocks. The original experimental data selected from the JNC-SDB were converted to the application conditions using the semi-quantitative scaling procedures. To illustrate the effect of the scaling procedures, and of related uncertainties, on the magnitude of the derived K_d-values, scaling procedures taking into account mineralogy as well as surface and solution speciation were applied sequentially, and all results were discussed in detail. This K_d-setting exercise allowed to predict the magnitude of K_d-values under the in-situ conditions, however the availability of experimental data that closely match the application conditions is limited for various reasons. The JNC-SDB and its classification scheme made it possible to obtain a quick overview of the available data, and to have suitable access to the respective K_d values.

Keywords: Sorption Database, Distribution Coefficient, K_d, K_d-setting, Horonobe Rocks, HLW Disposal

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収着データベースの適用による幌延岩石に対する収着分配係数の設定

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日本原子力研究開発機構（JAEA）では，高レベル放射性廃棄物地層処分研究開発の第２次取りまとめにおいて，その重要な基礎と位置づけられる幾つかのデータベースを整備してきた。これらのデータベースの一つが収着分配係数 K_d に関するデータベース（JNC-SDB）である。JAEA では，将来の性能評価におけるニーズへ対応するため，JNC-SDB の改良・更新を継続的に実施してきている。この開発計画の一環として，現在，実際の地質環境に対する K_d 設定におけるデータベース適用の有効性検討，データベースに含まれる K_d データの信頼度評価を進めている。

本報告書では，JNC-SDB を適用して，幌延岩石に対する Th, Np, Cs および Se の K_d 設定を試み，その適用性に関する検討を行った。JNC-SDB から関連する K_d データの抽出を行い，この K_d データ取得された実験条件と適用条件の違いを，半定量的なスケーリングファクターとして変換することで K_d が導出された。このスケーリングファクターによる設定手法と関連する不確実性が，K_d 設定に及ぼす影響を評価するため，評価対象となる岩石の鉱物組成，表面特性，核種の溶存化学種等の条件を考慮したスケーリングファクターを段階的に導出し，K_d 設定に及ぼす影響を詳細に評価した。この K_d 設定手法は，実際の地質環境条件での K_d の大きさを予測する手法として有効であるが，評価対象条件への関連付けが可能な実験データの存在に依存するなど，その適用範囲はある程度限定される。また，今回の K_d 設定への適用を通じて，JNC-SDB 及びその信頼度評価が，利用可能な関連データ集を速やかに抽出し，参照すべきデータを適切に選定する上で，有効な手法であることが確認された。

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1. Introduction

The Japan Atomic Energy Agency (JAEA) has been developing a number of databases that formed an important basis for the H12 performance assessment (PA) of high-level nuclear waste disposal in Japan (JNC, 2000). These databases include extensive compilations of sorption K_d data (JNC-SDB) (Shibutani et al., 1999). JAEA has been and is continuing to improve and update its PA-related databases, in particular the databases on sorption of radionuclides in view of potential future data needs (Suyama et al., 2004, Saito et al., 2007).

As part of this on-going development program, JAEA has focused on

- testing the usefulness of the existing databases to K_d-setting for possible PA-related applications;
- keeping the databases up-to-date and assuring the desired quality level.

JAEA is constructing of a generic underground research laboratory (URL) in a mudstone host formation at Horonobe, north-western Hokkaido, Japan. In this context, a first test and illustration was performed regarding the applicability of the JNC-SDB to the derivation of K_d-values for Th, Np, Cs, and Se valid for Horonobe rocks.

The purpose of this task is to test and illustrate the usefulness of the classified part of the JNC-SDB (see Ochs et al., 2007, Saito et al., 2008) for setting reference K_d-values in a site-specific situation. In general terms, this was done by applying the classified and reliable entries for Th, Np, Cs, and Se in the JNC-SDB to the derivation of K_d-values and their uncertainties for the two geological formations (Wakkanai, Koetoi) relevant for the Horonobe URL.

The related experimental K_d data selected from the JNC-SDB were converted to K_d-values for the application conditions using the semi-quantitative scaling procedures as described in the chaper 2. To illustrate the effect of the scaling procedures, and of related uncertainties, on the magnitude of the derived K_d-values, scaling procedures taking into account mineralogy as well as surface and solution speciation were applied sequentially, and all results were discussed in the chapter 3.

2. Approach for application of the SDB to K_d-setting for the Horonobe rocks

The NEA Sorption Project (NEA, 2005; see also Ochs et al., 2007) acknowledged and pointed out that distribution coefficients (K_d-values) are highly conditional parameters. The magnitude of K_d -values depends critically on all relevant geochemical conditions, such as number/type of surface sites, solution pH, and concentration of relevant dissolved solution components (e.g., carbonate). Because of the conditional nature of sorption data, K_d-values to be used in PA-calculations (or other assessments) need to correspond to the specific conditions that characterize the respective PA-setting. In principle, PA-specific K_d-values (henceforth termed "reference K_d") can be made available by two different approaches (which can be combined):

(a) sorption data can be measured under the specific (in situ) conditions that are relevant for PA to give directly reference K_d-values;

(b) sorption data that are available for other and/or simplified conditions can be used to derive reference K_d-values.

In most PA-applications, it is not possible to make sufficient data available by approach (a); often because the relevant geological/geochemical compartments are not directly accessible. Therefore, data from simplified or approximated systems are typically relied on (approach b). In order to derive reference K_d-values, the following approaches can be envisaged:

- In the past, reference K_d-values were often recommended on the basis of expert opinion, which typically was not quantitative and not transparent.
- TEA Sorption Project (NEA, 2005) recommends the use of thermodynamic sorption models (TSMs), because such models are the only method that takes both sorption reactions and solution speciation of radionuclides fully quantitatively into account. Unfortunately, reliable TSMs are only available for a very limited number of radionuclide (RN)/mineral systems.
- In the absence of reliable TSMs, Bradbury and Baeyens (1997, 2003a) and Ochs and Talerico (2004; see also Ochs et al., 2006) used semi-quantitative estimation procedures that explicity consider differences in sorption capacity as well as surface and solution speciation.

The present illustration of deriving reference K_d-values of Cs, Np, Se, and Th specific for the Wakkanai and Koetoi formations followed the general approach of Ochs and Talerico (2004). As primary data source, reliable entries in the JNC-SDB for sorption on relevant minerals were considered. Below, the various aspects of this approach are presented as follows:

- The general aspects considered are summarized in section 2.1;
- the relevant conditions for the K_d-setting and the sources of experimental data are discussed in sections 2.2 and 2.3, respectively;

- the detailed procedures that were used to scale experimental sorption data to the reference conditions are described in section 2.4;
- the treatment of data uncertainty is discussed in section 2.5.

2.1 General aspects

In general, the following sequence of steps was followed:

(1) The conditions relevant for K_d-setting (application conditions) were defined. In the present case, the data for the mineralogy of the Wakkanai and Koetoi formation and for the corresponding groundwater composition (see section 2.2 for details) were accepted as provided by JAEA; no uncertainties with respect to these data were considered.

(2) The speciation expected under the conditions of the reference groundwater from the borehole (HDB-6) was calculated for the RN considered to obtain an overview regarding relevant oxidation states and to evaluate the relative importance of the different solution constituents for RN speciation.

(3) Focussing on the data compiled in the JNC-SDB, a search was conducted for sets of original experimental data that
   i) are reliable,
   ii) had been obtained under conditions (mineralogy of the solid substrate, solution pH, etc.) that are similar enough to the present application conditions,
   iii) include sufficient sorption edge and/or isotherm data to allow an evaluation of important trends.

   In this context, the following remark should be made: Data derived for other PA-settings (given e.g. in compilations) are of limited use, because they typically represent derived data and are therefore associated with much larger uncertainties than experimental data which correspond directly to a given set of chemical conditions.

(4) Sets of experimental data for K_d-setting were selected. Where possible, several data sets were used that cover a certain variation of the most relevant conditions.

(5) The selected experimental data were converted to application conditions using the procedures described in section 2.4.

2.2 Relevant geochemical conditions for K_d-setting

The mineralogy and groundwater composition accepted for the present report as being representative for the Wakkanai and Koetoi formation is given in Appendix III. The Wakkanai and Koetoi formations are diatomaceous rocks (mudstone, shale) that contain approximately 20% clay minerals, predominantly 2:1 clays. According to the information provided in Appendix III, the corresponding groundwater (borehole HDB-6) is reducing and rich in dissolved carbonate.

In terms of sorption of the four RNs considered here, the clay mineral fraction (smectite, chlorite, kaolinite, illite) was considered to be the active component in case of both the Koetoi and Wakkanai formation. As a first approximation, the other minerals (silica/quartz, feldspars, pyrite) were considered to make no contribution to RN sorption.

Further details, such as assumptions made regarding cation exchange capacity (CEC), solution properties etc. are given at the relevant places of this report.

2.3 Data sources

Highest priority was given to the data contained in the JNC-SDB. The respective solid phase groups in the SDB included all groups that contained data on whole mudstone or similar complex substrates as well as groups that contained data for RN sorption on the relevant clay minerals smectite, chlorite, kaolinite, and illite. Specifically:

- mudstone
- bentonite
- other minerals.

These related K_d data in the JNC-SDB were classified according to the classification guideline, revision 4b (May 19, 2005); the respective results are documented in Saito et al.(2008). Where it appeared that the data sets contained in the JNC-SDB are not of sufficient quality and/or do not address a sufficiently wide range of chemical conditions, they were supplemented with experimental data sets available in the open literature. If such additional datasets were used, they were also classified according to the classification guideline, see also Saito et al.(2008).

Specific issues related to individual datasets used for K_d-setting are discussed in the sections dealing with the derivation of K_d-values for each individual RN (sections 3.1 to 3.4).

2.4 Conversion to application conditions

In general, the approach chosen by Ochs and Talerico (2004) was followed (see also Ochs et al., 2007; as well as Bradbury and Baeyens, 1997, 2003a). The scaling factors accounting for differences in sorption capacity and surface as well as solution chemistry in the experimental vs. application conditions are discussed below in sections 2.4.2 – 2.4.4. Beforehand, the more general issue of using batch data to derive K_d-values for intact rock are discussed in the following section.

2.4.1 Use of batch data to derive K_d-values for intact rock

Practically all sorption measurements are carried out in dilute suspensions. Reliable sorption measurements in intact material are extremely scarce due to experimental difficulties. This situation necessitates the use of sorption data from batch experiments to derive K_d-values valid for intact rock; i.e., the transfer of data from low to very high solid/water ratios.

While K_d is highly dependent on the chemical conditions (taken into account by the scaling factors discussed below in sections 2.4.2 – 2.4.4), it is in principle independent of the solid/water ratio, and no data conversion is necessary given that the available specific surface area or sorption site density per unit mass as well as the solution composition remain constant. This can be very difficult to assess in a fractured/heterogeneous rock (e.g., granite), but appears to be nearly established in the case of homogeneous porous media such as bentonite.

With regard to the available surface area, Bradbury and Baeyens (1998) measured similar BET values for loose and compacted (2000 kg/m^3) MX-80 and Montigel bentonites. The diffusion data by Kato et al. (1995) also suggest that no reduction of sorption-available surface area takes place upon compaction. Based on such evidence, it was concluded by e.g. Ochs et al. (2001), Bradbury and Baeyens (2002) and Ochs and Talerico (2004) that batch data can be directly applied to compacted systems, provided that any differences in solution composition are accounted for. Ochs and Talerico (2004; see also Ochs et al., 2007) derived K_d-values valid for compacted bentonite for a large number of RN, using scaling factors similar to the ones discussed below. From these K_d-values and D_e for HTO, they calculated the respective D_a-values and compared these to independent experimental D_a-values. This comparison indicated that no scaling factor is necessary to account for the transfer from batch to compacted systems, as long as the respective chemical conditions are taken into account.

From the information available, it is estimated for the present application that the relevant rock type (diatomaceous mudstone) can be treated in a 1st approximation as homogeneous porous medium, and that CF-exp→intact is unity. In particular, the following findings by Kemp et al. (2002) support this concept:

- First, fractures appear to be concentrated in discrete zones which may be the main areas of fault movement.
- More importantly, most fractures appear to be unmineralized, and in the few cases where mineralization was observed, only calcite was identified as infill. In terms of sorption, this means that fractures can be treated by using the bulk mineral composition.

2.4.2 Sorption capacity, mineralogy

The working hypothesis for the present K_d-setting is that the sorption capacity of the Wakkanai and Koetoi formation is determined by the respective content of clay minerals (smectite, chlorite, kaolinite, as well as illite). All available evidence suggests that these clay minerals are able to sorb radionuclides through surface complexation and ion exchange (see e.g. NEA, 2005).

To scale selected experimental sorption data to the present application conditions (i.e., a solid substrate representative of the Wakkanai and Koetoi formation in equilibrium with HDB-6 groundwater, a conversion or scaling factor (CF-min) based on the relative amount or sorption capacity of clay minerals present in a defined volume of the selected experimental systems vs. in the Wakkanai and Koetoi formation needed to be defined. Generally, the scaling factor CF-min can be based on:

- the exchange capacity of both solids, CEC (CF-CEC), section;
- the relative amount of clay minerals (CF-%clay),
- the relative (BET) surface area (CF-BET).

In the case of sorption by clays, such a factor can be based on the ratio of CEC per unit mass for the experimental and application system. Based on Table 5 in Kemp et al. (2002), an average CEC of about 20 meq/100 g can be estimated for a depth of about 200-400 m below ground in the boreholes HDB-1 and HDB-2. Some variation in the data can be observed, and it is also not clear, based on the information presently available to us, whether these data are compatible with the groundwater data from borehole HDB-6.

As a rough check, the CEC was therefore also calculated by considering typical CEC values for pure smectite, chlorite, kaolinite and illite and calculating a mass-weighted mean value for the mineralogical composition of the Wakkanai and Koetoi formation. The results are given in Appendix III and show that the above value is reasonable.

Scaling on the basis of CEC values was done using the following relation:

$$\text{CF-CEC} = \text{CEC (application)} / \text{CEC (data source)} \tag{2.1}$$

In this relation, CEC is used as a relative measure for total site density, based on the reasonable assumption that the density of surface complexation (edge) sites is proportional to the CEC.

Because of the uncertainty regarding CEC and the assumed relationship between CEC and surface complexation site density, data derivation was additionally based on the ratio of total clay content in both systems (eq. 2.2). Further, the BET-surface area was also considered (eq. 2.3) to obtain some information of the sensitivity of the conversion factor for sorption capacity on the actual measure used.

$$\text{CF-\%clay} = \text{\%clay (application)} / \text{\%clay (data source)} \tag{2.2}$$

$$\text{CF-BET} = \text{BET (application)} / \text{BET (data source)} \tag{2.3}$$

2.4.3 pH

The pH is the most critical geochemical parameter for the sorption of most elements as it determines

- the speciation of the sorbing element itself, in particular hydrolysis (relevant for Th, Np), as well as protonation-deprotonation in case of anions such as Se,
- the protonation-deprotonation of the surface complexation sites,
- the speciation and solubility behavior of major ligands (e.g., carbonate) and major cations (e.g., Ca) that have an important influence on sorption through complexation (e.g., carbonate complexation of Th and Np) and competition (e.g., Ca with Cs, but possibly also carbonate in case of Se).

For this reason, to the degree possible data sources were selected that allowed the selection of sorption data at pH values corresponding to the application conditions (in the data derivation tables in Appendix II, this is indicated by a pH-conversion factor of 1). Where this is not possible, scaling to the appropriate application pH can be done on the basis of additional data for the same RN, such as sorption edges on a montmorillonite. In such cases, scaling to the application pH was done using the conversion factor defined below:

$$\text{CF-pH} = K_d\,(\text{pH application}) / K_d\,(\text{pH data source}) \tag{2.4}$$

In contrast to Bradbury and Baeyens (2003a), CF-pH was interpreted by Ochs and Talerico (2004) as a factor addressing the overall surface/solution speciation. Thus, the conversion factor for additional radionuclide speciation effects defined below (CF-spec) addresses only those effects not included in CF-pH. In particular, CF-spec does not take into account hydrolysis.

2.4.4 Effects on radionuclide surface/solution speciation by dissolved ligands and major cations

As pointed out above, dissolved ligands and major cations can have a significant influence on radionuclide sorption. Therefore, scaling of K_d to application conditions should in principle be carried out in all cases where the source data correspond to a solution composition that is significantly different from that of the HDB-6 reference groundwater (which is nearly always the case). Only thermodynamic sorption models are capable of consistently taking into account all speciation effects, but such models are available for a few elements only. For the present application, it was attempted to account for variable solution compositions in a semi-quantitative, but fully traceable fashion. The following different processes need to be considered:

- RN sorption may decrease due to the formation of aqueous complexes with dissolved ligands (in case of Th, Np) or with dissolved cations (in case of Se). This is taken into account by the conversion factor CF-spec. For Cs with its simple solution chemistry, this is not a relevant process.

- In case of Cs (and probably also Se) sorption takes mainly place through weak (electrostatic) interaction (cation or anion exchange on the layer surface, outer-sphere complexation at the edge surface). Here, RN sorption may also decrease due to competition by major cations (Cs) or anions (Se). This is taken into account by the conversion factor CF-cmp.

CF-spec:

The formal definition of the factor CF-spec is accepted from Ochs and Talerico (2004).

$$\text{CF-spec} = F_{sorb}\text{ (application) / } F_{sorb}\text{ (data source)} \tag{2.5a}$$

where

$$F_{sorb} = (RN_{tot} - RN_{cmp}) / RN_{tot} \tag{2.5b}$$

with RN_{tot} as the total dissolved concentration of a given radionuclide, and RN_{cmp} as the total concentration of all dissolved RN complexes evaluated as being competitive with regard to sorption. However, the application of this factor is not straightforward:

- First, the conversion factor CF-pH will already include one or more of the effects of speciation. The following differences in speciation are therefore not included in the factor CF-spec., as the effects would be counted twice:
    - As pointed out above, effects of RN hydrolysis will already be included in CF-pH.
    - Complexation of Th or Np with the carbonate ion (CO_3^{2-}) can differ between two solutions because of i) different total carbonate concentrations, or ii) different pH values leading to different concentrations of CO_3^{2-} even when total carbonate levels are the same. In case ii), the effect will also be included in the conversion factor CF-pH.
- Second, several elements, especially IV- and higher-valent actinides are known or suspected to form mixed hydroxo-carbonato complexes. By analogy, the formation of ternary RN-carbonato surface complexes at the clay edge sites can be assumed. For some cases, the existence of such complexes has been confirmed by spectroscopy (e.g. for U(VI) sorption on iron oxide by Bargar et al., 2001). Therefore, it is highly questionable in these cases whether the presence of carbonate should be counted as a competitive factor. This situation is complicated further by the uncertainties regarding the existence and importance of various simple and mixed An(IV)-carbonato complexes (see discussions in Yui et al., 1999; Lemire et al., 2001; Hummel et al., 2002; Guillaumont et al., 2003). Therefore, scaling of K_d to account for speciation was carefully evaluated for both Np and Th. As a basis for further evaluation, CF-spec was calculated twice in these cases, taking into account or neglecting competition by complexation involving carbonate ions.
    - CF-spec/a: Complexation of a radionuclide with carbonate is viewed as being fully competitive with respect to sorption.

- o CF-spec/b: Complexation of a radionuclide with carbonate is viewed as being not competitive with respect to sorption.

CF-cmp:

As pointed out at the beginning of this section, CF-cmp is only relevant in the case of the relatively weakly sorbing Cs and Se. Th and Np sorb mainly through the formation of strong inner-sphere surface complexes and are not notably influenced by competing cations such as Ca. CF-cmp is defined as

$$\text{CF-cmp} = \Sigma_{\text{competing cations/anions}}\,(\text{data source}) / \Sigma_{\text{competing cations/anions}}\,(\text{application}) \qquad (2.6)$$

2.4.5 Summary of scaling factors

Overall scaling of experimental sorption data to the application conditions defined for the Wakkanai and Koetoi formations is done by combining the individual conversion factors discussed above:

$$\text{CF-overall} = \text{CF-min} \times \text{CF-pH} \times \text{CF-spec} \times \text{CF-cmp} \qquad (2.7)$$

As discussed, some of these may only be important in some cases (such as CF-cmp in the case of Cs). For reasons of transparency, and to illustrate the effects of the various scaling factors, the overall scaling procedures listed below were applied in a step-wise fashion:

$$\text{CF-1} = \text{CF-min} \times \text{CF-pH} \qquad (2.8a)$$

$$\text{CF-2} = \text{CF-min} \times \text{CF-pH} \times \text{CF-spec} \qquad (2.8b)$$

$$\text{CF-3} = \text{CF-min} \times \text{CF-pH} \times \text{CF-spec} \times \text{CF-cmp} \qquad (2.8c)$$

where CF-min is represented by each CF-CEC, CF-%clay, and CF-BET. Also, both CF-spec/a and CF-spec/b were compared where relevant. The results for each scaling step are given in Appendix II. The recommended procedure for K_d-setting as well as the resulting values for the Wakkanai and Koetoi formations are discussed in sections 3.1-3.4.

2.5 Uncertainties

The treatment of uncertainties follows closely the approach taken by Ochs and Talerico (2004). There is no obvious reason for choosing between quantifying uncertainties as an error on a linear scale (i.e, K_d ± error) vs. a logarithmic scale (i.e, log K_d ± log error). Following the procedure chosen in NEA (2005), the latter type of representation was adopted for the present purpose. On a linear scale, this translates to K_d multiplied/divided by an uncertainty factor UF:

$$\log K_d\ (\text{upper, lower limit}) = \log K_d \pm \log \text{uncertainty, or} \qquad (2.9a)$$

$$K_d\ \text{upper limit} = K_d \times \text{UF and } K_d\ \text{lower limit} = K_d / \text{UF} \qquad (2.9b)$$

Uncertainties are generally evaluated in a way that makes it likely that the indicated limits encompass all possible values. Where data are more uncertain, this is discussed specifically.
The following uncertainty factors (log errors) are considered:

(1) Uncertainty of source data (UF-starting K_d)

For good quality experimental data an uncertainty of log K_d ± 0.2 log units is proposed based on NEA (2005). This gives an uncertainty factor

→ UF-starting $K_d = 1.6$

(2) Uncertainty introduced by scaling to application conditions

- scaling for sorption capacity (UF-min):

  It is estimated that CEC can be measured within an uncertainty of ca. 10 %, and that SOH density can be scaled via CEC again within an uncertainty of ca. 20%. This gives an overall uncertainty of ± 30% or about a factor of 2 between highest and lowest value. This uncertainty is also accepted for sorption capacity conversions based on %clay or BET. Thus, we propose

  → UF-min = 1.4

- scaling for pH (UF-pH):

  This is only needed where CF-pH $\neq 1$, i.e., where scaling to application pH had to be done via additional data and equation (2.4). Because CF-pH contains uncertainties of two K_d values (which are read off at pH-data source and pH-application, respectively), an uncertainty log starting $K_d \pm 2 \times 0.2$ log units is used:

  → UF-pH conversion = 2.5

- scaling for speciation (UF-spec):

  Following the evaluation by Hummel et al. (2002), who propose a factor of 2 between highest and lowest value, a UF-spec = 1.4 is used. Note, however, that this is the uncertainty associated with the use of a given, self-consistent TDB. If certain species are missing or erroneous (see e.g. the discussion on mixed actinide OH-CO_3 complexes above), uncertainties could be much higher. Also, this UF does not take into account any inappropriate evaluation of CF-spec, as discussed in section 2.1.4.4 (this had to be evaluated with consistency examinations and "what-if" calculations using CF-spec/a and CF-spec/b as described above, rather than via formal uncertainties).

- scaling for competition by major cations/anions (UF-cmp):

  It is assumed that the sum of cation or anion concentration in each system can be known or predicted within 10%, giving an overall uncertainty of about ± 20%.

  → UF-cmp = 1.2

- scaling for batch data to conditions in intact rock (UF-exp→ intact):

  Arguments for the applicability of the K_d-values derived in this report to intact rock are presented in section 2.4.1. Accordingly, CF-exp→intact is unity and no UF is proposed for this conversion. This holds for application conditions as defined in section 2.2. Therefore, an additional uncertainty factor could be introduced to acknowledge uncertainties in the application conditions (i.e., in the mineral and porewater composition). Such an uncertainty factor can only be defined following a detailed assessment of the conditions (and their possible variations) to be considered in K_d-setting. For the present illustrative exercise in K_d-setting, such uncertainties have not been considered.

3 Derivation of K_d-values for the Horonobe rocks

K_d-values applicable to the conditions of the Wakkanai and Koetoi formations at the projected location of JAEA's Horonobe URL were derived using the estimation methods described above. The approach taken with regard to selecting sources of experimental data is discussed in section 2.3.

3.1 Thorium

Thorium is an actinide element that exists exclusively in the +IV state in aqueous solutions. Like other actinide elements, it shows a strong tendency to form hydroxo- and carbonate-, but also fluoro- and sulfate complexes. Based on the available evidence (see references cited below), sorption of Th on clay minerals is taking place mainly through inner-sphere surface complexation. Because of the strong tendency toward hydrolysis, sorption edges of Th(IV) on clay minerals reach a plateau already at very low pH values (see data in Bradbury and Baeyens, 2003a).

The relevant groundwater (HDB-6) for K_d-setting is given in Appendix III, the corresponding speciation of Th calculated with the JNC-TDB_011213c2 is completely dominated by the species $Th(OH)_3CO_3^-$ (see Appendix II). This is confirmed by additional calculations using the thermodynamic data given in Hummel et al. (2002). Note that questions regarding the identity of the mixed hydroxo-carbonato complex are not definitely resolved (Hummel et al., 2002). Therefore, the magnitude of the scaling factor CF-spec/a, and thus of the corresponding calculated K_d, will also be dependent on the thermodynamic data in the underlying TDB.

In the JNC-SDB database six references are found for the solid phase groups *mudstone* and *other minerals* (see Appendix I). According to the guideline for evaluating and categorizing the reliability of K_d values in the JNC-SDB (revision 4b, May 2005; Saito et al., 2005), the data obtained by Legoux et al. (1992) and Östhols (1995) were considered to be the most reliable data sources. The classification of the data for Th, as well as an evaluation regarding the consistency among each other and with independent data is provided in Saito et al. (2008). Lieser et al. (1990) do not give sufficient detail regarding the mineral composition of the sediment used.

Legoux et al. (1992) measured the sorption of Thorium in a synthetic (reconstituted) groundwater, equilibrated with a substrate (mineral soil) consisting of 9% clay minerals (illite, smectite, kaolinite and palygorskite) and 91% quartz. Mineral composition, final solution composition and pH are comparable, to a first approximation, with the corresponding parameters considered for the Koetoi or Wakkanai formations. Unfortunately, Legoux et al. (1992) measured only one datapoint.

Because the JNC-SDB does not contain any further datasets that are suitable for deriving K_d-values of Th, according to our evaluation, the sorption data obtained by Bradbury and Baeyens (2003a) were used in addition (see Figure 3.1 in Saito et al.(2008)). They present a sorption edge of thorium obtained on SWy-1 montmorillonite in a simple electrolyte (0.1 M $NaClO_4$). Although this dataset is not included in the present version of the JNC-SDB, it was classified in the same way as the entries of the JNC-SDB (see Saito et al., 2008).

For illustration, and because amorphous SiO_2 appears to be the main component of some rocks at the Horonobe URL site, the data by Östhols (1995) were considered. Östhols (1995) studied the sorption of thorium from a simple $NaClO_4$ solution at acidic pH on amorphous SiO_2 (Aerosil OX 200) as substrate. In comparison to the values derived from the data by Legoux et al. (1992) and Bradbury and Baeyens (2003a), the K_d-values derived from the data by Östhols (1995) show the importance of the clay mineral fraction in the Wakkanai and Koetoi formation for Th sorption. Thus, the K_d-values derived from the data by Östhols (1995) can be viewed as minimum values representative of rock layers that consist exclusively of silica.

The results of the derivation of K_d-values for the present application conditions are given in Table 3.1. The values derived on the basis of the scaling factor CF-2b (%clay) are considered to be the most relevant. Treating Th complexation with carbonate as fully competitive would lead to extremely small values in some systems and is not considered to be meaningful.

As is to be expected based on the underlying data (see discussion above as well as section 3.2.1 in Saito, 2008), the K_d-values derived on the basis of the different selected experimental datasets spread over about two orders of magnitude. The K_d-values derived from the data by Legoux et al. (1992) are not considered further, because only one experimental datapoint is provided by these authors. Finally, the K_d-values derived from the data by Östhols (1995) and Baston et al. (1992a) are preferred over K_d-values derived from the data by Bradbury and Baeyens, based on the greater similarity to the URL-application conditions in terms of aqueous chemistry. Assuming the contributions of clay minerals and silica to be additive results in a recommended K_d value of 0.88 m^3/kg. The lower limit is taken from the calculations based on Baston et al. (1992a), the upper limit from the calculations based on Bradbury and Baeyens (2003a). This gives, taking into account all uncertainties potentially introduced by data scaling (uncertainty factors UF) the following mean values for Wakkanai/Koetoi formation:

recommended K_d *= 0.88* m^3/kg*, lower limit: 0.03* m^3/kg*, upper limit ca. 180* m^3/kg

The recommended values are roughly in agreement with the recommended values for Np(IV). However, the spread in the data is not satisfying and should be improved. Based on the data presently contained in the JNC-SDB, this situation cannot easily be resolved, however. It is therefore recommended to include further data, in particular data measured by PSI on Opalinus Clay samples.

Table 3.1: Overview of K_d-setting for Th. See section 2.4 and Appendix II for details

K_d-Derivation Th(IV) Legoux et al. (1992)

Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**
	HDB-6	**HDB-6**
Predicted K_d: CF-1 (CEC)	570.04	570.04
Pred. K_d: CF-1 (BET)	56.23	47.40
Pred. K_d: CF-1 (% clay)	218.52	171.01
Pred. K_d: CF-2a (CEC))	86.06	86.06
Pred. K_d: CF-2a (BET)	8.49	7.16
Pred. K_d: CF-2a (% clay)	32.99	25.82
Pred. K_d: CF-2b (CEC)	570.04	570.04
Pred. K_d: CF-2b (BET)	56.23	47.40
Pred. K_d: CF-2b (% clay)	218.52	171.01

K_d-Derivation Th(IV) Bradbury&Baeyens (2003)

Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**
	HDB-6	**HDB-6**
Pred. K_d: CF-1 (% clay)	57.77	45.21
Pred. K_d: CF-2a (% clay)	0.06	0.04
Pred. K_d: CF-2b (% clay)	57.77	45.21

K_d-Derivation Th(IV) Östhols (1995)

Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**
	HDB-6	**HDB-6**
Pred. K_d: CF-1 (% SiO_2) [1]	0.62	0.65
Pred. K_d: CF-2a (% SiO_2)	5.78E-07	6.08E-07
Pred. K_d: CF-2b (% SiO_2)	0.62	0.65
Pred. K_d: CF-1 (100% SiO_2)	1.09	1.09
Pred. K_d: CF-2a (100% SiO_2)	1.01E-06	1.01E-06
Pred. K_d: CF-2b (100% SiO_2)	1.09	1.09

[1] corresponding to ca. 57-60 % silica, see Appendix III

K_d-Derivation Th(IV) (Baston 1992a)

Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**
	HDB-6	**HDB-6**
Predicted K_d: CF-1 (CEC)	0.57	0.57
Pred. K_d: CF-1 (% clay)	0.26	0.20
Pred. K_d: CF-2a (CEC))	0.01	0.01
Pred. K_d: CF-2a (% clay)	0.01	4.18E-03
Pred. K_d: CF-2b (CEC)	0.57	0.57
Pred. K_d: CF-2b (% clay)	0.26	0.20

3.2 Neptunium

Neptunium is an actinide element that may exist in the +IV and +V oxidation state in normal aqueous solutions depending on the redox conditions. In terms of sorption and solubility, the behavior of the +IV-valent state can be viewed as being similar to that of Th as a first approximation. The chemical behavior of the +V-valent state differs significantly from that (cf. Lemire et al., 2001; Guillaumont et al, 2003), showing a less pronounced tendency towards hydrolysis and correspondingly higher solubility and lower sorption.

The speciation of Np(IV) in the carbonate-rich HDB-6 groundwater as calculated using the JNC-TDB_011213c2 is dominated by the $Np(OH)_2(CO_3)_2^{2-}$ complex (see Appendix III), no other species appear to be relevant. Note in this context that the JNC-TDB does contain mixed hydroxo-carbonato complexes, while Guillaumont et al. (2003) only confirm their existence but give no stability constants (reportedly due to the lack of sufficient reliable experimental data).

Appendix I gives an overview of the data sources considered. Under the solid phase groups *bentonite*, *mudstone* and *other minerals*, the JNC-SDB contains a large number of K_d values for the sorption of Np on silica, clays, and related minerals, as well as on a number of sediments. However, many of the entries refer to Np(V). Further, in most cases where Np(IV) is indicated, the redox conditions are not defined well enough. This had already become apparent in the classification for the entries in the *bentonite* group carried out previously (Ochs et al., 2007). No supplementary literature sources for the sorption of Np(IV) on relevant minerals could be found.

Within the solid phase group *mudstone*, the study by Lieser and Mühlenweg (1988) appeared to be the most promising. In all other cases, redox conditions are either oxidizing or not well enough defined to be useful for K_d-setting of Np(IV). Lieser and Mühlenweg (1988) used a reducing groundwater and confirmed the +IV oxidation state of Np with TTA extraction. However, the initial concentration of Np was not sufficiently low to avoid precipitation, and the respective entries are rated *unreliable*.

Therefore, the data by Baston et al. (1999) on Kunigel-V1 were selected for K_d-setting of Np(IV). This study contains the only reliable data for the sorption of Np(IV) on relevant minerals. Because of its relatively low proportion of clay minerals to silica, Kunigel-V1 is considered as a reasonably close surrogate for the relevant mudstones.

The results of the K_d-derivation are summarized in Table 3.2. Relying again on the scaling factor CF-2b (%clay), an average K_d-value of about 3.6 m^3/kg is calculated. This compares reasonably well with the value derived for Th. As in the case of Th, assuming that complexation with carbonate would be fully competitive with respect to sorption (CF-2a) would lead to very small, meaningless values. In the case of Np(IV), this is compounded by the uncertainties regarding the stability of mixed hydroxo-carbonato complexes.

Taking into account all uncertainties potentially introduced by data scaling (uncertainty factors UF), the following is obtained (mean values for Wakkanai/Koetoi formation):

recommended $K_d = 3.6\ m^3/kg$, *lower limit:* $0.5\ m^3/kg$, *upper limit* $27\ m^3/kg$

Because only one data source is available, the uncertainties are smaller than in the case of Th. While the data source appears to be reasonably well matched to the application conditions, the recommended values above should also be re-evaluated if any new results are obtained for Th (using e.g. further data available in the literature). Based on the information considered so far, it cannot be excluded with absolute certainty that sorption may be underestimated in the experiments by Baston and co-workers.

Table 3.2: Overview of K_d-setting for Np. See section 2.4 and Appendix II for details

Data source Baston et al. (1999): Smectite

Overview Pred. K_d [m^3/kg]	**Koetoi[3]**	**Wakkanai[3]**
	HDB-6	**HDB-6**
Pred. K_d: CF-1 (CEC)	2.73	2.73
Pred. K_d: CF-1 (%clay)	4.11	3.21
Pred. K_d: CF-2a (CEC)	0.12	0.12
Pred. K_d: CF-2a (% clay)	0.18	0.14
Pred. K_d: CF-2b (CEC)	2.73	2.73
Pred. K_d: CF-2b (% clay)	4.11	3.21

3.3 Cesium

As an alkaline element, Cesium exists almost exclusively as Cs^+ ion in aqueous solutions. Sorption on clay minerals takes place by ion exchange typically occurring on the layer surface. In the case of illitic clays, additional ion exchange sites with a higher affinity for Cs exist at the frayed edge sites (FES) of these minerals (Poinssot et al., 1999; see also the note by Ochs, 1997, and references therein). Due to steric reasons, only some cations (mainly K^+, NH_4^+, H^+) are able to compete with Cs for these sites.

An overview of the available data sources is provided in Appendix I. Under the solid phase groups *bentonite*, *mudstone* and *other minerals*, the JNC-SDB contains a large number of K_d values for the sorption of Cs on clays and related minerals including illite, as well as on a number of sediments.

Because of the important role that illite can play for Cs sorption, the data on illite by Gorgeon (1994) were selected for K_d derivation. As supplementary source dataset for illite, the data by Poinssot et al. (1999) were considered additionally. It is admitted that the simple solutions used as background electrolyte in these experiments, which contained only Na as major ion, represent somewhat of a disadvantage for K_d derivation. As most representative dataset for a smectite-dominated system, the data by Sato and Shibutani (1994) for Kunigel-V1 were selected from the JNC-SDB.

A summary of the results of the K_d-derivation is given in Table 3.3. Because Cs is sorbing via ion exchange, competition by other (major) cations for ion exchange sites needs to be taken into account. In the case of source data for smectite, simply all major cations need to be considered. On the other hand, Cs sorption on illite takes place mainly on the FES, as long as Cs is present in trace concentrations (Poinssot et al., 1999). Therefore, when source data for illite were used, calculations were done by considering (i) only competition by sufficiently small cations (K^+, NH_4^+) as well as (ii) by considering competition by all cations. Because the solutions in the experiments with illite contained only Na (based on the information available), approach (i) proved to be not feasible (the corresponding correction factors are meaningless, see Appendix II). It further appears from the data of Poinssot et al. (1999) that Cs sorption on the FES shows a small but distinct pH-dependence; this was accepted for the present K_d-derivation.

When K_d-values are being derived on the basis of sorption data for illite, the underlying assumption is that sorption of trace amounts of Cs occurs at the FES of illite. Therefore, the scaling factor CF-min should include only the proportion of illite (and not of the sum of all clay minerals) that is available in the rocks of the Wakkanai and Koetoi formations. This was also followed for the scaling factors CF-CEC and CF-BET.

Using the scaling factor CF-3a (%illite); i.e., assuming that Cs will sorb on illite and that all major cations may be competitive gives a mean K_d of about 1.1 m^3/kg. Applying the scaling factor CF-3 to the data of Sato and Shibutani (1994) results in much smaller values. The reason may be that the competition by major cations is overestimated in this case, because the difference in cation concentration between source and application system is very large in this case. However, this value is tentatively kept as lower limit (upper limit is based on illite).

Following the above, and taking into account all uncertainties potentially introduced by data scaling (uncertainty factors UF), the following is obtained (mean values for Wakkanai/Koetoi formation):

recommended $K_d = 1.1\ m^3/kg$*, lower limit:* $1\times10^{-4}\ m^3/kg$*, upper limit* $6\ m^3/kg$

Table 3.3: Overview of K_d-setting for Cs. See section 2.4 and Appendix II for details

Data source Gorgeon (1994): Illite

Overview Pred. K_d [m^3/kg]	Koetoi	Wakkanai
	HDB-6	HDB-6
Pred. K_d: CF-1 (CEC)	0.41	0.41
Pred. K_d: CF-1 (BET)	0.05	0.05
Pred. K_d: CF-1 (% clay)	0.72	0.56
Pred. K_d: CF-1 (% Illite)	0.22	0.22
Pred. K_d: CF-3 (CEC)	1.73	1.73
Pred. K_d: CF-3 (BET)	0.20	0.20
Pred. K_d: CF-3 (% clay)	3.02	2.36
Pred. K_d: CF-3 (% Illite)	0.92	0.92

Data source Sato and Shibutani (1994): Kunigel V1

Overview Pred. K_d [m^3/kg]	Koetoi	Wakkanai
	HDB-6	HDB-6
Pred. K_d: CF-1 (CEC)	0.28	0.28
Pred. K_d: CF-1 (BET)	0.14	0.12
Pred. K_d: CF-1 (% clay)	0.43	0.33
Pred. K_d: CF-3 (CEC)	3.21E-04	3.21E-04
Pred. K_d: CF-3 (BET)	1.56E-04	1.31E-04
Pred. K_d: CF-3 (%clay)	4.82E-04	3.77E-04

Data source PSI Report (1999): Illite

Overview Pred. K_d [m^3/kg]	0.01 M $NaClO_4$		0.1 M $NaClO_4$		1 M $NaClO_4$	
	Koetoi	Wakkanai	Koetoi	Wakkanai	Koetoi	Wakkanai
	HDB-6	HDB-6	HDB-6	HDB-6	HDB-6	HDB-6
Pred. K_d: CF-1 (CEC)	5.42	5.42	0.91	0.91	0.12	0.12
Pred. K_d: CF-1 (BET)	4.12	4.12	0.70	0.70	0.09	0.09
Pred. K_d: CF-1 (% clay)	58.38	45.69	9.85	7.71	1.24	0.97
Pred. K_d: CF-1 (% Illite)	17.77	17.77	3.00	3.00	0.38	0.38
Pred. K_d: CF-3a (CEC)	0.23	0.23	0.38	0.38	0.48	0.48
Pred. K_d: CF-3a (BET)	0.17	0.17	0.29	0.29	0.37	0.37
Pred. K_d: CF-3a (% clay)	2.46	1.92	4.14	3.24	5.21	4.08
Pred. K_d: CF-3a (% Illite)	0.75	0.75	1.26	1.26	1.59	1.59

3.4 Selenium

Selenium is a group-VI element. Dissolved Se species in aqueous solution can exist in the oxidation states +VI, +IV, and –II, depending on the redox state. Speciation calculations for Se in the HDB-6 groundwater using the JNC-TDB (see Appendix III) indicate that only Se(-II) is relevant under these conditions. The calculated speciation is very simple with HSe^{-1} as the only relevant species. However, it needs to be pointed out that many potentially relevant species of Se(-II) treated in Olin et al. (2005) are not included in the present version of the JNC-TDB. Inclusion of further Se species in the underlying TDB could change the results for Se given in this report.

While some information is available on the sorption behavior of the oxidized forms of Se (see the modeling exercise presented in NEA, 2005), very little is known for Se(-II) in terms of sorption reactions. In the absence of any evidence to the contrary, the following is assumed for the present application:

i) Sorption of HSe^{-1} takes place at the edge surface of clays, rather than at the layer surfaces carrying a permanent negative charge.

ii) The sorption behavior of HSe^{-1} can as a first approximation be assumed to be similar to that of the selenate anion (see NEA, 2005). This implies that HSe^{-1} forms only weakly bound outer-sphere complexes with the edge surface functional groups, and that these complexes are subject to competition by other dissolved cations, such as sulfate and carbonate species.

An overview of the data sources for Se is provided in Appendix I. Under the solid phase groups *bentonite*, *mudstone* and *other minerals*, the JNC-SDB contains mainly data obtained for Se(VI) or Se(IV) under oxidizing or ill-defined redox conditions. The only relevant data for the present application are given by Ticknor et al. (1988), who present sorption data for the sorption of Se(-II) on kaolinite and chlorite. No additional relevant data could be found in the open literature.

Table 3.4 and Figure 3.1 summarize the results of the K_d-derivation based on the sorption data by Ticknor et al. (1988). Based on the presently available information, it is estimated that the K_d-values derived from the data for chlorite are more representative for sorption onto the rocks of the Wakkanai and Koetoi formations, which appear to be dominated by 2:1 clays. However, it needs to be noted in this regard that the chlorite used by Ticknor et al. (1988) is reported to have a CEC of only 1.7 meq/100 g. Use of a more typical CEC for chlorite (about 25 meq/100 g) would lead to a decrease of the calculated K_d-values of about a factor of 20.

Based on the scaling factor CF-3 (%clay), and taking into account the data for both kaolinite and chlorite as well as all uncertainties potentially introduced by data scaling (uncertainty factors UF), the following is obtained (mean values for Wakkanai/Koetoi formation):

recommended $K_d = 8.2\times10^{-5}$ m^3/kg*, lower limit:* 7×10^{-6} m^3/kg*, upper limit* 9×10^{-4} m^3/kg

Table 3.4: Overview of K_d-setting for Se. See section 2.4 and Appendix II for details

Data source Ticknor et al. (1988): Kaolinite

	100% SCSSS[1]		10% SCSSS	
Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**
Kaolinite	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Pred. Kd: CF-1 (CEC)	0.01	0.01	0.02	0.02
Pred. Kd: CF-1 (BET)	0.01	4.72E-03	0.01	0.01
Pred. Kd: CF-1 (%clay)	1.91E-03	1.49E-03	2.99E-03	2.34E-03
Pred. Kd: CF-3 (CEC)	8.19E-04	8.19E-04	3.65E-04	3.65E-04
Pred. Kd: CF-3 (BET)	3.87E-04	3.26E-04	1.72E-04	1.45E-04
Pred. Kd: CF-3 (%clay)	1.32E-04	1.03E-04	5.87E-05	4.59E-05

Data source Ticknor et al. (1988): Chlorite

	100% SCSSS		10% SCSSS	
Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**
Chlorite	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Pred. Kd: CF-1 (CEC)	0.08	0.08	0.16	0.16
Pred. Kd: CF-1 (BET)	0.02	0.01	0.03	0.03
Pred. Kd: CF-1 (%clay)	1.66E-03	1.30E-03	3.22E-03	2.52E-03
Pred. Kd: CF-3 (CEC)	5.85E-03	5.85E-03	3.23E-03	3.23E-03
Pred. Kd: CF-3 (BET)	1.18E-03	9.96E-04	6.53E-04	5.50E-04
Pred. Kd: CF-3 (%clay)	1.14E-04	8.95E-05	6.32E-05	4.94E-05

1) Standard Canadian Shield Saline Solution

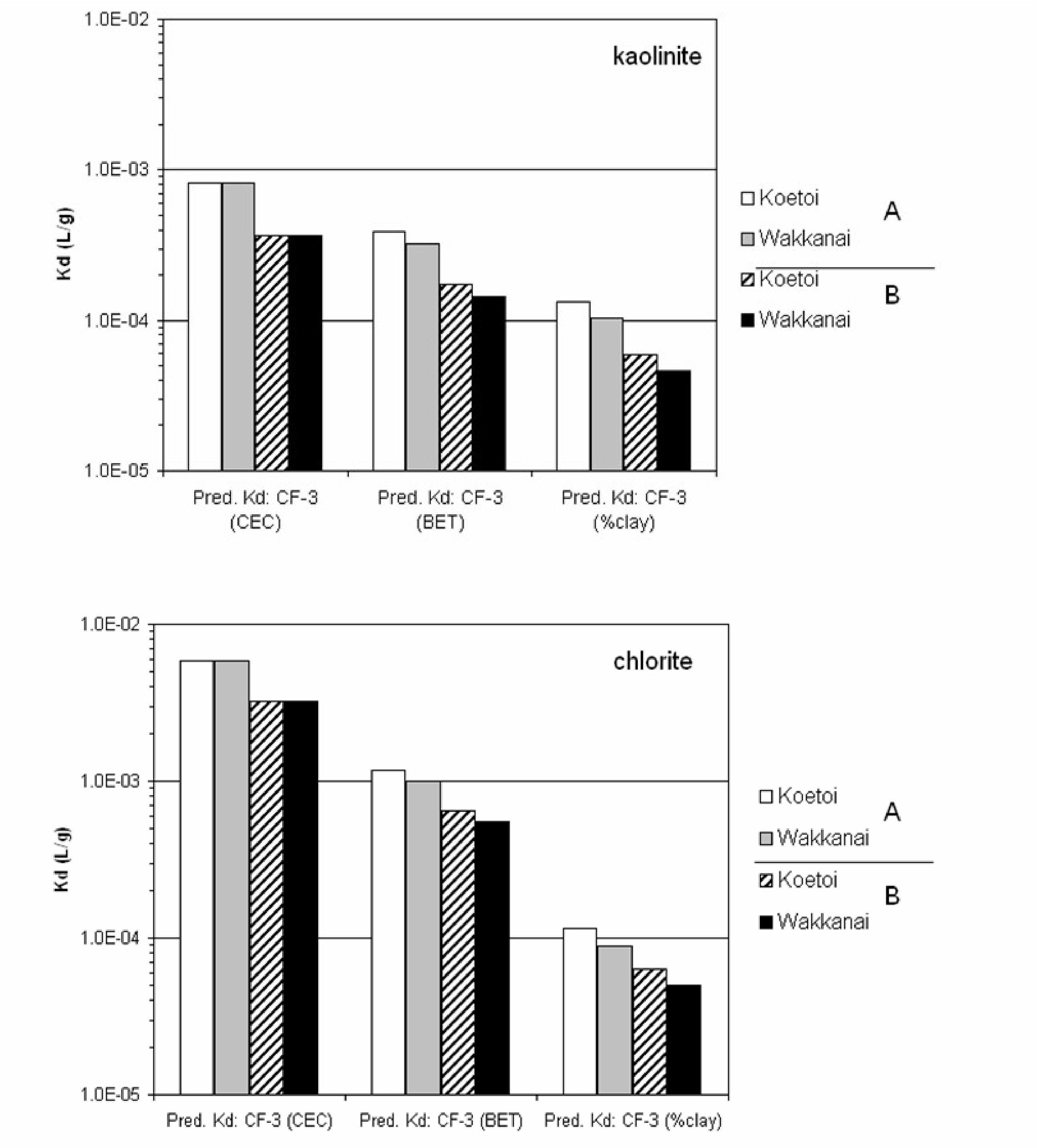

Figure 3.1: Summary of K_d-setting for Se. See Table 3.4 for numerical values and explanations (A = 100% SCSSS, B = 10% SCSSS).

4. Summary and recommendations

The present exercise in K_d-setting shows that;

- The scaling procedures coupled with the JNC-SDB is applicable to predict the magnitude of K_d-values under the in-situ conditions, however the availability of experimental data that closely match the application conditions is limited for various reasons
- The JNC-SDB is a very valuable tool, in particular, it allows to obtain a quick overview of the available data, and to have fast access to the respective experimental values.

On the basis of the experiences made in the present K_d-setting exercise, a number of recommendations can be made:

- The additional data sources used for the present K_d-setting exercise should be included in the JNC-SDB. A further improvement for better plotting options and/or to consult the original literature would be expected to allows to easily identify suitable datasets.
- The K_d-derivation clearly showed the potentially strong influence of calculated RN speciation under experimental and in-situ conditions on the outcome of the derivation procedures and calculations. It is therefore strongly recommended to update the JNC-TDB to include all up-to-date, relevant stability constants. This holds especially for Se.
- As the work at the foreseen site of the Horonobe URL progresses, the application (in-situ) conditions (mineralogy, groundwater composition) for the Wakkanai and Koetoi formations should be better defined and the respective uncertainties should be quantified.
- Finally, these approaches should be tested through the comparison with actual experimental data to be obtained for in-situ conditions in future experimental programs.

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Appendix I

Overview of sources for sorption data

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Sources of sorption data for thorium in JNC-SDB

Reference in JNC-SDB *1	Solid phase	Mineralogy reported	Solution	Soln. details	Remark	classification *2
Solid phase group bentonite						
Allard et al.(1979b)	bentonite/quartz(10:90)	—	groundwaters	yes	—	yes*
Baston et al.(1991)	clays	yes	cement waters	no	unsuitable solutions, not enough information (solution)	yes*
Bond and Tweed(1991)	clay	yes	cement waters	no	only modeling study	not evaluated
Ueta(1998)	kunigel V1	— —	distilled water, seawater, simple electrolyte	$NaHCO_3$	—	not evaluated
Solid phase group mudstone						
Legoux et al.(1992)	soil A	yes	synthetic groundwater	yes (Ref.)	used for K_d derivation	yes
Lieser et al.(1990)	sediments	no	sediment groundwater	no	not enough information (mineral, solution)	yes
Meier et al.(1994)	marl	no	sediment groundwater	no	not enough information (mineral, solution)	unreliable
Solid phase group other minerals						
Hunter et al.(1988)	goethite	no	UV irrad. seawater	no	not enough information (mineral, solution)	no
Östhols(1995)	SiO2 (Aerosil OX200)	—	simple electrolyte	$NaClO_4$	used for K_d derivation (minimal sorption)	yes
Righetto et al.(1988)	aluminium oxide	—	simple electrolyte	$NaClO_4$	mineral not relevant	no

* some datapoints unreliable

Supplementary sources of sorption data

Reference in JNC-SDB *1	Solid phase	Mineralogy reported	Solution	Sol. details	Remark	classification *2
Bradbury and Baeyens (2003a)	SWy-1 montmorillonite	yes	simple electrolyte	$NaClO_4$	used for K_d derivation	yes

*1) see JNC-SDB (http://migrationdb.jaea.go.jp)
*2) classification based on the guideline to evaluate the reliability of Kd data (see Ochs et al.,2007, Saito et al.,2008)

Sources of sorption data for neptunium in JNC-SDB

Reference in JNC-SDB *1	Solid phase	Mineralogy reported	Solution	Soln. details	Remark	classification *2
Solid phase group bentonite						
Allard et al.(1979b)	bentonite/quartz	—	groundwater	yes	not enough information (redox conditions)	yes
Ames et al.(1981)	smectite	no	synthetic groundwaters	yes	Np(V), oxidizing conditions	unreliable
Ashida et al.(1999)	smectite	no	simple electrolyte	NaCl	Np(IV), not enough information (mineral)	not evaluated*
Barney(1981)	basaltic mineral	no	synthetic groundwaters	yes	Np(IV)/(V), not enough information (mineral)	unreliable
Baston et al.(1997)	kunigel V1	—	deionized water	no	Np oxidation state not known	yes
Baston et al.(1999)	kunigel V1	—	deionized water	yes	Np(IV) (Ref.), redox conditions reducing, used for K_d derivation	yes
Gorgeon(1994)	illite, smectite	no	simple electrolytes	$NaClO_4$	Np oxidation state not known, aerobic conditions	yes
Higgo et al.(1983)	illite/kaolinite, smectite	no	seawater	no	not enough information (mineral, solution, redox conditions)	yes
Kitamura et al.(2002)	smectite	no	simple electrolyte	NaCl	Np(IV) or (V), redox conditions reducing, not enough information (mineral)	unreliable
Kozai et al.(1994)	kunipia F	—	simple electrolyte	$Ca/NaClO_4$	Np oxidation state not known, aerobic conditions, soln. conc. unknown	yes
Kozai et al.(1995)	bentonite, smectite	no	simple electrolyte	$NaClO_4$	not enough information (mineral, redox conditions)	unreliable
Kozai et al.(1996)	smectite	no	simple electrolyte	$NaClO_4$	not enough information (mineral, redox conditions)	unreliable
Meijer et al.(1990)	montmorillonite	no	distilled water	no	Np oxidation state not known, aerobic conditions	unreliable
Morgan et al.(1987)	bentonite	—	demineralized water	no	not enough information (mineral, solution, redox conditions)	unreliable
Ohe et al.(1993)	kunigel V1	yes	simple electrolytes	NaCl	Np(V)	yes
Relyea et al.(1978)	illite, kaolinite, montmorillonite, vermicullite	no	simple electrolytes	NaCl, $NaHCO_3$, $CaCl_2$	Np(V)	unreliable
Sakamoto et al.(1990)	bentonite	no	simple electrolytes	$NaClO_4$	Np(V)	not evaluated
Salter et al.(1981)	smectite	yes (Ref.)	groundwaters	yes	Np(V), oxidizing conditions	yes
Salter(1982)	bentonite	—	groundwater	no	Np oxidation state not known, not enough information (solution)	unreliable
Shade et al.(1994)	bentonite	—	simple electrolyte	HCl/NaOH	Np oxidation state not known, aerobic conditions	yes
Stammose et al.(1992)	clay	yes (Ref.)	simple electrolytes	$NaClO_4$	Np(V)	yes
Ticknor(1993)	illite, kaolinite	no	synthetic groundwaters	yes	Np oxidation state not known, aerobic conditions	yes
Torstenfelt et al.(1988)	bentonite, illite	no	groundwater	yes	Np oxidation state not known, aerobic conditions	yes
Tsukamoto et al.(1994)	kunigel V1	yes	simple electrolyte	no	Np(V)	unreliable
Yamaguchi et al.(1991)	kunibond	—	simple electrolytes	$NaClO_4$	not enough information (redox conditions)	yes*
Solid phase group mudstone						
Barney and Anderson(1979)	argillites	no	groundwater	no	not enough information (mineral, solution, redox conditions)	unreliable
Barney and Brown(1979)	argillites	no	synthetic groundwater	no	not enough information (mineral, solution, redox conditions)	unreliable
Berry et al.(1990a)	mudstone	no	synthetic groundwaters	yes	Np(V) (Ref.), not enough information (mineral, redox conditions)	unreliable
El-Naggar et al.(2000)	shale, silt	no	synthetic groundwater	no	Np(IV) or (V), not enough information (mineral, solution, redox condition)	unreliable
Higgo et al.(1987)	sediments	no	seawater	no	Np oxidation state not known, aerobic conditions, not enough information (mineral, solution)	unreliable
Kim et al.(1994)	marl & sandy sediments	no	groundwater	no	Np oxidation state not known, reducing conditions, not enough information (mineral, solution)	unreliable
Legoux et al.(1992)	soils	yes	synthetic groundwater	yes (Ref.)	Np(V) (Ref.)	unreliable
Lieser and Muhlenweg(1988)	sediments	no	natural groundwater	yes	Np(IV), not enough information (mineral)	unreliable
Mackenzie et al.(1983)	sediments	no	deionized water	no	Np oxidation state not known, aerobic conditions and positiv Eh values	unreliable
Sakamoto et al.(1990)	loam	no	simple electrolyte	$NaClO_4$	Np(V)	yes
Sakamoto(1994)	loam	no	simple electrolyte	$NaClO_4$	Np(V)	yes
Tachi et al.(1999a)	mudstone	no	distilled water	no	Np oxidation state not known, reducing conditions, not enough information (mineral, solution)	yes
Tanaka and Muraoka(1998)	soils	no	deionized water	yes	Np oxidation state not known, aerobic conditions	yes
Tanaka and Muraoka(1999)	soils	no	equilibrated solution	yes	Np(V)	unreliable
Tanaka et al.(1999)	soil	no	simple electrolyte	$NaNO_3$	Np(V)	unreliable
Solid phase group other minerals						
Francis and Bondietti(1979)	dolomite, gypsum	no	deionized water	no	Np(V)	no
Higgo et al.(1983)	amorphous Mn and Fe, birnessite/todorokite calcite, calcite/quartz	no	seawater	no	not enough information (mineral, solution, redox conditions)	no
Kaukonen et al.(1993)	hornblendite	yes	groundwater, allard water	yes	Np(IV)/(V), oxidizing and reducing conditions, mineral not relevant	no
Nakayama and Sakamoto(1991)	biotite, goethite hematite, magnetite	no	simple electrolyte	$NaNO_3$	Np(V)	no
Nakayama et al.(1986)	quartz	—	distilled water	no	Np oxidation state not known, aerobic conditions, not enough information (solution)	no
Relyea et al.(1978)	albite, anorthite, augite, etc.	no	simple electrolytes	NaCl, $NaHCO_3$, $CaCl_2$	Np(V)	no
Ticknor(1993)	calcite, chlorite, epidote, goethite, etc.	no	synthetic groundwaters	yes	Np oxidation state not known, aerobic conditions, not enough information (minerals)	no
Torstenfelt et al.(1988)	albite, anorthite, hornblendite, microcline	no	groundwater	yes	Np oxidation state not known, aerobic conditions, not enough information (minerals)	no
Meijer et al.(1990)	hematite, goethite, romanechite, etc.	no	distilled water	no	Np oxidation state not known, aerobic conditions, not enough information (mineral, solution)	no
Shade et al.(1994)	iron silicate	no	simple electrolyte	HCl/NaOH	Np oxidation state not known, aerobic conditions, not enough information (mineral)	no
Tanaka et al.(2002)	loess	no	deionized water	no	Np(V)	no

* some datapoints unreliable

Supplementary sources of sorption data

none

*1) see JNC-SDB (http://migrationdb.jaea.go.jp)
*2) classification based on the guideline to evaluate the reliability of Kd data (see Ochs et al.,2007, Saito et al.,2008)

Sources of sorption data for cesium in JNC-SDB

Reference in JNC-SDB *1	Solid phase	Mineralogy reported	Solution	Soln. details	Remark	classification *2
Solid phase group bentonite						
Allard et al.(1979b)	bentonite/quartz(10:90)	—	simple electrolytes	yes	—	not evaluated
Ames et al.(1980)	clay, smectite	no	groundwaters, simple electr	no	not enough information (mineral, solution)	unreliable
Ames et al.(1981)	smectite	no	groundwaters, simple electr	yes	not enough information (mineral)	unreliable
Andersson et al.(1983)	bentonite, illite, kaolinite	no	groundwater	yes	not enough information (minerals)	yes
Barney(1981)	basaltic mineral	no	synthetic groundwaters	yes	not enough information (minerals)	unreliable
Benischek et al.(1992b)	bentonite, calzonite, clays montmorillonite, smectite	no	cement solution	no	unsuitable solution, not enough information (mineral, solution)	unreliable
Berry et al.(1988a)	clays	no	synthetic clay water	no	not enough information (mineral, solution)	unreliable
Cho et al.(1996)	bentonite, illite, kaolinite	no	synthetic waters	yes	not enough information (mineral)	unreliable
Erdal et al.(1977)	bentonite	—	groundwaters	yes (Ref.)	not enough information (solution)	yes
Eriksen and Jansson(1996)	bentonite	—	groundwaters	yes	—	not evaluated
Gorgeon(1994)	illite, kaolinite, smectite	yes (Ref.)	simple electrolytes	NaCl	used for K_d derivation	yes
Hsu and Chang(1994)	bentonite	-	deionized water	no	not enough information (solution)	yes
Inoue and Morisawa(1975)	clays	no	tap water	yes	not enough information (mineral)	unreliable
Jedinakova-Krizova(1998)	bentonite	—	synthetic groundwater	yes	—	yes
Kawaguchi et al.(1989)	bentonite	—	distilled water	yes	—	yes
Konishi et al.(1988)	bentonite	—	deionized water, synthetic g	no	not enough information (solution)	yes*
Murali and Mathur(1999)	bentonite	—	natural groundwater	no	not enough information (solution)	unreliable
Muurinen et al.(1985)	MX-80	— —	synthetic groundwater with EDTA, simple electrolytes	yes	—	yes
Nowak(1979)	bentonite	—	simple electrolyte	yes	—	no
Ohnuki et al.(1992)	smectite	no	chloride solution	no	not enough information (mineral, solution)	unreliable
Ohnuki(1994b)	kaolinite	no	simple electrolyte	NaOAc	not enough information (mineral)	yes
Onodera et al.(1994)	smectite	no	nitrous acid solution, iron ion solution	HNO_3	not enough information (mineral)	yes*
Poinssot et al. 1999	illite	yes	simple electrolytes	NaClO4	used for Kd derivation	no
Oscarson et al.(1994)	bentonite	—	synthetic groundwater	yes	—	unreliable
Relyea et al.(1978)	kaolinite, montmorillonite, illite, vermicullite	no	simple electrolytes	yes	not enough information (minerals)	not evaluated
Salter et al.(1981)	smectite	no	groundwaters	yes	not enough information (mineral)	yes
Salter(1982)	bentonite	no	groundwater	no	not enough information (mineral, solution)	unreliable
Sato and Shibutani(1994)	kunigel V1	—	distilled water	no	used for K_d derivation	yes*
Ticknor et al.(1991)	illite, kaolinite	no	synthetic groundwater	no	not enough information (mineral, solution)	unreliable
Yucel et al.(1996)	clay	no	distilled water	no	not enough information (mineral, solution)	yes
Shade et al.(1994)	bentonite	—	simple electrolyte	HCl/NaOH	no information about solution concentration	yes
Solid phase group mudstone						
Ashida et al.(1999)	mudstone	no	simple electrolyte	NaCl	not enough information (mineral)	yes
Barney and Anderson(1979)	argillites	no	groundwater	no	not enough information (mineral, solution)	unreliable
Barney and Brown(1979)	argillites	no	groundwater	no	not enough information (mineral, solution)	unreliable
Daniels(1981)	argillites	no	different groundwaters	no	not enough information (mineral, solution)	yes
Duursma(1973)	marine sediments	no	natural seawater	yes	not enough information (mineral), mineral not relevant	unreliable
Erdal et al.(1977)	alluvium sediments	no	groundwater	no	not enough information (mineral, solution), mineral not relevant	yes
Erdal et al.(1979b)	different ARG_CN	no	simple electrolytes	yes	not enough information (mineral)	yes
Erdal et al.(1979d)	argillite, alluvium	no	groundwater	no	not enough information (mineral, solution)	yes
Erdal(1980)	aquifer, aquitard	no	Brine, Wilcox	no	not enough information (mineral, solution), mineral not relevant	unreliable
Fujikawa and Fukui(1997)	shale	no	simple electrolytes		not enough information (mineral)	unreliable
Higgo et al.(1987)	sediments	no	seawater	no	not enough information (mineral)	yes
Inoue and Morisawa(1975)	silt	no	tap water	yes	not enough information (mineral)	unreliable
Kamel and Ibrahim(1998)	soils	no	natural canal water	yes	not enough information (mineral)	no
Konishi et al.(1988)	loam	no	synthetic groundwater, distilled water	no	not enough information (mineral, solution)	yes
Legoux et al.(1992)	soils	yes	synthetic groundwater	yes (Ref.)	—	yes
Mackenzie et al.(1983)	sediments	no	deionized water	no	not enough information (mineral, solution)	unreliable
Maclean et al.(1978)	shale	no	synthetic groundwater	yes	not enough information (mineral), mineral not relevant	yes
Mollah and Ullah(1998)	soils	no	groundwater	yes	not enough information (mineral)	yes
Rajec et al.(1998)	sedimentary rocks	no	dilute solutions	no	not enough information (mineral, solutions)	no
Relyea et al.(1978)	shales	no	simple electrolytes	yes	not enough information (mineral), mineral not relevant	no
Strezov et al.(2000)	soil	no	groundwater	yes	not enough information (mineral)	yes*
Yamamoto et al.(1989)	loams and soils	no	distilled water	no	not enough information (minerals, solution)	no
Solid phase group other minerals						
Andersson et al.(1983)	apatite, biotite, calcite, chlorite, muscovite, etc.	no	groundwater	yes	not enough information (minerals)	no
Cho et al.(1996)	zeolite	no	simple electrolytes	yes	not enough information (mineral), mineral not relevant	no
Erdal et al.(1979d)	quartz	no	groundwater	no	not enough information (mineral, solution)	no
Fujikawa and Fukui(1997)	calcite, hematite, magnetite	no	simple electrolytes	NaCl, Na_2CO_3, $NaHCO_3$, $NaSO_4$	not enough information (minerals), minerals not relevant	no
Hsu and Chang(1994)	humic acid	no	deionized water	no	not enough information (mineral, solution), mineral not relevant	no
Kitamura et al.(1997)	microcline	no	simple electrolytes	$NaClO_4$	not enough information (mineral), mineral not relevant	no
Maclean et al.(1978)	biotite, dolomite limestone	no	synthetic groundwater and solution, nat. groundwater	yes	not enough information (minerals), minerals not relevant	no
Meyer et al.(1990)	clinoptilolite	yes	simple electrolyte	yes	mineral not relevant	no
Nowak(1979)	hectorite	no	simple electrolyte	yes	not enough information (mineral), mineral not relevant	no
Ohnuki(1994b)	chlorite, halloysite, etc.	no	simple electrolyte	NaOAc	not enough information (minerals), minerals not relevant	no
Relyea et al.(1978)	albite, anorthite, etc.	no	simple electrolytes	yes	not enough information (minerals), minerals not relevant	no
Ticknor et al.(1991)	chlorite, epidote, goethite, gypsum, muscovite, etc.	no	synthetic groundwater	HCl/NaOH	no information about solution concentration	no
Torstenfelt et al.(1981)	apatite, biotite, calcite, muscovite, orthoclase, etc.	no	groundwater	no	not enough information (minerals, solution)	no
Shade et al.(1994)	iron silicate	no	simple electrolyte	yes	not enough information (mineral), mineral not relevant	no

* some datapoints unreliable

*1) see JNC-SDB (http://migrationdb.jaea.go.jp)
*2) classification based on the guideline to evaluate the reliability of Kd data (see Ochs et al.,2007, Saito et al.,2008)

Sources of sorption data for selenium in JNC-SDB

Reference in JNC-SDB *1	Solid phase	Mineralogy reported	Solution	Soln. details	Remark	classification *2
Solid phase group bentonite						
Barney(1981)	basaltic mineral	no	synthetic groundwaters	yes	mineral not relevant	unreliable
Salter et al.(1981)	smectite	no	groundwater	yes	oxidizing conditions, not enough information (mineral)	yes
Shibutani et al.(1994)	kunigel V1, kunipia F	—	simple electrolyte	NaCl	oxidizing conditions	yes*
Tachi et al.(1999c)	kunigel V1	—	simple electrolytes	NaCl	—	yes*
Ticknor et al.(1988)	kaolinite	yes	groundwaters	SCSSS	used for K_d derivation	yes
Solid phase group mudstone						
Fujikawa and Fukui(1997)	shale	no	simple electrolytes	NaCl, Na_2CO_3, $NaSO_4$	not enough information (mineral, redox conditions), mineral not relevant	unreliable
Legoux et al.(1992)	soils	yes	synthetic groundwater	yes (Ref.)	not enough information (redox conditions)	yes*
Solid phase group other minerals						
Davis and Leckie(1980)	$Fe(OH)_3$	—	simple electrolyte	$NaNO_3$	Se(VI), mineral not relevant	no
Fujikawa and Fukui(1997)	calcite, hematite, magnetite	no	simple electrolytes	NaCl, Na_2CO_3, $NaHCO_3$, $NaSO_4$	not enough information (mineral, redox conditions), mineral not relevant	no
Hayes et al.(1988)	goethite, HFO	no	simple electrolytes	$NaNO_3$	Se(IV)/(VI), not enough information (mineral), mineral not relevant	no
Shibutani et al.(1994)	a-FeOOH, Al(OH)3, albite, feldspar, pyrite, quartz	no	simple electrolyte	NaCl	not enough information (redox conditions) mineral not relevant	no
Tachi et al.(1998)	clinoptilolite, lignite	no	simple electrolyte	NaCl	not enough information (mineral, redox conditions)	no
Ticknor and McMurry(1996)	goethite	no	groundwaters	yes	Se(IV), not enough information (mineral), mineral not relevant	no
Ticknor et al.(1988)	calcite, chlorite, epidote, goethite, gypsum, hematite, muscovite, quartz	yes	groundwaters	SCSSS[1]	Se(-II)/(IV)/(VI), used for K_d derivation	yes

1) Standard Canadian Shield Saline Solution

Supplementary sources of sorption data

none

*1) see JNC-SDB (http://migrationdb.jaea.go.jp)
*2) classification based on the guideline to evaluate the reliability of Kd data (see Ochs et al.,2007, Saito et al.,2008)

* some datapoints unreliable

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Appendix II

K_d derivation tables and radionuclide speciation

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Speciation

Filename	mudstone_HDB-6_5b_Th(2)		Legoux et al.(1992)_A_Th(1)
	TDB:	JNCTDB_011213c2	Nagra-PSI 2001
		Nagra-PSI 2001	

Th(IV) speciation (Legoux et al., 1992)

System		**Application**		**Data Source**
Substrate		**Koetoi**	**Wakkanai**	**Clay mineral, Sample A**
Solution		**HDB-6**		**Synthetic Groundwater**
Th(IV) added	(mol/kg)	4.06E-11	4.06E-11	4.00E-11
pH		6.75	6.75	7.6
pCO_2		-0.58	-0.58	-2.96
Th(IV) dissolved	(mol/kg)	4.06E-11	4.06E-11	4.00E-11
Th^{+4}	(mol/kg)	2.04E-20	2.04E-20	5.59E-24
$Th(OH)_4$	(mol/kg)	2.81E-15	2.81E-15	1.29E-13
ThF_3^+	(mol/kg)	4.69E-19	4.69E-19	0.00E+00
ThF_4	(mol/kg)	5.91E-21	5.91E-21	0.00E+00
ThF_5^-	(mol/kg)	1.51E-23	1.51E-23	0.00E+00
ThF_6^{2-}	(mol/kg)	1.57E-27	1.57E-27	0.00E+00
$Th(OH)_3CO_3^-$	(mol/kg)	4.06E-11	4.06E-11	3.99E-11
$Th(CO_3)_5^{-6}$	(mol/kg)	7.78E-17	7.78E-17	5.15E-26
$Th(SO_4)_3^{2-}$	(mol/kg)	2.24E-27	2.24E-27	0.00E+00
∑ competitive Th complexes (Th-cmp) with Th-CO_3	(mol/kg)	4.06E-11	4.06E-11	3.99E-11
Th tot-(Th-cmp)	(mol/kg)	1.99E-14	1.99E-14	1.30E-13
(Th tot- (Th-cmp)) / Th tot (CF-spec/a)		**4.91E-04**	**4.91E-04**	**3.25E-03**
ThF_3^+	(mol/kg)	4.69E-19	4.69E-19	0.00E+00
ThF_4	(mol/kg)	5.91E-21	5.91E-21	0.00E+00
ThF_5^-	(mol/kg)	1.51E-23	1.51E-23	0.00E+00
ThF_6^{2-}	(mol/kg)	1.57E-27	1.57E-27	0.00E+00
$Th(OH)_3CO_3^-$	(mol/kg)	4.06E-11	4.06E-11	3.99E-11
$Th(CO_3)_5^{-6}$	(mol/kg)	7.78E-17	7.78E-17	5.15E-26
$Th(SO_4)_3^{-2}$	(mol/kg)	2.24E-27	2.24E-27	0.00E+00
∑ competitive Th complexes (Th-cmp) without Th-CO_3	(mol/kg)	4.75E-19	4.75E-19	0.00E+00
Th tot-(Th-cmp) without Th-CO4	(mol/kg)	4.06E-11	4.06E-11	4.00E-11
(Th tot- (Th-cmp)) / Th tot (CF-spec/b)		**1.00E+00**	**1.00E+00**	**1.00E+00**

K_d-Derivation Th(IV) Legoux et al. (1992), page 1/2

Overview Pred. K_d [m^3/kg]	Koetoi[3]	Wakkanai[3]
	HDB-6	HDB-6
Predicted K_d: CF-1 (CEC)	570.04	570.04
Pred. K_d: CF-1 (BET)	56.23	47.40
Pred. K_d: CF-1 (% clay)	218.52	171.01
Pred. K_d: CF-2a (CEC))	86.06	86.06
Pred. K_d: CF-2a (BET)	8.49	7.16
Pred. K_d: CF-2a (% clay)	32.99	25.82
Pred. K_d: CF-2b (CEC)	570.04	570.04
Pred. K_d: CF-2b (BET)	56.23	47.40
Pred. K_d: CF-2b (% clay)	218.52	171.01

Th(IV) K_d-derivation		**Conditions**					**Conversion (C) / Uncertainty (U)**	
		Data source[1]	**Additional information[2]**		**Application**		**CF**	
					Mudstone		**Mudstone**	
Solution		**Synthetic Groundwater**	**0.1 M NaClO4**		**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Substrate		**Clay mineral, Sample A**	**SWy-1**	**SWy-1**	**Koetoi[3]**	**Wakkanai[3]**	**Koetoi[3]**	**Wakkanai[3]**
Experimental K_d	(m^3/kg)	100						
Conversion Mineralogy (CF-min)								
CEC	(meq/100g)	3	87	87	20.00	20.00	6.67	6.67
BET	(m^2/g)	8.6			5.66	4.77	0.66	0.55
% clay		9			23.00	18.00	2.56	2.00
Conversion pH (CF-pH)								
pH		7.6	7.60	6.75	6.75	6.75		
Kd for 0.1 M NaClO4 (pH conversion)[2]		100	294	251			0.86	0.86
Conversion Speciation (CF-spec)								
CF-spec/a		3.25E-03			4.91E-04	4.91E-04	0.15	0.15
CF-spec/b		1.00			1.00	1.00	1.00	1.00
Conversion Competition (Anionic or Cationic) (CF-cmp)	*irrelevant*							

(1) K_d value from Th(IV) sorption datapoint Legoux et al. (1992) K_d=100 m^3/kg
(2) K_d values from Th(IV) sorption edge (Bradbury and Baeyens, 2003a), p.63
(3) Values of the avarage composition (Table Mineralogy 1)

Th(IV) K_d-derivation via CEC							**CF**	
CF-1 (CEC)							5.70	5.70
Speciation								
CF-2a (CEC)							0.86	0.86
CF-2b (CEC)							5.70	5.70
							UF	
Predicted K_d: CF-1 (CEC)	(m^3/kg)				**570.04**	**570.04**		
UF-starting K_d							1.6	1.6
UF-min							1.4	1.4
UF-pH conversion							2.5	2.5
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				3162.11	3162.11		
K_d lower limit	(m^3/kg)				102.76	102.76		
positive error bar					*2592.06*	*2592.06*		
negative error bar					*467.28*	*467.28*		
Predicted K_d: CF-2a (CEC)	(m^3/kg)				**86.06**	**86.06**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				668.38	668.38		
K_d lower limit	(L/g)				11.08	11.08		
positive error bar					*582.31*	*582.31*		
negative error bar					*74.98*	*74.98*		
Predicted K_d: CF-2b (CEC)	(m^3/kg)				**570.04**	**570.04**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				4426.95	4426.95		
K_d lower limit	(m^3/kg)				73.40	73.40		
positive error bar					*3856.91*	*3856.91*		
negative error bar					*496.64*	*496.64*		

K_d-Derivation Th(IV) Legoux et al. (1992), page 2/2

Th(IV) K_d-derivation via BET							**CF**	
CF-1 (BET)							0.56	0.47
Speciation								
CF-2a (BET)							0.08	0.07
CF-2b (BET)							0.56	0.47
							UF	
Predicted K_d: CF-1 (BET)	(m^3/kg)				**56.23**	**47.40**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
Kd upper limit	(m^3/kg)				311.89	262.91		
Kd lower limit	(m^3/kg)				10.14	8.54		
positive error bar					*255.66*	*215.52*		
negative error bar					*46.09*	*38.85*		
Predicted K_d: CF-2a (BET)	(m^3/kg)				**8.49**	**7.16**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				65.92	55.57		
K_d lower limit	(m^3/kg)				1.09	0.92		
positive error bar					*57.44*	*48.42*		
negative error bar					*7.40*	*6.23*		
Predicted K_d: CF-2b (BET)	(m^3/kg)				**56.23**	**47.40**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				436.65	368.08		
K_d lower limit	(m^3/kg)				7.24	6.10		
positive error bar					*380.42*	*320.68*		
negative error bar					*48.99*	*41.29*		

Th(IV) K_d-derivation via % clay							**CF**	
CF-1 (%clay)							2.19	1.71
Speciation								
CF-2a (% clay)							0.33	0.26
CF-2b (% clay)							2.19	1.71
							UF	
Predicted K_d: CF-1 (% clay)	(m^3/kg)				**218.52**	**171.01**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				1212.14	948.63		
K_d lower limit	(m^3/kg)				39.39	30.83		
positive error bar					*993.62*	*777.62*		
negative error bar					*179.12*	*140.18*		
Predicted K_d: CF-2a (% clay)	(m^3/kg)				**32.99**	**25.82**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				256.21	200.51		
K_d lower limit	(m^3/kg)				4.25	3.32		
positive error bar					*223.22*	*174.69*		
negative error bar					*28.74*	*22.49*		
Predicted K_d: CF-2b (% clay)	(m^3/kg)				**218.52**	**171.01**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				1697.00	1328.09		
K_d lower limit	(m^3/kg)				28.14	22.02		
positive error bar					*1478.48*	*1157.07*		
negative error bar					*190.38*	*148.99*		

Speciation

Filename mudstone_HDB-6_5b_Th(3) Östhols(1995)_Th(1)
TDB: JNCTDB_011213c2
(Nagra-PSI 2001)

Th(IV) speciation (Östhols, 1995)

System		**Application**		**Data Source**
Substrate		**Koetoi**	**Wakkanai**	**Aerosil OX 200 (SiO_2)**
Solution		**HDB-6**		**0.1 M $NaClO_4$**
Th(IV) added	(mol/kg)	3.50E-06	3.50E-06	3.45E-06
pH		6.75E+00	6.75E+00	2.77E+00
pCO_2		-5.80E-01	-5.80E-01	0.00E+00
Th(IV) dissolved	(mol/kg)	3.50E-06	3.50E-06	3.45E-06
Th^{+4}	(mol/kg)	1.76E-15	1.76E-15	3.46E-06
$Th(OH)_4$	(mol/kg)	2.42E-10	2.42E-10	3.41E-16
ThF_3^+	(mol/kg)	4.04E-14	4.04E-14	0.00E+00
ThF_4	(mol/kg)	5.09E-16	5.09E-16	0.00E+00
ThF_5^-	(mol/kg)	1.30E-18	1.30E-18	0.00E+00
ThF_6^{2-}	(mol/kg)	1.35E-22	1.35E-22	0.00E+00
$Th(OH)_3CO_3^-$	(mol/kg)	3.50E-06	3.50E-06	0.00E+00
$Th(CO_3)_5^{-6}$	(mol/kg)	6.71E-12	6.71E-12	0.00E+00
$Th(SO_4)_3^{2-}$	(mol/kg)	1.93E-22	1.93E-22	0.00E+00
∑ competitive Th complexes (Th-cmp) with Th-CO_3	(mol/kg)	3.50E-06	3.50E-06	0.00E+00
Th tot-(Th-cmp)	(mol/kg)	3.25E-12	3.25E-12	3.45E-06
(Th tot- (Th-cmp)) / Th tot (CF-spec/a)		**9.29E-07**	**9.29E-07**	**1.00E+00**
ThF_3^+	(mol/kg)	4.04E-14	4.04E-14	0.00E+00
ThF_4	(mol/kg)	5.09E-16	5.09E-16	0.00E+00
ThF_5^-	(mol/kg)	1.30E-18	1.30E-18	0.00E+00
ThF_6^{2-}	(mol/kg)	1.35E-22	1.35E-22	0.00E+00
$Th(OH)_3CO_3^-$	(mol/kg)	3.50E-06	3.50E-06	0.00E+00
$Th(CO_3)_5^{-6}$	(mol/kg)	6.71E-12	6.71E-12	0.00E+00
$Th(SO_4)_3^{-2}$	(mol/kg)	1.93E-22	1.93E-22	0.00E+00
∑ competitive Th complexes (Th-cmp) without Th-CO_3	(mol/kg)	4.09E-14	4.09E-14	0.00E+00
Th tot-(Th-cmp) without Th-CO4	(mol/kg)	3.50E-06	3.50E-06	3.45E-06
(Th tot- (Th-cmp)) / Th tot (CF-spec/b)		**1.00E+00**	**1.00E+00**	**1.00E+00**

K_d-Derivation Th(IV) Östhols (1995)

Overview Pred. K_d [m^3/kg]	Koetoi[3]	Wakkanai[3]
	HDB-6	HDB-6
Pred. K_d: CF-1 (% SiO_2)	0.62	0.65
Pred. K_d: CF-2a (% SiO_2)	5.78E-07	6.08E-07
Pred. K_d: CF-2b (% SiO_2)	0.62	0.65
Pred. K_d: CF-1 (100% SiO_2)	1.09	1.09
Pred. K_d: CF-2a (100% SiO_2)	1.01E-06	1.01E-06
Pred. K_d: CF-2b (100% SiO_2)	1.09	1.09

Th(IV) K_d-derivation		Conditions					Conversion (C) / Uncertainty (U)	
		Data source[1]	Additional information[2]		Application		CF	
					Mudstone		Mudstone	
Solution		0.1 M $NaClO_4$	0.1 M $NaClO_4$		HDB-6	HDB-6	HDB-6	HDB-6
Substrate		Aerosil OX 200 (SiO_2)	SWy-1	SWy-1	Koetoi[3]	Wakkanai[3]	Koetoi[3]	Wakkanai[3]
Experimental K_d	(m^3/kg)	0.42						
Conversion Mineralogy (CF-min)								
%SiO_2		100.00			57.00	60.00	0.57	0.60
%SiO_2 (100%)		100.00			100.00	100.00	1.00	1.00
Conversion pH (CF-pH)								
pH		2.77	2.77	6.75	6.75	6.75		
K_d for 0.1 M NaClO4 (pH conversion)[2]		0.42	95	251			2.63	2.63
Conversion Speciation (CF-spec)								
CF-spec/a		1.00			9.29E-07	9.29E-07	9.29E-07	9.29E-07
CF-spec/b		1.00			1.00	1.00	1.00	1.00
Conversion Competition (Anionic or Cationic) (CF-cmp)	irrelevant							

(1) K_d value from Th(IV) sorption datapoint Osthols(1995)

(2) K_d values from Th(IV) sorption edge (Bradbury and Baeyens, 2003a), p.63

(3) Values of the avarage composition (Table Mineralogy 1)

Th(IV) K_d-derivation via % SiO_2							CF	
CF-1 (%SiO_2)							1.5	1.6
Speciation								
CF-2a (%SiO_2)							1.39E-06	1.47E-06
CF-2b (%SiO_2)							1.50	1.58
							UF	
Predicted K_d: CF-1 (%SiO_2)	(m^3/kg)				**0.62**	**0.65**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				3.45	3.63		
K_d lower limit	(m^3/kg)				0.11	0.12		
positive error bar					*2.83*	*2.98*		
negative error bar					*0.51*	*0.54*		
Predicted K_d: CF-2a (%SiO_2)	(m^3/kg)				**5.78E-07**	**6.08E-07**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				0.00	0.00		
K_d lower limit	(m^3/kg)				0.00	0.00		
positive error bar					*0.00*	*0.00*		
negative error bar					*0.00*	*0.00*		
Predicted K_d: CF-2b (%SiO_2)	(m^3/kg)				**0.62**	**0.65**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				4.83	5.09		
K_d lower limit	(m^3/kg)				0.08	0.08		
positive error bar					*4.21*	*4.43*		
negative error bar					*0.54*	*0.57*		

Th(IV) K_d-derivation via 100% SiO_2							CF	
CF-1 (100% SiO_2)							2.6	2.6
Speciation								
CF-2a (100% SiO_2)							2.44E-06	2.44E-06
CF-2b (100% SiO_2)							2.63	2.63
							UF	
Predicted K_d: CF-1 (100% SiO_2)	(m^3/kg)				**1.09**	**1.09**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				6.06	6.06		
K_d lower limit	(m^3/kg)				0.20	0.20		
positive error bar					*4.96*	*4.96*		
negative error bar					*0.89*	*0.89*		
Predicted K_d: CF-2a (100% SiO_2)	(m^3/kg)				**1.01E-06**	**1.01E-06**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				0.00	0.00		
K_d lower limit	(m^3/kg)				0.00	0.00		
positive error bar					*0.00*	*0.00*		
negative error bar					*0.00*	*0.00*		
Predicted K_d: CF-2b (100% SiO_2)	(m^3/kg)				**1.09**	**1.09**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				8.48	8.48		
K_d lower limit	(m^3/kg)				0.14	0.14		
positive error bar					*7.39*	*7.39*		
negative error bar					*0.95*	*0.95*		

Speciation

Filename mudstone_HDB-6_5b_Th(4) Bradbury&Baeyens(2003a)_Th(1)
TDB: JNCTDB_011213c2

Th(IV) speciation (Bradbury&Baeyens, 2003a)

System		**Application**		**Data Source**
Substrate		**Koetoi**	**Wakkanai**	**Na-SWy1montmorillonite**
Solution		**HDB-6**		**0.1 M $NaClO_4$**
Th(IV) added	(mol/kg)	1.01E-09	1.01E-09	1.00E-09
pH		6.75E+00	6.75E+00	6.75E+00
pCO_2		-5.80E-01	-5.80E-01	0.00E+00
Th(IV) dissolved	(mol/kg)	1.02E-09	1.02E-09	1.00E-09
Th^{+4}	(mol/kg)	5.10E-19	5.10E-19	1.17E-15
$Th(OH)_4$	(mol/kg)	7.03E-14	7.03E-14	1.00E-09
ThF_3^+	(mol/kg)	1.17E-17	1.17E-17	0.00E+00
ThF_4	(mol/kg)	1.48E-19	1.48E-19	0.00E+00
ThF_5^-	(mol/kg)	3.77E-22	3.77E-22	0.00E+00
ThF_6^{2-}	(mol/kg)	3.92E-26	3.92E-26	0.00E+00
$Th(OH)_3CO_3^-$	(mol/kg)	1.01E-09	1.01E-09	0.00E+00
$Th(CO_3)_5^{-6}$	(mol/kg)	1.95E-15	1.95E-15	0.00E+00
$Th(SO_4)_3^{2-}$	(mol/kg)	5.59E-26	5.59E-26	0.00E+00
∑ competitive Th complexes (Th-cmp) with Th-CO_3	(mol/kg)	1.01E-09	1.01E-09	0.00E+00
Th tot-(Th-cmp)	(mol/kg)	9.98E-13	9.98E-13	1.00E-09
(Th tot- (Th-cmp)) / Th tot (CF-spec/a)		**9.83E-04**	**9.83E-04**	**1.00E+00**
ThF_3^+	(mol/kg)	1.17E-17	1.17E-17	0.00E+00
ThF_4	(mol/kg)	1.48E-19	1.48E-19	0.00E+00
ThF_5^-	(mol/kg)	3.77E-22	3.77E-22	0.00E+00
ThF_6^{2-}	(mol/kg)	3.92E-26	3.92E-26	0.00E+00
$Th(OH)_3CO_3^-$	(mol/kg)	1.01E-09	1.01E-09	0.00E+00
$Th(CO_3)_5^{-6}$	(mol/kg)	1.95E-15	1.95E-15	0.00E+00
$Th(SO_4)_3^{-2}$	(mol/kg)	5.59E-26	5.59E-26	0.00E+00
∑ competitive Th complexes (Th-cmp) without Th-CO_3	(mol/kg)	1.19E-17	1.19E-17	0.00E+00
Th tot-(Th-cmp) without Th-CO4	(mol/kg)	1.01E-09	1.01E-09	1.00E-09
(Th tot- (Th-cmp)) / Th tot (CF-spec/b)		**1.00E+00**	**1.00E+00**	**1.00E+00**

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K_d-Derivation Th(IV) Bradbury&Baeyens (2003a)

Overview Pred. K_d [m^3/kg]	**Koetoi[3]**	**Wakkanai[3]**
	HDB-6	**HDB-6**
Pred. K_d: CF-1 (% clay)	57.773	45.214
Pred. K_d: CF-2a (% clay)	0.057	0.044
Pred. K_d: CF-2b (% clay)	57.773	45.214

Th(IV) K_d-derivation		**Conditions**					**Conversion (C) / Uncertainty (U)**	
		Data source[1]	**Additional information[1]**		**Application**		**CF**	
					Mudstone		**Mudstone**	
Solution		**0.1 M $NaClO_4$**	**0.1 M $NaClO_4$**		**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Substrate		**SWy-1**	**SWy-1**	**SWy-1**	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**
Experimental K_d	(m^3/kg)	251						
Conversion Mineralogy (CF-min)								
%clay		100			23	18	0.23	0.18
Conversion pH (CF-pH)								
pH		6.75	6.75	6.75	6.75	6.75		
Kd for 0.1 M NaClO4 (pH conversion)[2]		251	251	251			1	1
Conversion Speciation (CF-spec)								
CF-spec/a		1.00			9.83E-04	9.83E-04	9.83E-04	9.83E-04
CF-spec/b		1			0.99999999	0.99999999	0.99999999	0.99999999
Conversion Competition (Anionic or Cationic) (CF-cmp)	irrelevant							

(1) K_d values from Th(IV) sorption edge (Bradbury and Baeyens, 2003a), p.63

(2) Values of the avarage composition (Table Mineralogy 1)

Th(IV) K_d-derivation via % clay							**CF**	
CF-1 (% clay)							0.23	0.18
Speciation								
CF-2a (% clay)							2.26E-04	1.77E-04
CF-2b (% clay)							0.23	0.18
							UF	
Predicted K_d: CF-1 (% clay)	(m^3/kg)				**57.77**	**45.21**		
UF-starting K_d							1.6	1.6
UF-min							1.4	1.4
UF-total							2.2	2.2
K_d upper limit	(m^3/kg)				128.19	100.32		
K_d lower limit	(m^3/kg)				26.04	20.38		
positive error bar					*70.42*	*55.11*		
negative error bar					*31.74*	*24.84*		
Predicted K_d: CF-2a (% clay)	(m^3/kg)				**0.06**	**0.04**		
UF-starting K_d							1.6	1.6
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							3.1	3.1
K_d upper limit	(m^3/kg)				0.18	0.14		
K_d lower limit	(m^3/kg)				0.02	0.01		
positive error bar					*0.12*	*0.09*		
negative error bar					*0.04*	*0.03*		
Predicted K_d: CF-2b (% clay)	(m^3/kg)				**57.77**	**45.21**		
UF-starting K_d							1.6	1.6
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							3.1	3.1
K_d upper limit	(m^3/kg)				179.47	140.45		
K_d lower limit	(m^3/kg)				18.60	14.56		
positive error bar					*121.69*	*95.24*		
negative error bar					*39.18*	*30.66*		

Speciation

Filename mudstone_HDB-6_5b_Th(5) Baston(1992a)_Th
Baston(1992a)_Th_NAPSI
TDB: JNCTDB_011213c2 (Nagra-PSI 2001)

Th(IV) speciation (Baston, 1992a)

System		**Application**		**Data Source**
Substrate		**Koetoi**	**Wakkanai**	**London Clay**
Solution		**HDB-6**		**Cement eq. water**
Th(IV) added	(mol/kg)	2.03E-11	2.03E-11	2.00E-11
pH		6.75	6.75	8.1
pCO_2		-0.58	-0.58	-4.39
Th(IV) dissolved	(mol/kg)	2.03E-11	2.03E-11	2.00E-11
Th^{+4}	(mol/kg)	1.02E-20	1.02E-20	1.22E-24
$Th(OH)_4$	(mol/kg)	1.41E-15	1.41E-15	4.72E-13
ThF_3^+	(mol/kg)	2.343E-19	2.343E-19	0.00E+00
ThF_4	(mol/kg)	2.95E-21	2.95E-21	0.00E+00
ThF_5^-	(mol/kg)	7.55E-24	7.55E-24	0.00E+00
ThF_6^{2-}	(mol/kg)	7.83E-28	7.83E-28	0.00E+00
$Th(OH)_3CO_3^-$	(mol/kg)	2.03E-11	2.03E-11	1.95E-11
$Th(CO_3)_5^{-6}$	(mol/kg)	3.89E-17	3.89E-17	7.78E-28
$Th(SO_4)_3^{2-}$	(mol/kg)	1.12E-27	1.12E-27	1.39E-26
∑ competitive Th complexes (Th-cmp) with $Th\text{-}CO_3$	(mol/kg)	2.03E-11	2.03E-11	1.95E-11
Th tot-(Th-cmp)	(mol/kg)	9.96E-15	9.96E-15	4.70E-13
(Th tot- (Th-cmp)) / Th tot (CF-spec/a)		**4.91E-04**	**4.91E-04**	**2.35E-02**
ThF_3^+	(mol/kg)	2.34E-19	2.34E-19	0.00E+00
ThF_4	(mol/kg)	2.95E-21	2.95E-21	0.00E+00
ThF_5^-	(mol/kg)	7.55E-24	7.55E-24	0.00E+00
ThF_6^{2-}	(mol/kg)	7.83E-28	7.83E-28	0.00E+00
$Th(OH)_3CO_3^-$	(mol/kg)	2.03E-11	2.03E-11	1.95E-11
$Th(CO_3)_5^{-6}$	(mol/kg)	3.89E-17	3.89E-17	7.78E-28
$Th(SO_4)_3^{-2}$	(mol/kg)	1.12E-27	1.12E-27	1.39E-26
∑ competitive Th complexes (Th-cmp) without $Th\text{-}CO_3$	(mol/kg)	2.37E-19	2.37E-19	1.39E-26
Th tot-(Th-cmp) without Th-CO4	(mol/kg)	2.03E-11	2.03E-11	2.00E-11
(Th tot- (Th-cmp)) / Th tot (CF-spec/b)		**1.00E+00**	**1.00E+00**	**1.00E+00**

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K_d-Derivation Th(IV) (Baston 1992a)

Overview Pred. K_d [m^3/kg]	Koetoi[3]	Wakkanai[3]
	HDB-6	HDB-6
Predicted K_d: CF-1 (CEC)	0.57	0.57
Pred. K_d: CF-1 (% clay)	0.26	0.20
Pred. K_d: CF-2a (CEC))	0.01	0.01
Pred. K_d: CF-2a (% clay)	0.01	4.18E-03
Pred. K_d: CF-2b (CEC)	0.57	0.57
Pred. K_d: CF-2b (% clay)	0.26	0.20

Th(IV) K_d-derivation		**Conditions**					**Conversion (C) / Uncertainty (U)**	
		Data source[1]	**Additional information[2]**		**Application**		**CF**	
					Mudstone		**Mudstone**	
Solution		**Cement eq. water**	**0.1 M NaClO4**		**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Substrate		**London Clay**	**SWy-1**	**SWy-1**	**Koetoi[3]**	**Wakkanai[3]**	**Koetoi[3]**	**Wakkanai[3]**
Experimental K_d	(m^3/kg)	1.1						
Conversion Mineralogy (CF-min)								
CEC	(meq/100g)	27.5			20.00	20.00	0.73	0.73
BET	(m^2/g)	-			5.66	4.77	-	-
% clay		70.8			23.00	18.00	0.32	0.25
Conversion pH (CF-pH)								
pH		8.1	8.1	6.75	6.75	6.75		
Kd for 0.1 M NaClO4 (pH conversion)[2]		1.1	351	251			0.72	0.72
Conversion Speciation (CF-spec)								
CF-spec/a		0.02			4.91E-04	4.91E-04	0.02	0.02
CF-spec/b		1.00			1.00	1.00	1.00	1.00
Conversion Competition (Anionic or Cationic) (CF-cmp)	*irrelevant*							

(1) K_d value from Th(IV) sorption datapoint Baston (1992a) K_d=1.1 m^3/kg

(2) K_d values from Th(IV) sorption edge (Bradbury and Baeyens, 2003a), p.63

(3) Values of the avarage composition (Table Mineralogy 1)

Th(IV) K_d-derivation via CEC							**CF**	
CF-1 (CEC)							0.52	0.52
Speciation								
CF-2a (CEC)							0.01	0.01
CF-2b (CEC)							0.52	0.52
							UF	
Predicted K_d: CF-1 (CEC)	(m^3/kg)				**0.57**	**0.57**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				3.18	3.18		
K_d lower limit	(m^3/kg)				0.10	0.10		
positive error bar					*2.61*	*2.61*		
negative error bar					*0.47*	*0.47*		
Predicted K_d: CF-2a (CEC)	(m^3/kg)				**0.01**	**0.01**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				0.09	0.09		
K_d lower limit	(L/g)				0.00	0.00		
positive error bar					*0.08*	*0.08*		
negative error bar					*0.01*	*0.01*		
Predicted K_d: CF-2b (CEC)	(m^3/kg)				**0.57**	**0.57**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				4.45	4.45		
K_d lower limit	(m^3/kg)				0.07	0.07		
positive error bar					*3.88*	*3.88*		
negative error bar					*0.50*	*0.50*		
positive error bar					*3.88*	*3.88*		
negative error bar					*0.50*	*0.50*		

Th(IV) K_d-derivation via % clay							**CF**	
CF-1 (%clay)							0.23	0.18
Speciation								
CF-2a (% clay)							4.86E-03	3.80E-03
CF-2b (% clay)							0.23	0.18
							UF	
Predicted K_d: CF-1 (% clay)	(m^3/kg)				**0.26**	**0.20**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				1.42	1.11		
K_d lower limit	(m^3/kg)				0.05	0.04		
positive error bar					*1.16*	*0.91*		
negative error bar					*0.21*	*0.16*		
Predicted K_d: CF-2a (% clay)	(m^3/kg)				**5.35E-03**	**4.18E-03**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				0.04	0.03		
K_d lower limit	(m^3/kg)				0.00	0.00		
positive error bar					*0.04*	*0.03*		
negative error bar					*0.00*	*0.00*		
Predicted K_d: CF-2b (% clay)	(m^3/kg)				**0.26**	**0.20**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-speciation							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				1.987	1.555E+00		
K_d lower limit	(m^3/kg)				0.033	2.579E-02		
positive error bar					*1.73*	*1.36*		
negative error bar					*0.22*	*0.17*		

Speciation

Filename mudstone_HDB-6_5b_Np(2) Baston(1999)_Np(1)
TDB: JNCTDB_011213c2

Np(IV) speciation (Baston et al., 1999)

System		**Application**		**Data Source**
Substrate		**Koetoi**	**Wakkanai**	**Kunigel V1**
Solution		**HDB-6**		**Dist. equil. water**
Np(IV) added	(mol/kg)	6.09E-09	6.09E-09	6.00E-09
pH		6.75	6.75	10.4
pCO_2		-0.58	-0.58	-6.34
Np^{+4} dissolved	(mol/kg)	6.09E-09	6.09E-09	6.00E-09
Np^{+4}	(mol/kg)	3.82E-25	3.82E-25	4.16E-40
$Np(OH)_4$	(mol/kg)	2.64E-10	2.64E-10	6.00E-09
$Np(OH)^{3+}$	(mol/kg)	7.97E-20	7.97E-20	2.12E-30
Np(V)-species	(mol/kg)	1.23E-13	1.23E-13	1.57E-15
$Np(OH)_2(CO_3)_2^{2-}$	(mol/kg)	5.82E-09	5.82E-09	2.85E-12
$Np(CO_3)_5^{6-}$	(mol/kg)	2.72E-15	2.72E-15	1.23E-24
$Np(SO_4)^{2+}$	(mol/kg)	1.16E-23	1.16E-23	1.42E-35
$Np(SO_4)_2$	(mol/kg)	1.89E-27	1.89E-27	4.05E-37
∑ competitive Np complexes (Np-cmp) with $Np-CO_3$	(mol/kg)	5.82E-09	5.82E-09	2.85E-12
Np tot-(Np-cmp)	(mol/kg)	2.64E-10	2.64E-10	6.00E-09
(Np tot- (Np-cmp)) / Np tot (CF-spec/a)		**0.04**	**0.04**	**1.00**
Np(V)-species	(mol/kg)	1.23E-13	1.23E-13	1.57E-15
$Np(SO_4)^{2+}$	(mol/kg)	1.16E-23	1.16E-23	1.42E-35
$Np(SO_4)_2$	(mol/kg)	1.89E-27	1.89E-27	4.05E-37
∑ competitive Np complexes (Np-cmp) without $Np-CO_3$	(mol/kg)	1.23E-13	1.23E-13	1.57E-15
Np tot-(Np-cmp) without $Np-CO_3$	(mol/kg)	6.09E-09	6.09E-09	6.00E-09
(Np tot- (Np-cmp)) / Np tot (CF-spec/b)		**1.00**	**1.00**	**1.00**

K_d-derivation Np(IV) on Smectite Baston et al. (1999), page 1/2

Overview Pred. K_d [m^3/kg]	**Koetoi[3]**	**Wakkanai[3]**
	HDB-6	**HDB-6**
Pred. K_d: CF-1 (CEC)	2.73	2.73
Pred. K_d: CF-1 (%clay)	4.11	3.21
Pred. K_d: CF-2a (CEC)	0.12	0.12
Pred. K_d: CF-2a (% clay)	0.18	0.14
Pred. K_d: CF-2b (CEC)	2.73	2.73
Pred. K_d: CF-2b (% clay)	4.11	3.21

Np(IV) Kd-derivation		**Conditions**					**Conversion (C) / Uncertainty (U)**	
		Data source[1]	**Additional information[2]**		**Application**		**CF**	
					Mudstone		**Mudstone**	
Solution		**Dist. equil. water**	**0.1 M $NaClO_4$**		**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Substrate		**Kunigel V1**	**SWy-1**	**SWy-1**	**Koetoi[3]**	**Wakkanai[3]**	**Koetoi[3]**	**Wakkanai[3]**
Experimental K_d	(m^3/kg)	14.60						
Conversion Mineralogy (CF-min)								
CEC[4]	(meq/100g)	60.1			20.00	20.00	0.33	0.33
BET		35			5.66	4.77	0.16	0.14
% clay		46			23	18	0.50	0.39
Conversion pH (CF-pH)								
pH		10.4	10.4	6.75	6.75	6.75		
K_d for Th in 0.1 M NaClO4 (pH conversion)[2]		5.7	351	197			0.56	0.56
Conversion Speciation (CF-spec)								
CF-2a		1.00			0.04	0.04	0.04	0.04
CF-2b		1.00			1.00	1.00	1.00	1.00
Conversion Competition (Cationic) (CF-cmp)	*irrelevant*							

(1) K_d value from Np(IV) sorption data table Baston (1999), L:S =20:1, room temp.,
(2) K_d values from Th(IV) sorption edge (Bradbury and Baeyens, 2003a), p.63
(3) Values of the avarage composition (Table Mineralogy 1)
(4) CEC value of data source from Sasaki et al. (1995)

Np(IV) K_d-derivation via CEC					**Koetoi**	**Wakkanai**	**CF**	
CF-1 (CEC)							**0.19**	**0.19**
Speciation								
CF-2a							**0.01**	**0.01**
CF-2b							**0.19**	**0.19**
							UF	
Predicted K_d: CF-1 (CEC)	(m^3/kg)				**2.73**	**2.73**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				15.16	15.16		
K_d lower limit	(m^3/kg)				0.49	0.49		
positive error bar					*12.42*	*12.42*		
negative error bar					*2.24*	*2.24*		
Predicted K_d: CF-2a (CEC)	(m^3/kg)				**0.12**	**0.12**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				0.92	0.92		
K_d lower limit	(m^3/kg)				0.02	0.02		
positive error bar					*0.80*	*0.80*		
negative error bar					*0.10*	*0.10*		
Predicted K_d: CF-2b (CEC)	(m^3/kg)				**2.73**	**2.73**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				21.22	21.22		
K_d lower limit	(m^3/kg)				0.35	0.35		
positive error bar					*18.49*	*18.49*		
negative error bar					*2.38*	*2.38*		

K_d-derivation Np(IV) on Smectite Baston et al. (1999), page 2/2

Np(IV) K_d-derivation via BET					**Koetoi**	**Wakkanai**	**CF**	
CF-1 (CEC)							**0.09**	**0.08**
Speciation								
CF-2a							**0.00**	**0.00**
CF-2b							**0.09**	**0.08**
							UF	
Predicted K_d: CF-1 (BET)	(m^3/kg)				**1.33**	**1.12**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				7.36	6.20		
K_d lower limit	(m^3/kg)				0.24	0.20		
positive error bar					*6.03*	*5.08*		
negative error bar					*1.09*	*0.92*		
Predicted K_d: CF-2a (BET)	(m^3/kg)				**0.06**	**0.05**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				0.45	0.38		
K_d lower limit	(m^3/kg)				0.01	0.01		
positive error bar					*0.39*	*0.33*		
negative error bar					*0.05*	*0.04*		
Predicted K_d: CF-2b (CEC)	(m^3/kg)				**1.33**	**1.12**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				10.30	8.68		
K_d lower limit	(m^3/kg)				0.17	0.14		
positive error bar					*8.98*	*7.57*		
negative error bar					*1.16*	*0.97*		

Np(IV) K_d-derivation via % clay					**Koetoi**	**Wakkanai**	**CF**	
CF-1 (%clay)							**0.28**	**0.22**
Speciation								
CF-2a (% clay)							**0.01**	**0.01**
CF-2b (% clay)							**0.28**	**0.22**
							UF	
Predicted K_d: CF-1 (% clay)	(m^3/kg)				**4.11**	**3.21**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-min							1.4	1.4
UF-total							5.5	5.5
K_d upper limit	(m^3/kg)				22.77	17.82		
K_d lower limit	(m^3/kg)				0.74	0.58		
positive error bar					*18.67*	*14.61*		
negative error bar					*3.37*	*2.63*		
Predicted K_d: CF-2a (% clay)	(m^3/kg)				**0.18**	**0.14**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				1.38	1.08		
K_d lower limit	(m^3/kg)				0.02	0.02		
positive error bar					*1.20*	*0.94*		
negative error bar					*0.16*	*0.12*		
Predicted K_d: CF-2b (% clay)	(m^3/kg)				**4.11**	**3.21**		
UF-starting K_d							1.6	1.6
UF-pH conversion							2.5	2.5
UF-speciation							1.4	1.4
UF-min							1.4	1.4
UF-total							7.8	7.8
K_d upper limit	(m^3/kg)				31.88	24.95		
K_d lower limit	(m^3/kg)				0.53	0.41		
positive error bar					*27.77*	*21.74*		
negative error bar					*3.58*	*2.80*		

Speciation

Filename	mudstone_HDB-6_5b_Cs	Gorgeon(1994)_Cs
	TDB: JNCTDB_011213c2	

Cs(I) speciation (Gorgeon, 1994)

System		**Application**		**Data Source**
Substrate		**Koetoi**	**Wakkanai**	**Na-Illite**
Solution		**HDB-6**		**1 M NaCl**
Cs^{+1} added	(mol/kg)	2.00E-02	2.00E-02	2.00E-02
pH		6.75	6.75	6.6
pCO_2		-0.58	-0.58	-
CEC		20.00	20.00	122.00
BET		5.66	4.77	97.00
Cs^{+1} dissolved	(mol/kg)	2.00E-02	2.00E-02	2.00E-02
Na^+	(mol/kg)	2.28E-01	2.28E-01	1.00E+00
K^+	(mol/kg)	2.08E-03	2.08E-03	0.00E+00
NH_4^+	(mol/kg)	7.89E-03	7.89E-03	0.00E+00
∑ competitive cations in solution with Na^+ (C-cmp/a)	(mol/kg)	2.38E-01	2.38E-01	1.00E+00
Na^+	(mol/kg)	2.28E-01	2.28E-01	1.00E+00
K^+	(mol/kg)	2.08E-03	2.08E-03	0.00E+00
NH_4^+	(mol/kg)	7.89E-03	7.89E-03	0.00E+00
∑ competitive cations in solution without Na^+ (C-cmp/b)	(mol/kg)	9.97E-03	9.97E-03	0.00E+00

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K_d-derivation Cs(I) Gorgeon (1994), page 1/2

Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**
	HDB-6	**HDB-6**
Pred. K_d: CF-1 (CEC)	0.41	0.41
Pred. K_d: CF-1 (BET)	0.05	0.05
Pred. K_d: CF-1 (% clay)	0.72	0.56
Pred. K_d: CF-1 (% Illite)	0.22	0.22
Pred. K_d: CF-3 (CEC)	1.73	1.73
Pred. K_d: CF-3 (BET)	0.20	0.20
Pred. K_d: CF-3 (% clay)	3.02	2.36
Pred. K_d: CF-3 (% Illite)	0.92	0.92

Cs(I) K_d-derivation		**Conditions**					**Conversion (C) / Uncertainty (U)**	
		Data source[1]	**Additional Information**[1]		**Application**		**CF**	
					Mudstone		**Mudstone**	
Solution		**1 M NaCl**	**1 M NaCl**	**1 M NaCl**	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Substrate		**Illite**	**Illite**	**Illite**	**Koetoi**[2]	**Wakkanai**[2]	**Koetoi**[2]	**Wakkanai**[2]
Experimental K_d	(m^3/kg)	2.82						
Conversion Mineralogy (CF-min)								
CEC	(meq/100g)	21.2			2.80	2.80	0.13	0.13
BET	(m^2/g)	111.5			1.69	1.69	0.02	0.02
% clay		100			23.00	18.00	0.23	0.18
% Illite		100			7.00	7.00	0.07	0.07
Conversion pH (CF-pH)								
pH		6.87	6.87	6.75	6.75	6.75		
K_d for 1 M NaCl (pH conversion)[1]			2.82	3.12			1.11	1.11
Conversion Speciation (CF-spec)	*irrelevant*							
Conversion Competition (Cationic) (CF-cmp)								
∑ competitive cations in soln. with Na^+ (CF-cmp/a)	mol/l	1.00			0.24	0.24	4.20	4.20
∑ competitive cations in soln. without Na^+ (CF-cmp/b)	mol/l	0.00E+00			9.97E-03	9.97E-03	0	0

(1) K_d values from data table Gorgeon (1994) given as log Kd
(2) Values of the avarage composition (Table Mineralogy 1)

Cs(I) K_d-derivation via CEC			**Koetoi**	**Wakkanai**	**CF**	
CF-1 (CEC)					0.15	0.15
Competition						
CF-3 (CEC)					0.61	0.61
					UF	
Predicted K_d: CF-1 (CEC)	(m^3/kg)		**0.41**	**0.41**		
UF-starting K_d					1.6	1.6
UF-pH conversion					2.5	2.5
UF-min					1.4	1.4
UF-total					5.5	5.5
K_d upper limit	(m^3/kg)		2.29	2.29		
K_d lower limit	(m^3/kg)		0.07	0.07		
positive error bar			*1.87*	*1.87*		
negative error bar			*0.34*	*0.34*		
Predicted K_d: CF-3 (CEC)	(m^3/kg)		**1.73**	**1.73**		
UF-starting K_d					1.6	1.6
UF-cations conversion					2.5	2.5
UF-pH conversion					2.5	2.5
UF-min					1.4	1.4
UF-total					13.9	13.9
K_d upper limit	(m^3/kg)		24.02	24.02		
K_d lower limit	(m^3/kg)		0.12	0.12		
positive error bar			*22.29*	*22.29*		
negative error bar			*1.61*	*1.61*		

K_d-derivation Cs(I) Gorgeon (1994), page 2/2

Cs(I) K_d-derivation via BET			**Koetoi**	**Wakkanai**	**CF**	
CF-1 (BET)					0.02	0.02
Competition						
CF-3 (BET)					0.07	0.07
					UF	
Predicted K_d: CF-1 (BET)	(m^3/kg)		**0.05**	**0.05**		
UF-starting K_d					1.6	1.6
UF-pH conversion					2.5	2.5
UF-min					1.4	1.4
UF-total					5.5	5.5
K_d upper limit	(m^3/kg)		0.26	0.26		
K_d lower limit	(m^3/kg)		0.01	0.01		
positive error bar			*0.22*	*0.22*		
negative error bar			*0.04*	*0.04*		
Predicted K_d: CF-3 (BET)	(m^3/kg)		**0.20**	**0.20**		
UF-starting K_d					1.6	1.6
UF-pH conversion					2.5	2.5
UF-cmp					1.2	1.2
UF-min					1.4	1.4
UF-total					6.7	6.7
K_d upper limit	(m^3/kg)		1.33	1.33		
K_d lower limit	(m^3/kg)		0.03	0.03		
positive error bar			*1.13*	*1.13*		
negative error bar			*0.17*	*0.17*		

Cs(I) K_d-derivation via % clay			**Koetoi**	**Wakkanai**	**CF**	
CF-1 (% clay)					0.25	0.20
Competition						
CF-3 (% clay)					1.07	0.84
					UF	
Predicted K_d: CF-1 (% clay)	(m^3/kg)		**0.72**	**0.56**		
UF-starting K_d					1.6	1.6
UF-pH conversion					2.5	2.5
UF-min					1.4	1.4
UF-total					5.5	5.5
K_d upper limit	(m^3/kg)		3.98	3.11		
K_d lower limit	(m^3/kg)		0.13	0.10		
positive error bar			*3.26*	*2.55*		
negative error bar			*0.59*	*0.46*		
Predicted K_d: CF-3 (% clay)	(m^3/kg)		**3.02**	**2.36**		
UF-starting K_d					1.6	1.6
UF-pH conversion					2.5	2.5
UF-cmp					1.2	1.2
UF-min					1.4	1.4
UF-total					6.7	6.7
K_d upper limit	(m^3/kg)		20.08	15.71		
K_d lower limit	(m^3/kg)		0.45	0.35		
positive error bar			*17.06*	*13.35*		
negative error bar			*2.56*	*2.01*		

Cs(I) K_d-derivation via % Illite			**Koetoi**	**Wakkanai**	**CF**	
CF-1 (% Illite)					0.08	0.08
Competition						
CF-3 (% Illite)					0.33	0.33
					UF	
Predicted K_d: CF-1 (% Illite)	(m^3/kg)		**0.22**	**0.22**		
UF-starting K_d					1.6	1.6
UF-pH conversion					2.5	2.5
UF-min					1.4	1.4
UF-total					5.5	5.5
K_d upper limit	(m^3/kg)		1.21	1.21		
K_d lower limit	(m^3/kg)		0.04	0.04		
positive error bar			*0.99*	*0.99*		
negative error bar			*0.18*	*0.18*		
Predicted K_d: CF-3 (% Illite)	(m^3/kg)		**0.92**	**0.92**		
UF-starting K_d					1.6	1.6
UF-pH conversion					2.5	2.5
UF-cmp					1.2	1.2
UF-min					1.4	1.4
UF-total					6.7	6.7
K_d upper limit	(m^3/kg)		6.11	6.11		
K_d lower limit	(m^3/kg)		0.14	0.14		
positive error bar			*5.19*	*5.19*		
negative error bar			*0.78*	*0.78*		

Speciation

Filename mudstone_HDB-6_5b_Cs PSI(1999)_0.1MNaClO4_Cs
TDB: JNCTDB_011213c2

Cs(I) speciation (Poinssot et al., 1999; PSI-Bericht)

System		**Application**		**Data Source**		
Substrate		**Koetoi**	**Wakkanai**	**Na-Illite**		
Solution		**HDB-6**		**0.01 M $NaClO_4$**	**0.1 M $NaClO_4$**	**1 M $NaClO_4$**
Cs(I) added	(mol/kg)	1.00E-08	1.00E-08	1.00E-08	1.00E-08	1.00E-08
pH		6.75	6.75	6.6	6.6	6.6
pCO_2		-0.58	-0.58	-	-	-
CEC		20.00	20.00	122.00	122.00	122.00
BET		5.66	4.77	97.00	97.00	97.00
Cs^{+1} dissolved	(mol/kg)	1.00E-08	1.00E-08	1.00E-08	1.00E-08	1.00E-08
Na^+	(mol/kg)	2.28E-01	2.28E-01	1.00E-02	1.00E-01	1.00E+00
K^+	(mol/kg)	2.08E-03	2.08E-03	4.70E-06	1.50E-05	0.00E+00
NH_4^+	(mol/kg)	7.89E-03	7.89E-03	0.00E+00	0.00E+00	0.00E+00
∑ competitive cations in solution with Na^+ (CF-cmp/a)	(mol/kg)	2.38E-01	2.38E-01	1.00E-02	1.00E-01	1.00E+00
Na^+	(mol/kg)	2.28E-01	2.28E-01	1.00E-02	1.00E-01	1.00E+00
K^+	(mol/kg)	2.08E-03	2.08E-03	4.70E-06	1.50E-05	0.00E+00
NH_4^+	(mol/kg)	7.89E-03	7.89E-03	0.00E+00	0.00E+00	0.00E+00
∑ competitive cations in solution without Na^+ (CF-cmp/b)	(mol/kg)	9.97E-03	9.97E-03	4.70E-06	1.50E-05	0.00E+00

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K_d-derivation Cs(I) on Illite PSI Report (1999), page 1/2

Overview Pred. K_d [m^3/kg]	A		B		C	
	Koetoi	Wakkanai	Koetoi	Wakkanai	Koetoi	Wakkanai
	HDB-6	HDB-6	HDB-6	HDB-6	HDB-6	HDB-6
Pred. K_d: CF-1 (CEC)	5.42	5.42	0.91	0.91	0.12	0.12
Pred. K_d: CF-1 (BET)	4.12	4.12	0.70	0.70	0.09	0.09
Pred. K_d: CF-1 (% clay)	58.38	45.69	9.85	7.71	1.24	0.97
Pred. K_d: CF-1 (% Illite)	17.77	17.77	3.00	3.00	0.38	0.38
Pred. K_d: CF-3a (CEC)	0.23	0.23	0.38	0.38	0.48	0.48
Pred. K_d: CF-3a (BET)	0.17	0.17	0.29	0.29	0.37	0.37
Pred. K_d: CF-3a (% clay)	2.46	1.92	4.14	3.24	5.21	4.08
Pred. K_d: CF-3a (% Illite)	0.75	0.75	1.26	1.26	1.59	1.59
Pred. K_d: CF-3b (CEC)	0.00	0.00	0.00	0.00	0.00	0.00
Pred. K_d: CF-3b (BET)	0.00	0.00	1.05E-03	1.05E-03	0.00	0.00
Pred. K_d: CF-3b (% clay)	0.03	0.02	0.01	0.01	0.00	0.00
Pred. K_d: CF-3b (% Illite)	0.01	0.01	4.51E-03	4.51E-03	0.00	0.00

Cs(I) K_d-derivation (Illite)		Conditions					Conversion (C) / Uncertainty (U) Factor(F)					
		Data source[1]			Application		CF for A		CF for B		CF for C	
		A	B	C	Mudstone		Mudstone		Mudstone		Mudstone	
Solution		0.01 M $NaClO_4$	0.1 M $NaClO_4$	1 M $NaClO_4$	HDB-6	HDB-6	HDB-6	HDB-6	HDB-6	HDB-6	HDB-6	HDB-6
Substrate		Na-Illite[3]	Na-Illite[3]	Na-Illite	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**
Experimental K_d	(m^3/kg)	236.05	39.81	5.01								
Conversion Mineralogy (CF-min)												
CEC[5]	(meq/100g)	122.00	122.00	122.00	2.80	2.80	0.02	0.02	0.02	0.02	0.02	0.02
BET[4]	(m^2/g)	97.00	97.00	97.00	1.69	1.69	0.02	0.02	0.02	0.02	0.02	0.02
% clay		93.00	93.00	93.00	23.00	18.00	0.25	0.19	0.25	0.19	0.25	0.19
% Illite		93.00	93.00	93.00	7.00	7.00	0.08	0.08	0.08	0.08	0.08	0.08
Conversion pH (CF-pH)	*irrelevant*											
Conversion Speciation (CF-spec)	*irrelevant*											
Conversion Competition (Cationic) (CF-cmp)												
∑ competitive cations in soln. with Na^+ (CF-cmp/a)	(mol/l)	0.01	0.10	1.00	0.24	0.24	0.04	0.04	0.42	0.42	4.20	4.20
∑ competitive cations in soln. without Na^+ (CF-cmp/b)	(mol/l)	4.70E-06	1.50E-05	0.00	9.97E-03	9.97E-03	4.72E-04	4.72E-04	1.51E-03	1.51E-03	0.00	0.00

(1) K_d value from Cs(I) sorption datapoint from Poinssot et al. (1999), PSI Report; Kd value from graph at pH = 6.63; [Cs] = 1.0E-8 M
(2) Values of the avarage composition (Table Mineralogy 1)
(3) Conditioned Na-Illite; clay mineral composition: 93% illite and 7% kaolinite
(4) BET value of non-treated illite
(5) CEC value of treated Na-illite; pH 7.1

		A		B		C		Koetoi	Wakkanai	Koetoi	Wakkanai	Koetoi	Wakkanai
Cs(I) K_d-derivation via CEC		**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**	**CF for A**		**CF for B**		**CF for C**	
CF-1 (CEC)								0.02	0.02	0.02	0.02	0.02	0.02
Competition													
CF-3a (CEC)								0.00	0.00	0.01	0.01	0.10	0.10
CF-3b (CEC)								1.08E-05	1.08E-05	3.45E-05	3.45E-05	0.00	0.00
								UF		**UF**		**UF**	
Predicted K_d: CF-1 (CEC)	(m^3/kg)	**5.42**	**5.42**	**0.91**	**0.91**	**0.12**	**0.12**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.2	2.2	2.2	2.2	2.2	2.2
K_d upper limit	(m^3/kg)	12.02	12.02	2.03	2.03	0.26	0.26						
K_d lower limit	(m^3/kg)	2.44	2.44	0.41	0.41	0.05	0.05						
positive error bar		*6.60*	*6.60*	*1.11*	*1.11*	*0.14*	*0.14*						
negative error bar		*2.98*	*2.98*	*0.50*	*0.50*	*0.06*	*0.06*						
Predicted K_d: CF-3a (CEC)		**0.23**	**0.23**	**0.38**	**0.38**	**0.48**	**0.48**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-cmp								1.2	1.2	1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.7	2.7	2.7	2.7	2.7	2.7
K_d upper limit		0.61	0.61	1.02	1.02	1.29	1.29						
K_d lower limit		0.09	0.09	0.14	0.14	0.18	0.18						
positive error bar		*0.38*	*0.38*	*0.64*	*0.64*	*0.80*	*0.80*						
negative error bar		*0.14*	*0.14*	*0.24*	*0.24*	*0.30*	*0.30*						
Predicted K_d: CF-3b (CEC)		**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-cmp								1.2	1.2	1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.7	2.7	2.7	2.7	2.7	2.7
K_d upper limit		0.01	0.01	0.00	0.00	0.00	0.00						
K_d lower limit		0.00	0.00	0.00	0.00	0.00	0.00						
positive error bar		*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*						
negative error bar		*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*						

		A		B		C		Koetoi	Wakkanai	Koetoi	Wakkanai	Koetoi	Wakkanai
Cs(I) K_d-derivation via BET		**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**	**CF for A**		**CF for B**		**CF for C**	
CF-1 (BET)								0.02	0.02	0.02	0.02	0.02	0.02
Competition													
CF-3a (BET)								0.00	0.00	0.01	0.01	0.07	0.07
CF-3b (BET)								0.00	0.00	0.00	0.00	0.00	0.00
								UF		**UF**		**UF**	
Predicted K_d: CF-1 (BET)	(m^3/kg)	**4.12**	**4.12**	**0.70**	**0.70**	**0.09**	**0.09**						
UF-starting K_d								1.585	1.585	1.585	1.585	1.585	1.585
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.2	2.2	2.2	2.2	2.2	2.2
K_d upper limit	(m^3/kg)	9.15	9.15	1.54	1.54	0.19	0.19						
K_d lower limit	(m^3/kg)	1.86	1.86	0.31	0.31	0.04	0.04						
positive error bar		*5.02*	*5.02*	*0.85*	*0.85*	*0.11*	*0.11*						
negative error bar		*2.26*	*2.26*	*0.38*	*0.38*	*0.05*	*0.05*						
Predicted K_d: CF-3a (BET)		**0.17**	**0.17**	**0.29**	**0.29**	**0.37**	**0.37**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-cmp								1.2	1.2	1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.7	2.7	2.7	2.7	2.7	2.7
K_d upper limit		0.46	0.46	0.78	0.78	0.98	0.98						
K_d lower limit		0.07	0.07	0.11	0.11	0.14	0.14						
positive error bar		*0.29*	*0.29*	*0.49*	*0.49*	*0.61*	*0.61*						
negative error bar		*0.11*	*0.11*	*0.18*	*0.18*	*0.23*	*0.23*						
Predicted K_d: CF-3b (BET)		**0.00**	**0.00**	**1.05E-03**	**1.05E-03**	**0.00E+00**	**0.00E+00**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-cmp								1.2	1.2	1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.7	2.7	2.7	2.7	2.7	2.7
K_d upper limit		0.01	0.01	0.00	0.00	0.00	0.00						
K_d lower limit		7.30E-04	7.30E-04	3.93E-04	3.93E-04	0.00	0.00						
positive error bar		*0.00*	*0.00*	*0.00*	*1.74E-03*	*0.00*	*0.00*						
negative error bar		*1.21E-03*	*1.21E-03*	*6.53E-04*	*6.53E-04*	*0.00*	*0.00*						

K_d-derivation Cs(I) on Illite PSI Report (1999), page 2/2

		A		B		C		Koetoi	Wakkanai	Koetoi	Wakkanai	Koetoi	Wakkanai
Cs(I) K_d-derivation via % clay		**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**	**CF for A**		**CF for B**		**CF for C**	
CF-1 (% clay)								0.25	0.19	0.25	0.19	0.25	0.19
Competition													
CF-3a (% clay)								0.01	0.01	0.10	0.08	1.04	0.81
CF-3b (% clay)								0.00	0.00	0.00	0.00	0.00	0.00
								UF		**UF**		**UF**	
Predicted K_d: CF-1 (% clay)	(m^3/kg)	**58.38**	**45.69**	**9.85**	**7.71**	**1.24**	**0.97**						
UF-starting K_d								1.585	1.585	1.585	1.585	1.585	1.585
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.2	2.2	2.2	2.2	2.2	2.2
K_d upper limit	(m^3/kg)	129.53	101.37	21.85	17.10	2.75	2.15						
K_d lower limit	(m^3/kg)	26.31	20.59	4.44	3.47	0.56	0.44						
positive error bar		*71.15*	*55.69*	*12.00*	*9.39*	*1.51*	*1.18*						
negative error bar		*32.07*	*25.10*	*5.41*	*4.23*	*0.68*	*0.53*						
Predicted K_d: CF-3a (% clay)		**2.46**	**1.92**	**4.14**	**3.24**	**5.21**	**4.08**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-cmp								1.2	1.2	1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.7	2.7	2.7	2.7	2.7	2.7
K_d upper limit		6.54	5.12	11.02	8.63	13.88	10.86						
K_d lower limit		0.92	0.72	1.55	1.22	1.96	1.53						
positive error bar		*4.08*	*3.20*	*6.88*	*5.39*	*8.66*	*6.78*						
negative error bar		*1.53*	*1.20*	*2.59*	*2.02*	*3.25*	*2.55*						
Predicted K_d: CF-3b (% clay)		**0.03**	**0.02**	**0.01**	**0.01**	**0.00**	**0.00**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-cmp								1.2	1.2	1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.7	2.7	2.7	2.7	2.7	2.7
K_d upper limit		0.07	0.06	0.04	0.03	0.00	0.00						
K_d lower limit		0.01	0.01	0.01	0.00	0.00	0.00						
positive error bar		*0.05*	*0.04*	*0.02*	*0.02*	*0.00*	*0.00*						
negative error bar		*0.02*	*0.01*	*0.01*	*0.01*	*0.00*	*0.00*						

		A		B		C		Koetoi	Wakkanai	Koetoi	Wakkanai	Koetoi	Wakkanai
Cs(I) K_d-derivation via % Illite		**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**	**CF for A**		**CF for B**		**CF for C**	
CF-1 (% Illite)								0.08	0.08	0.08	0.08	0.08	0.08
Competition													
CF-3a (% Illite)								3.17E-03	3.17E-03	0.03	0.03	0.32	0.32
CF-3b (% Illite)								3.55E-05	3.55E-05	1.13E-04	1.13E-04	0.00	0.00
								UF		**UF**		**UF**	
Predicted K_d: CF-1 (% Illite)	(m^3/kg)	**17.77**	**17.77**	**3.00**	**3.00**	**0.38**	**0.38**						
UF-starting K_d								1.585	1.585	1.585	1.585	1.585	1.585
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.2	2.2	2.2	2.2	2.2	2.2
K_d upper limit	(m^3/kg)	39.42	39.42	6.65	6.65	0.84	0.84						
K_d lower limit	(m^3/kg)	8.01	8.01	1.35	1.35	0.17	0.17						
positive error bar		*21.66*	*21.66*	*3.65*	*3.65*	*0.46*	*0.46*						
negative error bar		*9.76*	*9.76*	*1.65*	*1.65*	*0.21*	*0.21*						
Predicted K_d: CF-3a (% Illite)		**0.75**	**0.75**	**1.26**	**1.26**	**1.59**	**1.59**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-cmp								1.2	1.2	1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.7	2.7	2.7	2.7	2.7	2.7
K_d upper limit		1.99	1.99	3.36	3.36	4.22	4.22						
K_d lower limit		0.28	0.28	0.47	0.47	0.60	0.60						
positive error bar		*1.24*	*1.24*	*2.10*	*2.10*	*2.64*	*2.64*						
negative error bar		*0.47*	*0.47*	*0.79*	*0.79*	*0.99*	*0.99*						
Predicted K_d: CF-3b (% Illite)		**0.01**	**0.01**	**0.00**	**0.00**	**0.00**	**0.00**						
UF-starting K_d								1.6	1.6	1.6	1.6	1.6	1.6
UF-cmp								1.2	1.2	1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4	1.4	1.4
UF-total								2.7	2.7	2.7	2.7	2.7	2.7
K_d upper limit		0.02	0.02	0.01	0.01	0.00	0.00						
K_d lower limit		3.15E-03	3.15E-03	1.69E-03	1.69E-03	0.00	0.00						
positive error bar		*0.01*	*0.01*	*0.01*	*0.01*	*0.00*	*0.00*						
negative error bar		*0.01*	*0.01*	*2.82E-03*	*2.82E-03*	*0.00*	*0.00*						

Speciation

Filename mudstone_HDB-6_5b_Cs PW_Sato&Shibutani(1994)_JNCTDB
TDB: JNCTDB_011213c2

Cs(I) speciation (Sato & Shibutani, 1994)

System		**Application**		**Data Source**
Substrate		**Koetoi**	**Wakkanai**	**Kunigel V1**
Solution		**HDB-6**		**Dist. equil. water**
Cs^{+1} added	(mol/kg)	7.52E-05	7.52E-05	7.52E-05
pH		6.75	6.75	6.92
pCO_2		-0.58	-0.58	-
CEC		20.00	20.00	60.10
BET		5.66	4.77	-
Cs^{+1} dissolved	(mol/kg)	7.52E-05	7.52E-05	7.52E-05
Ca^{+2}	(mol/kg)	2.09E-03	2.09E-03	9.45E-05
Fe^{+2}	(mol/kg)	1.52E-05	1.52E-05	-
Fe^{+3}	(mol/kg)	6.42E-14	6.42E-14	-
Mg^{+2}	(mol/kg)	5.87E-03	5.87E-03	-
Mn (all ox. states)	(mol/kg)	3.69E-07	3.69E-07	-
Na^{+}	(mol/kg)	2.31E-01	2.31E-01	1.86E-04
K^{+}	(mol/kg)	2.11E-03	2.11E-03	2.07E-06
Sr^{+2}	(mol/kg)	3.01E-05	3.01E-05	-
NH_4^{+}	(mol/kg)	7.89E-03	7.89E-03	0.00E+00
∑ competitive cations in solution with Na^{+} (C-cmp/a)	(mol/kg)	2.49E-01	2.49E-01	2.82E-04
Ca^{+2}	(mol/kg)	2.09E-03	2.09E-03	9.45E-05
Fe^{+2}	(mol/kg)	1.52E-05	1.52E-05	-
Fe^{+3}	(mol/kg)	6.42E-14	6.42E-14	-
Mg^{+2}	(mol/kg)	5.87E-03	5.87E-03	-
Mn (all ox. states)	(mol/kg)	3.69E-07	3.69E-07	-
Na^{+}	(mol/kg)	2.31E-01	2.31E-01	1.86E-04
K^{+}	(mol/kg)	2.11E-03	2.11E-03	2.07E-06
Sr^{+2}	(mol/kg)	3.01E-05	3.01E-05	-
NH_4^{+}	(mol/kg)	7.89E-03	7.89E-03	0.00E+00
∑ competitive cations in solution without Na^{+} (C-cmp/b)	(mol/kg)	1.80E-02	1.80E-02	9.66E-05

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K_d-derivation Cs(I) on Kunigel-V1 Sato and Shibutani (1994), page 1/2

Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**
	HDB-6	**HDB-6**
Pred. K_d: CF-1 (CEC)	0.28	0.28
Pred. K_d: CF-1 (BET)	0.14	0.12
Pred. K_d: CF-1 (% clay)	0.43	0.33
Pred. K_d: CF-3 (CEC)	3.21E-04	3.21E-04
Pred. K_d: CF-3 (BET)	1.56E-04	1.31E-04
Pred. K_d: CF-3 (%clay)	4.82E-04	3.77E-04

Cs(I) K_d-derivation (Smectite)		**Conditions**			**Conversion (C) / Uncertainty (U)**	
		Data source[1]	**Application**		**CF**	
			Mudstone		**Mudstone**	
Solution[5]		Dist. equil. water	HDB-6	HDB-6	HDB-6	HDB-6
Substrate		Kunigel-V1	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**
Experimental K_d	(m^3/kg)	0.85				
Conversion Mineralogy (CF-min)						
CEC[4]	(meq/100g)	60.10	20.00	20.00	0.33	0.33
BET[6]	m^2/g	35.00	5.66	4.77	0.16	0.14
% clay[3]		46.00	23.00	18.00	0.50	0.39
Conversion pH (CF-pH)	*irrelevant*					
Conversion Speciation (CF-spec)	*irrelevant*					
Conversion Competition (Cationic) (CF-cmp)						
∑ competitive cations in soln. with Na^+ (CF-cmp/a)	(mol/l)	2.82E-04	0.25	0.25	1.13E-03	1.13E-03
∑ competitive cations in soln. without Na^+ (CF-cmp/b)	(mol/l)	9.66E-05	0.02	0.02	5.36E-03	5.36E-03

(1) K_d value from SDB database, Sato and Shibutani (1994), at pH = 6.92; [Cs] = 7.52E-5 M

(2) Values of the avarage composition (Table Mineralogy 1)

(3) clay mineral composition of data source from Sasaki et al. (1995): smectite 46-49%, quartz 29-38% and other trace impurities

(4) CEC value of data source from Sasaki et al. (1995)

(5) [Na^+] calculated with Phreeqci Ion Exchange with Kunigel V1 equilibrated in distilled water (S:W = 2 g/l)

(6)Value from 'Minerals in Soil Environments; J.B. Dixon and S.B. Weed; Soil Science Society of America'

				Koetoi	**Wakkanai**
Cs(I) K_d-derivation via CEC		Koetoi	Wakkanai	**CF**	
CF-1 (CEC)				**0.33**	**0.33**
Competition					
CF-3a (CEC)				**3.77E-04**	**3.77E-04**
				UF	
Predicted K_d: CF-1 (CEC)	(m^3/kg)	**0.28**	**0.28**		
UF-starting K_d				1.6	1.6
UF-min				1.4	1.4
UF-total				2.2	2.2
K_d upper limit	(m^3/kg)	0.63	0.63		
K_d lower limit	(m^3/kg)	0.13	0.13		
positive error bar		*0.35*	*0.35*		
negative error bar		*0.16*	*0.16*		
Predicted K_d: CF-3 (CEC)	(m^3/kg)	**3.21E-04**	**3.21E-04**		
UF-starting K_d				1.6	1.6
UF-cmp				1.2	1.2
UF-min				1.4	1.4
UF-total				2.7	2.7
K_d upper limit	(m^3/kg)	8.54E-04	8.54E-04		
K_d lower limit	(m^3/kg)	1.21E-04	1.21E-04		
positive error bar		*5.33E-04*	*5.33E-04*		
negative error bar		*2.00E-04*	*2.00E-04*		

K_d-derivation Cs(I) on Kunigel-V1 Sato and Shibutani (1994), page 2/2

				Koetoi	Wakkanai
Cs(I) K_d-derivation via BET		**Koetoi**	**Wakkanai**	**CF**	
CF-1 (BET)				**0.16**	**0.14**
Competition					
CF-3 (BET)				**1.83E-04**	**1.54E-04**
				UF	
Predicted K_d: CF-1 (BET)	(m^3/kg)	**0.14**	**0.12**		
UF-starting K_d				1.6	1.6
UF-min				1.4	1.4
UF-total				2.2	2.2
K_d upper limit	(m^3/kg)	0.31	0.26		
K_d lower limit	(m^3/kg)	0.06	0.05		
positive error bar		*0.17*	*0.14*		
negative error bar		*0.08*	*0.06*		
Predicted Kd: CF-3 (BET)	(m^3/kg)	**1.56E-04**	**1.31E-04**		
UF-starting K_d				1.6	1.6
UF-cmp				1.2	1.2
UF-min				1.4	1.4
UF-total				2.7	2.7
K_d upper limit	(m^3/kg)	4.15E-04	3.50E-04		
K_d lower limit	(m^3/kg)	5.85E-05	4.93E-05		
positive error bar		*2.59E-04*	*2.18E-04*		
negative error bar		*9.73E-05*	*8.20E-05*		

				Koetoi	Wakkanai
Cs(I) K_d-derivation via % clay		**Koetoi**	**Wakkanai**	**CF**	
CF-1 (% clay)				**0.50**	**0.39**
Competition					
CF-3 (% clay)				**0.00**	**0.00**
				UF	
Predicted Kd: CF-1 (% clay)	(m^3/kg)	**0.43**	**0.33**		
UF-starting K_d				1.6	1.6
UF-min				1.4	1.4
UF-total				2.2	2.2
K_d upper limit	(m^3/kg)	0.94	0.74		
K_d lower limit	(m^3/kg)	0.19	0.15		
positive error bar		*0.52*	*0.41*		
negative error bar		*0.23*	*0.18*		
Predicted Kd: CF-3 (% clay)	(m^3/kg)	**4.82E-04**	**3.77E-04**		
UF-starting K_d				1.6	1.6
UF-cmp				1.2	1.2
UF-min				1.4	1.4
UF-total				2.7	2.7
K_d upper limit	(m^3/kg)	1.28E-03	1.00E-03		
K_d lower limit	(m^3/kg)	1.81E-04	1.42E-04		
positive error bar		*8.02E-04*	*6.27E-04*		
negative error bar		*3.01E-04*	*2.36E-04*		

Speciation

Filename mudstone_HDB-6_5b_Se(2) Ticknor(1988)_100%_Se(Kaolinit)_redox_H
Ticknor(1988)_10%_Se(Kaolinit)_redox_H
TDB: JNCTDB_011213c2

Se(-II) speciation (Ticknor et al., 1988)

System		**Application**		**Data Source**	
Substrate		**Koetoi**	**Wakkanai**	**Kaolinite**	
Solution		**HDB-6**		**SCSSS^1 100%**	**SCSSS 10%**
Se(-II) added	(mol/kg)	8.87E-11	8.87E-11	9.28E-11	8.79E-11
pH		6.75	6.75	9.5	9.5
pCO_2		-0.58	-0.58	-	-
Se(-II) dissolved	(mol/kg)	8.87E-11	8.87E-11	9.28E-11	8.79E-11
HSe^{-1}	(mol/kg)	8.86E-11	8.86E-11	9.28E-11	8.79E-11
H_2Se	(mol/kg)	8.69E-14	8.69E-14	1.47E-16	1.62E-16
Se^{-2}	(mol/kg)	1.56E-18	1.56E-18	4.96E-16	7.98E-16
CF-spec		**1.00E+00**	**1.00E+00**	**1.00E+00**	**1.00E+00**
Se(IV) dissolved	(mol/kg)	2.694E-32	2.694E-32	1.53E-35	1.10E-37
$HSeO_3^-$	(mol/kg)	2.55E-32	2.55E-32	8.55E-37	3.71E-39
SeO_3^{-2}	(mol/kg)	1.42E-33	1.42E-33	1.44E-35	1.07E-37
H_2SeO_3	(mol/kg)	2.01E-36	2.01E-36	0.00E+00	0.00E+00
S(-II)-ions	(mol/kg)	8.46E-11	8.46E-11	2.57E-05	7.83E-04
SiO_4-ions	(mol/kg)	1.14E-03	1.14E-03	2.32E-04	2.20E-05
PO_4-ions	(mol/kg)	1.29E-06	1.29E-06	-	-
CO_3-ions	(mol/kg)	4.15E-02	4.15E-02	-	-
SO_4-ions	(mol/kg)	6.34E-06	6.34E-06	2.69E-03	3.28E-05
∑ competitive Anions in solution (CF-cmp)	(mol/kg)	**4.27E-02**	**4.27E-02**	**2.95E-03**	**8.37E-04**

1) Standard Canadian Shield Saline Solution

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Kd-Derivation Se(-II) Ticknor et al. (1988)

	Data source A		Data source B	
Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**
Kaolinite	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Pred. K_d: CF-1 (CEC)	0.01	0.01	0.02	0.02
Pred. K_d: CF-1 (BET)	0.01	4.72E-03	0.01	0.01
Pred. K_d: CF-1 (% clay)	1.91E-03	1.49E-03	2.99E-03	2.34E-03
Pred. K_d: CF-3 (CEC)	8.19E-04	8.19E-04	3.65E-04	3.65E-04
Pred. K_d: CF-3 (BET)	3.87E-04	3.26E-04	1.72E-04	1.45E-04
Pred. K_d: CF-3 (%clay)	1.32E-04	1.03E-04	5.87E-05	4.59E-05

Se(II) K_d-derivation (Kaolinite)		**Conditions**				**Conversion (C) / Uncertainty (U)**		**Conversion (C) / Uncertainty (U)**	
		Data source[1]		**Application**		**CF for A**		**CF for B**	
		A	**B**	**Mudstone**		**Mudstone**		**Mudstone**	
Solution		**100%SCSSS**	**10%SCSSS**	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Substrate		**Kaolinite**	**Kaolinite**	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**
Experimental K_d	(m^3/kg)	8.30E-03	0.013						
Conversion Mineralogy (CF-min)									
CEC	(meq/100g)	13.99	13.99	20.00	20.00	1.43	1.43	1.43	1.43
BET	(m^2/g)	8.38	8.38	5.66	4.77	0.67	0.57	0.67	0.57
% clay		100	100	23.00	18.00	0.23	0.18	0.23	0.18
Conversion pH (CF-pH)									
pH		9.5	9.5	6.75	6.75				
K_d for pH conversion[3] (*tentative*)						1	1	1	1
Conversion Speciation (CF-spec)	*irrelevant (no relevant species included in JNC-TDB)*								
Conversion Competition (Anionic) (CF-cmp)									
∑ competitive anions in solution		2.95E-03	8.37E-04	4.27E-02	4.27E-02	0.07	0.07	0.02	0.02

(1) K_d values from data table Ticknor et al. (1988) given in ml/g

(2) Values of the avarage composition (Table Mineralogy 1)

(3) Based on speciation of Se(-II)

				A		B					
Se(-II) K_d-derivation via CEC				Koetoi	Wakkanai	Koetoi	Wakkanai	**CF for A**		**CF for B**	
CF-1 (CEC)								1.43	1.43	1.43	1.43
Competition											
CF-3 (CEC)								0.10	0.10	0.03	0.03
								UF		**UF**	
Predicted K_d: CF-1 (CEC)	(m^3/kg)			**0.01**	**0.01**	**0.02**	**0.02**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-min								1.4	1.4	1.4	1.4
UF-total								5.5	5.5	5.5	5.5
K_d upper limit	(m^3/kg)			0.07	0.07	0.10	0.10				
K_d lower limit	(m^3/kg)			0.00	0.00	0.00	0.00				
positive error bar				*0.05*	*0.05*	*0.08*	*0.08*				
negative error bar				*0.01*	*0.01*	*0.02*	*0.02*				
Predicted Kd: CF-3 (CEC)	(m^3/kg)			**8.19E-04**	**8.19E-04**	**3.65E-04**	**3.65E-04**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-cmp								1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4
UF-total								6.7	6.7	6.7	6.7
K_d upper limit	(m^3/kg)			0.01	0.01	0.00	0.00				
K_d lower limit	(m^3/kg)			0.00	0.00	0.00	0.00				
positive error bar				*0.00*	*0.00*	*0.00*	*0.00*				
negative error bar				*0.00*	*0.00*	*0.00*	*0.00*				

				A		B					
Se(-II) K_d-derivation via BET				Koetoi	Wakkanai	Koetoi	Wakkanai	**CF for A**		**CF for B**	
CF-1 (BET)								0.67	0.57	0.67	0.57
Competition											
CF-3 (BET)								0.05	0.04	0.01	0.01
								UF		**UF**	
Predicted K_d: CF-1 (BET)	(m^3/kg)			**5.60E-03**	**4.72E-03**	**8.77E-03**	**7.40E-03**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-min								1.4	1.4	1.4	1.4
UF-total								5.5	5.5	5.5	5.5
K_d upper limit	(m^3/kg)			0.03	0.03	0.05	0.04				
K_d lower limit	(m^3/kg)			0.00	0.00	0.00	0.00				
positive error bar				*0.03*	*0.02*	*0.04*	*0.03*				
negative error bar				*0.00*	*0.00*	*0.01*	*0.01*				
Predicted K_d: CF-3 (BET)	(m^3/kg)			**3.87E-04**	**3.26E-04**	**1.72E-04**	**1.45E-04**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-cmp								1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4
UF-total								6.7	6.7	6.7	6.7
K_d upper limit	(m^3/kg)			2.57E-03	2.17E-03	1.15E-03	9.66E-04				
K_d lower limit	(m^3/kg)			5.81E-05	4.90E-05	2.59E-05	2.18E-05				
positive error bar				*2.19E-03*	*1.84E-03*	*9.74E-04*	*8.21E-04*				
negative error bar				*3.29E-04*	*2.77E-04*	*1.46E-04*	*1.23E-04*				

				A		B					
Se(-II) K_d-derivation via % clay				Koetoi	Wakkanai	Koetoi	Wakkanai	**CF for A**		**CF for B**	
CF-1 (% clay)								0.23	0.18	0.23	0.18
Competition											
CF-3 (% clay)								0.02	0.01	0.00	0.00
								UF		**UF**	
Predicted K_d: CF-1 (% clay)	(m^3/kg)			**1.91E-03**	**1.49E-03**	**2.99E-03**	**2.34E-03**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-min								1.4	1.4	1.4	1.4
UF-total								5.5	5.5	5.5	5.5
K_d upper limit	(m^3/kg)			1.06E-02	8.29E-03	1.66E-02	1.30E-02				
K_d lower limit	(m^3/kg)			3.44E-04	2.69E-04	5.39E-04	4.22E-04				
positive error bar				*8.68E-03*	*6.79E-03*	*1.36E-02*	*1.06E-02*				
negative error bar				*1.56E-03*	*1.22E-03*	*2.45E-03*	*1.92E-03*				
Predicted K_d: CF-3 (% clay)	(m^3/kg)			**1.32E-04**	**1.03E-04**	**5.87E-05**	**4.59E-05**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-cmp								1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4
UF-total								6.7	6.7	6.7	6.7
K_d upper limit	(m^3/kg)			8.78E-04	6.87E-04	3.90E-04	3.06E-04				
K_d lower limit	(m^3/kg)			1.98E-05	1.55E-05	8.81E-06	6.90E-06				
positive error bar				*7.46E-04*	*5.84E-04*	*3.32E-04*	*2.60E-04*				
negative error bar				*1.12E-04*	*8.77E-05*	*4.98E-05*	*3.90E-05*				

K_d-Derivation Se(-II) Ticknor et al. (1988)

	Data source A		Data source B	
Overview Pred. K_d [m^3/kg]	**Koetoi**	**Wakkanai**	**Koetoi**	**Wakkanai**
Chlorite	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Pred. K_d: CF-1 (CEC)	0.08	0.08	0.16	0.16
Pred. K_d: CF-1 (BET)	0.02	0.01	0.03	0.03
Pred. K_d: CF-1 (% clay)	1.66E-03	1.30E-03	3.22E-03	2.52E-03
Pred. K_d: CF-3 (CEC)	5.85E-03	5.85E-03	3.23E-03	3.23E-03
Pred. K_d: CF-3 (BET)	1.18E-03	9.96E-04	6.53E-04	5.50E-04
Pred. K_d: CF-3 (%clay)	1.14E-04	8.95E-05	6.32E-05	4.94E-05

Se(II) K_d-derivation (Chlorite)		**Conditions**				**Conversion (C) / Uncertainty (U)**		**Conversion (C) / Uncertainty (U)**	
		Data source[1]		**Application**		**CF for A**		**CF for B**	
		A	**B**	**Mudstone**		**Mudstone**		**Mudstone**	
Solution		**100%SCSSS**	**10%SCSSS**	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**	**HDB-6**
Substrate		**Chlorite**	**Chlorite**	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**	**Koetoi[2]**	**Wakkanai[2]**
Experimental K_d	(m^3/kg)	7.20E-03	0.014						
Conversion Mineralogy (CF-min)									
CEC	(meq/100g)	1.7	1.7	20.00	20.00	11.76	11.76	11.76	11.76
BET	(m^2/g)	2.38	2.38	5.66	4.77	2.38	2.00	2.38	2.00
% clay		100	100	23.00	18.00	0.23	0.18	0.23	0.18
Conversion pH (CF-pH)									
pH		10.5	10.5	6.75	6.75				
K_d for pH conversion[2] (*tentative*)						1	1	1	1
Conversion Speciation (CF-spec)	*irrelevant*								
Conversion Competition (Anionic) (CF-cmp)									
∑ competitive anions in solution		2.95E-03	8.37E-04	0.04	0.04	0.07	0.07	0.02	0.02

(1) K_d values from data table Ticknor et al. (1988) given in ml/g

(2) Values of the avarage composition (Table Mineralogy 1)

				A		B		Koetoi	Wakkanai	Koetoi	Wakkanai
Se(-II) K_d-derivation via CEC				Koetoi	Wakkanai	Koetoi	Wakkanai	**CF for A**		**CF for B**	
CF-1 (CEC)								11.76	11.76	11.76	11.76
Competition											
CF-3 (CEC)								0.81	0.81	0.23	0.23
								UF		**UF**	
Predicted K_d: CF-1 (CEC)	(L/g)			**0.08**	**0.08**	**0.16**	**0.16**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-min								1.4	1.4	1.4	1.4
UF-total								5.5	5.5	5.5	5.5
K_d upper limit	(L/g)			0.47	0.47	0.91	0.91				
K_d lower limit	(L/g)			0.02	0.02	0.03	0.03				
positive error bar				*0.39*	*0.39*	*0.75*	*0.75*				
negative error bar				*0.07*	*0.07*	*0.14*	*0.14*				
Predicted K_d: CF-3 (CEC)	(L/g)			**0.01**	**0.01**	**3.23E-03**	**3.23E-03**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-cmp								1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4
UF-total								6.7	6.7	6.7	6.7
K_d upper limit	(L/g)			0.04	0.04	0.02	0.02				
K_d lower limit	(L/g)			8.79E-04	8.79E-04	4.85E-04	4.85E-04				
positive error bar				*0.03*	*0.03*	*0.02*	*0.02*				
negative error bar				*0.00*	*0.00*	*0.00*	*0.00*				

				A		B					
Se(-II) K_d-derivation via BET				Koetoi	Wakkanai	Koetoi	Wakkanai	**CF for A**		**CF for B**	
CF-1 (BET)								2.38	2.00	2.38	2.00
Competition											
CF-3 (BET)								0.16	0.14	0.05	0.04
								UF		**UF**	
Predicted K_d: CF-1 (BET)	(L/g)			**0.02**	**0.01**	**0.03**	**0.03**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-min								1.4	1.4	1.4	1.4
UF-total								5.5	5.5	5.5	5.5
K_d upper limit	(L/g)			0.09	0.08	0.18	0.16				
K_d lower limit	(L/g)			3.08E-03	2.60E-03	0.01	5.06E-03				
positive error bar				*0.08*	*0.07*	*0.15*	*0.13*				
negative error bar				*0.01*	*0.01*	*0.03*	*0.02*				
Predicted K_d: CF-3 (BET)	(L/g)			**1.18E-03**	**9.96E-04**	**6.53E-04**	**5.50E-04**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-cmp								1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4
UF-total								6.7	6.7	6.7	6.7
K_d upper limit	(L/g)			0.01	0.01	4.34E-03	3.66E-03				
K_d lower limit	(L/g)			1.77E-04	1.50E-04	9.80E-05	8.26E-05				
positive error bar				*0.01*	*0.01*	*3.69E-03*	*3.11E-03*				
negative error bar				*1.00E-03*	*8.46E-04*	*5.55E-04*	*4.67E-04*				

				A		B					
Se(-II) K_d-derivation via % clay				Koetoi	Wakkanai	Koetoi	Wakkanai	**CF for A**		**CF for B**	
CF-1 (% clay)								0.23	0.18	0.23	0.18
Competition											
CF-3 (% clay)								0.02	0.01	4.51E-03	3.53E-03
								UF		**UF**	
Predicted K_d: CF-1 (% clay)	(L/g)			**1.66E-03**	**1.30E-03**	**3.22E-03**	**2.52E-03**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-min								1.4	1.4	1.4	1.4
UF-total								5.5	5.5	5.5	5.5
K_d upper limit	(L/g)					0.02	0.01				
K_d lower limit	(L/g)					5.80E-04	4.54E-04				
positive error bar						*0.01*	*0.01*				
negative error bar						*2.64E-03*	*2.07E-03*				
Predicted K_d: CF-3 (% clay)	(L/g)			**1.14E-04**	**8.95E-05**	**6.32E-05**	**4.94E-05**				
UF-starting K_d								1.6	1.6	1.6	1.6
UF-pH conversion								2.5	2.5	2.5	2.5
UF-cmp								1.2	1.2	1.2	1.2
UF-min								1.4	1.4	1.4	1.4
UF-total								6.7	6.7	6.7	6.7
K_d upper limit	(L/g)			7.61E-04	5.96E-04	4.20E-04	3.29E-04				
K_d lower limit	(L/g)			1.72E-05	1.34E-05	9.49E-06	7.43E-06				
positive error bar				*6.47E-04*	*5.06E-04*	*3.57E-04*	*2.80E-04*				
negative error bar				*9.72E-05*	*7.61E-05*	*5.37E-05*	*4.20E-05*				

Appendix III

Information on application conditions

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Quantification of mineral composition
(Based on normative calculation)

	Koetoi	Wakkanai
Quartz	9	11
Albite	4	5
K-feldspar	2	3
Illite	7	7
Smectite	11	8
Kaolinite	1	3
Chlorite	4	b.d.
Pyrite	1	4
Resid. $SiO2$	48	49

Data in wt%, b.d.=below detection

Estimated groundwater compositions for borehole HDB-6 (GL -450m)

TDB	011213c2.tdb	
Temp（℃）	25	
pH	6.752	
pe	-2.804	
Eh（mV）	-166	
log P_{CO2}	-2.081	
Ionic strength	2.579E-01	
Electrical balance（eq）	6.762E-15	
Elements	mol/L	mg/L
Na	2.279E-01	5239.42
K	2.077E-03	81.21
Mg	5.784E-03	140.61
Cl	2.202E-01	7806.09
Br	5.632E-04	45.00
Ca	2.093E-03	83.93
C	4.098E-02	491.76
S	6.250E-06	0.20
F	1.053E-05	0.20
Fe	1.524E-05	0.85
Si	1.141E-03	32.05
N	7.777E-03	108.88
P	1.266E-06	0.04
Sr	2.967E-05	2.60
Mn	3.640E-07	0.02
Al	3.706E-07	0.01
Dissolved species	mol/L	mg/L
HCO_3^-	2.989E-02	1823.29
CO_3^-	2.037E-05	1.22
SO_4^{2-}	4.375E-06	0.42
N_2	-	-
NH_4^+	7.761E-03	139.70
Fe^{2+}	1.523E-05	0.85
$H_4SiO_4(aq)$	1.139E-03	109.34
HPO_4^{2-}	5.060E-07	0.04
PO_4^{3-}	7.623E-12	0.00
Saturation Index		
calcite	0.00	
amorphous silica	-0.20	
siderite	0.00	
pyrite	0.00	

Mineral compositions

			Koetoi			Wakkanai		
Mineral	Standard CEC [*meq/100g*]	Standard BET [m^2/g]	weight %	Calc. CEC [*meq/g*]	Calc. BET [m^2/g]	weight %	Calc. CEC [*meq/g*]	Calc. BET [m^2/g]
Quartz			9			11		
Albite			4			5		
K-feldspar			2			3		
Illite	40 a	24.2 c	7	2.80	1.69	7	2.80	1.69
Smectite	110 a	35	11	12.10	3.85	8	8.80	2.80
Kaolinite	5 b	9.1 c	1	0.05	0.09	3	0.15	0.27
Chlorite	25 b	0.5 d	4	1.00	0.02	b.d.		
Pyrite			1			4		
Res. SiO_2			48			49		
Total			87			90		
Total CEC and BET	180	68.8	23	20.00	5.66	18	20.00	4.77
Total SiO_2			57			60		
Calculated				15.95			11.75	

b.d.=below detection

a Minerals in Soil Environments; J.B. Dixon and S.B. Weed; Soil Science Society of America
b Physical and Chemical Hydrogeology; P.A. Domenico and F.W. Schwartz; John Wiley & Sons
c Clays and Clay Minerals (1996), 44 (5), 609-623
d Eleventh Annual V.M. Goldschmidt Conference (2001)

国際単位系（SI）

表１．SI 基本単位

基本量	SI 基本単位	
	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd

表２．基本単位を用いて表されるSI組立単位の例

組立量	SI 基本単位	
	名称	記号
面積	平方メートル	m^2
体積	立法メートル	m^3
速さ，速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	m/s^2
波数	毎メートル	m-1
密度（質量密度）	キログラム毎立法メートル	kg/m^3
質量体積（比体積）	立法メートル毎キログラム	m^3/kg
電流密度	アンペア毎平方メートル	A/m^2
磁界の強さ	アンペア毎メートル	A/m
（物質量の）濃度	モル毎立方メートル	mol/m^3
輝度	カンデラ毎平方メートル	cd/m^2
屈折率	（数の）　1	1

表５．SI 接頭語

乗数	接頭語	記号	乗数	接頭語	記号
10^{24}	ヨタ	Y	10^{-1}	デシ	d
10^{21}	ゼタ	Z	10^{-2}	センチ	c
10^{18}	エクサ	E	10^{-3}	ミリ	m
10^{15}	ペタ	P	10^{-6}	マイクロ	μ
10^{12}	テラ	T	10^{-9}	ナノ	n
10^{9}	ギガ	G	10^{-12}	ピコ	p
10^{6}	メガ	M	10^{-15}	フェムト	f
10^{3}	キロ	k	10^{-18}	アト	a
10^{2}	ヘクト	h	10^{-21}	ゼプト	z
10^{1}	デカ	da	10^{-24}	ヨクト	y

表３．固有の名称とその独自の記号で表されるSI組立単位

組立量	SI 組立単位			
	名称	記号	他のSI単位による表し方	SI基本単位による表し方
平面角	ラジアン(a)	rad		$m\cdot m^{-1}=1$(b)
立体角	ステラジアン(a)	sr(c)		$m^2\cdot m^{-2}=1$(b)
周波数	ヘルツ	Hz		s^{-1}
力	ニュートン	N		$m\cdot kg\cdot s^{-2}$
圧力，応力	パスカル	Pa	N/m^2	$m^{-1}\cdot kg\cdot s^{-2}$
エネルギー，仕事，熱量	ジュール	J	N・m	$m^2\cdot kg\cdot s^{-2}$
工率，放射束	ワット	W	J/s	$m^2\cdot kg\cdot s^{-3}$
電荷，電気量	クーロン	C		s・A
電位差（電圧），起電力	ボルト	V	W/A	$m^2\cdot kg\cdot s^{-3}\cdot A^{-1}$
静電容量	ファラド	F	C/V	$m^{-2}\cdot kg^{-1}\cdot s^4\cdot A^2$
電気抵抗	オーム	Ω	V/A	$m^2\cdot kg\cdot s^{-3}\cdot A^{-2}$
コンダクタンス	ジーメンス	S	A/V	$m^{-2}\cdot kg^{-1}\cdot s^3\cdot A^2$
磁束	ウエーバ	Wb	V・s	$m^2\cdot kg\cdot s^{-2}\cdot A^{-1}$
磁束密度	テスラ	T	Wb/m^2	$kg\cdot s^{-2}\cdot A^{-1}$
インダクタンス	ヘンリー	H	Wb/A	$m^2\cdot kg\cdot s^{-2}\cdot A^{-2}$
セルシウス温度	セルシウス度(d)	℃		K
光束	ルーメン	lm	cd・sr(c)	$m^2\cdot m^{-2}\cdot cd=cd$
照度	ルクス	lx	lm/m^2	$m^2\cdot m^{-4}\cdot cd=m^{-2}\cdot cd$
（放射性核種の）放射能	ベクレル	Bq		s^{-1}
吸収線量，質量エネルギー分与，カーマ	グレイ	Gy	J/kg	$m^2\cdot s^{-2}$
線量当量，周辺線量当量，方向性線量当量，個人線量当量，組織線量当	シーベルト	Sv	J/kg	$m^2\cdot s^{-2}$

(a) ラジアン及びステラジアンの使用は、同じ次元であっても異なった性質をもった量を区別するときの組立単位の表し方として利点がある。組立単位を形作るときのいくつかの用例は表４に示されている。

(b) 実際には、使用する時には記号rad及びsrが用いられるが、習慣として組立単位としての記号“1”は明示されない。

(c) 測光学では、ステラジアンの名称と記号srを単位の表し方の中にそのまま維持している。

(d) この単位は、例としてミリセルシウス度m℃のようにSI接頭語を伴って用いても良い。

表４．単位の中に固有の名称とその独自の記号を含むSI組立単位の例

組立量	SI 組立単位		
	名称	記号	SI 基本単位による表し方
粘度	パスカル秒	Pa・s	$m^{-1}\cdot kg\cdot s^{-1}$
力のモーメント	ニュートンメートル	N・m	$m^2\cdot kg\cdot s^{-2}$
表面張力	ニュートン毎メートル	N/m	$kg\cdot s^{-2}$
角速度	ラジアン毎秒	rad/s	$m\cdot m^{-1}\cdot s^{-1}=s^{-1}$
角加速度	ラジアン毎平方秒	rad/s^2	$m\cdot m^{-1}\cdot s^{-2}=s^{-2}$
熱流密度，放射照度	ワット毎平方メートル	W/m^2	$kg\cdot s^{-3}$
熱容量，エントロピー	ジュール毎ケルビン	J/K	$m^2\cdot kg\cdot s^{-2}\cdot K^{-1}$
質量熱容量（比熱容量），質量エントロピー	ジュール毎キログラム毎ケルビン	J/(kg・K)	$m^2\cdot s^{-2}\cdot K^{-1}$
質量エネルギー（比エネルギー）	ジュール毎キログラム	J/kg	$m^2\cdot s^{-2}\cdot K^{-1}$
熱伝導率	ワット毎メートル毎ケルビン	W/(m・K)	$m\cdot kg\cdot s^{-3}\cdot K^{-1}$
体積エネルギー	ジュール毎立方メートル	J/m^3	$m^{-1}\cdot kg\cdot s^{-2}$
電界の強さ	ボルト毎メートル	V/m	$m\cdot kg\cdot s^{-3}\cdot A^{-1}$
体積電荷	クーロン毎立方メートル	C/m^3	$m^{-3}\cdot s\cdot A$
電気変位	クーロン毎平方メートル	C/m^2	$m^{-2}\cdot s\cdot A$
誘電率	ファラド毎メートル	F/m	$m^{-3}\cdot kg^{-1}\cdot s^4\cdot A^2$
透磁率	ヘンリー毎メートル	H/m	$m\cdot kg\cdot s^{-2}\cdot A^{-2}$
モルエネルギー	ジュール毎モル	J/mol	$m^2\cdot kg\cdot s^{-2}\cdot mol^{-1}$
モルエントロピー，モル熱容量	ジュール毎モル毎ケルビン	J/(mol・K)	$m^2\cdot kg\cdot s^{-2}\cdot K^{-1}\cdot mol^{-1}$
照射線量（Ｘ線及びγ線）	クーロン毎キログラム	C/kg	$kg^{-1}\cdot s\cdot A$
吸収線量率	グレイ毎秒	Gy/s	$m^2\cdot s^{-3}$
放射強度	ワット毎ステラジアン	W/sr	$m^4\cdot m^{-2}\cdot kg\cdot s^{-3}=m^2\cdot kg\cdot s^{-3}$
放射輝度	ワット毎平方メートル毎ステラジアン	$W/(m^2\cdot sr)$	$m^2\cdot m^{-2}\cdot kg\cdot s^{-3}=kg\cdot s^{-3}$

表６．国際単位系と併用されるが国際単位系に属さない単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1h =60 min=3600 s
日	d	1 d=24 h=86400 s
度	°	1°=(π/180) rad
分	’	1’=(1/60)°=(π/10800) rad
秒	”	1”=(1/60)’=(π/648000) rad
リットル	l、L	$1l=1\ dm^3=10^{-3}m^3$
トン	t	$1t=10^3\ kg$
ネーパ	Np	1Np=1
ベル	B	1B=(1/2)ln10(Np)

表７．国際単位系と併用されこれに属さない単位でSI単位で表される数値が実験的に得られるもの

名称	記号	SI 単位であらわされる数値
電子ボルト	eV	$1eV=1.60217733(49)\times10^{-19}J$
統一原子質量単位	u	$1u=1.6605402(10)\times10^{-27}kg$
天文単位	ua	$1ua=1.49597870691(30)\times10^{11}m$

表８．国際単位系に属さないが国際単位系と併用されるその他の単位

名称	記号	SI 単位であらわされる数値
海里		1海里=1852m
ノット		1ノット=1海里毎時=(1852/3600)m/s
アール	a	$1\ a=1\ dam^2=10^2m^2$
ヘクタール	ha	$1\ ha=1\ hm^2=10^4m^2$
バール	bar	$1\ bar=0.1MPa=100kPa=1000hPa=10^5Pa$
オングストローム	Å	$1\ Å=0.1nm=10^{-10}m$
バーン	b	$1\ b=100fm^2=10^{-28}m^2$

表９．固有の名称を含むCGS組立単位

名称	記号	SI 単位であらわされる数値
エルグ	erg	$1\ erg=10^{-7}\ J$
ダイン	dyn	$1\ dyn=10^{-5}N$
ポアズ	P	$1\ P=1\ dyn\cdot s/cm^2=0.1Pa\cdot s$
ストークス	St	$1\ St=1cm^2/s=10^{-4}m^2/s$
ガウス	G	$1\ G \triangleq 10^{-4}T$
エルステッド	Oe	$1\ Oe \triangleq (1000/4\pi)A/m$
マクスウェル	Mx	$1\ Mx \triangleq 10^{-8}Wb$
スチルブ	sb	$1\ sb=1cd/cm^2=10^4cd/m^2$
ホト	ph	$1\ ph=10^4lx$
ガル	Gal	$1\ Gal=1cm/s^2=10^{-2}m/s^2$

表10．国際単位に属さないその他の単位の例

名称	記号	SI 単位であらわされる数値
キュリー	Ci	$1\ Ci=3.7\times10^{10}Bq$
レントゲン	R	$1\ R = 2.58\times10^{-4}C/kg$
ラド	rad	$1\ rad=1cGy=10^{-2}Gy$
レム	rem	$1\ rem=1\ cSv=10^{-2}Sv$
X線単位		$1X\ unit=1.002\times10^{-4}nm$
ガンマ	γ	$1\gamma=1\ nT=10^{-9}T$
ジャンスキー	Jy	$1\ Jy=10^{-26}W\cdot m^{-2}\cdot Hz^{-1}$
フェルミ		$1\ fermi=1\ fm=10^{-15}m$
メートル系カラット		$1\ metric\ carat = 200\ mg = 2\times10^{-4}kg$
トル	Torr	1 Torr = (101 325/760) Pa
標準大気圧	atm	1 atm = 101 325 Pa
カロリー	cal	
ミクロン	μ	$1\ \mu=1\mu m=10^{-6}m$

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