



## Evaluating and Categorizing the Reliability of Distribution Coefficient Values in the Sorption Database (4)

Tadahiro SUYAMA, Charlotte GANTER, Susanne KUNZE  
Yukio TACHI and Michael OCHS

Geological Isolation Research Unit  
Geological Isolation Research and Development Directorate

February 2011

Japan Atomic Energy Agency

日本原子力研究開発機構

JAEA-Data/Code

本レポートは独立行政法人日本原子力研究開発機構が不定期に発行する成果報告書です。  
本レポートの入手並びに著作権利用に関するお問い合わせは、下記あてにお問い合わせ下さい。  
なお、本レポートの全文は日本原子力研究開発機構ホームページ (<http://www.jaea.go.jp>)  
より発信されています。

独立行政法人日本原子力研究開発機構 研究技術情報部 研究技術情報課  
〒319-1195 茨城県那珂郡東海村白方白根 2 番地 4  
電話 029-282-6387, Fax 029-282-5920, E-mail:ird-support@jaea.go.jp

This report is issued irregularly by Japan Atomic Energy Agency  
Inquiries about availability and/or copyright of this report should be addressed to  
Intellectual Resources Section, Intellectual Resources Department,  
Japan Atomic Energy Agency  
2-4 Shirakata Shirane, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195 Japan  
Tel +81-29-282-6387, Fax +81-29-282-5920, E-mail:ird-support@jaea.go.jp

© Japan Atomic Energy Agency, 2010

Evaluating and Categorizing the Reliability of Distribution Coefficient Values  
in the Sorption Database (4)

Tadahiro SUYAMA<sup>※</sup>, Charlotte GANTER<sup>\*</sup>, Susanne KUNZE<sup>\*</sup>,  
Yukio TACHI and Michael OCHS<sup>\*</sup>

Geological Isolation Research Unit  
Geological Isolation Research and Development Directorate  
Japan Atomic Energy Agency  
Tokai-mura, Naka-gun, Ibaraki-ken

(Received December 13, 2010)

Sorption of radionuclides in bentonites and rocks is one of the key processes in the safe geological disposal of radioactive waste. Japan Atomic Energy Agency (JAEA) has developed sorption database (JAEA-SDB) which includes extensive compilation of sorption  $K_d$  data by batch experiments, extracted from published literatures. JAEA published the first SDB as an important basis for the H12 performance assessment (PA), and has been continuing to improve and update the SDB in view of potential future data needs, focusing on assuring the desired quality level and practical applications to  $K_d$ -setting for the geological environment. The JAEA-SDB includes more than 24,000  $K_d$  data which are related with various conditions and methods, and different reliabilities. Accordingly, the quality assuring (QA) and classifying guideline/criteria has been developed in order to evaluate the reliability of each  $K_d$  value. The reliability of  $K_d$  values of key radionuclides for bentonite, mudstone, granite and Fe-oxide/hydroxide, Al-oxide/hydroxide has been already evaluated. These QA information has been made available to access through the web-based JAEA-SDB since March, 2009. In this report, the QA/classification of selected entries in the JAEA-SDB, focusing on key radionuclides (Th, Np, Am, Se and Cs) sorption on tuff existing widely in geological environment, was done following the approach/guideline defined in our previous report. As a result, the reliability of 560  $K_d$  values was evaluated and classified. This classification scheme is expected to make it possible to obtain quick overview of the available data from the SDB, and to have suitable access to the respective data for  $K_d$ -setting in PA.

Keywords: Sorption Database, Distribution Coefficient,  $K_d$ , Reliability, Quality Assurance, Geological Disposal

---

<sup>※</sup> Collaborating Engineer

<sup>\*</sup> BMG ENGINEERING LTD, Switzerland

収着データベースに登録された収着分配係数の信頼度評価 (4)

日本原子力研究開発機構  
地層処分研究開発部門  
地層処分基盤研究開発ユニット

陶山 忠宏<sup>\*</sup>, Charlotte GANTER<sup>\*</sup>, Susanne KUNZE<sup>\*</sup>, 舘 幸男, Michael OCHS<sup>\*</sup>

(2010年12月13日受理)

放射性廃棄物の地層処分安全評価において、人工バリアであるベントナイトや天然バリアである岩石中での核種の収着現象は、核種の移行遅延を支配する重要な現象である。日本原子力研究開発機構 (JAEA) では、バッチ法収着試験によって得られた収着分配係数を公開文献から抽出・整理して収着データベース (JAEA-SDB) として整備を進めてきた。最初の収着データベースを、地層処分研究開発第2次取りまとめの性能評価の重要な基盤情報として整備して以降、将来の性能評価におけるニーズへの対応を念頭に、データベースに含まれる  $K_d$  データの信頼度評価、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に着目して、データベースの改良・更新を継続的に実施してきている。

JAEA-SDB に登録されている  $K_d$  データは 24,000 データを超え、様々な実験条件や手法によって得られた信頼度の異なるデータが含まれる。このため、個々の  $K_d$  データの信頼性を評価することを目的に、信頼度評価とそのレベル分けに関するガイドライン/基準が開発された。これまでに、このガイドラインに基づき、ベントナイト系、泥岩系、花崗岩系および鉄やアルミニウムの酸化物/水酸化物系の主要核種の  $K_d$  データを対象に信頼度評価を実施した。これらの信頼度評価結果は、信頼度情報に基づくデータ抽出機能等を付加した Web アプリケーションによるデータベースを通じて、2009年3月以降利用可能である。

本報告書では、JAEA-SDB に含まれる重要核種 (Th, Np, Am, Se, Cs) の  $K_d$  データのうち、地質環境に広く存在する凝灰岩系岩石を対象として、これまで報告してきた信頼度評価手法に従って評価を実施した。その結果として、560 の  $K_d$  データに対して、新たな信頼度情報が付与された。この信頼度評価手法は、収着データベースから利用可能な関連データ群を速やかに抽出し、 $K_d$  データ設定の際に参照すべきデータを適切に選定する上で、有効な手法となると考えられる。

---

核燃料サイクル工学研究所 (駐在) : 〒319-1194 茨城県那珂郡東海村村松 4-33

<sup>\*</sup>技術開発協力員

<sup>\*</sup> BMG ENGINEERING LTD, スイス連邦共和国

Contents

1. Introduction.....	1
2. Reliability of JAEA-SDB: Classification Guideline .....	2
2.1 Introduction, description of main criteria.....	2
2.2 Description of checkpoints within each main criteria .....	3
2.2.1 General .....	3
2.2.2 Criteria I: Completeness of documentation and type of $K_d$ information .....	3
2.2.3 Criteria II: Technical and scientific quality of reported data.....	5
2.2.4 Criteria III: Consistency of data.....	17
2.3 Overall classification.....	18
3. Classification of selected entries for tuff in the JAEA-SDB.....	20
3.1 Criteria I and II.....	21
3.1.1 Americium .....	22
3.1.2 Cesium .....	33
3.1.3 Neptunium .....	39
3.1.4 Selenium.....	45
3.1.5 Thorium.....	48
3.2 Criteria III.....	51
3.2.1 Evaluation of data for americium .....	51
3.2.2 Evaluation of data for selenium .....	52
3.2.3 Evaluation of data for thorium and neptunium .....	53
4. Summary .....	54
References .....	55
Appendix :     Summary tables for $K_d$ classification .....	61

目 次

1. はじめに .....	1
2. JAEA-SDB データの信頼性評価ガイドライン .....	2
2.1 クライテリアについて .....	2
2.2 それぞれのクライテリアにおけるチェックポイントについて.....	3
2.2.1 クライテリアの概要 .....	3
2.2.2 クライテリア I:文献などの記述の網羅性と分配係数の情報タイプの評価 .....	3
2.2.3 クライテリア II:個々の登録データの技術的および科学的観点からの評価 .....	5
2.2.4 クライテリア III:データ相互間の整合性からの評価 .....	17
2.3 総合的な評価としてのクラス分けについて .....	18
3. 凝灰岩に対する選択核種のクラス分け .....	20
3.1 クライテリア I およびクライテリア II .....	21
3.1.1 アメリシウム(Am) .....	22
3.1.2 セシウム(Cs).....	33
3.1.3 ネプツニウム(Np) .....	39
3.1.4 セレン(Se) .....	45
3.1.5 トリウム(Th) .....	48
3.2 クライテリア III .....	51
3.2.1 アメリシウムについてのデータの評価.....	51
3.2.2 セレンについてのデータの評価.....	52
3.2.3 トリウムとネプツニウムについてのデータの評価.....	53
4. おわりに .....	54
参考文献 .....	55
付録： K <sub>d</sub> 値クラス分けのまとめ表 .....	61

Figure Contents

<b>Figure 3.2.1</b>	Overview of sorption data for Am on tuff.....	51
<b>Figure 3.2.2</b>	Overview of sorption data for Se on tuff.....	52
<b>Figure 3.2.3</b>	Overview of sorption data for Th and Np(IV) on tuff.....	53

Table Contents

<b>Table 2.3.1</b>	Weighting of individual checkpoints under Criteria II .....	19
<b>Table 2.3.2</b>	Overall classes of reliability for Criteria II .....	19
<b>Table 2.3.3</b>	The classification system .....	19

This is a blank page.



## 1. Introduction

Sorption and diffusion of radionuclides in buffer materials (bentonite) and host rocks (rock matrix) are the key processes in the safe geological disposal of radioactive waste, because migration of radionuclides in these barrier materials is expected to be diffusion-controlled and retarded by sorption processes. Sorption and diffusion of radionuclides on these barrier materials depends critically on relevant geochemical conditions, especially  $K_d$  values are highly conditional parameters (e.g., NEA, 2001; 2005). It is therefore necessary to understand the detailed/coupled processes of diffusion and sorption in compacted bentonite/intact rock, and to develop the database containing extensive compilation of sorption  $K_d$  data and the mechanistic/predictive model/database, so that reliable parameters can be set under a variety of geochemical conditions relevant to performance assessment (PA).

Japan Atomic Energy Agency (JAEA) has developed the sorption databases (SDB), which were firstly developed as an important basis for the H12 performance assessment (JNC, 1999; Shibutani et al., 1999). JAEA has been and is continuing to improve and update the SDB/DDB in view of potential future data needs, focusing on;

- 1) updating of sorption data (Suyama and Sasamoto, 2004; Saito et al., 2007)
- 2) assuring the desired quality level (Ochs et al., 2007; Saito et al., 2008; Ochs et al., 2010)
- 3) testing and applying of the databases to parameter-setting (Ochs et al., 2008).

To extract the respective  $K_d$  data for PA-related  $K_d$  setting using JAEA-SDB, which contains more than 24,000  $K_d$  data as well as the corresponding experimental conditions, the quality assuring (QA) and classifying guideline/criteria has been developed (Ochs et al., 2007). Based on the guideline, the reliability of  $K_d$  values of key radionuclides for bentonite (Ochs et al., 2007), mudstone (Saito et al., 2008), and granite, Fe-oxide/hydroxide, Al-oxide/hydroxide (Ochs et al., 2009) has been already evaluated. The web-based sorption and diffusion database system (JAEA-SDB/DDB) has been developed to utilize quality assuring procedure and to allow effective application for parameter setting (Tachi et al., 2010; <http://migrationdb.jaea.go.jp>).

In this report, the selected  $K_d$  data in the JAEA-SDB for key radionuclides (Th, Np, Am, Se, Cs) on tuff existing widely in Japanese geological environments was classified based on the QA guideline (chapter 2; Ochs et al., 2007). Evaluated results of selected entries for tuff in the JAEA-SDB are presented for three categorized criteria in chapter 3;

Criteria I - Completeness of documentation and type of  $K_d$  information

Criteria II - Quality of reported data

Criteria III- Consistency of data

The details of the evaluation and classification for the selected entries of the SDB are listed in the appendix.

## 2. Reliability of JAEA-SDB: Classification Guideline

### 2.1 Introduction, description of main criteria

The reliability of  $K_d$  values in the JAEA-SDB can be assessed using the following three main criteria. The three main criteria are listed in the expected sequence of application during a classification of entries in the JAEA-SDB. Criteria I-a and I-b are related to documentation and data entry, whereas the technical and scientific quality of an entry is addressed by criteria II and III.

#### **Criteria I — Completeness of documentation and type of $K_d$ information:**

- a) It needs to be verified that the documentation of each entry is detailed enough to allow further examination according to the main criteria II-III. At this point, only the completeness of the documentation is examined; the appropriateness of the reported data and approaches is evaluated under criteria II below.
- b) This point takes also into account that the reliability of data input to the JAEA-SDB will be substantially high if  $K_d$  values are directly available in table format in comparison to literature that reports e.g. %-adsorbed values in a graph. The latter way of reporting requires the operator to i) manually read values off a graph and ii) to calculate  $K_d$  from the %-adsorbed and Solid/water ratio (s/w) values given, which significantly increases the likelihood of an operator error during data input.

#### **Criteria II — Quality of reported data**

This is the most important issue from a technical and scientific point of view. This criteria encompasses an evaluation of the appropriateness of the experimental system to produce reliable  $K_d$  data. The methods used (or lacking) for determining experimental uncertainty are also examined for each literature source. Further, it is considered whether the data represent single-point measurements or are part of e.g. an isotherm, which would provide additional support for their reliability.

#### **Criteria III — Consistency of data:**

While the previous two main criteria address the reliability of each  $K_d$  entry in the JAEA-SDB, criteria No. III requires an examination of the level of support that

other  $K_d$  values in similar systems can lend to the entry under consideration. Any disagreement with data from related systems will have to be evaluated as well. It could be argued that this kind of data examination may be left to the user of the JAEA-SDB. However, the classification of data entries in the JAEA-SDB in terms of reliability adds an aspect of quality that is above that for a pure compilation, and users may expect that the listed  $K_d$  values passed some kind of check for internal consistency.

Internal consistency means that data from different sources should not be in obvious disagreement. An example would be the dependency on pH of  $K_d$  values for a certain radionuclide, which should be approximately similar in all studies. Similarly, if many studies indicate e.g. stronger sorption of U(IV) than of Th(IV), for any study that indicates the opposite an appropriate explanation should be given. If no good reason can be found, such deviations make a study less reliable. These types of considerations will only be possible for sufficiently well researched elements.

## **2.2 Description of checkpoints within each main criteria**

### **2.2.1 General**

Each entry in the JAEA-SDB (each  $K_d$  value identified in the JAEA-SDB by a unique ID) should be evaluated and classified individually. Because many studies report  $K_d$  values under different experimental conditions, it is not sufficient to evaluate all data based on a given reference globally. Depending on conditions, different entries related to a given study may receive a different rating.

### **2.2.2 Criteria I: Completeness of documentation and type of $K_d$ information**

The checkpoints under I-a are used for a screening prior to a further classification. Failure to satisfy these checkpoints will not be used (unreliable).

**I-a.1** Are all mandatory fields completed? Here it is only verified that all fields have been completed by the operator; an entry "not reported" is counted, therefore. The following entries are considered mandatory:

- element
- solid phase
- solution composition
- atmosphere
- pH (or other information that allows to derive pH, e.g. portlandite equilibrium)

- pe/redox condition (only in case of redox-sensitive systems)
- method of pe control (only in case of redox sensitive systems and imposed reducing conditions)
- initial radionuclide (RN) concentration (except for RN that are not solubility controlled)
- method for phase separation
- type of experiment, if different from batch
- In case of missing entries, the corresponding  $K_d$  is excluded from further evaluation and classified as unreliable (until remedied by operator). If all fields are completed, proceed to I-a.2.

**I-a.2** Is all mandatory information provided? Here it is evaluated whether critical information is provided or lacking completely. The quality of the information provided is evaluated under criteria II. In addition to the information listed under I-a.1, further mandatory information includes:

- units
- In case of missing mandatory information, the corresponding  $K_d$  is excluded from further evaluation and classified as unreliable. If all fields are completed, proceed to I-b.

**I-b** Does the type of  $K_d$  information provided require manipulation by the operator?

→ The following levels are distinguished:

- class 1: table with  $K_d$  values given
- class 2: table with % sorbed given  
table with residual concentration given
- class 3: linear graph  $K_d$
- class 4: linear graph % sorbed  
linear graph residual concentration
- class 5: logarithmic graph  $K_d$
- class 6: logarithmic graph % sorbed  
logarithmic graph residual concentration

### 2.2.3 Criteria II: Technical and scientific quality of reported data

It is generally assumed that the entries presently contained in the JAEA-SDB correspond to a minimum quality standard; i.e. are assumed to be basically reliable. The different checkpoints regarding experimental quality are designed to distinguish different levels of reliability. However, if in case of critical checkpoints even the requirements leading to the lowest rating are not met, the respective entry should be classified as unreliable (indicated for each checkpoint).

#### II-a Solid phase (substrate)

It is evaluated whether the solid phase has been sufficiently characterized. This is equally important for properly designing experiments, as well as for using the measured  $K_d$  values. In general, three types of key information are required:

- Information about major mineral composition.
- Information about accessory minerals or impurities.
- Information about surface characteristics: Minimum is a measure of sorption capacity per mass of sorbent, such as CEC or a different measure of site density per mass.

However, the amount of information required to sufficiently characterize a given solid phase also depends on the complexity of the substrate:

1. It needs to be known whether a substrate consists of a single pure mineral phase, or whether it contains impurities or additional minerals. In general, some measure of site density per mass (e.g. CEC) needs to be known to properly design experiments, in particular with respect to achieving reasonable surface loading.
2. In case of simple substrates (pure minerals), no further information is necessary.
3. In case of complex substrates (i.e., where significant impurities are present, or where a substrate is composed of several minerals), and in particular in case of natural samples, detailed information on composition has to be provided in addition.
4. In cases where sample treatment (such as crushing or sieving) had been performed, the respective information on particle size also needs to be provided (see II-f). Where any chemical treatments (e.g. acid washing to remove calcite; but also change of redox conditions in case of redox-sensitive substrates, see II-c) had been applied, the applied method and resulting mineralogy should be given as well.

5. In case of many commercially available substrates (e.g., MX-80 or Kunigel-V1 bentonite; standard clay minerals from the Clay Minerals Society, such as SWy-1; Min-U-Sil SiO<sub>2</sub>, etc.) detailed solid phase information is widely known and can be retrieved from a large number of publications. Therefore, characterization of such solids is not required for each entry in the JAEA-SDB; i.e., level A or B can be reached even if such information is not reported. Note that this holds only when such solids have been used as received. Where washing procedures etc. have been applied, the procedures and resulting changes still need to be documented.

→ Three levels of reliability:

A) Major and minor mineralogy as well as surface characteristics are known.

For example: The substrate is a single, well-defined mineral; or comprehensively characterized complex mineral assemblage. Either no sample treatment has been carried out, or it is described in detail and the result are documented.

B) Major mineralogy as well as surface characteristics are known.

For example: The substrate is a single mineral that may contain impurities (such as a non-purified clay mineral) or a complex mineral assemblage where additional impurities could be present. Sample treatment may have led to minor changes in mineralogy.

C/D) Information on both major mineralogy or surface characteristics is lacking.

For example: There is no information on CEC (or another measure of sorption capacity); or the substrate is a natural clay sample where it is not clear whether it is smectite, kaolinite, or illite; or a non-characterized soil or crushed rock. Sample treatment may have led to major changes in mineralogy that are not documented.

## **II-b** Adjustment and control of pH

One of the most important solution parameters controlling radionuclide(RN) sorption is pH. It needs to be known to interpret  $K_a$  values, but also for proper experimentation: The pH needs to be known to evaluate the solubility limits of radionuclides and some major ions, as well as the stability of certain mineral phases (in particular carbonates). Further, pH has to be approximately constant during a sorption experiment in order to reach

equilibrium of sorption reactions. There are two basically different approaches in sorption experiments with regard to pH control:

1. The pH is not controlled, but allowed to reach an equilibrium value according to the experimental conditions and is then measured at the end of the experiment. In this case, it is important that the pH has been verified after experimentation, in order to know its equilibrium value.
2. The pH is controlled during the experiment by acid-base addition and/or buffers. Where it is desired to determine  $K_a$  values as a function of pH, this cannot be avoided. In this case, it needs to be shown (or known from the literature) that the added acids, bases, or buffers do not interfere with RN reactions at the surface (which obviously influence sorption) or with RN reactions in solution (which influence sorption through changing the RN speciation). Therefore, use of a non-inert pH buffer at unspecified concentration levels leads to a classification as unreliable.

→ Four levels of reliability:

- A) To achieve rating A it is sufficient, but required, that the pH is verified at the end of the experiment. This is based on the assumption that equilibrium or at least a stable state of near-equilibrium conditions has been achieved (see also II-a, II-d, and II-j). In such systems, a determination of the experimental end pH will represent an adequate measure of the actual equilibrium pH. Second, rating A is given where the successful use of inert buffers has been demonstrated (e.g. by measuring  $K_a$  in the presence and absence of buffers at some pH, or by showing through speciation calculations that the buffer does not influence RN behavior). In some cases, level A may also apply if a non-inert buffer is part of the experimental setup (see the example of  $K_a$  determination as a function of carbonate concentration under point C).
- B) The final pH is reported, but only a pH range (within 1 pH unit) is given instead of a discrete pH value (the same assumptions regarding equilibrium can be made as for level A above). Rating B also applies in cases where only the initial pH is provided, but the experimental system is well buffered (for example, because a inert buffer is used, or because of the presence of a natural buffer system, such as carbonate).
- C) Only the initial pH is provided, no attempt is made to control final pH. All cases where non-inert pH-buffers are being added. Note that this

refers to the addition of an additional complexing ligand, such as acetate, for the control of pH. On the other hand, if a sorption experiment is carried out where  $K_d$  is measured as a function of carbonate concentration and this is simultaneously used to control pH, level A applies (given that the effect of carbonate on  $K_d$  is documented).

- D) Only a range (within 1 pH unit) of initial pH is provided, no information on final pH is given.
- If a lower quality than required for level D is evident, the respective entry is excluded from further evaluation as unreliable. If a non-inert buffer (e.g. acetate or carbonate) is used at unspecified concentration levels, the respective entry is excluded from further evaluation as unreliable.

#### **II-c** Redox conditions

Here it needs to be differentiated between systems that are not redox-sensitive and systems that are. Within the redox-sensitive systems, it needs to be further taken into account whether only the sorbing RN is redox-sensitive or whether other components of the system (such as solid phase or groundwater components) are redox-sensitive as well.

In this sense, checkpoint II-c deals with the redox control of the sorbing RN, not with redox control of an overall redox-sensitive system. If the experimental system comprises a range of redox-sensitive dissolved (e.g. organics) and solid (e.g. Fe- and Mn-phases) components, imposing redox conditions different from the original level may influence many redox-equilibria simultaneously. In such a case it can be very difficult to ascertain equilibrium or to know which solid phases are present. Such effects on solution and solid phase chemistry are addressed by checkpoints II-a and II-d. It also needs to be pointed out in this context that "imposed redox condition" does not necessarily refer only to imposing reducing conditions by adding a reducing agent, it also includes imposing oxidizing conditions by e.g. transferring a reduced natural sediment to the laboratory and exposing it to  $O_2$  (as a matter of fact, the latter may be the more common problem).

Given the focus of this checkpoint on redox control of sorbing radionuclides explained above, two different requirements on data quality can be distinguished. Levels of reliability reflect the degree to which these two



requirements are met:

1. Reliability regarding control and confirmation of the redox status of the sorbing RN.
2. Reliability regarding the absence of unwanted side effects, such as changes in RN speciation induced by the addition of a reducing agent.

→ Two levels of reliability:

A/B) Level A/B applies to entries in the JAEA-SDB where it is demonstrated that both of the above requirements are met: This includes the following cases:

- Systems which are not redox-sensitive in terms of sorption and where no reducing agents needed to be added (i.e., where the sorbing RN can take on only one oxidation state in aqueous solutions).
- Redox-sensitive systems that have been pre-equilibrated with and are being kept at ambient conditions.
- Experiments where reducing conditions are imposed on redox-sensitive RN (in otherwise stable systems) and where similar results are obtained using several reducing agents.

C/D) Level C/D applies to entries in the JAEA-SDB where meeting the above requirements may not have been demonstrated, but can be assumed with high certainty. This includes the following cases:

- Reducing conditions imposed on redox-sensitive RN (in otherwise stable systems) using one reducing agent that can be estimated (e.g. from experience or from the literature) to be effective and to be sufficiently inert with respect to influencing RN behavior.
- In cases where complexing reducing agents have been used, level C/D still can be achieved if the influence of the reducing agent on RN speciation has been estimated.
- All cases where redox conditions may be less well defined than for level A/B, but where it can be assumed that no significant artifacts regarding RN behavior are introduced and where the oxidation state of RN has been measured independently (in some cases, this may include low-O<sub>2</sub> conditions with a subsequent confirmation of RN oxidation state). Evaluating the reliability of such measurements is likely to require an expert decision by the operator.

→ If a lower quality than required for level C/D is evident, the respective entry is excluded from further evaluation as unreliable. For example, cases where it has been attempted to achieve reducing conditions only by minimizing the level of O<sub>2</sub> (e.g., by performing experiments in a N<sub>2</sub>

atmosphere) generally should be labeled "unreliable" (except where the oxidation state of a RN somehow has been confirmed, see description of level C/D). Also, if a strongly complexing reducing agent (such as many organic acids) is used at unspecified concentration levels, the respective entry is excluded from further evaluation as unreliable.

**II-d** Final solution composition

Note that solution composition includes dissolved carbonate concentration, which may be controlled through, or expressed as pCO<sub>2</sub>. Added pH-buffers or reducing agents are also included, and are addressed in checkpoints II-b and II-c.

→ Two levels of reliability:

A/B) The final solution composition is known (either from direct measurements or from the initial experimental setup and speciation calculations) and corresponds to equilibrium or is otherwise well constrained. All major components are included in the analysis. Relevant minor components (e.g. traces of carbonate or of other complexing ligands) may only be estimated. Some minor components may be unknown. In case of natural water samples, solutions are (or can be) shown to be charge balanced (within 5 %). The information on final solution composition can be obtained from i) analyses of the actual sorption samples or from ii) using pre-equilibrated solutions that had been analyzed prior to the actual sorption experiments.

C/D) The critical major solution components are known, or can be estimated approximately. There may be unknown minor components and/or less critical major components. In case of natural water samples, solutions are approximately charge balanced (within 10 %).

→ If a lower quality than required for level C/D is evident, the respective entry is excluded from further evaluation as unreliable.

**II-e** Temperature

Here, it is evaluated whether temperature is specified and kept constant.

→ Two levels of reliability:

A/B) Temperature is approximately specified (e.g. room temperature) and constant, or varied in a controlled fashion.

C/D) Temperature is not specified at all (i.e., it is not clear whether the experiments had been performed at room temperature or not).

**II-f** Liquid/Solid ratio (L/S) and grain size

It is evaluated whether enough solid had been added to avoid a significant influence by the vessel walls (see II-m), and to ensure sample reproducibility and representativeness in case of complex substrates, especially in case of large grain sizes: It is estimated that in cases where less than ca. 100 mg of solid (this value depends on grain size) has been added to each experimental vessel, sample reproducibility and representativeness becomes difficult to achieve in case of complex or crushed samples.

→ Two levels of reliability:

A/B) Enough solid had been added to each vessel to assume that

a) [surface area sorbent] » [surface area vessel], i.e. that at least 5 m<sup>2</sup> of sorbent surface had been added to each vessel, and to assume that

b) samples are reproducible and representative.

What is enough substrate clearly depends on specific surface area and homogeneity. Fulfilling the above two requirements is typically not a problem in case of relatively homogeneous sorbents with a high specific surface area (such as clay minerals or bentonite), where "enough" may mean at least ca. 100 mg. On the other hand, "enough" may mean at least one to several grams in case of rocks (depending on specific surface area, grain size and complexity of the sample).

C/D) Any other than the above.

**II-g** Sorption value

It is evaluated whether an appropriate experimental design had been employed to avoid sorption values near 0% or 100%, which can lead to higher experimental uncertainty. This problem can be addressed by choosing an appropriate L/S ratio (see II-f) or/and an appropriate initial concentration of RN ([RN]) (see II-h). However, the choice of [RN] is more restricted by solubility and analytical detection limits.

A) The sorption value is in the range of 5% - 95% sorbed.

B) The sorption value is inside the range of 2% - 98% sorbed.

C/D) Any other than the above.

**II-h** Initial RN concentration ([RN])

This parameter is used to evaluate the likelihood of a possible supersaturation of RN-phases:

→ Three levels of reliability:

A) RN is not solubility limited, or initial [RN] was clearly (at least a factor of 5) below the solubility limit. Note that factor 5 does not take into account uncertainties in RN solubility; i.e., if the solubility of a given RN cannot be estimated with more certainty than e.g.  $10^{-6}$  to  $10^{-8}$  M, then initial [RN] has to be  $\leq 2 \times 10^{-9}$  M for rating A to apply.

B) Initial [RN] was clearly below the solubility limit, but maybe less than a factor of 5 (see above).

C/D) [RN] was very small, and in all likelihood below their maximum solubility, but the solubility limit cannot be established clearly due to missing information (solution composition) or lacking thermodynamic data.

→ Note that the solubility limit can be defined on either thermodynamic calculations or on experimental data obtained under the relevant conditions.

→ If initial RN concentration had been clearly above the respective solubility limit, the respective entry is excluded from further evaluation as unreliable.

**II-i** Phase separation

Here, the appropriateness of phase separation is evaluated: Note that in cases where colloids or other artifacts are important, different phase separation methods will not lead to the same results. Identical or very similar results with different efficient methods are probably the best direct proof of absence of important colloid effects; hence such studies are rated A. Rating B would be given for methods that can be presumed to remove colloids, but where no direct proof as in A is given.

→ Three levels of reliability:

A) Identical (very similar) results are obtained with different methods of phase separation, where at least one method needs to be efficient in terms of colloids removal (ultrafiltration or high-speed centrifugation).

Accordingly, the best comparison would be between two efficient methods, such as ultrafiltration and high-speed centrifugation.

Note that such a comparison of phase separation methods is not required for each individual  $K_d$  value: For example: If the absence of artifacts has been demonstrated for some representative samples of a study by comparing an efficient and a standard method of phase separation, the rating A may be given to all datapoints of this study, even if they correspond to the standard method only.

- B) Only one, but efficient method (high-speed centrifugation, ultrafiltration) is used, and there is no evidence for artifacts such as colloid effects or significant sorption to the filter.
- C/D) Only one general method (normal centrifugation, membrane filtration with nominal pore sizes of 0.01~0.45  $\mu\text{m}$ ) is used, and there is no evidence for artifacts such as colloid effects or significant sorption to the filter.
- If no phase separation is used, or in case of obvious evidence for artifacts (colloid effect, adsorption on filter) the respective entry is excluded from further evaluation as unreliable.

## II-j Reaction time

- Two levels of reliability:
- A/B) Identical (similar) results are obtained with different reaction times, or some other demonstration of near-equilibrium is provided (e.g. separate kinetic experiments).
- C/D) Only one, but reasonably long reaction time is used. What is “reasonably long” is highly dependent on the experimental system: In general, the time needed to reach equilibrium will increase with the complexity of the sorbing substrate and the strength of sorption. Sorption of Sr onto a pure clay mineral through ion exchange can be assumed to be complete within a day; sorption of a trivalent actinide onto a complex substrate may need several days to weeks for completion. In the absence of kinetic information, operator expert decisions will be required to assess this point. If possible, reaction times reported for similar systems included in the JAEA-SDB could be used to evaluate what is reasonably long. Further, even for the most simple systems a reaction time of 1 day is considered as minimum

requirement.

- If the requirement for level C/D is not met (i.e., if the reaction time cannot be assumed to be reasonably long), the respective entry is excluded from further evaluation as unreliable.

**II-k** Agitation method

- Two levels of reliability:

A/B) Appropriate agitation is required in all cases, except where enough kinetic information is provided to show that equilibrium has been reached. Shaking is the preferred method, as use of stir bars can lead to abrasion of samples. In case of simple and well crystallized substrates (such as Al-oxide) or of substrates with very small grain size that are easily suspended, stir bars can also be accepted.

C/D) Any other than the above.

**II-l** RN loading

Ideal are values as a function of RN loading (i.e.,  $K_d$  values that form part of an isotherm), otherwise low loading is preferred. RN loading (e.g. in moles RN/kg substrate) refers to the amount of RN adsorbed in relation to the amount of different surface sites available. It is known from classical isotherms (e.g. Langmuir) that a linear sorption can only be assumed if sufficient unoccupied sites are present. In case of simple substrates (including some bentonites), the linear portion of an isotherm extends to fairly high RN loading. There are other cases where  $K_d$  depends significantly on RN loading over many orders of RN concentration.

- Three levels of reliability:

A) At least one isotherm has been determined (for a constant solution composition and L/S), and at least some experiments have been carried out using trace level RN concentration (i.e., at least some data are included within a linear sorption region).

B) No isotherm is available, but at least a limited variation of initial [RN] or L/S has been carried out, and some experiments have been carried out using trace level RN concentration (i.e., some data are included within a linear sorption region).

C/D) No variation as in A or B has been carried out.

**II-m** Reaction vessels

High-density polyethylene (HDPE) or Teflon are preferred over normal PE, which is preferred over glass, which may lead to sorption of radionuclides by the vessel walls. Especially at high or very low pH, glass dissolution and release of dissolved or colloidal silica may also occur. On the other hand, glass is more gas-tight (especially than PE); if that is of experimental relevance. Corrections for sorption on vessel walls should not be necessary if blank tests show that it can be neglected.

Correction for sorption on vessel walls may be needed to estimate  $K_d$  values correctly in some cases, but only in cases where a) sorption on the vessel is much stronger than on the solid sorbent, or b) if the vessel offers a significant surface area in comparison to the sorbent (see II-f). If that is not the case, the sorption on the added solid will be much greater than on the vessel in a system where both solid and vessel are present. It is further an erroneous assumption that sorption on the vessel will be same in i) the absence of the solid (no competition for RN by solid) as ii) in the presence of the solid (strong competition for RN by solid). The sorption on the walls is typically much smaller in ii) than in i). Therefore, the overall mistake is often bigger if sorption on the vessel wall is accounted for than if it is neglected.

If effects of vessel walls are corrected for, it has to be done by extracting any RN sorbed to vessel walls after experimentation (e.g. by acid washing) and establishing a complete mass balance.

→ Three levels of reliability:

- A) An appropriate vessel has been used (taking into account sorption as well as tightness with respect to CO<sub>2</sub> or O<sub>2</sub>, where required), and corrections for sorption on vessel wall have been performed or no sorption on vessel wall has been observed by blank tests. If effects of vessel walls are corrected for, it has to be done by extracting any RN sorbed to vessel walls after experimentation (e.g. by acid washing) and establishing a complete mass balance. If the sorption on vessel wall has been determined as significantly lower (at least two orders of magnitude in terms of  $K_d$ ) than the actual  $K_d$  value and thus corrections for sorption on vessel wall have not been performed, such a case would also correspond to level A
- B) An appropriate vessel has been used, and corrections for sorption on vessel walls have not been performed.

C/D) The vessel used may have been not appropriate (this is often the case with glass, see above), or corrections for sorption on vessel wall have been performed based on a blank test only (i.e., without verifying that sorption on vessel walls is relevant in the presence of a solid added, thus possibly leading to overcorrection).

## II-n Uncertainty estimates

In general, uncertainties based on repeated experiments (i.e., actual observations of  $K_d$ ) are preferred over uncertainties based on error propagation, as the latter is an estimate based on a type of extrapolation. Thus, the difference between levels of reliability is mainly based on the amount of actual information gained by repetitions: For level A, the entire experiment is repeated; for level B, only sampling and analysis are repeated; for C, no repetitions are carried out.

Values that are based on repetitive experiments are preferred over single experimental data points. Note, however, that this checkpoint refers to single-point  $K_d$  values and may be overruled by data being part of e.g. pH-edge, isotherm, kinetic experiment, etc., which may provide independent evidence of good reproducibility or systematic errors (see checkpoint II-o).

→ Four levels of reliability:

- A) Uncertainties in  $K_d$  are derived based on entire, replicated sorption experiments (i.e., at least duplicate experiments).
- B) Uncertainties in  $K_d$  are derived based on single sorption experiments that are sampled and analyzed repeatedly. This may be supplemented by error propagation.
- C) Uncertainties in  $K_d$  are based on error propagation of estimated analytical and/or procedural uncertainties.
- D) No error estimate is given, no repeated sampling is done.

## II-o Parameter variation

Studies with a systematic variation of key parameters are much more valuable and reliable than single  $K_d$  measurements. In this context, key parameters are those that influence sorption (for example, chemical parameters such as RN concentration, pH,  $pCO_2$ , but also temperature, L/S, or grain size in case of crushed substrates), but not parameters that only help to determine the experimental framework (such as vessel type or reaction



time). In particular, variation of key parameters allows improved detection of experimental problems and systematic errors. Especially the latter are not detected by repeating experiments under identical conditions. In the application of this checkpoint, care has to be taken to take into account the characteristics of the particular system studied. For example, more parameter variation may be required to show clear trends in a complicated system in comparison to a simpler one. On the other hand, the pH and carbonate concentration in experiments with calcite are quite constrained by the solid itself, and only limited variations are possible.

- Four levels of reliability:
- A) Both RN surface loading (isotherm) as well as a chemical parameter, such as pH or  $p\text{CO}_2$  (edge), or e.g. [Na] in case of ion exchange, are varied systematically.
- B) Either RN concentration (isotherm) and/or chemical parameters, such as pH or  $p\text{CO}_2$  (edge), or e.g. [Na] in case of ion exchange (i.e., at least two parameters in total), are varied. These variations are less systematic than in A, but still allow to observe trends.
- C) As B, but only one parameter in total is varied.
- D) No parameter variation is done.

#### 2.2.4 Criteria III: Consistency of data

Here it will be evaluated whether data from a particular study can be supported by other studies. Comparisons should only be made with studies that are at least as (or more) reliable than the study under investigation, based on criteria I and II. In many cases, only approximate consistencies or inconsistencies may be apparent, because of different conditions used in the different studies.

- Therefore, the evaluation of criteria III will only be reported in the form of a comment. Any such comments will be included both in a classification report as well as in the corresponding rating summary sheets.
- If the  $K_d$  values under investigation are clearly inconsistent with the majority of related reliable studies, and if the reason for this observation cannot be explained, they may also be labeled unreliable based on criteria III. As this requires an expert decision by the operator, the underlying reasoning needs to be clearly documented.

### 2.3 Overall classification

The above criteria are applied to an overall classification system as follows:

- The three criteria I-III are evaluated separately, the respective results are reported separately as well.
- Criteria I: The checkpoints under I-a are used in a yes/no screening fashion, entries not fulfilling I-a are labeled as unreliable and are not evaluated further.
- Criteria I-b is then used to assign classes 1-6 for documentation.
- Criteria II: a) The datasets that pass Criteria I are again classified according to a 6-level system, where classes 1-6 represent the highest and lowest levels of reliability. To ensure a minimum quality level, certain checkpoints are regarded as critical (marked with \* in Table 2.3.1). If the quality of the data does not correspond to the respective minimum requirements, the entries are not to be used and are classified as unreliable.
- b) To facilitate transparent averaging of all checkpoints, the following numerical system is suggested: A=3, B=2, C=1, D=0 (A/B=3 and C/D=0 in some cases).
- c) Initially, checkpoints II-b, II-c, II-d, and II-h are evaluated (indicated in bold letters below). If an entry is rated unreliable for any of these checkpoints, it is excluded from further evaluation.
- d) Weighting of individual checkpoints at this level is done according to the factors given in Table 2.3.1 below.
- e) The total sum of points obtained for Criteria II is then used to indicate the level of reliability. With the present system, the maximum number of points would be 183, leading to an overall classification as follows (Table 2.3.2):

Table 2.3.1 Weighting of individual checkpoints under Criteria II.

checkpoint	description	weighting factor
II-a	solid phase (substrate)	A-C/D × 2
<b>*II-b</b>	pH	A-D × 8
<b>*II-c</b>	redox conditions	A/B-C/D × 8
<b>*II-d</b>	final solution composition	A/B-C/D × 8
II-e	temperature	A/B-C/D × 1
II-f	L/S, grain size	A/B-C/D × 2
II-g	sorption value	A-C/D × 2
<b>*II-h</b>	initial RN concentration	A-/CD × 8
*II-i	phase separation	A-C/D × 8
*II-j	reaction time	A/B-C/D × 2
II-k	agitation	A/B-C/D × 1
II-l	RN loading	A-C/D × 2
II-m	reaction vessel	A-C/D × 1
II-n	uncertainty estimates	A-D × 2
II-o	parameter variation	A-D × 8

\* indicates critical checkpoints with minimum requirements;

**bold letters** indicate the checkpoints to be evaluated initially

Table 2.3.2 Overall classes of reliability for Criteria II

points	rating
183-151	class 1
150-121	class 2
120-91	class 3
90-61	class 4
60-31	class 5
30-0	class 6

- Criteria III: Criteria III is used to qualitatively assess consistency with other studies. In case of clear inconsistencies, an entry may be labeled as unreliable.
- Overall, the following classification system is used, with Criteria II as the main basis for assessing the reliability of entries in the JAEA-SDB.

Table 2.3.3 The classification system

Criteria	classification
I-a	accept/reject
I-b	6 classes of $K_d$ information
<b>II</b>	<b>6 classes of data quality and reliability</b>
III	qualitative level of consistency with other studies

### 3. Classification of selected entries for tuff in the JAEA-SDB

This section presents the classification results for selected entries in the JAEA-SDB covering the datasets for the sorption of Th, Np, Am, Se and Cs on tuff.

- An overview of the results as well as the corresponding numerical rating is given in the Appendix.
- For transparency and ease of presentation, all results of Criteria I and II are presented in tabular form, using the format of the following table throughout. The results pertaining to Criteria III are discussed subsequently and are illustrated in the form of plots of  $K_d$  vs. a relevant master variable (typically pH), where applicable.
- According to the established classification guideline, criteria I and checkpoints II-b, II-c, II-d, II-h were evaluated first. Classification and final numerical rating were only completed when an entry was evaluated as reliable based on these checkpoints. Otherwise, entries were labeled "unreliable" and were excluded from further evaluation. For most reliable entries, criteria III was evaluated as well.

### 3.1 Criteria I and II

Data table Element/#: REF: original reference JAEA-SDB version # – DATA: element/solid sorbent, datapoint # GUIDELINE: Revision # (date)		
Checkpoint <sup>1</sup> "SDB"/"REF"	Evaluation	Rating
I-a.1	Are all mandatory fields completed?	Yes/No
I-a.2	Is all mandatory information provided?	Yes/No
I-b	Type of K <sub>a</sub> information	class 1-6
II-a	Solid phase (substrate)	A-C/D
II-b	Adjustment and control of pH	A-D
II-c	Redox conditions.	A/B-C/D
II-d	Final solution composition	A/B-C/D
II-e	Temperature	A/B-C/D
II-f	Solid/water ratio (L/S) and grain size	A/B-C/D
II-g	Sorption value	A-C/D
II-h	Initial RN concentration [RN]	A-C/D
II-i	Phase separation	A-C/D
II-j	Reaction time	A/B-C/D
II-k	Agitation method	A/B-C/D
II-l	RN loading	A-C/D
II-m	Reaction vessels	A-C/D
II-n	Uncertainty estimates	A-D
II-o	Parameter variation	A-D

<sup>1</sup> Application of the checkpoint to the information given in the JAEA-SDB is indicated with "SDB".

"REF" indicates the additional application to the original reference indicated in each table.

3.1.1 Americium

Data table Am/1: REF: Barney (1982) JAEA-SDB version 3.1 DATA: Am/Tuff, #44934~44953 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A table with $K_d$ values is provided.	class 1
II-a SDB REF	Tuff as solid phase is indicated. SSA and CEC are given. The minerals present are reported. Further composition is not reported.	B
II-b SDB	Initial and end pH are indicated.	A
II-c SDB REF	Indicated redox state corresponds to the information in the reference. Redox state of Am is not given in the reference. Systems were pre-equilibrated. Am in the oxidation state (III) is reported. Am is not redox sensitive.	A/B
II-d REF	Experiments had been performed in synthetic groundwater. Final solution composition is not indicated.	C/D
II-e SDB	It is indicated that experiments had been performed at 23°C.	A/B
II-f SDB REF	The amount of solution/solid ratio is reported. It is indicated that surface area of tuff is $188 \pm 3$ [m <sup>2</sup> /g].	A/B
II-g SDB	The sorption values are calculated from $K_d$ and L/S ratios: • # 44934~44940 • # 44941~44951 • #44952, #44953	A B C/D
II-h SDB	Initial Am concentrations from $5.75 \times 10^{-10}$ to $1.83 \times 10^{-12}$ M are indicated. Based on data from Rai et al. (1999), the initial Am concentration is clearly below the solution limit, but maybe less than a factor of 5.	B
II-i SDB REF	As separation method filtration is indicated. Filtration through 30 Angstrom Amicon 50A ultrafilter is reported.	B
II-j SDB	A contact time of 14 days is indicated.	C/D
II-k REF	Continuous shaking (180 oscillations/min), method is not specified.	A/B
II-l REF	Isotherms were determined at different temperatures.	A
II-m REF	Polycarbonate centrifuge tube of 50[mL], sorption on vessel walls is not considered.	B
II-n REF	There is no error information reported.	D
II-o REF	Variation of solution composition (Na etc. variations).	C

Data table Am/2: REF: Baston et al. (1995b) JAEA-SDB version 3.1 DATA: Am/Tuff, #46684~46691 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	Oxidation state of Am and the contact time are not reported. It is reported that experiments were carried out in triplicate. One tube was analyzed regularly to monitor the approach to a steady state concentration of radionuclide.	Yes
I-b SDB	A table with $K_d$ values is given.	class 1

<b>II-a</b>	SDB	As solid phase tuff is indicated. It is noted that plagioclase and calcite are the major components of the tuff. Surface characteristics are not reported.	C/D
	REF	It is reported that only plagioclase is the major component of tuff.	
<b>II-b</b>	SDB	Initial and final pH values are indicated.	A
<b>II-c</b>	SDB	It is indicated that experiments had been conducted under nitrogen atmosphere and initial Eh values of 340[mV] are reported.	A/B
	REF	Am(+III) was used for experiments and Am is not redox sensitive.	
<b>II-d</b>	SDB	The solution composition of the synthetic groundwater and the concrete equilibrated synthetic groundwater is indicated.	A/B
<b>II-e</b>	SDB	The reaction temperature is not reported.	C/D
<b>II-f</b>	SDB	A L/S of 50[mL/g] is indicated. Although any information about the specific surface area is lacking, 1[g] of solid per reaction vial is assumed to be enough for tuff samples.	A/B
<b>II-g</b>	SDB	The sorption values are calculated from $K_d$ and L/S ratios: <ul style="list-style-type: none"> <li>• # 46686 (95% sorption)</li> <li>• # 46684 (96% sorption)</li> <li>• # 46685, # 46687~46691 (99~100% sorption)</li> </ul>	A B C/D
<b>II-h</b>	SDB	Initial Am concentrations of $4.0 \times 10^{-11}$ to $8.0 \times 10^{-11}$ M are indicated. Based on speciation calculations with Phreeqci 2.14.3 using the thermodynamic data of Hummel et al. (2002) the initial Am concentration is clearly below (factor >5) the solubility limit at pH 12.4 and 7.8 for the reported solutions, respectively.	A
<b>II-i</b>	SDB	Centrifugation at 1,500[g] for 30 minutes combined with two different filtration procedures was applied (0.45 $\mu$ m and 30,000 MWC0). The more effective the separation procedure, the higher were the $K_d$ values for the experiments with synthetic groundwater. These results indicate colloid formation which was not filtered off by 0.45 $\mu$ m filtration. <ul style="list-style-type: none"> <li>• # 46684, #46686</li> <li>• # 46685, #46687~46691</li> </ul>	unreliable A
<b>II-j</b>	SDB	There is no reaction time reported.	
	REF	It is reported that separate kinetic measurements had been performed to monitor the approach to steady state concentration of radionuclide, what indicates that reaction time was reasonably long. Datapoints with a timescale however are not reported.	C/D
<b>II-k</b>	REF	The reaction vials were continuously and gently agitated.	A/B
<b>II-l</b>	SDB	No variation in L/S or Am concentration had been performed.	C/D
<b>II-m</b>	SDB	Experiments were carried out in polypropylene centrifuge tubes. Sorption to the vessel walls was <0.5% in presence of solid phase.	A
<b>II-n</b>	SDB	Error estimates are indicated and are based on duplicate measurements.	A
<b>II-o</b>	SDB	No parameter variation had been done.	D

Data table Am/3: REF: Baston et al. (1998) JAEA-SDB version 3.1 DATA: Am/Tuff, #65952~65957 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	A table with $K_d$ values is provided.	class 1
II-a SDB	As solid phase tuff is indicated. SSA is given.	C/D
II-b SDB	The final pH is indicated.	A
II-c SDB	Am in the oxidation state (III) is reported. Experiments were conducted under strongly reducing conditions (Na-dithionite). Am is not redox sensitive.	A/B
II-d SDB	Experiments had been performed in de-ionized water which was equilibrated 4 weeks with the solid. Final solution composition is indicated.	A/B
II-e SDB	It is indicated that experiments had been performed at 60°C.	A/B
II-f SDB REF	The amount of L/S is indicated. It is not known from the reference how much solution and solid were taken respectively. Only the ratio is known.	C/D
II-g SDB	The sorption values are calculated from $K_d$ and L/S ratios. Sorption values of all data were 0.99~1.00%.	C/D
II-h SDB REF	An initial Am concentration of $1.00 \times 10^{-10}$ M is indicated. Solutions were filtered to ensure that no precipitates were in solution and solubility limit was not reached.	B
II-i SDB	It is indicated that three different combinations of separation methods were employed: 1. Centrifugation 1100[g] for 15min. 2. Centrifugation followed by filtration through a 0.45 $\mu$ m filter. 3. Centrifugation followed by filtration through a 0.45 $\mu$ m filter followed by filtration through a 10,000 MWCO filter	B
II-j SDB	A contact time of 122 days is indicated.	C/D
II-k REF	As agitation method the use of a shaker/incubator was reported.	A/B
II-l REF	No variations of initial Am concentration were done.	C/D
II-m REF	Polypropylene centrifuge tubes, sorption on vessel walls considered, RN sorbed to vessel walls were extracted by washing with HNO <sub>3</sub> and afterwards measured.	A
II-n SDB REF	Errors are indicated. Error information is based on statistics of counting only.	C
II-o REF	No parameter variation was done.	D

Data table Am/4: REF: REF: Berry et al. (2007) JAEA-SDB version 3.1 DATA: Am/Tuff, #46912~46917 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update of SDB required for I-a.2.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	Oxidation state of Am is not indicated. It is reported that the major aqueous species measured was Am(OH) <sub>2</sub> <sup>+</sup> with oxidation state +III.	Yes
I-b REF	A table with $K_d$ values is given.	class 1



II-a	SDB	As solid phase tuff is indicated. Mineral composition is reported, CEC or BET are not indicated.	C/D
	REF	Surface characteristics are not reported.	
II-b	SDB	Final pH values are indicated.	A
II-c	SDB	It is indicated that reducing conditions had been applied with final Eh values of $-390$ [mV]. Am is not redox sensitive and an oxidation state (+III) is reported.	C/D
	REF	Sodium dithionite ( $\text{Na}_2\text{S}_2\text{O}_4$ ) as reducing agent was added to the reaction mixtures. The effect of sodium dithionite on Am is difficult to estimate since no experiments with another reducing agent had been done. For this reason rating C/D is applied.	
II-d	SDB	The solution composition of tuff equilibrated distilled water (equilibration at $60^\circ\text{C}$ ) is indicated.	A/B
	REF	It is assumed that the same $\text{Na}_2\text{S}_2\text{O}_4$ concentration as in the batch experiments of Uranium was applied ( $2.5 \times 10^{-3}$ M).	
II-e	SDB	A temperature of $60^\circ\text{C}$ is indicated.	A/B
II-f	SDB	A L/S of $5$ [mL/g] is indicated. Although any information about the specific surface area is lacking, $1$ [g] of solid per reaction vial is assumed to be enough.	A/B
	REF		
II-g	SDB	The sorption values (calculated from $K_d$ and L/S ratios) are all $>99.8\%$ .	C/D
II-h	SDB	An initial Am concentration of $1.0 \times 10^{-10}$ M is indicated. Based on speciation calculations (for $60^\circ\text{C}$ ) with Phreeqci 2.12.5 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al. 2002) the initial Am concentration is clearly below (factor $>5$ ) the solubility limit at the reported pH of 9.2 (due to the $\text{AmSiO}(\text{OH})_3^{2+}$ and $\text{Am}(\text{CO}_3)_2^-$ species).	A
II-i	SDB	Centrifugation only and centrifugation combined with two different filtration procedures were applied ( $0.45 \mu\text{m}$ and $10,000$ MWCO). The more effective the separation procedure, the higher were the $K_d$ values. These results indicate colloid formation or sorption to the filter membranes.	unreliable

Data table Am/5: REF: Daniels et al. (1982)		
JAEA-SDB version 3.1 DATA: Am/Tuff, #49383~49402		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB Not all mandatory information is provided. pH, separation method, redox potential and a few initial RN concentrations are missing.	No
	REF The initial pH of the solutions used for experimentation and the actual pH during experimentation are not available. It is not clear whether the experimental systems had been at or near equilibrium.	

Data table Am/6: REF: Erdal et al. (1978) JAEA-SDB version 3.1 DATA: Am/Tuff, #50763~50768 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided. Initial RN concentration is missing.	No

Data table Am/7: REF: Erdal et al. (1979d) JAEA-SDB version 3.1 DATA: Am/Tuff, #50917, #50922 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided. pH and initial RN concentration is missing.	No

Data table Am/8: REF: Erdal (1980) JAEA-SDB version 3.1 DATA: Am/Tuff, #51063~51141 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A table with $K_d$ values is provided.	class 1
II-a SDB	As solid phase tuff is indicated. SSA and CEC are not given.	C/D
II-b SDB	pH values between 7 and 9 are given in the reference, Initial, end or both values are reported.	A
REF	For the data points #51075 and #51086 no pH values are given. These two points are therefore unreliable.	unreliable
II-c SDB	Experiments were conducted under atmospheric conditions. Am in the oxidation state (III) is reported. Am is not redox sensitive.	A/B
II-d SDB	Experiments had been performed in synthetic groundwater. Final solution composition is not indicated.	C/D
II-e SDB	It is indicated that experiments had been performed at 22 and 70°C.	A/B
II-f SDB	The amount of solution/solid ratio is reported. 20/1 water-to-rock ratio, 1[g] solid with 20[mL] solution.	A/B
II-g SDB	The sorption values are calculated from $K_d$ and L/S ratios: <ul style="list-style-type: none"> <li>• # 51063~51080, #51085~51090, #51093~51097, #51099~51102, #51119</li> <li>• # 51081~51084, #51107~51109, #51120, #51121, #51123~51125, #51127, #51129, #51130</li> <li>• Others</li> </ul>	A B C/D
II-h SDB	An initial Am concentration of $4.00 \times 10^{-7}$ M is indicated. According to the data given in Rai et al. (1999), the initial Am concentration given in the reference is above the solubility limit of americium between pH 7 and 9. UNRELIABLE. No further rating.	unreliable

Data table Am/9: REF: REF: Ikeda and Amaya (1998)		
JNC-SDB version 3.1 DATA: Am/Tuff, #53543~53550		
GUIDELINE: Revision 4b (May 19, 2005)		
* REMARK: Update of SDB required for checkpoints II-a, II-m and II-n		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A table with $K_d$ values is given.	class 1
II-a SDB	As solid phase tuff is indicated. Mineral composition and surface characteristics are not reported.	B
REF	Major mineral composition and chemical composition of tuff are indicated. A BET of 57[m <sup>2</sup> /g] is reported.	
II-b SDB	Initial and final pH values are indicated.	A
II-c SDB	It is indicated that reducing conditions had been applied with final Eh values of -190[mV] to -250[mV]. Am is not redox sensitive and an oxidation state (+III) is reported.	C/D
REF	Sodium dithionite (Na <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ) as reducing agent was added to the reaction mixtures. The effect of sodium dithionite on Am is difficult to estimate since no experiments with another reducing agent had been done. For this reason rating C/D is applied.	
II-d SDB	As water type seawater and distilled water are indicated. The solutions are 2×10 <sup>-4</sup> M to 1.2×10 <sup>-3</sup> M in sodiumdithionite, to keep reducing conditions.	A/B
REF	Final solution compositions are not given, but it is supposed that no essential changes take place in the case of seawater (#53543, #53548~53550). Major mineralogy and chemical composition of the tuff are available. Final solution composition with distilled water and the reported L/S can be estimated approximately (#53544~53547).	
II-e SDB	A temperature of 26°C is indicated.	A/B
II-f SDB	It is indicated that for reactions 0.1[g] of solid was added to either 49 or 50[mL] of solution. With a BET value of 57[m <sup>2</sup> /g], rating A/B is applied.	A/B
II-g SDB	The sorption values are calculated from $K_d$ and L/S ratios: <ul style="list-style-type: none"> <li>• #53546 (sorption value 98%)</li> <li>• #53543~53545 and #53547~53550 (sorption &gt;99%)</li> </ul>	B C/D
II-h SDB	Initial Am concentrations of 1.5×10 <sup>-10</sup> and 1.6×10 <sup>-10</sup> M are reported. Based on the data in Rai et al. (1999) it is assumed that initial Am concentration was clearly below (by a factor >5) the respective solubility limit for the reported data around pH 6 to 7.4.	A
II-i SDB	Two different filtration procedures were applied and similar results are reported: filtration with 0.45 μm membranes and with 10,000 MWCO-filters.	A
II-j SDB	A reaction time of 26 and 33 days is indicated. No further (kinetic) information is provided.	C/D
II-k REF	Samples were manually shaken every one to two weeks.	C/D
II-l SDB	No variation in L/S or Am concentration had been performed.	C/D
II-m REF	The experiments were carried out in teflon vessels. There is no information about blank measurements or sorption on vessel walls	B

		given.	
<b>II-n</b>	SDB	It is indicated that replicates are not reported. Error information is available for every datapoint.	B
	REF	Two repetitions are reported. It is unclear if the uncertainties are derived on the basis of replicated sorption experiments or are estimated analytical uncertainties.	
<b>II-o</b>	SDB	No parameter variation had been done.	D

Data table Am/10: REF: Meijer et al. (1990)			
JAEA-SDB version 3.1 DATA: Am/Tuff, #62087~62092			
GUIDELINE: Revision 4b (May 19, 2005)			
<b>Checkpoint</b>	<b>Evaluation</b>	<b>Rating</b>	
<b>I-a.1</b>	SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b>	SDB	Not all mandatory information is provided. Water type, solution/solid, pH, contact time, separation method are missing.	No

Data table Am/11: REF: Nakayama et al. (1986)			
JAEA-SDB version 3.1 DATA: Am/Tuff, #56816~56826			
GUIDELINE: Revision 4b (May 19, 2005)			
* REMARK: Update of SDB required for checkpoints I-a.2 and II-c.			
<b>Checkpoint</b>	<b>Evaluation</b>	<b>Rating</b>	
<b>I-a.1</b>	SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b>	SDB	It is indicated that redox state of Am and reaction temperature are not reported.	Yes
	REF	Batch sorption experiments had been performed at room temperature with Am(III).	
<b>I-b</b>	REF	A table with $K_d$ values is given.	class 1
<b>II-a</b>	SDB	As solid phase Ohya tuff with different mesh sizes (32~60 and <60) and Itado tuff with a mesh size of 32~60 are indicated. Mineral composition and surface characteristics are not reported. BET values are indicated.	C/D
	REF	Major mineral composition and chemical composition of the tuff samples are not reported.	
<b>II-b</b>	SDB	Final pH values are indicated.	A
<b>II-c</b>	SDB	It is indicated that experiments had been performed under aerobic conditions. Eh values are not reported. Am is not redox sensitive. The oxidation state of Am is not indicated.	A/B
	REF	It is reported that Am(III) was used for the experiments.	
<b>II-d</b>	SDB	As water type preequilibrated water and distilled water are indicated. Final solution compositions are not given.	unreliable
	REF	Final solution compositions are not reported. Since information about mineral composition is lacking as well, and because tuff may contain easily soluble minerals or impurities it is impossible to estimate the final solution composition.	

Data table Am/12: REF: Tanaka and Muraoka (1998) JAEA-SDB version 3.1 DATA: Am/Tuff, #62370 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update of SDB required for checkpoint II-i.		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	REF A table with the $K_d$ value is given.	class 1
II-a	SDB As solid phase tuff is indicated. Chemical (elemental) composition of the tuff and CEC are reported. REF Although tuff is a natural sample, no mineral assemblage is indicated.	C/D
II-b	SDB Initial and final pH values are indicated. The final pH covers a range within one pH unit. REF Final pH was measured after reaching the equilibrium.	B
II-c	SDB It is indicated that experiments had been done under aerobic conditions and a final Eh value of 220 to 270[mV] is given. Am is not redox sensitive. A redox state of +III is indicated.	A/B
II-d	SDB As water type tuff equilibrated water is indicated. A table with the final solution composition is provided.	A/B
II-e	SDB A temperature of 25°C is indicated.	A/B
II-f	SDB It is indicated that 0.1[g] of solid was added to 10[mL] of solution. BET values are not reported. Since tuff typically has a high specific surface area it is assumed that 0.1[g] of solid per reaction vial is enough.	A/B
II-g	SDB A sorption value of 99% was calculated from $K_d$ and L/S ratio.	C/D
II-h	SDB An initial Am concentration of $3.27 \times 10^{-7}$ M is reported. Based on speciation calculations with Phreeqci 2.14.3 using the thermodynamic data in NAGRA-PSI (Hummel et al., 2002) the initial Am concentration is still a factor of >5 below the solubility limit (due to the $\text{AmSiO}(\text{OH})_3^{2+}$ and $\text{Am}(\text{CO}_3)_2^-$ species).	A
II-i	SDB It is indicated that filtration with 50 nm membrane was applied.	A
II-j	SDB A reaction time of 7 days is indicated. REF Sorption kinetics of distribution coefficients for Am is provided. The $K_d$ values of the last two measurements are similar indicating near-equilibrium.	A/B
II-k	REF There is no information about sample agitation reported.	C/D
II-l	SDB No variation in L/S or Am concentration had been performed.	C/D
II-m	REF The experiments were carried out in teflon vessels. There is no information about blank measurements or sorption on vessel walls given.	B
II-n	SDB It is indicated that only one sample measurement had been performed. There is no error information given.	D
II-o	SDB No parameter variation had been done.	D

Data table Am/13: REF: Tanaka et al. (1998)		
JAEA-SDB version 3.1 DATA: Am/Tuff, #62377, #62383, #62407~62410, #62438~62442, #62469~62473		
GUIDELINE: Revision 4b (May 19, 2005)		
* REMARK: Update of SDB required for checkpoints I-b and II-i and II-j.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB REF	It is indicated that $K_d$ values are read out of a scanned figure. The diagrams are provided with logarithmic $K_d$ values.	class 5
II-a SDB REF	As solid phase tuff is indicated. Chemical composition of the tuff and CEC are reported. Although tuff is a natural sample, no mineral composition is indicated.	C/D
II-b SDB REF	Initial and final pH values are indicated. For the datapoints where final pH covers a range within one pH unit rating B is applied. For datapoint #62409 the pH range is exceeding one unit, however rating B is applied assuming the same quality as the other datapoints. <ul style="list-style-type: none"> <li>• #62377, #62383, #62438~62442, #62469~62473 (exact pH values given)</li> <li>• #62407, #62408, #62410 (range of one pH unit)</li> <li>• #62409 (range &gt;1 pH unit)</li> </ul> Final pH was measured after reaching the equilibrium.	A B B
II-c SDB	It is indicated that experiments had been done under aerobic conditions and final Eh values of 310[mV] are given. Am is not redox sensitive. A redox state of +III is indicated.	A/B
II-d SDB	As water type tuff equilibrated solution is indicated. A table with the final solution composition is provided for each datapoint.	A/B
II-e SDB	A temperature of 25°C is indicated.	A/B
II-f SDB	It is indicated that 0.1[g] of solid was added to 10[mL] of solution. BET values are not reported. Since tuff typically has a high specific surface area it is assumed that 0.1[g] of solid per reaction vial is enough.	A/B
II-g SDB	Rating is done based on %-sorbed values calculated from the information given in the SDB: <ul style="list-style-type: none"> <li>• #62410, #62441, #62442, #62473 (97.2 to 97.6% sorbed)</li> <li>• other datapoints (&gt;98% sorbed)</li> </ul>	B C/D
II-h SDB	An initial Am concentration of $8.0 \times 10^{-8}$ M is indicated. Based on speciation calculations with Phreeqci 2.14.3 using the thermodynamic data of Hummel et al. (2002) the initial Am concentration is at a pH up to 8.5 clearly below the solubility limit (due to the $\text{AmSiO}(\text{OH})_3^{2+}$ and $\text{Am}(\text{CO}_3)_2^-$ species). Datapoint #62410 with an end pH of 9.5~10.0 however is according to the calculations above the solubility limit and is therefore excluded from further evaluation.	A  unreliable
II-i SDB	It is indicated that filtration with 0.45 $\mu\text{m}$ membrane was applied.	C/D
II-j SDB REF	A reaction time of 7 days is indicated. Separate kinetic measurements demonstrate near-equilibrium was reached at the given reaction time.	A/B

II-k	REF	There is no information about sample agitation reported.	C/D
II-l	SDB	No variation in L/S or Am concentration had been performed.	C/D
II-m	REF	The experiments were carried out in teflon vessels. There is no information about blank measurements or sorption on vessel walls.	B
II-n	SDB	It is indicated that only one sample measurement had been performed. There is no error information given.	D
II-o	SDB	Am sorption had been measured at different pH values and at different Na and Ca concentration in solution.	B

Data table Am/14: REF: Tanaka and Muraoka(1999) JAEA-SDB version 3.1 DATA: Am/Tuff, #61653, #61654 GUIDELINE: Revision 4b (May 19, 2005)			
<b>Checkpoint</b>		<b>Evaluation</b>	<b>Rating</b>
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information are completed.	Yes
I-b	SDB	A figure with log $K_a$ values is provided.	class 5
II-a	SDB	It is indicated a physico-chemical properties of the tuff samples.	A
II-b	SDB	It is indicated pH of solution equilibrated with tuff samples. However pH of solution after sorption experiment is not reported.	B
II-c	SDB REF	It is reported that Eh is 450[mV]. It is considered that this experiment is carried out under air condition. Am(III) is not redox sensitive.	A/B
II-d	SDB REF	Initial solution composition is indicated. The final solution composition is not reported, but can be estimated based on major mineral components and initial solution composition.	A/B
II-e	SDB	It is indicated that the temperature is controlled at 25°C by using a water jacket.	A/B
II-f	SDB REF	It is indicated that L/S is 10[cm <sup>3</sup> ]/0.5[g]. It is considered that quantity of solid is little.	A/B
II-g	REF	The %-sorbed can be calculated with $K_a$ and L/S ratio. This data is 5~95%.	A
II-h	SDB REF	A value of $3.27 \times 10^{-7}$ [M] is indicated as initial Am concentration. Based on calculations using the JAEA-TDB (100331c0.tdb), solubility of Am(III) in the given equilibrated solution is $3.49 \times 10^{-6}$ [M].	A
II-i	SDB	Filtration through 0.45 μm membranes is indicated.	B
II-j	SDB REF	A reaction time of 7 days is indicated. No further (kinetic) information is provide.	C/D
II-k	REF	It is indicated that the samples are gently agitated on a shaker at 60[rpm] for 168 hours.	A/B
II-l	SDB	No variation in L/S or Am concentration had been performed.	C/D
II-m	REF	No information about vessel is indicated.	C/D
II-n	SDB	No information about error is indicated.	D
II-o	SDB	No parameter variation had been done.	D

Data table Am/15: REF: Thomas (1987) JAEA-SDB version 3.1 DATA: Am/Tuff, #60413~60423 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update of SDB required for I-a.2.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided: pH, Eh is missing, atmosphere conditions are indicated.	No

Data table Am/16: REF: Vine et al.(1980a) JAEA-SDB version 3.1 DATA: Am/Tuff, #61653, #61654 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	Initial Am concentration fields are not completed.	No
I-a.2 SDB	Initial Am concentration information is not completed.	No

Data table Am/17: REF: Wolfsberg et al. (1979) JAEA-SDB version 3.1 DATA: Tuff, Am: #61704~61709 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	Not all mandatory information is provided (initial RN concentration is missing). Some information on RN concentration is provided, but it is not clear whether this refers to experiments or stock solutions.	No

Data table Am/18: REF: Wolfsberg (1981) JAEA-SDB version 3.1 DATA: Am/Tuff, #61722~61727 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	Not all mandatory information is provided, initial RN concentration is missing. For experimental details, reference to Vine et al. (1980b) is made; however, the corresponding entry in the SDB also does not contain any information on initial RN concentration.	No



3.1.2 Cesium

Data table Cs/1: REF: Ashida et al. (1999)* JAEA-SDB version 3.1 DATA: Cs/Tuff, #62893, #62897 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	The $K_d$ values are extracted from graphs with a logarithmic scale.	class 5
II-a SDB	Tuff is reported as mineral phase without detailed mineralogic composition. BET is provided.	C/D
II-b SDB	Final pH values are reported (range within one pH unit).	B
II-c SDB	It is indicated that experiments had been performed under ambient conditions (air). Cs is not redox sensitive.	A/B
II-d SDB	As water type, 0.01 and 0.1 M NaCl-solution is indicated. Final solution compositions are not given.	C/D
II-e SDB	A temperature of 22°C is indicated.	A/B
II-f SDB REF	A L/S of 100[mL/g] is indicated. Based on the given specific surface area of the tuff sample, the mass of 1[g] tuff used for an experiment has a surface area of about 24[m <sup>2</sup> ].	A/B
II-g SDB	The sorption values were calculated based on the information given in the SDB. • # 2893 (96%) • #62897 (81%)	B A
II-h SDB	Initial Cs concentration is reported. Cs is not solubility limited.	A
II-i SDB	Filtration by 10,000 MWCO-filter is indicated.	B
II-j SDB REF	A reaction time of 30 days is indicated. The kinetics of sorption are not reported.	C/D
II-k REF	No information is provided for the agitation method.	C/D
II-l SDB	No isotherm, no variation of the Cs concentration and no variation of L/S are indicated.	C/D
II-m REF	There is no information about the reaction vessels or a correction for sorption on vessel walls given.	C/D
II-n REF	No replicates and no error estimates are reported.	D
II-o REF	NaCl concentration is varied.	C

Data table Cs/2: REF: Barney (1982) JAEA-SDB version 3.1 DATA: Cs/Tuff, #44989~45008 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	Table with $K_d$ values is provided.	class 1
II-a SDB REF	A solid phase tuff are indicated. SSA and CEC are given. The minerals present are reported. Further composition is not reported.	B
II-b SDB	Initial and end pH are indicated.	A
II-c SDB	Indicated redox state corresponds to the information in the reference. Redox state of Cs is not given in the reference.	A/B

	REF	Systems were pre-equilibrated. Cs in the oxidation state (I) is reported. Cs is not redox sensitive.	
II-d	REF	Experiments had been performed in synthetic groundwater. Final solution composition is not indicated.	C/D
II-e	SDB	It is indicated that experiments had been performed at 23°C.	A/B
II-f	SDB REF	The amount of L/S ratio is reported. It is indicated that surface area of tuff is $188 \pm 3$ [m <sup>2</sup> /g].	A/B
II-g	SDB	The sorption values were calculated based on the information given in the SDB. • #44989~44991 • #44992~45008	B C/D
II-h	SDB	Initial Cs concentrations from $9.54 \times 10^{-7}$ to $7.94 \times 10^{-9}$ M are indicated. Cs is not solubility limited.	A
II-i	SDB REF	As separation method filtration is indicated. Filtration through 30 Angstrom Amicon 50A ultrafilter is reported.	B
II-j	SDB	A contact time of 14 days is indicated.	C/D
II-k	REF	Continuous shaking (180 oscillations/min), method not specified.	A/B
II-l	REF	Isotherms were determined at different temperatures.	A
II-m	REF	Polycarbonate centrifuge tube 50[mL], sorption on vessel walls not considered.	B
II-n	REF	There is no error information reported.	D
II-o	REF	Variation of solution composition ([Na] etc. variations).	C

Data table Cs/3: REF: Daniels et al. (1982)

JAEA-SDB version 3.1 DATA: Cs/Tuff, #49551~49657

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB  REF	Not all mandatory information is provided. pH, separation method, redox potential and a few initial RN concentrations are missing.  The initial pH of the solutions used for experimentation and the actual pH during experimentation are not available. It is not clear whether the experimental systems had been at or near equilibrium.	No

Data table Cs /4: REF: Erdal et al. (1978)

JNC-SDB version 3.1 DATA: Cs/Tuff, #50937~#50942

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB  REF	Not all mandatory information is provided: pH and initial concentration are missing.  No further information could be found.	No

Data table Cs/5: REF: Maclean et al.(1978) JAEA-SDB version 3.1 DATA: Cs/Tuff, #56189 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information are completed.	Yes
I-b	SDB A table with $K_d$ values is provided.	class 1
II-a	SDB It is not indicated the composition and properties of mineral.	C/D
II-b	SDB Only initial pH of groundwater is reported.	D
II-c	SDB REF Redox conditions are not reported. It is considered that experiment is carried out under air condition. Cs(I) is not redox sensitive.	A/B
II-d	SDB REF Final composition of groundwater is not reported. Initial solution composition is indicated. The final solution composition is not reported, but can be estimated based on major mineral components and initial solution composition.	C/D
II-e	SDB A temperature of 25°C is reported.	A/B
II-f	SDB REF A solid/solution ratio is reported (1[g]/15[mL]). It is indicated that particle size of solid is 100~325 mesh.	A/B
II-g	REF The %-sorbed can be calculated with $K_d$ and L/S ratio. This data is 5~95%.	A
II-h	SDB A value of $2.8 \times 10^{-8}$ [M] is indicated as initial Cs concentration. Cs is not solubility limited.	A
II-i	SDB It is indicated that separation method is centrifuge (3000[rpm]/20~60 minutes) and filtration (0.1µm).	A
II-j	SDB REF A reaction time of 7 days is indicated. No further (kinetic) information is provide.	C/D
II-k	REF It is indicated that agitated method is shaker-table water bath and ~130 oscillations per minute for 48 hours.	A/B
II-l	SDB Initial Cs concentration is not varied.	C/D
II-m	REF It is indicated that experimental vessel is polycarbonate centrifuge tubes.	B
II-n	SDB No information about error is indicated.	C/D
II-o	SDB No parameter variation had been done.	D

Data table Cs/6: REF: Meijer et al. (1990) JAEA-SDB version 3.1 DATA: Cs/Tuff, #62101~62108 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided. Water type, pH, initial RN concentration and contact time are missing.	No

Data table Cs/7: REF: Meyer et al. (1990) JAEA-SDB version 3.1 DATA: Cs/Tuff, #56393~56407 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A table with $K_d$ values is provided.	class 1
II-a SDB REF	As solid phase tuff is indicated. SSA and CEC are not given. Some details of the composition of geological materials are reportedly given in Meyer et al. (1987).	C/D
II-b SDB	Final pH is indicated.	A
II-c SDB REF	An air/CO <sub>2</sub> atmosphere is indicated. Experiments were conducted in an atmosphere box with an overpressure of CO <sub>2</sub> to buffer the solution pH. System was pre-equilibrated. Cs in the oxidation state (I) is reported. Cs is not redox sensitive.	A/B
II-d REF	Experiments had been performed in NaCl solution with a small amount of NaHCO <sub>3</sub> . Final solution composition is not reported.	C/D
II-e SDB	It is indicated that no temperature is given.	C/D
II-f SDB REF	The solution/solid ratio is reported as 0.2[g] solid, 2[mL] solution. Since SSA is not given, the criterion cannot be evaluated.	C/D
II-g SDB	The %-sorbed can be calculated with $K_d$ and L/S ratio: <ul style="list-style-type: none"> <li>• #56393, #56394, #56398, #56406, #56407</li> <li>• #56401~56405</li> <li>• #56395~56397, #56399, #56400</li> </ul>	C/D B A
II-h SDB	An initial Cs concentration of $5.00 \times 10^{-9}$ M is indicated. Solubility limit has not been estimated. Cs is not solubility limited.	A
II-i SDB REF	As separation method centrifugation is indicated. Centrifugation 9000[rcf] for 30 minutes, after decantation a second centrifugation was done for 15 minutes.	C/D (update SDB)
II-j SDB REF	Contact times of 0.25~14 days are indicated. Equilibrium was reached within a few days. The experiments with a reaction time of 0.25 and 4 days may be haven not reached equilibrium. <ul style="list-style-type: none"> <li>• #56393, #56394, #56399, #56400, #56402, #56405</li> <li>• #56395~56398, #56401, #56403, #56404, #56406, #56407</li> </ul>	A/B unreliable
II-k REF	Not reported.	C/D
II-l REF	No isotherms and no variations of Cs concentrations are indicated.	C/D
II-m REF	No information about vessel material is reported. No information about consideration of losses to vessel walls is given.	C/D
II-n REF	It is indicated that there is no error information available.	D
II-o REF	No variations of conditions are indicated.	D

Data table Cs/8: REF: Park et al.(1992) JAEA-SDB version 3.1 DATA: Cs/tuff, #57249~57251 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	A table with $K_d$ values is given.	class 1
II-a SDB	Tuff is indicated as mineral phase; rough mineral composition and specific surface areas (BET) of the three grain size fractions are provided. Particle sizes of the fractions are given.	B
II-b SDB	Initial pH values are reported. It is not reported at which state of the experiment the pH was measured. The pH is listed in the table of groundwater composition. Since the synthetic groundwater is a well buffered system, rating B is given.	B
II-c SDB REF	It is indicated that redox conditions are not reported. No inert gas atmosphere is reported. Therefore it is assumed that the experiments were conducted under ambient conditions. Cs is not redox sensitive.	A/B
II-d SDB REF	The initial composition of the solution is given (synthetic groundwater). The composition of synthetic groundwater reported simulates the chemical composition of equilibrated natural groundwater from the tuff sampled.	A/B
II-e SDB	It is indicated that a reaction temperature of 25°C had been used.	A/B
II-f SDB	The BET surfaces of the tuff in three different grain sizes are indicated to be >30[m <sup>2</sup> /g]. Rating is done based on the calculated surface area of the added sorbent indicated. In all cases it is >5 [m <sup>2</sup> ] per reaction vessel.	A/B
II-g REF	The sorption values were calculated based on the information given in the SDB. The sorption values for all datapoints are >99.5%.	C/D
II-h SDB	Initial Cs-concentration of $8.4 \times 10^{-10}$ M is indicated. Cs is not solubility limited.	A
II-i SDB REF	Centrifugation is reported as separation method. It is reported that samples had been centrifuged for 10 minutes at 3,000[rpm].	C/D
II-j SDB REF	A reaction time of 14 days is indicated. For the three experiments the distribution ratios with time are illustrated in graphs with logarithmic time scales. It is unclear if near-equilibrium was reached.	C/D
II-k REF	Shaking is reported as agitation method.	A/B
II-l REF	No isotherm, no variation of the Cs concentration and no variation of the L/S is indicated.	C/D
II-m REF	It is indicated that glass vessels had been used for the experiments and corrections for sorption on the vessel walls had been performed based on a blank test.	C/D
II-n SDB	No replicates and no error estimates are reported.	D
II-o REF	Cs sorption on three different grain size fractions of the same tuff sample is reported.	C

Data table Cs/9: REF: Rogers and Meijer (1993) JAEA-SDB version 3.1 DATA: Cs/Tuff, #58575~58613 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	Not all mandatory information is provided; it is indicated that the initial RN concentration is missing. No further information could be found.	No

Data table Cs/10: REF: Thomas (1987) JAEA-SDB version 3.1 DATA: Cs/Tuff, #60430~60448 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided: pH, Eh is missing, atmosphere conditions are indicated.	No

Data table Cs/11: REF: Yamamoto et al.(1989) JAEA-SDB version 3.1 DATA: Cs/Tuff, #61769 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	Separation fields are not completed.	No
I-a.2 SDB	Separation information is not completed.	No

### 3.1.3 Neptunium

Data table Np/1: REF: Barney(1982) JAEA-SDB version 3.1 DATA: Np/Tuff, #45042~45061 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is completed.	Yes
I-b	SDB A table with $K_d$ values is provided.	class 1
II-a	SDB REF SSA and CEC of tuff are given. The minerals present are reported. Further composition is not reported.	B
II-b	SDB Initial and final pH are indicated.	A
II-c	SDB REF Indicated redox state corresponds to the information in the reference. These experiments are carried out under aerobic condition and controlled condition. It is used hydrazine as reducing agent under controlled condition. • #45042~45048, #45050, #45052, #45054 : Np(V) • #45049, #45051, #45053, #45055~45061 : Np(IV)	A C/D
II-d	SDB Experiments had been performed in synthetic groundwater. Final solution composition is not indicated.	C/D
II-e	SDB It is indicated that experiments has been performed at 23°C.	A/B
II-f	SDB REF The amount of solution/solid ratio is reported. Surface area 188[m <sup>2</sup> /g] in the tuff sample is available.	A/B
II-g	REF The %-sorbed can be calculated with $K_d$ and L/S ratio. This data is 5~95%.	A
II-h	SDB REF Initial Np concentrations are $5.71 \times 10^{-8} \sim 6.54 \times 10^{-8}$ [M] under aerobic condition, $6.31 \times 10^{-8} \sim 6.76 \times 10^{-8}$ [M] under reducing condition. Based on calculations using the thermodynamic database developed by JAEA (100331c1.tdb), in the case of aerobic condition, solubility of Np is $>1.95 \times 10^{-3}$ [M], in the case of reducing condition, $<8.0 \times 10^{-9}$ [M]. • #45042~45048, #45050, #45052, #45054 : Np(V) • #45049, #45051, #45053, #45055~45061 : Np(IV)	A unreliable
II-i	SDB REF As separation method filtration is indicated. Filtration through 30 Angstrom Amicon 50A ultrafilter is reported.	B
II-j	SDB A contact time of 14 days is indicated.	C/D
II-k	REF Continuous shaking (180 oscillations/min), method not specified.	A/B
II-l	SDB Isotherms were determined at different temperatures.	A
II-m	REF Polycarbonate centrifuge tube 50[mL], sorption on vessel walls not considered.	B
II-n	SDB There is no error information reported.	D
II-o	SDB Variation of solution composition (Na concentration etc. variations).	C

Data table Np/2: REF: Baston et al. (1997) and Berry et al.(2007) JAEA-SDB version 3.1 DATA: Np/Tuff, #46828~46831, #46940, #46941 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Update of SDB required for checkpoints II-a, II-c, II-d and II-i.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	A table with $K_a$ values is given.	class 1
II-a SDB	As solid phase, tuff is indicated. Major mineral composition is reported for datapoints #46940 and #46941 only, but is also valid for datapoints #46828~46831. Surface characteristics are not given. Since minor mineral composition is not indicated, surface characteristics cannot be estimated.	C/D
II-b SDB REF	Final pH values are reported. No use of any pH buffer is reported.	A
II-c SDB REF	The oxidation state of Np is not reported. It is indicated that experiments had been performed under nitrogen atmosphere with dithionite as reducing agent. Final Eh values are indicated. It is reported that Np(V) was reduced to Np(IV) with sodium dithionite prior to the adsorption experiments. O <sub>2</sub> levels were reportedly < 1[ppm]. All solutions had been de-oxygenated before experimentation. Levels of dithionite were monitored during the experiments, and were corrected where needed.	C/D
II-d SDB REF	As water type tuff equilibrated distilled water is indicated. Only for datapoints #46940 and #46941 the final solution composition of equilibration at 60°C resp. at room temperature is provided. The final solution compositions for datapoints #46828~46831 are identical to the compositions of datapoints #46940 and #46941.	A/B
II-e SDB	It is indicated that experiments had been done at 25 and 60°C.	A/B
II-f SDB	It is indicated that an L/S ratio of 5 with 300[mL] solution and 6[g] of solid phase had been used for the experiments.	A/B
II-g SDB	Sorption values are calculated from $K_a$ and L/S ratios: • #46828 (97% sorption) • #46829~46831, #46940, #46941 (>98% sorption)	A C/D
II-h SDB REF	Initial Np concentration of $6.0 \times 10^{-9}$ M is indicated. Based on speciation calculations with Phreeqci 2.14.3 using the thermodynamic database developed by JAEA (100331c1.tdb), the initial Np concentration may have been at, or slightly above, the solubility limit. The solutions were pre-filtered (0.45 μm) before being equilibrated with the solid. Presumably, Np-precipitates would have been removed in this way.	C/D
II-i SDB REF	Filtration through 10,000 MWCO or 0.45 μm membranes, or centrifugation at 1100[g] for 3 hours is indicated. Three liquid/solid separation techniques were employed: 1. Centrifugation at 1100[g] for 15 minutes with aliquots being removed from near the surface of the supernatant liquid 2. Centrifugation followed by filtration through a 0.45 μm filter	A



		3. Centrifugation followed by filtration first through a 0.45 $\mu\text{m}$ filter, and then through a 10,000 MWCO filter $K_d$ values were all in the same range, independent of the applied separation technique.	
<b>II-j</b>	SDB	A contact time of 120 days is indicated.	C/D
<b>II-k</b>	REF	Gentle agitation on a shaker is reported.	A/B
<b>II-l</b>	SDB	No variation in L/S or Np concentration had been performed.	C/D
<b>II-m</b>	REF	The experiments had been carried out in polypropylene centrifuge tubes. Sorption on vessel walls was not tested in case of Np. However, tests with Cm suggest that sorption on vessel walls can be neglected.	B
<b>II-n</b>	SDB	Error estimates are given, but it is indicated that no replicate measurements are available.	B
	REF	Error estimates are given, which are based on counting statistics only. Neptunium experiments were carried out in duplicate.	
<b>II-o</b>	SDB	Temperature had been varied (and as a result of the temperature change also the pH varied).	C

Data table Np/3: REF: Daniels et al.(1982)  
JAEA-SDB version 3.1 DATA: Np/Tuff, #49763~49769  
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	Initial Np concentration fields are not completed.	No
<b>I-a.2</b> SDB	Initial Np concentration information is not completed.	No

Data table Np/4: REF: Nakayama et al.(1986)  
JAEA-SDB version 2 . DATA: Np/Tuff, #56839~56844  
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is completed.	Yes
<b>I-b</b> SDB	A table with $K_d$ values is provided.	class 1
<b>II-a</b> SDB	Information of physic-chemical properties about tuff is not reported. However, source, mesh size and specific surface area are reported.	C/D
<b>II-b</b> SDB REF	Final pH is indicated. pH is adjusted before sorption experiments, during sorption experiment pH is not adjusted.	B
<b>II-c</b> SDB REF	It is not indicated about redox condition. Sorption experiment is supposed to be performed under aerobic condition. So, redox state of Np is considered as Np(V).	A/B
<b>II-d</b> SDB REF	There is no information about final solution composition and physico-chemical properties of tuff. It is impossible that final solution composition is predicted.	unreliable

Data table Np/5: REF: Rogers and Meijer(1993) JAEA-SDB version 3.1 DATA: Np/Tuff, #58614~58648 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is completed.	Yes
I-b	SDB A table with $K_d$ values is provided.	class 1
II-a	SDB Information of physico-chemical properties about tuff is not reported. However, source, particle size and specific surface area are reported.	C/D
II-b	SDB Final pH is indicated. REF No more information is reported as pH adjustment during sorption experiment.	B
II-c	SDB It is not indicated about redox condition. REF Sorption experiment is supposed to be performed under aerobic condition. So, redox state of Np is considered as Np(V).	A/B
II-d	SDB There is no information about final solution composition and physico-chemical properties of tuff. REF It is impossible that final solution composition is predicted.	unreliable

Data table Np/6: REF: Tanaka and Muraoka(1999) JAEA-SDB version 3.1 DATA: Np/Tuff, #62315 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information are completed.	Yes
I-b	SDB A figure with log $K_d$ values is provided.	class 5
II-a	SDB Physico-chemical properties of the tuff samples are indicated.	A
II-b	SDB It is indicated pH of solution equilibrated with tuff samples. However pH of solution after sorption experiment is not reported.	B
II-c	SDB It is reported that Eh is 450[mV]. REF It is considered that this experiment is carried out under air condition. So, redox state of Np is considered as Np(V).	A/B
II-d	SDB Initial solution composition is indicated. The final solution composition is not reported, but can be estimated based on major mineral components and initial solution composition.	A/B
II-e	SDB It is indicated that the temperature is controlled at 25°C by using a water jacket.	A/B
II-f	SDB It is indicated that L/S is 10[cm <sup>3</sup> ]/0.5[g]. REF It is considered that quantity of solid is little.	A/B
II-g	REF The %-sorbed can be calculated with $K_d$ and L/S ratio. This data is 5~95%.	A
II-h	SDB A value of $1.62 \times 10^{-3}$ [M] is indicated as initial Np concentration. REF Based on calculations using the thermodynamic data given JAEA (100331c1.tdb), solubility of Np(V) in the given equilibrated solution are $2.093 \times 10^{-3}$ [M].	A
II-i	SDB Filtration through 0.45 μm membranes is indicated.	B
II-j	SDB A reaction time of 7 days is indicated. REF No further (kinetic) information is provide.	C/D

II-k	REF	It is indicated that the solution containing the sample is gently agitated on a shaker at 60[rpm] for 168 hours.	A/B
II-l	SDB	Initial Np concentration is not varied.	C/D
II-m	REF	No information about vessel is indicated.	C/D
II-n	SDB	No information about error is indicated.	C/D
II-o	SDB	No parameter variation had been done..	D

Data table Np/7: REF: Tanaka et al.(1998)			
JAEA-SDB version 3.1 DATA: Np/Tuff, #62374, #62380, #62390~62394, #62422~62426, #62453~62458			
GUIDELINE: Revision 4b (May 19, 2005)			
<b>Checkpoint</b>		<b>Evaluation</b>	<b>Rating</b>
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB REF	It is indicated that $K_d$ values are read out of a scanned figure. The diagrams are provided with logarithmic $K_d$ values.	class 5
II-a	SDB REF	As solid phase tuff is indicated. Chemical composition and CEC are reported. Although tuff is a natural sample, no mineral composition is indicated.	C/D
II-b	SDB REF	Initial and final pH are reported. pH is adjusted using NaOH and HCl (data point #62390~62394). Other data points are not adjusted.	A
II-c	SDB REF	It is indicated that experiments had been done under aerobic conditions and final Eh values of 310[mV] are given. So, redox state of Np is considered as Np(V).	A/B
II-d	SDB	As water type tuff equilibrated solution is indicated. A table with the final solution composition is provided for each data point.	A/B
II-e	SDB	A temperature of 25°C is indicated.	A/B
II-f	SDB REF	It is indicated that 0.1[g] of solid was added to 10[mL] of solution. BET values are not reported. Since tuff typically has a high specific surface area it is assumed that 0.1[g] of solid per reaction vial is enough.	A/B
II-g	REF	Rating is done based on %-sorbed values calculated from the information given in the SDB: • #62374, #62380, #62392~62394, #62422, #62423, #62453~62457 • #62390, #62391, #62424~62426, #62458	A B
II-h	SDB REF	An initial Np concentration of $2.0 \times 10^{-4}$ [M] is indicated. Based on calculations using the thermodynamic data selected by JAEA (100331c1.tdb), solubility of Np(V) in the given equilibrated solution are $>8.2 \times 10^{-5}$ [M].	A
II-i	SDB	It is indicated that filtration with 0.45 μm membrane was applied.	C/D
II-j	SDB REF	A reaction time of 7 days is indicated. Separate kinetic measurements demonstrate near-equilibrium was reached at the given reaction time.	A/B
II-k	REF	It is indicated that agitation method is shaking by hand during experimental period.	A/B
II-l	SDB	No variation in L/S or initial Np concentration had been performed.	C/D

<b>II-m</b>	REF	The experiments were carried out in teflon vessels. There is no information about blank measurements or sorption on vessel walls.	B
<b>II-n</b>	SDB	It is indicated that only one sample measurement had been performed. There is no error information given.	D
<b>II-o</b>	SDB	Np sorption had been measured at different pH values and at different Na and Ca concentrations in test solutions.	B

Data table Np/8: REF: Thomas(1987)  
 JAEA-SDB version 3.1 DATA: Np/Tuff, #60456~60487  
 GUIDELINE: Revision 4b (May 19, 2005)

<b>Checkpoint</b>	<b>Evaluation</b>	<b>Rating</b>
<b>I-a.1</b>	SDB All mandatory fields are completed.	Yes
<b>I-a.2</b>	SDB Not all mandatory information is provided: pH, Eh is missing, atmosphere conditions are indicated.	No

3.1.4 Selenium

Data table Se/1: REF: Barney (1982)		
JAEA-SDB version 3.1 DATA: Se/Tuff, #45192~45210		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A table with $K_d$ values is provided.	class 1
II-a SDB REF	As solid phase tuff is indicated. SSA and CEC are given. The minerals present are reported. Further composition is not reported.	B
II-b SDB	Initial and end pH are indicated.	A
II-c SDB REF	Indicated redox state corresponds to the information in the reference. Eh is not reported. These experiments are carried out under aerobic condition and controlled condition. It is used hydrazine as reducing agent under controlled condition. • #45192, #45194~45198, #45202, #45209, #45210 : Se(-II) • #45193, #45199~45201, #45203~45208 : Se(VI)	unreliable A/B
II-d SDB	Experiments had been performed in synthetic groundwater. Final solution composition is not indicated.	C/D
II-e SDB	It is indicated that experiments has been performed at 23°C.	A/B
II-f SDB REF	The amount of solution/solid ratio is reported. Surface area 188[m <sup>2</sup> /g] in the tuff sample is available.	A/B
II-g REF	The %-sorbed can be calculated with $K_d$ and L/S ratio. • #45192 (<5%) • Others data (5~95%)	C/D A
II-h SDB	Initial Se concentrations are $2.80 \times 10^{-8}$ [M] under aerobic condition. Se(VI) is not solubility limited (Azuma et al., 1999). • #45193, #45199~45201, #45203~45208 : Se(VI)	A
II-i SDB REF	As separation method filtration is indicated. Filtration through 30 Angstrom Amicon 50A ultrafilter is reported.	B
II-j SDB	A contact time of 14 days is indicated.	C/D
II-k REF	Continuous shaking (180 oscillations/min), method not specified.	A/B
II-l SDB	Isotherms were determined at different temperatures.	A
II-m REF	Polycarbonate centrifuge tube 50[mL], sorption on vessel walls not considered.	B
II-n SDB	There is no error information reported.	D
II-o SDB	Variation of solution composition (Na concentration etc. variations).	C

Data table Se/2: REF: Conca and Triay(1996)		
JAEA-SDB version 3.1 DATA: Se/Tuff, #49374~49376		
GUIDELINE: Revision 4b (May 19, 2005)		
* REMARK: Update of SDB required for I-a.1.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	A table with $K_d$ values is provided.	class 1

<b>II-a</b>	SDB	Tuff is indicated as solid phase. Mineralogy is not indicated. Specific surface area is provided.	C/D
<b>II-b</b>	SDB	Final pH values are reported.	A
<b>II-c</b>	SDB REF	It is not reported experimental conditions. However, final Eh is reported (140~150 [mV]). It is considered that redox state of Se is Se(IV).	A/B
<b>II-d</b>	SDB	As water type J-13 Well water is indicated. The final solution composition of the equilibrated groundwater is not provided and cannot be estimated due to lacking mineralogy of the tuff sample.	unreliable

Data table Se/3: REF: Daniels et al. (1982)  
 JAEA-SDB version 3.1 DATA: Se/Tuff, #49826~49830  
 GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
<b>I-a.1</b>	SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b>	SDB REF	Not all mandatory information is provided. pH, separation method and redox potential are missing. The initial pH of the solutions used for experimentation and the actual pH during experimentation are not available. It is not clear whether the experimental systems had been at or near equilibrium.	No

Data table Se/4: REF: Shibutani et al. (1994)  
 JAEA-SDB version 3.1 DATA: Se/Tuff, # 59232~59255  
 GUIDELINE: Revision 4b (May 19, 2005)

\* REMARK: Update of SDB required for checkpoints I-a.2, II-d, II-f and II-h.

Checkpoint		Evaluation	Rating
<b>I-a.1</b>	SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b>	SDB	All mandatory information is provided.	Yes
<b>I-b</b>	SDB	It is indicated that $K_d$ values are provided as % sorbed.	class 2
<b>II-a</b>	SDB REF	Tuff is indicated as solid phase. Specific surface area is provided. Mineralogy of used tuff is plagioclases, smectite, clinoptilolite, heulandite, quartz, kaolinite, biotite, gypsum and pyrite, and a little of K-feldspar, illite, sericite, chlorite, amphibole and calcite.	C/D
<b>II-b</b>	SDB	Final pH values are reported (after a contact time of 14 days, which can be assumed to be enough to reach equilibrium).	A
<b>II-c</b>	SDB REF	It is indicated that experiments had been performed in an atmosphere with <1[ppm] of oxygen. It is reported that experiments had been performed under N <sub>2</sub> -atmosphere with <1[ppm] of oxygen present. Eh values are not reported. Due to the kinetic stability of added Se(IV) under ambient conditions, rating C/D is applied.	C/D
<b>II-d</b>	SDB REF	As water type 0.01 M NaCl solution is indicated. The final solution composition of the equilibrated groundwater is not provided. The final solution composition is not reported, but can be estimated based on major mineral components and initial solution composition.	C/D
<b>II-e</b>	SDB	Experiments had been conducted at room temperature.	A/B
<b>II-f</b>	SDB	A liquid/solid ratio of 20[mL/g] is reported.	A/B

	REF	The L/S ratio is indicated to be 2.5[mL/g]. With the indicated specific surface area of 57[m <sup>2</sup> /g] rating A/B is applied.	
II-g	SDB	The sorption values are calculated from K <sub>d</sub> and L/S ratios: <ul style="list-style-type: none"> <li>• #59234~59247, #59254, #59255 (26~83% sorption)</li> <li>• #59248~59253 (96% sorption)</li> <li>• #59232, #59233 (&gt;99% sorption)</li> </ul>	A B C/D
II-h	SDB	Initial Se concentration is indicated as 1.0×10 <sup>-4</sup> M. According to Phreeqci-calculations using the thermodynamic data in NAGRA-PSI thermodynamic database (Hummel et al., 2002), the reported Se concentration is clearly below the solubility limit.	C/D
II-i	SDB	It is reported that reaction mixtures were filtered with a 10,000 MWCO (Molecular Weight Cut-Off) ultrafilter.	B
II-j	SDB	A contact time of 14 days is indicated. This reaction time is considered to be reasonably long.	C/D
II-k	REF	Agitation method is shaking sometime during experimental period.	A/B
II-l	SDB	No variation in L/S or initial Se concentration is indicated.	C/D
II-m	REF	There is no information about the vessel type used for experimentation. It is indicated that blank measurements had been made, but it is not reported if corrections for sorption on the vessel walls had been performed.	C/D
II-n	SDB	No error estimates are reported. Only one replicate is indicated.	D
II-o	SDB	pH had been varied systematically.	C

Data table Se/5: REF: Thomas (1987)		
JAEA-SDB version 3.1 DATA: Se/Tuff, #60506~60526		
GUIDELINE: Revision 4b (May 19, 2005)		
<b>Checkpoint</b>	<b>Evaluation</b>	<b>Rating</b>
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided: pH, Eh is missing, atmosphere conditions are indicated.	No

3.1.5 Thorium

Data table Th/1: REF: Baston et al.(1994)		
JAEA-SDB version 3.1 DATA: Th/Tuff, #46560~46563		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	Eh fields are not completed.	Yes
I-a.2 SDB	All mandatory information is completed.	Yes
I-b SDB	A graph with log $K_d$ is provided.	class 5
II-a SDB	Tuff as solid phase is indicated. SSA and CEC are not given. The minerals present are reported. Further composition is not reported.	B
II-b SDB REF	Final pH value is given. One tube is monitored regularly over a 60~100 days period to monitor the pH and, if necessary, pH readjustments are carried out in all tubes (triplicated).	A
II-c SDB	All experiments were carried out in nitrogen atmosphere glove boxes. Th(IV) is not redox sensitive.	A/B
II-d SDB	The composition of the synthetic groundwater is not given.	unreliable

Data table Th/2: REF: Ishii et al.(2001)		
JAEA-SDB version 3.1 DATA: Th/Tuff, #65713, #65714		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	Eh fields are not completed.	Yes
I-a.2 SDB	All mandatory information is completed.	Yes
I-b SDB	A table with $K_d$ values is provided.	class 1
II-a SDB	Tuff as solid phase is indicated. SSA and CEC are given. The chemical composition is reported.	A
II-b SDB	Initial and equilibrium pH is indicated. It is not carried out pH adjustments.	A
II-c SDB REF	Redox conditions are not reported. It is considered that experiment is carried out under air condition. Th(IV) is not redox sensitive.	A/B
II-d SDB REF	An initial liquid composition is indicated. The final solution composition is not reported, but can be estimated based on major mineral components and initial solution composition.	A/B
II-e SDB	A temperature of 15°C is reported.	A/B
II-f SDB	In the case of Th, solid/solution is reported 1[g]/50[mL] or 1[g]/100[mL].	A/B
II-g REF	The %-sorbed can be calculated with $K_d$ and L/S ratio. All data are 5~95%.	A
II-h SDB REF	Initial Th concentration is decided by solubility calculation using solution composition and thermodynamic data.	A
II-i SDB	Filtration through 0.45 $\mu$ m membranes is indicated.	B
II-j SDB REF	A reaction time of 14 days is indicated. No further (kinetic) information is provide.	C/D
II-k REF	Samples are agitated continuously by a stirrer (50 strokes/minute) and shaking (1 times/day).	A/B



<b>II-1</b>	SDB REF	It is carried out three different initial Th concentrations. It is not indicated Th sorption isotherms.	B
<b>II-m</b>	REF	It is reported that reaction vessel is teflon or polypropylene. After sorption experiment, it is confirmed that Th is not sorbed onto vessel wall.	A
<b>II-n</b>	SDB	It is carried out in triplicate. It is reported $K_d$ error.	A
<b>II-o</b>	SDB	It is carried out in different solution and three different initial Th concentrations.	B

Data table Th/3: REF: Thomas (1987) JAEA-SDB version 3.1 DATA: Th/Tuff, #60554~60563 GUIDELINE: Revision 4b (May 19, 2005)		
<b>Checkpoint</b>	<b>Evaluation</b>	<b>Rating</b>
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	Not all mandatory information is provided: pH, Eh is missing, atmosphere conditions are indicated.	No

Data table Th/4: REF: Ueta (1998) JAEA-SDB version 3.1 DATA: Th/tuff, #61621~61628 GUIDELINE: Revision 4b (May 19, 2005)		
<b>Checkpoint</b>	<b>Evaluation</b>	<b>Rating</b>
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	$K_d$ values are provided in [mL/g].	class 1
<b>II-a</b> SDB REF	As solid phase tuff from Gifu-ken Tono is indicated. Major mineralogy and surface characteristics of the tuff are not reported. A surface area of 57[m <sup>2</sup> /g] is reported.	C/D
<b>II-b</b> SDB	Initial and final pH values are reported.	A
<b>II-c</b> SDB	Redox state of Th is not indicated. Experiments had been performed under aerobic conditions. Eh values are not reported. Th is not redox sensitive.	A/B
<b>II-d</b> SDB REF	Experiments had been performed in seawater and distilled water. Final solution compositions are not reported: • #61621~61624: due to lacking mineralogy the solution composition after equilibration with distilled water cannot be estimated. • #61625~61628: it is supposed that no essential changes take place with seawater. Carbonate concentrations of the solutions are reported. All solutions had been analysed after pre-equilibration.	unreliable C/D
<b>II-e</b> SDB	A temperature of 25°C is indicated.	A/B
<b>II-f</b> SDB	It is indicated that 1[g] of solid per reaction vial was used. With the indicated BET the total solid surface is 57[m <sup>2</sup> /vial].	A/B
<b>II-g</b> REF	The sorption values are calculated from $K_d$ and L/S ratios. For all datapoints the sorption is >98%.	C/D
<b>II-h</b> SDB	An initial Th concentration of $4.0 \times 10^{-8}$ M is indicated. Based on speciation calculations with Phreeqci 2.14.3 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al. 2002) and the JNC-TDB_011213c2, the initial Th	unreliable

	concentration is clearly above the solubility limit and datapoints are considered as unreliable.	
--	--	--

Data table Th/5: REF: Ueta et al. (1999) JAEA-SDB version 3.1 DATA: Th/tuff, #61629~61636 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	A table with $K_d$ values is given.	class 1
II-a SDB	As solid phase tuff from Gifu-ken Tono is indicated. Major mineralogy and surface characteristics of the tuff are not reported.	C/D
II-b SDB	Initial and final pH values are reported.	A
II-c SDB	Redox state of Th is not indicated. Experiments had been performed under aerobic conditions. However, Th is not redox sensitive.	A/B
II-d SDB	Experiments had been performed in seawater and distilled water. Final solution compositions are not reported: <ul style="list-style-type: none"> <li>• #61629~61632: due to lacking mineralogy the solution composition after equilibration with distilled water cannot be estimated.</li> <li>• #61633~61636: it is supposed that no essential changes take place with seawater.</li> </ul>	unreliable A/B
II-e SDB	A temperature of 25°C is indicated.	A/B
II-f SDB	It is indicated that 2[g] of tuff and 100[mL] of solution was used for the experiments.	A/B
REF	With the indicated BET for tuff from Gifu-ken Tono in Ueta (1998) the total surface/vial is 114[m <sup>2</sup> ].	
II-g SDB	The sorption values are calculated from $K_d$ and L/S ratios. They are 63~64% for the experiments with seawater #61633~61636.	A
II-h SDB	An initial Th concentration of $2.0 \times 10^{-9}$ M is indicated. Based on speciation calculations with Phreeqci 2.14.3 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al. 2002), the initial Th concentration is below the solubility limit but less than a factor of 5.	B
II-i SDB	Similar results were obtained by filtration over 0.45 μm membranes and filtration over a 10,000 MWCO filter (molecular weight cut-off).	A
II-j SDB	A contact time of 30 days is indicated.	C/D
II-k REF	The samples were shaken.	A/B
II-l SDB	No variation in L/S or initial Th concentration is indicated.	C/D
II-m REF	Type of reaction vial is not reported. Corrections for sorption on vessel wall have been done. Sorbed Th of the reaction vial was extracted by acid leaching and was corrected in $K_d$ calculations.	C/D
II-n SDB	<ul style="list-style-type: none"> <li>• No error information is available for data points #61633, #61636.</li> <li>• Error information based on duplicate measurements is available for datapoints # 61634, #61635</li> </ul>	D
		A
II-o SDB	No parameter variation is indicated.	D

### 3.2 Criteria III

Only the entries for Am, Np, Se and Th classified as reliable are being considered for criteria III. All unreliable entries, or entries where classification according to criteria I and II could not be completed, are excluded. Entries for Cs are not included in this analysis because the final cation concentration would have to be estimated or calculated in most cases before a meaningful comparison can be done.

#### 3.2.1 Evaluation of data for americium

The following entries are evaluated in this section; the respective data are shown in Figure 3.2.1.

Reference	Data table	Solid phase
Baston et al.(1995b)	Am/2	tuff
Ikeda and Amaya(1998)	Am/9	tuff
Tanaka and Muraoka(1998)	Am/12	tuff
Tanaka et al.(1998)	Am/13	tuff

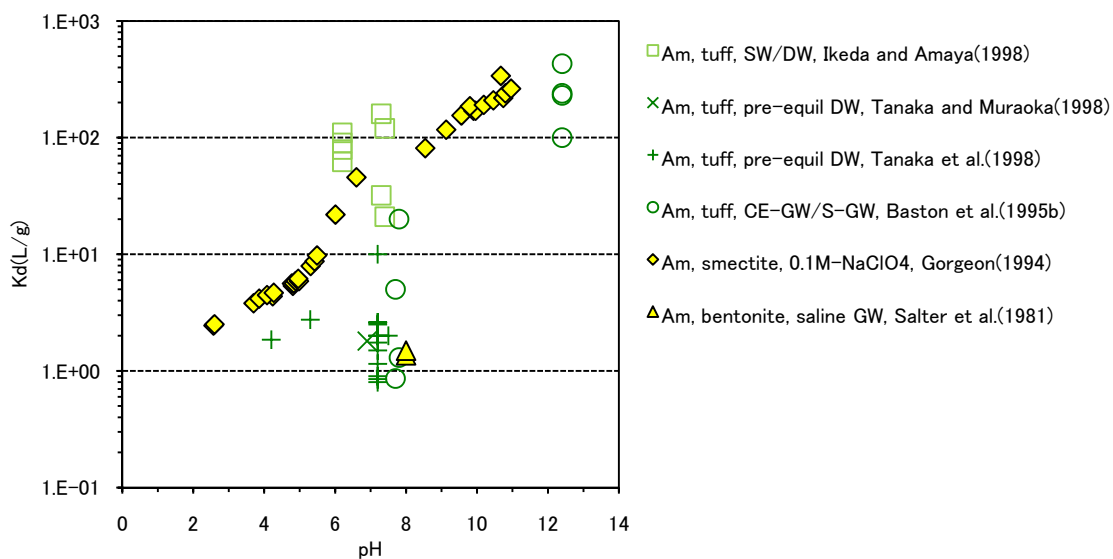


Figure 3.2.1 Overview of sorption data for Am on tuff. For comparison, sorption data for Am on smectite and bentonite are also shown. SW = seawater, DW = distilled water, CE-GW = concrete-equilibrated ground water, S-GW = synthetic ground water, GW = ground water.

Figure 3.2.1 summarizes the data for the sorption of Am on tuff, with those on smectite and bentonite. The  $K_d$  values measured by Tanaka et al. (1998) and Baston et al. (1995b) show a fairly clear trend of increasing  $K_d$  with increasing pH, which is consistent with the trend for smectite. The variation of  $K_d$  data observed at pH around 7 in Tanaka et al. (1998) can be explained by the difference of ionic strength. Considering the differences of experimental conditions, all  $K_d$  values of Am for tuff are evaluated as

being consistent with each other, and with the data for smectite and bentonite. Although the detailed mineralogical compositions of the tuff samples are not known, it can be assumed that tuff often contains clay minerals such as smectite as weathering products, resulting in the consistent sorption behavior.

### 3.2.2 Evaluation of data for selenium

The following entries are evaluated in this section; the respective data are shown in Figure 3.2.2.

Reference	Data table	Solid phase
Barney(1982)	Se/1	tuff
Shibutani et al. (1994)	Se/4	tuff

Figure 3.2.2 shows the available data for Se(IV)/Se(VI) sorption on tuff and related minerals (clay minerals and Fe minerals). Although  $K_d$  values lie in wide ranges, a fairly clear trend of decreasing  $K_d$  with increasing pH was found. It is difficult to evaluate because of lack of detailed information on the mineralogy of the tuff for both Shibutani et al. (1994) and Barney (1982), but they are approximately consistent with each other. As discussed in Shibutani et al. (1994), comparison of pH dependencies between tuff and its constituent minerals suggests that Fe minerals such as Fe-oxyhydroxide and pyrite contribute to sorption behavior of Se on tuff. Assuming that the data for granodiorite by Sato et al. (1997) refer to Se(IV), it would seem reasonable that the minerals in granodiorite have a lower sorption capacity for anions than tuff.

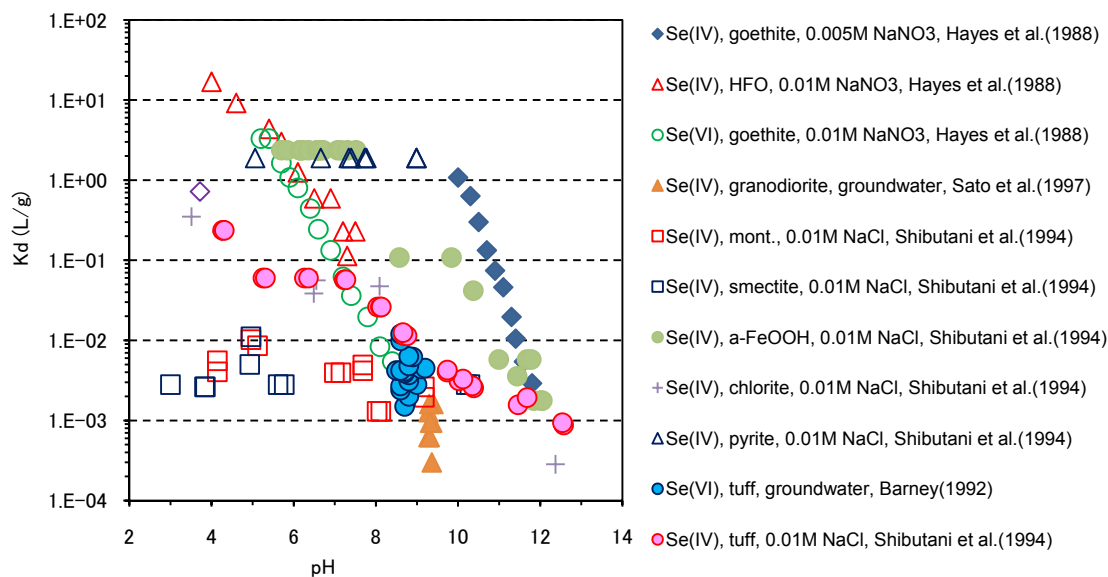


Figure 3.2.2 Overview of sorption data for Se on tuff. For comparison, sorption data for goethite, HFO and granodiorite are also shown. HFO = hydrous ferric oxide. Mont. = montmorillonite

### 3.2.3 Evaluation of data for thorium and neptunium

The following entries are evaluated in this section; the respective data are shown in Figure 3.2.3.

Reference	Data table	Solid phase
Ueta et al.(1999)	Th/5	tuff
Baston et al.(1997) and Berry et al.(2007)	Np/2	tuff

Figure 3.2.3 shows the available data for Th(IV)/Np(IV) sorption on tuff and related minerals (clay minerals and Fe minerals). It is noted that  $K_d$  values for tuff of Th(IV) by Ueta et al. (1999) and Np(IV) by Baston et al. (1997, 1999) are fairly consistent, and are similar with those on granodiorite and bentonite, reported by same authors. In comparison with the  $K_d$  values of Th on pure montmorillonite (SWy-1) obtained by Bradbury and Baeyens (2003) and those on goethite by Hunter et al. (1988), relatively low sorption on tuff has been observed for Th and for Np(IV). In all these cases, solution chemistry had been relatively complex as well as mineralogy of tuff samples, including presumably significant concentrations of carbonate, silicate, etc. Because the influence of such ligands on Th sorption is not known precisely, due to the lack of systematic sorption data, these data cannot be evaluated conclusively according to Criterion III, but they appear to be consistent among each other.

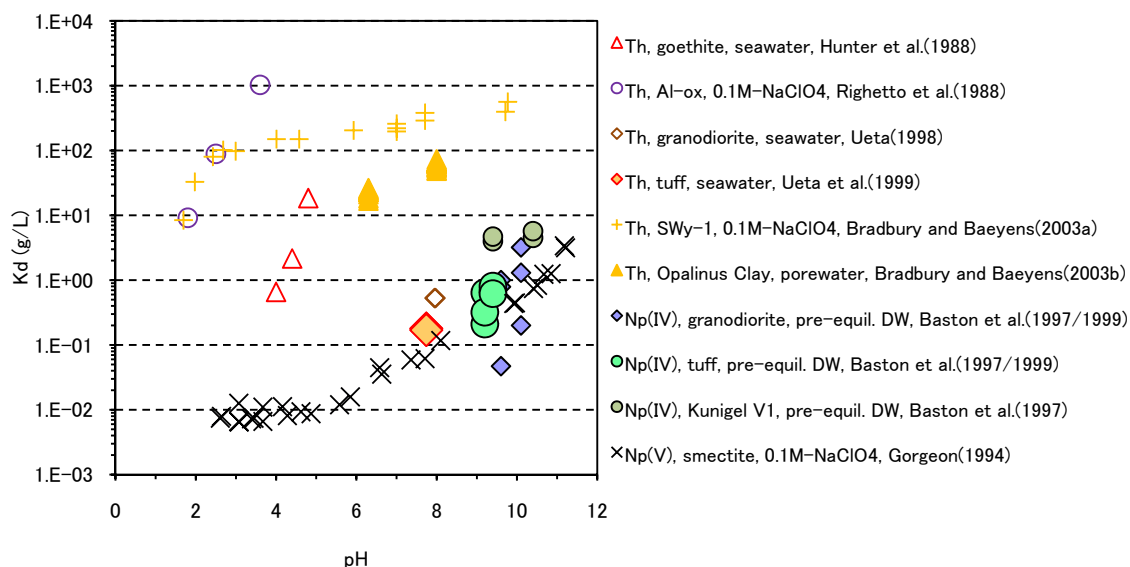


Figure 3.2.3 Overview of sorption data for Th and Np(IV) on tuff. For comparison, sorption data for Th and Np(IV), as well as for Am on metal oxide minerals, granitic rocks, various clays and clay minerals are also shown. DW = distilled water, GW = ground water, SBPW = synthetic bentonite porewater.

#### 4. Summary

The QA/classification of selected entries in the JAEA-SDB, focusing tuff existing widely in geological environment, was done following the approach/guideline defined in our previous report. As a result, the reliability of 560  $K_d$  values was evaluated and classified. The QA/classification for about 27.8 % for all  $K_d$  data (56.2 % for 5 key nuclides- Am, Cs, Np, Se, Th) in JAEA-SDB has been completed.

Based on the results of the fourth application of classification guideline to  $K_d$  data for tuff system (1st-bentonite, 2nd-mudstone, 3rd-granite), some conclusions can be drawn;

- The classification guideline allows a suitable classification of the  $K_d$  values on the basis of the completeness of documented key information and the quality of the underlying experimental methods and conditions.
- The classification scheme made it possible to obtain quick overview of the available data, and to provide suitable access to the respective  $K_d$  values for the PA-related  $K_d$ -setting.
- Finally, JAEA-SDB including QA information should be repeatedly tested through the application to various rocks and geochemical conditions, for example, sandstone and basaltic rocks.

## References

The notation of reference is according to JAEA-SDB reference, considering relation with JAEA-SDB.

- Azuma, J. , Shibata, M. , Yui, M. , Shibutani, T. , Notoya, S. and Yoshikawa, H. :  
 “Solubility and Speciation of Radioactive Elements of High-level Radioactive Waste Disposal System”, JNC Technical Report, JNC TN 8400 99-071 (1999) (in Japanese).
- Ashida, T. , Shibutani, T, Sato, H. , Tachi, Y. , Kitamura, A. and Kawamura, K. :  
 “Nuclide Migration Study in the QUALITY -Data Acquisitions for the Second Progress Report-”, JNC Technical Report, JNC TN8400 99-083 (1999) (in Japanese).
- Barney, G. S. : “Radionuclide Sorption on Basalt-Interbed Materials FY 1981 Annual Report”, BASALT WASTE ISOLATION PROJECT, RHO-BW-ST-35P (1982).
- Baston, G. M. N. , Berry, J. A. , Bond, K. A. , Boulton, K. A. and Linklater, C. M. : “Effects of cellulosic degradation products concentration on actinide sorption on tuffs from the Borrowdale Volcanic Group, Sellafield, Cumbria”, *Radiochim. Acta*, vol. 66/67, pp. 437-442 (1984).
- Baston, G. M. N. , Berry, J. A. , Brownsword, M. , Heath, T. G. , Tweed, C. J. and Williams, S. J. : “Sorption of Plutonium and Americium on Repository, Backfill and Geological Materials Relevant to the JNFL Low-Level Radioactive Waste Repository at Rokkasho-Mura”, *Mat. Res. Soc. Symp. Proc.*, vol. 353, pp. 957-964 (1995).
- Baston, G. M. N. , Berry, J. A. , Brownsword, M. , Heath, T. G. , Ilett, D. J. , Tweed, C. J. and Yui, M. : “The Effect of Temperature on the Sorption of Technetium, Uranium, Neptunium and Curium on Bentonite, Tuff and Granodiorite”, *Materials Research Society Symposia Proceedings*, vol.465, pp.805-812 (1997).
- Baston, G. M. N. ,Berry, J. A. ,Brownword, M., Cowper, M. M., Haworth, A., Heath, T. G., Ilett, D. J., McCrohon, R., Tweed and C.J. : “Sorption Studies of Radioelements on Geological Materials”, AEAT-3142(Revised), AEA Technology plc (1998).
- Berry, J. A. , Yui, M. and Kitamura, A. : “Sorption Studies of Radioelements on Geological Materials”, JAEA Technical Report, JAEA-Research 2007-074 (2007).
- Bradbury, M. H. and Baeyens, B. : “Near-field sorption data bases for compacted MX-80 bentonite for performance assessment of high-level radioactive waste repository in Opalinus Clay host rock”, *Nagra Technical*

- Report, Nagra NTB 02-18 (2003a).
- Bradbury, M. H. and Baeyens, B. : “Far-field sorption data bases for performance assessment of high-level radioactive waste repository in Opalinus Clay host rock”, Nagra Technical Report, Nagra NTB 02-19 (2003b).
- Conca, J. L. and Triay, I. R. : “Validity of Batch Sorption Data to Describe Selenium Transport through Unsaturated Tuff”, LA-12957-MS (1996).
- Daniels, W. R. , Wolfsberg, K. , Rumborg, R. S. , Ogaard, A. E. , Kerrisk, J. F. , Duffy, C. J. , Newton, T. W. , Thompson, J. L. , Bayhurst, B. P. , Bish, D. L. , Blacic, J. D. , Crowe, B. M. , Erdal, B. R. , Griffith, J. F. , Knight, S. D. , Lawrence, F. O. , Rumborg, V. L. , Skyes, M. L. , Thompson, G. M. , Travis, B. J. , Treher, E. N. , Vidale, R. J. , Walter, G. R. , Aguilar, R. D. , Cisneros, M. R. , Maestas, S. , Mitchell, A. J. , Oliver, P. Q. , Raybold, N. A. and Wanek, P. L. : “Summary Report on the Geochemistry of Yucca Mountain and Environs”, LA-9328-MS (1982).
- Erdal, B. R. , Daniel, W. R. , Hoffman, D. C. , Lawrence, F. O. and Wolfsberg, K. : “Sorption and migration of radionuclides in geologic media”, Mat. Res. Sym. Proc., vol.1, pp. 423-426 (1978).
- Erdal, B. R. : “Laboratory Studies of Radionuclide Distributions Between Selected Groundwaters and Geologic Media”, LA-8088-PR, LA-UR--80-437 (1980).
- Gorgeon, L. : “Contribution a la Modelisation Physico-Chimique de la Retention de Radioelements a via Longue par des Materiaux Argileux”, THESE de DOCTORAT de l'UNIVERSITE PARIS 6 (1994).
- Hayes, K. F. , Papelis, C. and Leckie, J. O. : “Modeling Ionic Strength Effects on Anion Adsorption at Hydrous Oxide/ Solution Interfaces”, J. Colloid and Interface Science, vol.125, No.2, pp. 717-726 (1988).
- Hummel, W. , Berner, U. , Curti, E. , Pearson, F. J. and Thoenen, T. : “Chemical thermodynamic data base (01/01)”, Universal Publishers, Parkland, Florida (2002).
- Hunter K. A. , Hawke D. J. , Choo L. K. : “Equilibrium Adsorption of Thorium by Metal Oxides in Marine Electrolytes”, Geochimica et Cosmochimica Acta, vol.52, pp. 627-636 (1988).
- Ikeda, T. and Amaya, T. : “Model Development of Chemical Evolution in Repository Vol.II Acquisition of Nuclide Migration Data in Near-Field”, PNC TJ 1281 98-003 (1998) (in Japanese).
- Ishii, T. , Inagawa, S. , Gunji, Y. , Skamoto, Y. , Takabe, S. , Ogawa, H. and Sasaki, T. : “Measurement of distribution coefficients for uranium series radionuclides under shallow land environment condition (I)”, Journal of Nuclear Fuel cycle



- and Environment, Atomic Energy Society of Japan, vol.8, no.1, pp. 55-63 (2001).
- Maclean, S. C. , Coles, D. G. and Weed, H. C. : “The Measurement of Sorption Ratios for Selected Radionuclides on Various Geologic Media”, UCID-17928 (1978).
- Meijer, A. , Triay, I. , Knight, S. and Cisneros, M. : “Sorption of Radionuclides on Yucca Mountain Tuffs”, Proceedings of the Topical Meeting on Nuclear and Hazardous Waste Management, pp.113-117 (1990).
- Meyer, R. E. , Arnold, W. D. , Case, F. I. , O'Kelly, G. D. O. and Land, J. F. : “Effects of Mineralogy on Sorption of Strontium and Cesium onto Calico Hills Tuff”, NUREG/CR—5463 (1990).
- Nakayama, S. , Moriyama, H. , Arimoto, H. and Higashi, K. : “Distribution Coefficients of Americium, Neptunium and Protoactinium for Selected Rocks”, The Memoris of the Faculth of Engineering, Kyoto University, vol.48, No.3, pp.275-283 (1986).
- NEA : “Using Thermodynamic Sorption Models for Guiding Radioelement Distribution Coefficient ( $K_d$ ) Investigations – A Status Report”. OECD/NEA, Paris (2001).
- NEA : “NEA Sorption Project. Phase II: Interpretation and Prediction of Radionuclide Sorption onto Substrates relevant for Radioactive Waste Disposal using Thermodynamic Sorption Models”. By Davis, J., Ochs, M., Olin, M., Payne, T., Tweed, C., OECD/NEA, Paris (2005).
- Ochs, M. , Saito, Y. , Kitamura, A. , Shibata, M. , Sasamoto, H. and Yui, M. : “Evaluating and categorizing the reliability of distribution coefficient values in the sorption database”, JAEA Technical Report, JAEA-Technology 2007-011 (2007).
- Ochs, M. , Kunze, S. , Saito, Y. , Kitamura, A. , Tachi, Y. and Yui, M. : “Application of the sorption database to  $K_d$ -setting for Horonobe rocks”, JAEA Technical Report, JAEA-Research 2008-017 (2008).
- Ochs, M. and Kunze, S. : “Revised Technical Report. Classification of selected entries of the JNC-SDB. Proposal for use of SDB and data acquisition.  $K_d$  setting for Th and Cs in Horonobe rocks. Data entry for Cs/MX-80 in the JNC-DDB”, Technical report for JAEA, 31 March 2008, BMG Engineering Ltd., Schlieren-Zurich, Switzerland, (2008).
- Ochs, M. , Suyama, T. , Kunze, S. , Tachi, Y. and Yui, M. : “Evaluating and categorizing the reliability of distribution coefficient values in the sorption database(3)”, JAEA Technical Report, JAEA-Data/Code 2009-021 (2010).
- Park, C. K. , Woo, S. I. , Tanaka, T. and Kamiyama, H. : “Sorption and Desorption Behavior of  $^{60}\text{Co}$ ,  $^{85}\text{Sr}$  and  $^{137}\text{Cs}$  in a Porous Tuff -Mechanisms and Kinetics-“, Journal of Nuclear Science and Technology, vol.29, No.12, pp. 1184-1193 (1992).
- Rai, D. , Rao, L. , Weger, H. T. , Felmy, A. R. , Choppin, G. R. and Yui, M. :

- “Thermodynamic data for predicting concentrations of Pu(III), Am(III), and Cm(III) in geologic environments”, JNC TN8400 99-010 (1999).
- Righetto L. , Bidoglio G. , Marcandalli B. , Bellobono I. R. : “Surface Interactions of Actinides with Alumina Colloids”, *Radiochimica Acta*, vol.44/45, pp.73-75 (1988).
- Rogers, P. S. Z. and Meijer, A. : “Dependence of Radionuclide Sorption on Sample Grading Surface Area, and Water Composition”, *High Level Radioactive Waste Management*, vol.2, pp.1509-1516 (1993).
- Saito, Y. , Ochs, M. , Jintoku, T. , Suyama, T. , Shibata, M. , Sasamoto, H. and Yui, M. : “Development of guideline for evaluating and categorizing the reliability of distribution coefficient values in the JNC sorption database”, JNC Technical Report, JNC TN8410 2005-011 (2005) (in Japanese).
- Saito, Y. , Ochs, M. , Suyama, T. , Kitamura, A. , Shibata, M. , Sasamoto, H. : “An update of the sorption database: Correction and addition of published literature data”, JAEA Technical Report, JAEA-Data/Code 2007-014 (2007) (in Japanese).
- Saito, Y. , Ochs, M. , Kunze, S. , Kitamura, A. , Tachi, Y. and Yui, M. : “Evaluating and categorizing the reliability of distribution coefficient values in the sorption database (2)”, JAEA Technical Report, JAEA-Technology 2008-018 (2008).
- Salter, P. F. , Ames, L. L. and McGarrah, J. E. : “Sorption of Selected Radionuclides on Secondary Minerals Associated with the Columbia River Basalts”, RHO-BWI-LD-43 (1981).
- Sato, H. , Shibutani, T. , Tachi, Y. , Ota, K. , Amano, K. and Yui, M. : “Diffusion Behavior of Nuclides Considering Pathways in Fractured Crystalline Rocks”, PNC Technical Report, PNC TN8410 97-127 (1997).
- Shibutani, T. , Nishikawa, Y. , Inui, S. , Uchidate, N. and Yui M. , : “Study of Adsorption of Selenium onto Rocks and Minerals”, PNC Technical Report, PNC TN8410 94-395 (1994) (in Japanese).
- Shibutani, T. , Shibata, M. and Suyama, T. : “Sorption Database of Radionuclides on Bentonite and Rocks”, JNC TN8410 99-050 (1999) (in Japanese).
- Suyama, T. and Sasamoto, H. : “A renewal of the JNC-Sorption database (JNC-SDB): Addition of literature data published from 1998 to 2003”, JNC Technical Report, JNC TN8410 2003-018 (2004) (in Japanese).
- Tachi, Y. , Shibutani, T. and Yoshikawa, H. : “Sorption Behavior of Neptunium on Rocks under Reducing Conditions”, JAEA Technical Report (2010) (in preparation).
- Tachi, Y. , Tochigi, Y. , Suyama, T. , Ochs, M. and Yui, M. : “Development of the sorption and diffusion database system for safety assessment of geological disposal”, JAEA Technical Report, JAEA-Data/Code 2008-034 (2009) (in Japanese).

- Tanaka, T. and Muraoka, S. : “Distribution Coefficients of TRU-Nuclides in Natural Barriers;Influence of Size of Colloidal Species”, Japan Atomic Energy Research Institute, JAERI-Research 98-017 (1998) (in Japanese).
- Tanaka, T. and Muraoka, S. : “Sorption Characteristics of <sup>237</sup>Np, <sup>238</sup>Pu and <sup>241</sup>Am in Sedimentary Materials”, Journal of Radioanalytical and Nuclear Chemistry, vol.240, No.1, pp. 177-182 (1999).
- Tanaka, T. , Takebe, S. , Ogawa, H. and Muraoka, S. : “Distribution Coefficients of <sup>237</sup>Np and <sup>241</sup>Am in Sedimentary Geological Formation”, Japan Atomic Energy Research Institute, JAERI-Research 98-018 (1998) (in Japanese).
- Thomas, K. W. : “Summary of Sorption Measurements Performed with Yucca Mountain, Nevada, Tuff Samples and Water from Well J-13”, LA-10960-MS (1987).
- Ueta, S. : “Development of Database System for Performance Assessment(III)”, JNC TJ1211 98-001 (1998) (in Japanese).
- Ueta, S. , Kato, H. , Kurosawa, S and Nakazawa, T. : “Development of Database System for Performance Assessment(III)”, JNC TJ8400 99-032 (1999) (in Japanese).
- Vine, E. N. , Aguilar, R. D. , Bayhurst, B. P. , Daniels, W. R. , DeViliers, S. J. , Erdal, B. R. , Lawrence, F. O. , Naestae, S. , Oliver, P. O. , Thompson, J. L. and Wolfsberg, K. : “Sorption-Desorption Studies on tuff. II. A Continuation of Studies with Samples from Jackass Flats, Nevada and Initial Studies with Samples from Yucca Mountain, Nevada”, Los Alamos National Laboratory report LA-8110-MS (1980b).
- Wolfsberg, K. , Bayhurst, B. P. , Crowe, B. M. , Daniels, W. R. , Erdal, B. R. , Lawrence, F. O. , Norris, A. E. and Smyth, J. R. : “Sorption-desorption studies on tuff: I. Initial studies with samples from the J-13 drill site, Jackass Flats, Nevada”, Los Alamos Scientific Laboratory Report, LA-7480-MS (1979).
- Wolfsberg, K. , Aguilar, R. D. , Bayhurst, B. P. , Daniels, W. R. , DeViliers, S. J. , Erdal, B. R. , Lawrence, F. O. , Maestas, S. , Mitchell, A. J. , et al. : “Sorption-desorption studies on tuff III. A continuation of studies with samples from Jackass Flats and Yucca Mountain, Nevada”, Los Alamos Scientific Laboratory Report, LA-8747-MS (1981).
- Yamamoto, T. , Takebe, S. , Ogawa, H. , Tanaka, T. , Mukai, M. , Komiya, T. , Yokomoto, S. and Wadac, T. : “Migration Behavior of Radionuclide in Soil Layer of Final Storage Site -Radionuclide Migration Test in Aerated Soil Layer by Precipitation-“, JAERI-M 89-189 (1989) (in Japanese).

This is a blank page.

Appendix  
Summary tables for  $K_d$  classification

This is a blank page.



JAEA-Data/Code 2010-026

Datapoint	Reference	I - Completeness of documentation and type of Kd		II - Technical and scientific quality of reported data														Rating II	comment/rating	Operator	Data	Classification Guideline			
		Rating ⇒ I-a: Yes/No, I-b: class 1-6		Checkpoints ⇒ level: A-D (numerical value: 3-0)/unreliable																					
		I-a.1	I-a.2	Rating I-a	Rating I-b	II-a	II-b	II-c	II-d	II-e	II-f	II-g	II-h	II-i	II-j	II-k	II-l						II-m	II-n	II-o
51114	Erdal (1980)	Yes	Yes	yes (can be used)	class 1	C/D	A)	A/B	C/D	A/B	A/B	C/D	A)	A)	C/D	C/D	C/D	B)	B)	unreliable	N.E.	C. Gantner/M. Ochs, BMG	March 2010	Revision 4b (May 19, 2005)	Am/8









# 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 <sup>2</sup>
体積	立方メートル	m <sup>3</sup>
速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	m/s <sup>2</sup>
波数	毎メートル	m <sup>-1</sup>
密度, 質量密度	キログラム毎立方メートル	kg/m <sup>3</sup>
面積密度	キログラム毎平方メートル	kg/m <sup>2</sup>
比体積	立方メートル毎キログラム	m <sup>3</sup> /kg
電流密度	アンペア毎平方メートル	A/m <sup>2</sup>
磁界の強さ	アンペア毎メートル	A/m
量濃度 <sup>(a)</sup> , 濃度	モル毎立方メートル	mol/m <sup>3</sup>
質量濃度	キログラム毎立方メートル	kg/m <sup>3</sup>
輝度	カンデラ毎平方メートル	cd/m <sup>2</sup>
屈折率 <sup>(b)</sup>	(数字の)	1
比透磁率 <sup>(b)</sup>	(数字の)	1

(a) 量濃度 (amount concentration) は臨床化学の分野では物質濃度 (substance concentration) ともよばれる。  
 (b) これらは無次元量あるいは次元1をもつ量であるが、そのことを表す単位記号である数字の1は通常は表記しない。

表3. 固有の名称と記号で表される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 <sup>(b)</sup>	rad	1 <sup>(b)</sup>	m/m
立体角	ステラジアン <sup>(b)</sup>	sr <sup>(c)</sup>	1 <sup>(b)</sup>	m <sup>2</sup> /m <sup>2</sup>
周波数	ヘルツ <sup>(d)</sup>	Hz		s <sup>-1</sup>
力	ニュートン	N		m kg s <sup>-2</sup>
圧力, 応力	パスカル	Pa	N/m <sup>2</sup>	m <sup>-1</sup> kg s <sup>-2</sup>
エネルギー, 仕事, 熱量	ジュール	J	N m	m <sup>2</sup> kg s <sup>-2</sup>
仕事率, 工率, 放射束	ワット	W	J/s	m <sup>2</sup> kg s <sup>-3</sup>
電荷, 電流量	クーロン	C		s A
電位差 (電圧), 起電力	ボルト	V	W/A	m <sup>2</sup> kg s <sup>-3</sup> A <sup>-1</sup>
静電容量	ファラド	F	C/V	m <sup>-2</sup> kg <sup>-1</sup> s <sup>4</sup> A <sup>2</sup>
電気抵抗	オーム	Ω	V/A	m <sup>2</sup> kg s <sup>-3</sup> A <sup>-2</sup>
コンダクタンス	ジーメンズ	S	A/V	m <sup>-2</sup> kg <sup>-1</sup> s <sup>3</sup> A <sup>2</sup>
磁束	ウェーバ	Wb	Vs	m <sup>2</sup> kg s <sup>-2</sup> A <sup>-1</sup>
磁束密度	テスラ	T	Wb/m <sup>2</sup>	kg s <sup>-2</sup> A <sup>-1</sup>
インダクタンス	ヘンリー	H	Wb/A	m <sup>2</sup> kg s <sup>-2</sup> A <sup>-2</sup>
セルシウス温度	セルシウス度 <sup>(e)</sup>	°C		K
光照度	ルーメン	lm	cd sr <sup>(c)</sup>	cd
放射線量	ルクス	lx	lm/m <sup>2</sup>	m <sup>-2</sup> cd
放射線種の放射能 <sup>(f)</sup>	ベクレル <sup>(d)</sup>	Bq		s <sup>-1</sup>
吸収線量, 比エネルギー分与, カーマ	グレイ	Gy	J/kg	m <sup>2</sup> s <sup>-2</sup>
線量当量, 周辺線量当量, 方向線量当量, 個人線量当量	シーベルト <sup>(g)</sup>	Sv	J/kg	m <sup>2</sup> s <sup>-2</sup>
酸素活性化	カタール	kat		s <sup>-1</sup> mol

(a) SI接頭語は固有の名称と記号を持つ組立単位と組み合わせても使用できる。しかし接頭語を付した単位はもはやコヒーレントではない。  
 (b) ラジアンとステラジアンは数字の1に対する単位の特別な名称で、量についての情報をつたえるために使われる。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である数字の1は明示されない。  
 (c) 測光学ではステラジアンという名称と記号srを単位の表し方の中に、そのまま維持している。  
 (d) ヘルツは周期現象についての、ベクレルは放射性核種の統計的過程についてのみ使用される。  
 (e) セルシウス度はケルビンの特別な名称で、セルシウス温度を表すために使用される。セルシウス度とケルビンの単位の大きさは同一である。したがって、温度差や温度間隔を表す数値はどちらの単位で表しても同じである。  
 (f) 放射性核種の放射能 (activity referred to a radionuclide) は、しばしば誤った用語で"radioactivity"と記される。  
 (g) 単位シーベルト (PV,2002,70,205) についてはCIPM勧告2 (CI-2002) を参照。

表4. 単位の中に固有の名称と記号を含む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
粘力のモーメント	パスカル秒	Pa s	m <sup>-1</sup> kg s <sup>-1</sup>
表面張力	ニュートンメートル	N m	m <sup>2</sup> kg s <sup>-2</sup>
角速度	ニュートン毎メートル	N/m	kg s <sup>-2</sup>
角加速度	ラジアン毎秒	rad/s	m m <sup>-1</sup> s <sup>-1</sup> =s <sup>-1</sup>
熱流密度, 放射照度	ラジアン毎秒毎秒	rad/s <sup>2</sup>	m m <sup>-1</sup> s <sup>-2</sup> =s <sup>-2</sup>
熱容量, エントロピー	ワット毎平方メートル	W/m <sup>2</sup>	kg s <sup>-3</sup>
比熱容量, 比エントロピー	ジュール毎ケルビン	J/K	m <sup>2</sup> kg s <sup>-2</sup> K <sup>-1</sup>
比エネルギー	ジュール毎キログラム毎ケルビン	J/(kg K)	m <sup>2</sup> s <sup>-2</sup> K <sup>-1</sup>
熱伝導率	ジュール毎キログラム	J/kg	m <sup>2</sup> s <sup>-2</sup>
体積エネルギー	ワット毎メートル毎ケルビン	W/(m K)	m kg s <sup>-3</sup> K <sup>-1</sup>
電界の強さ	ジュール毎立方メートル	J/m <sup>3</sup>	m <sup>3</sup> kg s <sup>-2</sup>
電荷密度	ボルト毎メートル	V/m	m kg s <sup>-3</sup> A <sup>-1</sup>
表面電荷	クーロン毎立方メートル	C/m <sup>3</sup>	m <sup>3</sup> s A
電束密度, 電気変位	クーロン毎平方メートル	C/m <sup>2</sup>	m <sup>2</sup> s A
誘電率	クーロン毎平方メートル	C/m <sup>2</sup>	m <sup>2</sup> s A
透磁率	ファラド毎メートル	F/m	m <sup>3</sup> kg <sup>-1</sup> s <sup>4</sup> A <sup>2</sup>
モルエネルギー	ヘンリー毎メートル	H/m	m kg s <sup>-2</sup> A <sup>-2</sup>
モルエントロピー, モル熱容量	ジュール毎モル	J/mol	m <sup>2</sup> kg s <sup>-2</sup> mol <sup>-1</sup>
照射線量 (X線及びγ線)	ジュール毎モル毎ケルビン	J/(mol K)	m <sup>2</sup> kg s <sup>-2</sup> K <sup>-1</sup> mol <sup>-1</sup>
吸収線量率	クーロン毎キログラム	C/kg	kg <sup>-1</sup> s A
放射線強度	グレイ毎秒	Gy/s	m <sup>2</sup> s <sup>-3</sup>
放射線輝度	ワット毎ステラジアン	W/sr	m <sup>3</sup> m <sup>-2</sup> kg s <sup>-3</sup> =m <sup>2</sup> kg s <sup>-3</sup>
酵素活性濃度	ワット毎平方メートル毎ステラジアン	W/(m <sup>2</sup> sr)	m <sup>2</sup> m <sup>-2</sup> kg s <sup>-3</sup> =kg s <sup>-3</sup>
	カタール毎立方メートル	kat/m <sup>3</sup>	m <sup>3</sup> s <sup>-1</sup> mol

表5. SI接頭語

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

表6. SIに属さないが、SIと併用される単位

名称	記号	SI単位による値
分	min	1 min=60s
時	h	1 h=60 min=3600 s
日	d	1 d=24 h=86 400 s
度	°	1°=(π/180) rad
分	'	1'=(1/60)°=(π/10800) rad
秒	"	1"=(1/60)'=(π/648000) rad
ヘクタール	ha	1 ha=1 hm <sup>2</sup> =10 <sup>4</sup> m <sup>2</sup>
リットル	L, l	1 L=1 l=1 dm <sup>3</sup> =10 <sup>3</sup> cm <sup>3</sup> =10 <sup>-3</sup> m <sup>3</sup>
トン	t	1 t=10 <sup>3</sup> kg

表7. SIに属さないが、SIと併用される単位で、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単位で表される数値
電子ボルト	eV	1 eV=1.602 176 53(14)×10 <sup>-19</sup> J
ダルトン	Da	1 Da=1.660 538 86(28)×10 <sup>-27</sup> kg
統一原子質量単位	u	1 u=1 Da
天文単位	ua	1 ua=1.495 978 706 91(6)×10 <sup>11</sup> m

表8. SIに属さないが、SIと併用されるその他の単位

名称	記号	SI単位で表される数値
バール	bar	1 bar=0.1 MPa=100 kPa=10 <sup>5</sup> Pa
水銀柱ミリメートル	mmHg	1 mmHg=133.322 Pa
オングストローム	Å	1 Å=0.1 nm=100 pm=10 <sup>-10</sup> m
海里	M	1 M=1852 m
バイン	b	1 b=100 fm <sup>2</sup> =(10 <sup>-12</sup> cm) <sup>2</sup> =10 <sup>-28</sup> m <sup>2</sup>
ノット	kn	1 kn=(1852/3600) m/s
ネーパ	Np	SI単位との数値的な関係は、対数量の定義に依存。
ベベル	B	
デジベル	dB	

表9. 固有の名称をもつCGS組立単位

名称	記号	SI単位で表される数値
エルグ	erg	1 erg=10 <sup>-7</sup> J
ダイン	dyn	1 dyn=10 <sup>-5</sup> N
ポアズ	P	1 P=1 dyn s cm <sup>-2</sup> =0.1 Pa s
ストークス	St	1 St=1 cm <sup>2</sup> s <sup>-1</sup> =10 <sup>-4</sup> m <sup>2</sup> s <sup>-1</sup>
スチルブ	sb	1 sb=1 cd cm <sup>-2</sup> =10 <sup>-4</sup> cd m <sup>-2</sup>
ファ	ph	1 ph=1 cd sr cm <sup>-2</sup> 10 <sup>4</sup> lx
ガル	Gal	1 Gal=1 cm s <sup>-2</sup> =10 <sup>-2</sup> ms <sup>-2</sup>
マクスウェル	Mx	1 Mx=1 G cm <sup>2</sup> =10 <sup>-8</sup> Wb
ガウス	G	1 G=1 Mx cm <sup>-2</sup> =10 <sup>-4</sup> T
エルステッド <sup>(c)</sup>	Oe	1 Oe ≐ (10 <sup>3</sup> /4π) A m <sup>-1</sup>

(c) 3元系のCGS単位系とSIでは直接比較できないため、等号「≐」は対応関係を示すものである。

表10. SIに属さないその他の単位の例

名称	記号	SI単位で表される数値
キュリー	Ci	1 Ci=3.7×10 <sup>10</sup> Bq
レントゲン	R	1 R=2.58×10 <sup>-4</sup> C/kg
ラド	rad	1 rad=1 cGy=10 <sup>-2</sup> Gy
レム	rem	1 rem=1 cSv=10 <sup>-2</sup> Sv
ガンマ	γ	1 γ=1 nT=10 <sup>-9</sup> T
フェルミ	f	1 f=1 fm=10 <sup>-15</sup> m
メートル系カラット		1メートル系カラット=200 mg=2×10 <sup>-4</sup> kg
トル	Torr	1 Torr=(101 325/760) Pa
標準大気圧	atm	1 atm=101 325 Pa
カロリ	cal	1 cal=4.1868 J (「15°C」カロリ), 4.1868 J (「IT」カロリ), 4.184 J (「熱化学」カロリ)
マイクロン	μ	1 μ=1 μm=10 <sup>-6</sup> m

