

Evaluating and Categorizing the Reliability of Distribution Coefficient Values in the Sorption Database(2)

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March 2008

Japan Atomic Energy Agency

日本原子力研究開発機構

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(Received January 18, 2008)

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

The JNC-SDB includes more than 24,000 K_d data which have a great variety of K_d and related experimental information from many different literatures. Accordingly, the quality assuring (QA) and classifying criteria for K_d has been developed in order to evaluate the reliability of each K_d value. The reliability of K_d values for bentonite system has been already evaluated.

In this report, the QA/classification of selected entries in the JNC-SDB, especially of K_d values for mudstone systems to use in the K_d -derivation exercise for Horonobe rocks, was done following the approach defined in our previous report. As a result, the reliability of 1,056 K_d values was evaluated and classified with numerical rating. 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 , Classification, Reliability, HLW Disposal

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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 (2)

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

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(2008 年 1 月 18 日受理)

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

JNC-SDB に登録されている K_d は 24,000 データを超え、膨大な文献データから収集された様々な条件での幅広い K_d データと関連する実験条件等の情報が含まれている。このため、各々の K_d データの信頼性を評価するため、 K_d の品質確認とクラス分けの手法の開発を進めてきた。また、この手法に基づき、ベントナイト系の K_d データを対象に信頼性評価を行った結果を既に報告した。

本報告書においては、JNC-SDB に含まれる K_d データのうち、特に幌延岩石を対象にした K_d 設定検討への活用を念頭に、泥岩系の K_d データを主な対象として、前報告書にて設定した手法に従って信頼性評価を行った。その結果、1,056 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集を速やかに抽出し、 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。

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1. Introduction

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

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

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

As part of this on-going development program, a project to classify the entries in the JNC-SDB according to defined QA-criteria has been started. The JNC-SDB includes more than 24,000 K_d data which have a great variety of K_d and related experimental information from many different literatures. Accordingly, the quality assuring (QA) and classifying criteria for K_d has been developed in order to evaluate the reliability of each K_d value (Saito et al., 2005). The reliability of K_d values for bentonite system has been already evaluated (Ochs et al., 2007).

In this report, the QA/classification of selected entries in the JNC-SDB, especially of K_d values for mudstone systems to use in the K_d -derivation exercise for Horonobe rocks (Ochs et al., 2008), was done following the approach defined in our previous report. The K_d values for the sorption of Th, Np, Se, Cs, Pu and Am on mudstone, bentonite and related minerals.

In the chapter 2, the QA criteria and classification scheme defined in our previous report (Ochs et al., 2007) are described. And in the chapter 3, classifications of selected entries for mudstone and related minerals in the JNC-SDB are described by each item. In the appendix, the details of the evaluation and classifications for the selected entries of the SDB are listed.

2. Reliability of JNC-SDB: Classification Guideline

2.1 Introduction, description of main criteria

The reliability of K_d values in the JNC-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 JNC-SDB. Criteria Ia and Ib are related to documentation and data entry, whereas the technical and scientific quality of an entry is addressed by criteria II and III.

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 criterion II below.
- b) This point takes also into account that the reliability of data input to the JNC-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) ratio values given, which significantly increases the likelihood of an operator error during data input.

II Quality of reported data

This is the most important issue from a technical and scientific point of view. This criterion 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.

III Consistency of data:

While the previous two main criteria address the reliability of each K_d entry in the JNC-SDB, criterion 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 JNC-SDB. However, the classification of data entries in the JNC-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 criterion

2.2.1 General

Each entry in the JNC-SDB (each K_d value identified in the JNC-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 Criterion 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 to 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 Ia.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 criterion II. In addition to the information listed under Ia.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 Ib.

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 Criterion II: Technical and scientific quality of reported data

It is generally assumed that the entries presently contained in the JNC-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 SiO₂, 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 JNC-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_d 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_d 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_d 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_d 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 O₂ (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 JNC-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 JNC-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-O₂ 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 O₂ (e.g., by performing experiments in a N₂ 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 pCO₂. 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 Solid/water ratio (S/W) 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 m² 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 S/W 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 μm) 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 JNC-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 S/W), 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 S/W 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_2 or O_2 , 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, S/W, 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 pCO_2 (edge), or e.g. $[\text{Na}]$ in case of ion exchange, are varied systematically.
- B) Either RN concentration (isotherm) and/or chemical parameters, such as pH or pCO_2 (edge), or e.g. $[\text{Na}]$ 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 Criterion 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 criterion 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 criterion 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.
- Criterion 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. Criterion I-b is then used to assign classes 1-6 for documentation.
- Criterion II:
 - a) The datasets that pass Criterion 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 Criterion 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 Criterion II.

checkpoint	description	weighting factor
II-a	solid phase (substrate)	A-C/D × 2
* II-b	pH	A-D × 8
* II-c	redox conditions	A/B-C/D × 8
* II-d	final solution composition	A/B-C/D × 8
II-e	temperature	A/B-C/D × 1
II-f	S/W, grain size	A/B-C/D × 2
II-g	sorption value	A-C/D × 2
* II-h	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 Criterion 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

- Criterion III: Criterion 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 Criterion II as the main basis for assessing the reliability of entries in the JNC-SDB

Table 2.3.3 The classification system

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

3 Classification of selected entries for mudstone and related minerals in the JNC-SDB

This section presents the classification results for selected entries in the JNC-SDB covering the datasets for the sorption of Th, Np, Se, Se, Pu and Am on mudstone and related minerals that were mainly used for the K_d -setting exercise discussed in Ochs et al.(2008).

- 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 Criterion 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, criterion 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, criterion III was evaluated as well.

3.1 Criteria I and II

Data table Element/#: REF: original reference		
JNC-SDB version # – DATA: element/solid sorbent, datapoint #		
GUIDELINE: Revision # (date)		
Checkpoint ¹ "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_d 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 (S/W) 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

¹ Application of the checkpoint to the information given in the JNC-SDB is indicated with "SDB".
"REF" indicates the additional application to the original reference indicated in each table.

3.1.1. Thorium

Data table Th/1: REF: Lieser et al. (1990) JNC-SDB version 2 – DATA: Th/Mudstone, # 56105-56107 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 REF	It is indicated that the distribution between size fractions is used for calculation of K_d values. It is a linear graph with indication of relative concentrations c/c_0 of Th in percent in the effluent groundwater (c_0 = total initial conc. of Th in the groundwater).	class 4
II-a SDB REF	It is indicated that Elster glacial sediment (specific surface area: 0.003) and Weichsel glacial sediment (specific surface area: 0.01) has been used. No mineral composition is available, only the chemical compositions of the sediments are listed in a table.	C/D
II-b SDB	Initial and final pH-values are given.	A
II-c SDB	It is indicated that all groundwaters and sediments are kept under 99% argon and 1% carbon dioxide. Th is not redox sensitive.	A/B
II-d SDB REF	It is indicated that solutions are low and medium salinity groundwaters. The final solution compositions after equilibration with the corresponding sediments are listed in a table. The concentrations are given for unfiltered, 0.45 μm filtered and ultrafiltered groundwater solutions.	A/B
II-e SDB	Temperature is not specified.	C/D
II-f SDB	A solution/solid ratio of 2.5 mL/g is indicated. 100 g solid are added to 250 mL solution.	A/B
II-g SDB	Based on the information given in the SDB, and on a solution/solid ratio of 2.5 mL/g, sorption values between 97.4-99.5 % sorbed can be calculated. <ul style="list-style-type: none"> Datapoints 56105, 56107 Datapoint 56106 	C/D B
II-h SDB REF	The initial Th concentrations are reported to be 1.0×10^{-11} M in all three groundwaters: Based on thermodynamic calculations with PHREEQC Interactive 2.12.5 (database: JNC-TDB_011213c2 and NAGRA-PSI) for the groundwaters G1,	A

		G8 and G9 the indicated initial [Th] is below the calculated solubility limits: <i>Calculated solubility limits for ThO₂ in mol/kg</i>													
		<table><tr><td></td><td>JNC-TDB_011213c2</td><td>NAGRA-PSI</td></tr><tr><td>G1 a) unfiltered</td><td>2.44 × 10⁻⁷</td><td>2.57 × 10⁻⁷</td></tr><tr><td>G8 a) unfiltered</td><td>1.87 × 10⁻⁶</td><td>1.97 × 10⁻⁶</td></tr><tr><td>G9 a) unfiltered</td><td>1.11 × 10⁻⁶</td><td>1.20 × 10⁻⁶</td></tr></table>			JNC-TDB_011213c2	NAGRA-PSI	G1 a) unfiltered	2.44 × 10 ⁻⁷	2.57 × 10 ⁻⁷	G8 a) unfiltered	1.87 × 10 ⁻⁶	1.97 × 10 ⁻⁶	G9 a) unfiltered	1.11 × 10 ⁻⁶	1.20 × 10 ⁻⁶
	JNC-TDB_011213c2	NAGRA-PSI													
G1 a) unfiltered	2.44 × 10 ⁻⁷	2.57 × 10 ⁻⁷													
G8 a) unfiltered	1.87 × 10 ⁻⁶	1.97 × 10 ⁻⁶													
G9 a) unfiltered	1.11 × 10 ⁻⁶	1.20 × 10 ⁻⁶													
		The calculated solubility limits agree with the solubility data given in Rai et al. (1999).													
II-i	REF	Samples are analyzed without filtration, after filtration through membrane filters (Millipore) of 0.45 µm pore size and after ultrafiltration through filter sets (Millipore Immersible CX-30) of 0.002 µm pore size. Sorption values from the different methods are similar.	A												
II-j	SDB	It is indicated that a contact time of 14 days had been used.	C/D												
II-k	REF	Sufficient mixing had been achieved, considering the relatively long reaction time. For mixing the closed reaction vessels are slowly turned over head (1 revolution / 3 min.).	A/B												
II-l	SDB	Only one datapoint is available for each groundwater.	C/D												
II-m	REF	No description of reaction vessels is available. However, a sufficient amount of sediment (400 g/L) is used in the experiments and therefore no correction for vessel walls is necessary in case of all experiments.	B												
II-n	SDB	No repeated sampling is done and no uncertainties are reported.	D												
II-o	SDB	Only one datapoint is available for each groundwater.	D												

Data table Th/2: REF: Legoux et al. (1992)		
JNC-SDB version 2 – DATA: Th/Mudstone, # 56055		
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	It is indicated that tables with K _d are given.	class 1
II-a SDB	The solid phase is indicated as soil A. The mineralogical composition and specific surface of the sample are given in a table.	A
II-b SDB	Initial and final pH is indicated.	A
II-c SDB	It is indicated that no redox conditions are reported.	

	REF	No reducing agents are added to the experiment and no inert gas atmosphere is reported. Therefore it is assumed that the experiment is conducted under ambient conditions. Thorium is not redox sensitive.	A/B
II-d	REF	The final solution composition is reported.	A/B
II-e	SDB	It is indicated that no temperature is reported.	C/D
II-f	SDB	A L/S ratio of 10:1 (10 mL/1 g) is indicated.	A/B
	REF	A specific surface area (BET) of 8.6 m ² /g is reported. The grain sizes of the sample is between 150 and 500 µm.	
II-g	SDB	Based on the information given in the SDB, a sorption value of 99.99 %-sorbed can be calculated.	C/D
II-h	SDB	An initial Th concentration of 4×10 ⁻¹¹ M is indicated.	A
	REF	Based on the solubility data given in Rai et al. (1999), the experiments are considered to be undersaturated with respect to ThO ₂ (s) by a factor of 5 or more.	
II-i	SDB	Centrifugation and ultrafiltration with 0.025 and 0.002 µm Millipore filters is reported. Centrifugation is done at 4000 rpm prior to filtration.	A
II-j	SDB	It is indicated that contact time is 2 days.	C/D
II-k	REF	Samples are agitated continuously.	A/B
II-l	SDB	No variation of initial [Th] or S/W has been carried out.	C/D
II-m	REF	The experiments are carried out in polypropylene vessels. It is reported that sorption to the vessel wall has been corrected for. No information about the correction procedure is available. It is assumed that the correction is based on the data obtained of a blank experiment.	C/D
II-n	REF	The reported error represents the standard deviation of the average of at least four experimental repetitions.	A
II-o	SDB	No parameter variation is indicated.	D

Data table Th/3: REF: Östhols (1995)

JNC-SDB version 2 – DATA: Th/Other minerals, # 57172-57220

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	It is indicated that tables with % sorption are given.	class 2
II-a	SDB	It is indicated that SiO ₂ (Aerosil OX200) had been used.	A
II-b	SDB	Final pH-values are given.	A
II-c	REF	It is indicated that during all titrations water-saturated N ₂ is bubbled through the solutions. Th is not redox sensitive.	A/B
II-d	SDB	It is indicated that solutions consisted of 0.1 M and 1.0 M NaClO ₄ . Due to the simplicity of the given solutions, the final solution composition can be estimated.	A/B
II-e	SDB	It is indicated that a temperature of $25 \pm 0.6^{\circ}\text{C}$ had been used.	A/B
II-f	SDB	The BET surface area is indicated to be 169.3 m ² /g. Rating is done based on the calculated surface area of the added sorbent indicated. In all cases it is $> 5 \text{ m}^2$.	A/B
II-g	SDB	Rating is done based on %-sorbed values calculated from the information given in the JNC-SDB: <ul style="list-style-type: none"> Datapoints 57199, 57205, 57208, 57209, 57213, 57219 (<1.7%, > 98.88%) All other datapoints (between 5.09%- 93.4%) 	C/D A
II-h	SDB	The following initial Th concentrations are indicated: <ul style="list-style-type: none"> 0.1 M NaClO₄: initial [Th] = $3.45 \times 10^{-6} \text{ M}$ 1.0 M NaClO₄: initial [Th] = $1.00 \times 10^{-6} \text{ M}$ $3.18 \times 10^{-6} \text{ M}$ $6.33 \times 10^{-6} \text{ M}$ $3.00 \times 10^{-5} \text{ M}$ $3.16 \times 10^{-6} \text{ M}$ <p>Based on the solubility data given in Rai et al. (1999), initial [Th] in the experiments with 0.1 M and 1.0 M NaClO₄ at the indicated acidic pH values are far below the solubility limit given by ThO₂(s).</p>	A
II-i	SDB	It is indicated that all samples had been centrifuged for 20 min. at 19000 rpm.	B
II-j	SDB	It is indicated that a contact time of at least 24 hours had been used.	C/D
II-k	REF	For mixing, the samples are shaken for at least 24 hours.	A/B
II-l	SDB	[Th] and the S/W have been varied.	B
II-m	REF	Experiments are performed in glass vessels. A blank titration is made using an appropriate [Th]. At a pH of 3.5 the losses to vessel walls are around 20%. Information about a possibly performed correction is not available.	C/D

II-n	REF	It is indicated that forward (alkaline direction) and reverse titration had been performed. The corresponding uncertainties of % adsorbed Th are given as error bars in a graph.	B
II-o	SDB	Distribution ratios are determined for six Th concentrations; pH is also varied (sorption edge).	A

Data table Th/4: REF: Bradbury & Baeyens (2003)* JNC-SDB version 2 – DATA: Th/Na-SWy1 montmorillonite, # 67039-67054 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: The literature was classified assuming the same experimental conditions as described in Lauber et al. (2000) and Baeyens and Bradbury (1997)			
Checkpoint		Evaluation	Rating
I-a.1	REF	All mandatory fields are completed.	Yes
I-a.2	REF	All mandatory information is provided.	Yes
I-b	REF	A sorption edge graph with logarithmic K_d values is given.	class 5
II-a	REF	Purified Na-SWy1 montmorillonite with determined mineralogical composition and characteristics is used for the experiments.	A
II-b	REF	Final pH-values are measured.	A
II-c	REF	Experiments are carried out in an inert atmosphere glove box ($\text{CO}_2 < 10^{-5.5}$ bar). Th is not redox sensitive.	A/B
II-d	REF	A 0.1 M NaClO_4 -solution is used.	A/B
II-e	REF	It is not specified at which temperature experiments had been performed. It is assumed that experiments had been made at ambient temperature.	C/D
II-f	REF	Enough solid had been added to each vessel (0.42 g/L).	A/B
II-g	REF	Rating is done based on %-sorbed values calculated from sixteen K_d -values (pH-range 1-12) out of the sorption edge graph. Sorption values are in the range of 78% and 99.5%. <ul style="list-style-type: none"> Datapoints: 67039, 67040, 67043 Datapoints: 67041, 67042, 67044, 67046 Datapoints: 67045, 67047-67054 	A B C/D
II-h	REF	The initial Th concentration is reported to be $< 10^{-9}$ M. According to the data of Rai et al. (1999), in a pH range of 1-8.5, the reported Th concentration is below the solubility limit. Datapoints above pH 8.5 are close or above the solubility limit and are	B unreliable

		considered as unreliable.	
II-i	REF	It is reported that samples had been centrifuged for 60 min. at 95,000g max.	B
II-j	REF	Only one reaction time is reported.	C/D
II-k	REF	For mixing the samples, the tubes are shaken end-over-end for 7 days.	A/B
II-l	REF	No variation in [Th] or the S/W is indicated. A sorption isotherm on MX-80 bentonite is reported. However these data are not considered for the classification of Th on Swy1 montmorillonite.	C/D
II-m	REF	Experiments are performed in polyethylene vessels. A maximum uncertainty in the log K_d values of ~0.05 log units due to wall sorption is indicated.	A
II-n	REF	Estimates of the maximum error in each operation in similar batch sorption tests to those performed in Lauber et al. (2000) have been done.	C
II-o	REF	Experiments are performed with constant [Th] at various pH values.	B

Data table Th/5: REF: Meier et al. (1994)

JNC-SDB version 2 – DATA: Th /Mudstone, # 62232 – 62236

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: it is indicated that no information on initial and final pH, final solution composition, phase separation, initial and final Eh and atmosphere/ redox condition are given.	No
REF	No further information is available. Thorium is not redox sensitive.	unreliable

Data table Th/6: REF: Ishii et al. (2001)

JNC-SDB version 2 – DATA: Th /Mudstone, # 65701 – 65704

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	Tables with K_d are given.	class 1
II-a SDB	The solid phase is reported as loam(I) and loam(II). Physico- chemical properties and specific surface of loams are given in a table.	A
II-b SDB	Initial pH values are reported. Final pH values are not reported.	C

II-c	SDB	It is reported that experiments are done under atmosphere and controlled atmosphere. Also, Th is not a redox-sensitive element.	A/B
II-d	SDB	The final chemical properties of spring and synthesized rain water are reported.	A/B
II-e	SDB	A temperature of 15°C is reported.	A/B
II-f	SDB REF	Solution/solid ratios are reported for 50mL/1g or 100mL/1g. A specific surface area (BET) of 99.5 or 43.9 m ² /g are reported.	A/B
II-g	SDB	Based on the information given in the SDB, and on a solution/solid ratio of 100ml/g, sorption values between 98.7%- 99.9% sorbed can be calculated.	C/D
II-h	SDB REF	The initial Th concentrations are reported to be 8.0×10^{-8} M, 4.3×10^{-7} M, 8.6×10^{-7} M. Based on thermodynamic calculations with CHESS (Chemical Equilibrium with Species and Surface, database: Yamaguchi JAERI-Data/Code 2000-031, 2000), the indicated initial [Th] is below the calculated solubility limits (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Th).	B
II-i	SDB	The membrane filtration with pore size of 0.45μm is used.	C/D
II-j	SDB REF	It is indicated that contact time is 14 days. This reaction time is reasonably long. The kinetics of sorption is not tested.	C/D
II-k	REF	The batch sorption experiments are continuously performed by shaking (50rpm). And handshakes are performed once a day.	A/B
II-l	REF	[Th] and the W/S have been varied.	B
II-m	REF	The experiments are carried out in polypropylene or Teflon. The sorption on vessel wall has been determined as lower than 5% than the actual value and thus corrections for sorption on vessel wall have not been performed.	B
II-n	SDB	Uncertainties are reported (n=3). -)Datapoints: 65701, 65702, 65704 Uncertainties are not reported. -)Datapoint: 65703	A D
II-o	SDB	The initial pH and initial Th concentration are varied.	B

3.1.2 Neptunium

Data table Np/1: REF: Lieser and Mühlenweg (1988) JNC-SDB version 2 – DATA: Np/Mudstone, # 56095 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	It is indicated that K_d values are tabulated.	class 1
II-b SDB	Both initial and final pH values are indicated.	A
II-c SDB REF	Reducing conditions and initial and final Eh values are indicated. As additional information it is indicated that Np(V) is reduced to Np(IV) during groundwater circulation (column experiment). Original redox potentials of the groundwaters are reported to be between -100 mV and + 200 mV. The original concentration of molecular oxygen is indicated to be < 0.06 mmol/L. All experiments under anaerobic conditions are performed in inert gas boxes filled with a mixture of 99% Ar and 1% CO ₂ . The oxygen content in these inert gas boxes is reported to be between 0.02 and 0.05%. Eh and pH are continuously monitored during the experiments. No reducing agent is reported. Final amount of Np(IV) is determined by extraction with TTA in xylene.	C/D
II-d SDB REF	Natural groundwater is indicated as input solution; final solution compositions are provided. K_d values of seven different natural groundwaters are reported. All groundwaters are characterized.	A/B
II-h SDB REF	The initial Np concentration is indicated to be 4.0×10^{-9} M in groundwater G7. Based on calculations with PHREEQC-2.12.5 (databases: JNC-TDB_011213c2 and NAGRA-PSI) for the indicated groundwater, the initial [Np(IV)] is above the calculated solubility limits. In addition, the calculated data indicate that the main species is Np(V) given the reported Eh of 80 mV. Apparent sorption due to the formation of sparingly soluble species of Np(IV) that are precipitated and held back by the sediments is reported. The formation of colloids and precipitate lead to erroneous K_d values.	unreliable

Data table Np/2: REF: Barney and Anderson (1979) JNC-SDB version 2 – DATA: Np /Mudstone, # 44274 – 44279 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: it is indicated that no information on final solution composition is given.	No
REF	No further information is available. The initial composition of groundwater is not reported. The final solution composition can not be estimated.	unreliable

Data table Np/3: REF: Barney and Brown (1979) JNC-SDB version 2 – DATA: Np /Mudstone, # 44340 – 44342 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: it is indicated that no information on final solution composition, Eh (and pH) at beginning or end of the experiments, experimental redox/atmosphere conditions and the initial RN concentration are given.	No
REF	No further information is available. The initial composition of groundwater is not reported. The final solution composition can not be estimated.	unreliable

Data table Np/4: REF: Berry et al. (1990a) JNC-SDB version 2 – DATA: Np /Mudstone, # 48144 – 48172 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: it is indicated that no information on Eh at beginning or end of the experiments and contact time are given.	No
REF	No further information is available.	unreliable

Data table Np/5: REF: Higgo et al.(1987) JNC-SDB version 2 – DATA: Np /Mudstone, # 53249 – 53260 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: it is indicated that no information on final solution composition, Eh at beginning or end of the experiments and contact time are given.	No
REF	No further information is available.	unreliable

Data table Np/6: REF: Kim et al. (1994) JNC-SDB version 2 – DATA: Np /Mudstone, # 53968 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: it is indicated that no information on separation and final solution composition are given.	No
REF	No further information is available.	unreliable

Data table Np/7: REF:Legoux et al.(1992) JNC-SDB version 2 – DATA: Np /Mudstone, # 56023 – 56026 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	Tables with K_d are given.	class 1
II-a SDB	Four soils with known mineral composition are indicated. CEC value and specific surface area are reported.	A
II-b SDB	Initial and final pH values are indicated.	A
REF	No use of any pH-buffer is reported.	
II-c SDB	It is indicated that no redox conditions are reported. There is no information about Eh. Experiments are carried out with Np (V).	C/D
REF	No reducing agents are added to the experiment and no inert gas atmosphere is reported. Therefore it is assumed that the experiment is conducted under	

		ambient conditions.	
II-d	REF	The final solution composition is reported.	A/B
II-e	SDB	A temperature is not reported.	C/D
II-f	SDB REF	Solution/solid ratio is 10mL/g. The used mass of 1g soil (A, B, C, D) has a surface area of about 6.6 to 14.7m ² .	A/B
II-g	SDB	The sorption value is between 43.18% and 85.61% (calculated with W/S and K _d values).	A
II-h	SDB REF	Initial [Np] is 5.0×10 ⁻¹² M. Based on speciation calculations (for 25° C) with PHREEQC using the thermodynamic data in JNC-TDB the initial [Np] are below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Np).	B
II-i	SDB	The centrifugation is performed at 4000rpm followed by ultrafiltration through 0.025 and 0.002µm Millipore filters is indicated.	A
II-j	SDB	A reaction time of 2 days is indicated.	C/D
II-k	REF	Agitation is carried out in reaction time.	A/B
II-l	REF	No isotherms, no variation of the Np concentration is indicated.	C/D
II-m	REF	The experiments are carried out in polypropylene vessels. It is reported sorption to the vessel wall has been corrected for. No information about the correction procedure is available. It is assumed that the correction is based on the data obtained of a blank experiment.	C/D
II-n	REF	The reported error represents the standard deviation of the average of at least four experimental repetitions.	A
II-o	REF	No parameter variation is indicated.	D

Data table Np/8: REF: Mackenzie et al.(1983)

JNC-SDB version 2 – DATA: Np /Mudstone, # 56147 – 56150

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: it is indicated that no information about final solution composition is given.	No
REF	No further information is available.	unreliable

Data table Np/9: REF: Sakamoto et al. (1990) JNC-SDB version 2 – DATA: Np /Mudstone, # 58697 –58703 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 REF	It is indicated that K_d values are scanned from a graphical presentation. The K_d –axis is in logarithmic form.	class 5
II-a SDB REF	The solid phase is TAKADATE loam which is hydrated halloysite 40% and quartz 60%. It is reported that CEC is measured between pH 2 and 10 by NH_4^+ ion saturation (Wada and Okada, 1977). Specific surface area is not reported. The loam contains a small amount of colored minerals such as mica, olivine and feldspar.	B
II-b SDB	Ranges (1 pH-unit) of final pH values are given.	B
II-c SDB REF	There is no information about Eh. The experiment is conducted under atmospheric conditions. Experiments are carried out with Np(V). No reducing agents are added to the experiment and no inert gas atmosphere is reported.	A/B
II-d REF	The initial composition is indicated. The final solution composition is not reported.	C/D
II-e SDB	Temperatures of 30°C are reported.	A/B
II-f SDB REF	Solution/solid ratios are 100mL/g. Solid masses of 0.05g are added to a liquid volume of 5 mL.	C/D
II-g SDB	Based on the information given in the JNC-SDB, all sorption values are calculated to lie in the range 18.37- 87.50% sorbed.	A
II-h SDB REF	An initial [Np] of 1.0×10^{-5} M is indicated. Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the experiments are considered to be below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Np).	B
II-i SDB	The phase separation is carried out by centrifugation of 3000g for 20 min.	C/D
II-j SDB	A reaction time of 7 days is indicated.	C/D
II-k REF	Samples are shaken for 7 days at 30°C. This reaction time is reasonably long.	A/B
II-l REF	No variation is indicated for either W/S or [Np].	C/D
II-m REF	The loam is added to the solution in polyethylene container. The experiments without loam are also carried out to examine whether neptunium adsorbs to	A

		the container wall.	
II-n	REF	Error of K_d is not reported, no replicated are performed.	D
II-o	REF	Only pH is varied.	C

Data table Np/10: REF: Sakamoto (1994) JNC-SDB version 2 – DATA: Np /Mudstone, # 58718 – 58731 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 REF	It is indicated that K_d values are scanned from a graphical presentation. A linear graph % sorbed K_d are provided.	class 4
II-a	SDB REF	It is reported that CEC is measured 10-30 meq/100g. Specific surface area is reported to 130m ² /g. The solid phase is TAKADATE loam which is hydrated halloysite 40% and quartz 60%. The loam contains a small amount of colored minerals such as mica, olivine and feldspar.	B
II-b	SDB	Ranges (0.5 or 1 pH-unit) of final pH values are given.	B
II-c	SDB REF	It is indicated that no redox conditions are reported. There is no information about Eh. Experiments are carried out with Np(V). No reducing agents are added to the experiment and no inert gas atmosphere is reported. Therefore it is assumed that the experiment is conducted under ambient conditions.	A/B
II-d	REF	The initial composition is indicated in Sakamoto et al. (1990). The final solution composition is not reported.	C/D
II-e	SDB	Temperatures of 30°C are reported.	A/B
II-f	SDB REF	Solution/solid ratios are 100mL/g. Solid masses of 0.05g are added to a liquid volume of 5 mL.	C/D
II-g	SDB	Based on the information given in the SDB, all sorption values are calculated to lie in the range 15.97-85.07% sorbed.	A
II-h	SDB REF	An initial [Np] of 6.0×10^{-6} M is indicated. Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the experiments are considered to be below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Np).	B

II-i	SDB	The phase separation is carried out by centrifugation of 3000g for 20 min.	C/D
II-j	SDB	A reaction time of 7 days is indicated. This reaction time is reasonably long.	C/D
II-k	REF	Samples are shaken for 7 days at 30°C.	A/B
II-l	REF	No variation is indicated for either W/S or [Np].	C/D
II-m	REF	The loam is added to the solution in polyethylene container. The experiments without loam are also carried out to examine whether neptunium adsorbs to the container wall.	A
II-n	REF	Error of K_d is not reported, no replicate is performed.	D
II-o	REF	Only pH is varied.	C

Data table Np/11: REF: Tachi et al. (1999a) JNC-SDB version 2 – DATA: Np /Mudstone, # 59864 – 59893 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	K_d is given in tabular form.	class 1
II-a	SDB	CEC and specific surface area are not reported.	C/D
	REF	The solid phase is mudstone which is product at TOMAI in Miyagi prefecture. Information about mineral composition and chemical composition are given.	
II-b	SDB	Initial as well as final pH are given.	A
	REF	HCl or NaOH are used to adjust pH.	
II-c	SDB	Initial and final Eh values are indicated. It is further indicated that 0.01M $\text{Na}_2\text{S}_2\text{O}_4$ is used as reducing agent. Experiments are performed under Ar (O_2 : <1ppm). The oxidation state of Np is not indicated. The initial oxidation state of Np is not given.	C/D
II-d	REF	The major initial solution composition is reported (Na^+ , SiO_2 , Fe, SO_4^{2-}).	C/D
II-e	SDB	Temperatures of 25°C are reported.	A/B
II-f	SDB	Solution/solid ratios are 50mL/g.	A/B
	REF	Solid masses of 2g are added to a liquid volume of 100mL.	
II-g	SDB	The %-sorbed can be calculated with K_d and W/S ratio: -) Datapoints 59864-59866, 59879-59881: between 89.1% and 91.5% is sorbed -) Datapoints 59867-59869, 59883-59884: between 97.5% and 97.9% is sorbed	A B

		-) Datapoints 59870-59878, 59882, 59885-59893: between 98.0% and 99.8% is sorbed	C/D
II-h	SDB REF	An initial [Np] of 2.0×10^{-9} M is indicated. Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the experiments are considered to be below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Np).	B
II-i	SDB	The phase separation is carried out by filtration with 10000 MWCO membranes.	B
II-j	SDB	A reaction time of 1, 7, 14, 21 and 35 days are indicated. Similar results are obtained with 14, 21 and 35 days. -) Datapoints: 59864-59869, 59879-59887 -) Datapoints: 59870-59878, 59888-59893	C/D A/B
II-k	REF	Samples are shaken for 1, 7, 14, 21 and 35 days at 30°C.	A/B
II-l	REF	No variation is indicated for either W/S or [Np].	C/D
II-m	REF	The mudstone is added to the solution in Teflon container. The experiments without mudstone are also carried out to examine whether neptunium adsorbs to the container wall.	A
II-n	REF	Error of K_d is not reported. 3 replicates are performed.	D
II-o	REF	It is indicated that contact time and Eh are varied.	B

Data table Np/12: REF: Tanaka and Muraoka (1999)

JNC-SDB version 2 – DATA: Np /Mudstone, # 62312 - 62314

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
II-h SDB REF	An initial [Np] of 1.62×10^{-3} M is indicated. Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the experiments are considered to be above the solubility limit.	unreliable

Data table Np/13: REF: Tanaka and Muraoka (1998) JNC-SDB version 2 – DATA: Np /Mudstone, # 62353 - 62355 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	Tables with K_d are given.	class 1
II-a SDB	CEC and chemical composition are reported about the ando soil, yellowish soil and reddish soil.	B
REF	Humic substance and humic acid are reported. Surface area are not reported.	
II-b SDB	Initial pH values and final pH values (as range < 1 pH unit) are reported.	B
II-c SDB	It is reported that experiments are done under air; i.e., under oxidizing conditions.	A/B
II-d SDB	Physico-chemical properties of the equilibrated solution are reported.	A/B
II-e SDB	A temperature of 25°C is reported.	A/B
II-f SDB	Solution/solid ratio is 20mL/g.	A/B
REF	The used mass of 0.5g soil is added to liquid volumes (de-ionized water) of 10mL. It is assumed that enough solid had been added to each vessel.	
II-g SDB	The sorption value is between 14.53% and 67.74% (calculated with W/S and K_d values).	A
II-h SDB	An initial [Np] of 1.62×10^{-4} M is indicated.	B
REF	Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the experiments are considered to be below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Np).	
II-i SDB	The 5000MWCO filters are used for phase separation.	A
II-j SDB	A reaction time of 7 days is indicated.	A/B
REF	Identical (similar) results are obtained with different reaction times (>48 hours).	
II-k REF	The sample is shaking for 7 days.	A/B
II-l REF	No isotherms, no variation of the Np concentration is indicated.	C/D
II-m REF	The reaction vessel is made from teflon. Corrections for sorption on vessel walls are not mentions.	B
II-n SDB	Error of K_d is not reported, no replicated are performed.	D
II-o REF	Only pH (end) is varied.	C

Data table Np/14: REF: Tanaka et al. (1999) JNC-SDB version 2 – DATA: Np /Mudstone, # 62805 - 62809 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: it is indicated that no information on phase separation is given.	No
REF	No further information is available.	unreliable

Data table Np/15: REF: El-Naggar et al. (2000) JNC-SDB version 2 – DATA: Np /Mudstone, # 63027 - 63046 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: it is indicated that no information on Eh, contact time, initial Np concentration and final solution composition are given.	No
REF	No further information is available. The Eh is not a sensitive parameter for Cs, but the phase separation method and final solution composition are key points which are missing in the reference.	unreliable

Data table Np/16: REF: Kitamura et al. (2001) JNC-SDB version 2 – DATA: Np /Bentonite, # 65073 – 65107 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	Tables with K_d are given.	class 1
II-a SDB	The solid phase is reported as a purified Na-Smectite. The bentonite sample of Kunipia-F(Kunimine Industries Co.), which is commercially purified from Kunigel-V, is used as a starting material for purification of smectite.	A
II-b SDB	Final pH values are reported.	A
II-c SDB	Experiments are performed under N_2 . The oxidation state of Np is indicated as +IV or +V. Final Eh values are provided, as well as the reducing agent used	

REF	(0.01M Na ₂ S ₂ O ₄). Reagent of NaHCO ₃ is also added for ranging a total carbonate concentration from 0.09M to 1.0M. O ₂ levels are reportedly <1 ppm. A TTA-extraction method is applied to the determination of the oxidation state of neptunium.	C/D
II-d SDB	A NaCl and NaHCO ₃ are reported as input solution; final solution compositions are reported in the additional file “solution composition”.	A/B
II-e SDB	A temperature of 22 ± 3°C is reported.	A/B
II-f SDB	A solution/solid ratio of 100 mL/g is reported. 0.2 g solid are added to 20 mL solution. From Shibutani et al.(1999), the BET (outer) surface areas are 50 - 58 m ² /g for a purified Na-Smectite.	A/B
II-g SDB	Based on the information given in the JNC-SDB, and on a solution/solid ratio that may range from 100 mL/g, sorption values between 1.3 - 72.9 % sorbed can be calculated. <ul style="list-style-type: none"> • Datapoints 65073-65088, 65090, 65092- 65103, 65105-65107 • Datapoints 65089, 65091 • Datapoint 65104 	A B C/D
II-h SDB REF	Initial Np concentration is 1.0×10 ⁻⁶ M. Based on calculations (Kitamura and Tomura, 2003) using the thermodynamic data (in JNC-TDB and OECD/NEA-TDB) and the data given in Yamaguchi et al.(1991) as a function of pH and dissolved carbonate concentration , it is estimated that initial Np concentration is considered to be below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Np).	B
II-i SDB	10000MWCO filters are used for phase separation. This method is considered to be efficient for removal of colloids.	B
II-j SDB	It is reported that contact time is 16 or 42 days for different datapoints. Similar results are obtained with different reaction times.	A/B
II-k REF	The Samples are gently shaken for 16 or 42 days (during the entire experiment) to attain sorption equilibrium.	A/B
II-l SDB	All experiments are presumably conducted at the same S/W and initial RN concentration.	C/D
II-m REF	The experiments are carried out in polypropylene tubes. And corrections for sorption on vessel walls have not been performed.	B
II-n SDB REF	No information is given with regard to errors. Error estimates are not reported. It is not clear, whether repeated sampling is done.	D

II-o SDB	Reaction time (16 days or 42days) and total carbonate concentration (from 0.09M to 1.0M) are varied.	B
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Data table Np/17: REF: Kitamura and Tomura (2003) JNC-SDB version 2 – DATA: Np /Bentonite, # 64869 – 64974 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	Tables with K_d are given.	class 1
II-a SDB	The solid phase is reported as a purified Na-Smectite. The bentonite sample of Kunipia-F(Kunimine Industries Co.), which is commercially purified from Kunigel-V, is used as a starting material for purification of smectite.	A
II-b SDB	Initial pH ranges and final pH values are reported.	A
II-c SDB REF	Experiments are performed under N_2 . The oxidation state of Np is reported as +IV or +V. Final Eh values are provided, as well as the reducing agent used ($0.01M Na_2S_2O_4$) or nothing. Reagent of $NaHCO_3$ is also added for ranging a total carbonate concentration from 0.04M to 1.0M. O_2 levels are reportedly <1 ppm. A TTA-extraction method is applied to the determination of the oxidation state of neptunium. -) Datapoints 64955 –64974 -) Datapoints 64869 –64954	A/B C/D
II-d SDB	$NaCl$ and $NaHCO_3$ are reported as input solution; main solution compositions are indicated in the additional file “solution composition”.	C/D
II-e SDB	A temperature of 25°C is reported.	A/B
II-f SDB REF	A solution/solid ratio of 100, 1000 and 20 mL/g are reported. 0.02g, 0.2g and 1 g solid are added to 20 mL solution. The 0.02g solid is not satisfactory for reproducibility and representativeness. From Shibutani et al.(1999), the BET (outer) surface areas are 50–58 m^2/g for a purified Na-Smectite. -) Datapoints 64869–64904, 64930–64974 -) Datapoints 64905–64929	A/B C/D
II-g SDB	Solution/solid ratios are reported; 20, 100 and 1000 mL/g, sorption values between 0.2 – 97.1 % sorbed can be calculated.	

	<ul style="list-style-type: none"> Datapoints: 64869, 64925, 64963 Datapoints: 64870–64924, 64926–64962, 64964–64972, 64974 Datapoints: 64973 	B A C/D
II-h SDB	<p>Initial Np concentration is 1.3×10^{-6} (in the presence of air), 1.3×10^{-7} and 6.3×10^{-8} M. Based on calculations (Kitamura and Tomura, 2003) using the thermodynamic data (in JNC-TDB and OECD/NEA-TDB) and the data given from Neck et al.(1992) in the presence of air, it is estimated that initial Np is at least five-fold below the solubility in the samples with pH <ca. 10(except the case in the presence of air).</p> <p>-) Datapoints: 64869–64954</p> <p>-) Datapoints: 64955–64974</p>	A B
II-i SDB	10000MWCO filters are used for phase separation. And membrane filtrations with pore size of $0.45 \mu\text{m}$ and 3000MWCO filters are partly used in order to compare with samples. There is the direct proof about absence of important colloid effects.	A
II-j SDB	It is indicated that contact time is 14, 15, 28, 29, 30, 92 or 156 days for different datapoints. Similar results are broadly obtained with different reaction times.	A/B
II-k REF	Samples are shaken by orbital shaker at 70 rpm for 14, 15, 28, 29, 30, 92 or 156 days (during the entire experiment).	A/B
II-l SDB	A limited variation of initial Np concentration has been used, including some experiments at trace concentrations.	B
II-m REF	The experiments are carried out in polypropylene tubes. And corrections for sorption on vessel walls have not been performed.	B
II-n SDB	<p>Uncertainties in K_d are derived based on duplicate experiments. Uncertainties in K_d of the case in the presence of air are derived based on experiments.</p> <p>-) Datapoints: 64869–64954</p> <p>-) Datapoints: 64955–64974</p>	A B
II-o SDB	Solid/water ratio, reaction time and total carbonate concentration are varied.	B

3.1.3 Selenium

Data table Se/1: REF: Ticknor et al. (1988) JNC-SDB version 2 – DATA: Se/Bentonite, # 60751-60759 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed	Yes
I-a.2 SDB REF	Separation of the samples is not reported. It is reported, that aliquots of the aqueous phases are taken for the radiometric analysis. Phase separation is performed by high-speed centrifugation (oral communication with T. T. Vandergraaf).	Yes
I-b SDB	A table with log K_d values is provided.	class 1
II-a SDB REF	As solid phase, Kaolinite is indicated and a detailed chemical composition of the mineral is available. Surface characteristics (CEC and specific surface area) are reported. It is reported that the Kaolinite is used as received from the supplier (KGa-1 from Source Clays Repository of the Clay Minerals Society, Columbia, Missouri).	A
II-b SDB REF	Initial as well as final pH values are reported. The solution pH is determined with litmus paper. No pH correction with buffer is performed after hydrazine addition.	B
II-c SDB	Redox conditions are reported for each experiment. Experiments are performed under aerobic conditions, under nitrogen and under reducing conditions (addition of hydrazine under nitrogen atmosphere). All experiments are conducted in pre-equilibrated systems. Initial and final Eh values are given in the SDB. <ul style="list-style-type: none"> • # 60753-60755 (aerobic conditions, Se(IV)) • # 60756-60758 (nitrogen atmosphere, Se(IV)) • # 60751, 60752 and 60759 (Se(-II), hydrazine, nitrogen atmosphere). Only one reducing agent is used. 	A/B A/B C/D
II-d SDB REF	As water type, 1%, 10% and 100% SCSSS (Standard Canadian Shield saline solution, synthetic brine) is indicated. Under reducing conditions, the solutions are 0.08 M in hydrazine. Final solution compositions are not given, but it is supposed that no essential	A/B

		changes take place with 10% and 100% SCSSS. Chlorite and muscovite are reported to be of high purity and final solution compositions with the reported S/W and 1% SCSSS can be estimated approximately.	C/D
II-e	SDB	A temperature of 22°C is indicated.	A/B
II-f	SDB REF	A liquid/solid ratio of 25 mL/g is indicated. It is reported that standard-scale experiments used 10 mL of solution and 0.4 g of solid.	A/B
II-g	SDB	The sorption value (calculated from K_d and S/W ratios) ranges from 25% to 68%.	A
II-h	SDB	Initial Se concentrations between 4.43×10^{-11} and 8.84×10^{-11} M are given. Based on speciation calculations (for 25°C) with PHREEQC 2.12.5 using the thermodynamic data in JNC-TDB_011213c2 the initial Se concentrations are below the solubility limit.	A
II-i	REF	It is indicated that no specific separation is reported. High-speed centrifugation of the samples is used for phase separation (oral communication with T. T. Vandergraaf).	B
II-j	SDB REF	A reaction time of 14 days is indicated. No further (kinetic) information is provided.	C/D
II-k	REF	The samples are intermittently agitated.	A/B
II-l	SDB	No variation in S/W or initial Se concentration is indicated.	C/D
II-m	REF	The experiments are carried out in polypropylene centrifuge tubes. Sorption on vessel walls is not tested and no corrections had been done.	C/D
II-n	REF	No error information is available.	D
II-o	SDB	Only the SCSSS salinity is varied.	C

Data table Se/2: REF: Ticknor et al. (1988)

JNC-SDB version 2 – DATA: Se/Other Minerals, # 60706-60714 (Se/Chlorite) and # 60760-60768 (Se/Muscovite)

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed	Yes
I-a.2 SDB REF	Separation of the samples is not reported. It is reported, that aliquots of the aqueous phases are taken for the radiometric analysis. Phase separation is performed by high-speed	

		centrifugation (oral communication with T. T. Vandergraaf).	Yes
I-b	SDB	A table with log K_d values is provided.	class 1
II-a	SDB	As solid phases, chlorite and muscovite are indicated and a detailed mineral composition is listed. Surface characteristics (CEC values and specific surface areas) are reported.	A
	REF	It is indicated that chlorite and muscovite are obtained as bulk mineral samples from Wards Natural Science Limited. The samples are further treated. It is indicated that chlorite and muscovite are of high purity.	
II-b	SDB	Initial as well as final pH values are indicated.	B
	REF	The solution pH is determined with litmus paper. No pH correction with buffer is performed after hydrazine addition.	
II-c	SDB	Redox conditions are reported for each experiment. Experiments are performed under aerobic conditions, under nitrogen and under reducing conditions with addition of hydrazine under nitrogen atmosphere. All experiments are conducted in pre-equilibrated systems. Initial and final Eh values are given in the JNC-SDB.	
		• # 60708, 60709, 60712, 60761, 60764, 60768 (aerobic conditions, Se(IV))	A/B
		• # 60707, 60710, 60714, 60760, 60765, 60767 (nitrogen atmosphere, Se(IV))	A/B
		• # 60706, 60711, 60713, 60762, 60763, 60766 (hydrazine, nitrogen atmosphere, Se(-II), only one reducing agent is indicated)	C/D
II-d	SDB	As water type, 1%, 10% and 100% SCSSS (Standard Canadian Shield saline solution, synthetic brine) is indicated. Under reducing conditions, the solutions are 0.08 M in hydrazine.	
		Final solution compositions are not given, but it is supposed that no essential changes take place with 10% and 100% SCSSS.	A/B
		Chlorite and muscovite are reported to be of high purity and final solution compositions with the reported S/W and 1% SCSSS can be estimated approximately.	C/D
II-e	SDB	A temperature of 22°C is indicated.	A/B
II-f	SDB	A liquid/solid ratio of 25 mL/g is indicated.	
	REF	It is reported that standard-scale experiments used 10 mL of solution and 0.4 g of solid.	A/B
II-g	SDB	The sorption value (calculated from K_d and S/W ratios) ranges between 8% and 75%.	A

II-h	SDB	Initial Se concentrations between 4.43×10^{-11} and 1.21×10^{-10} are given. Based on speciation calculations (for 25°C) with PHREEQC 2.12.5 using the thermodynamic data in JNC-TDB_011213c2 the initial Se concentrations are below the solubility limit.	A
II-i	SDB REF	It is indicated that no specific separation is reported. High-speed centrifugation of the samples is used for phase separation (oral communication with T. T. Vandergraaf).	B
II-j	SDB REF	A reaction time of 14 days is indicated. No further (kinetic) information is provided.	C/D
II-k	REF	The samples are intermittently agitated.	A/B
II-l	SDB	No variation in S/W or initial Se concentration is indicated.	C/D
II-m	REF	The experiments are carried out in polypropylene centrifuge tubes. Sorption on vessel walls is not tested and no corrections had been done.	C/D
II-n	REF	No error information is available.	D
II-o	SDB	Only the SCSSS salinity is varied.	C

Data table Se/3: REF: Ticknor et al. (1988)

JNC-SDB version 2 – DATA: Se/Other Minerals, Illite-Muscovite, #67055-67063

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	-	-
I-a.2 REF	It is reported, that aliquots of the aqueous phases are taken for the radiometric analysis. Phase separation is performed by high-speed centrifugation (oral communication with T. T. Vandergraaf).	Yes
I-b REF	A table with log K_d values is provided.	class 1
II-a REF	As solid phase illite-muscovite obtained from a drill core (Cigar Lake, Saskatchewan) is reported. A detailed mineral composition of the mineral sample and its specific surface area are available. The sample is crushed but not purified.	B
II-b REF	Initial as well as final pH values are reported. The solution pH is determined with litmus paper. No pH correction with buffer is performed after hydrazine addition.	B
II-c REF	Redox conditions are reported for each experiment. Experiments are performed under aerobic conditions, under nitrogen and under reducing	

		<p>conditions with addition of hydrazine under nitrogen atmosphere. All experiments are conducted in pre-equilibrated systems. Initial and final Eh values are given.</p> <ul style="list-style-type: none"> aerobic conditions, Se(IV): # 67055, 67056, 67061 nitrogen atmosphere, Se(IV): # 67057, 67058, 67062 hydrazine, nitrogen atmosphere (only one reducing agent has been used): # 67059, 67060, 67063 	<p>A/B</p> <p>A/B</p> <p>C/D</p>
II-d	REF	<p>As water type, 1%, 10% and 100% SCSSS (Standard Canadian Shield saline solution, synthetic brine) is reported. Under reducing conditions, the solutions are 0.08 M in hydrazine.</p> <p>Final solution compositions are not given, but it is supposed that no essential changes take place with 10% and 100% SCSSS. : #67055-67060</p> <p>Chlorite and muscovite are reported to be of high purity and final solution compositions with the reported S/W and 1% SCSSS can be estimated approximately. : #67061-67063</p>	<p>A/B</p> <p>C/D</p>
II-e	REF	A temperature of 22°C is indicated.	A/B
II-f	REF	It is reported that standard-scale experiments used 10 mL of solution and 0.4 g of solid. This corresponds to a liquid/solid ratio of 25 mL/g.	A/B
II-g	REF	Sorption values (calculated from K_d and S/W ratios) range from 19% to 58%.	A
II-h	REF	<p>Initial Se concentrations between 5.65×10^{-11} and 8.56×10^{-11} M are given.</p> <p>Based on speciation calculations (for 25°C) with PHREEQC 2.12.5 using the thermodynamic data in JNC-TDB_011213c2 the initial Se concentrations are below the solubility limit.</p>	A
II-i	REF	High-speed centrifugation of the samples is used for phase separation (oral communication with T. T. Vandergraaf).	B
II-j	REF	<p>A reaction time of 14 days is indicated. This reaction time is reasonably long.</p> <p>No further (kinetic) information is provided.</p>	C/D
II-k	REF	The samples are intermittently agitated.	A/B
II-l	REF	No variation in S/W or initial Se concentration is indicated.	C/D
II-m	REF	The experiments are carried out in polypropylene centrifuge tubes. Sorption on vessel walls is not tested and no corrections had been done.	C/D
II-n	REF	No error information is available.	D
II-o	SDB	Only the SCSSS salinity is varied.	C

Data table Se/4: REF: Fujikawa and Fukui (1997b) JNC-SDB version 2 – DATA: Se /Mudstone, # 51979 - 52002 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: it is indicated that no information on Eh, separation method and final solution composition are given.	No
REF	No further information is available.	unreliable

Data table Se/5: REF: Legoux et al. (1992) JNC-SDB version 2 – DATA: Se/Mudstone, # 56039 - 56042 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	Tables with K_d are given.	class 1
II-a SDB	The solid phase is indicated as soil (A, B, C and D). Mineralogical composition, specific surfaces and cationic exchange capacity (CEC) are reported.	A
II-b SDB	Initial pH values and final pH values are reported.	A
II-c SDB REF	It is indicated that no redox conditions are reported. There is no information about Eh. Redox of Se is reported VI. Se is in solution in the forms of SeO_4^{2-} . No reducing agents are added to the experiment and no inert gas atmosphere is reported. Therefore it is assumed that the experiment is conducted under ambient conditions.	C/D
II-d REF	The final solution composition is reported.	A/B
II-e SDB	A temperature is not reported.	C/D
II-f SDB REF	It is indicated that a W/S ratio of 10 mL/g had been used. The specific solid mass (1g) and solution volume (10ml) are reported. The soil mass of 1g has a surface area of 6.6-14.7m ² .	A/B
II-g SDB	The sorption value is between 19.4% and 93.0% (calculated with W/S and K_d values).	A
II-h SDB	The value of initial concentration is 2.0×10^{-7} M. Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the experiments are considered to be below the	

		<p>solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Se).</p> <p>-) Datapoints: 56039, 56041, 56042</p> <p>And it is estimated that the initial Se concentration may have been at, or slightly above, the solubility limit.</p> <p>-) Datapoints: 56040</p>	<p>B</p> <p>unreliable</p>
II-i	SDB	Ultrafiltration through 0.002µm and 0.025µm and membranes, as well as centrifugation at 4000rpm is reported.	A
II-j	SDB	It is indicated that contact time is 2 days. This reaction time is reasonably long.	C/D
II-k	REF	Samples are agitated continuously.	A/B
II-l	SDB	No variation of initial [Se] or S/W has been carried out.	C/D
II-m	REF	The experiments are carried out in polypropylene vessels. It is reported sorption to the vessel wall has been corrected for. No information about the correction procedure is available. It is assumed that the correction is based on the data obtained of a blank experiment.	C/D
II-n	SDB	The reported error represents the standard deviation of the average of at least four experimental repetitions.	A
II-o	SDB	No parameter variation is indicated.	D

3.1.4 Cesium

Data table Cs/1: REF: Barney and Anderson (1979) JNC-SDB version 2 – DATA: Cs /Mudstone, # 44256 – 44261 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: it is indicated that no information on “Adjustment and control of pH”, final solution composition and atmosphere/ redox condition are given.	No
REF	No further information is available.	unreliable

Data table Cs/2: REF: Barney and Brown (1979) JNC-SDB version 2 – DATA: Cs /Mudstone, # 44331 – 44333 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: it is indicated that no information on final solution composition is given.	No
REF	No further information is available.	unreliable

Data table Cs/3: REF: Daniels (1981) JNC-SDB version 2 – DATA: Cs /Mudstone, # 50063 – 50078 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	Tables with K_d are given.	class 1
II-a SDB REF	The solid phase is reported as Eleana argillite. Additional Eleana argillite is crushed in the controlled-atmosphere boxes. Physico- chemical properties and specific surface are not reported.	C/D
II-b SDB	Initial pH value and final pH value are reported. -) Datapoints: 50063, 50064, 50066, 50071, 50073, 50074	A

	Initial pH value is reported. -) Datapoints: 50065, 50067-50070, 50072, 50075-50078	C
II-c SDB	It is reported that experiments are done under atmosphere and controlled atmosphere. Also, Cs is not a redox-sensitive element.	A/B
II-d SDB REF	The final composition of the solution is not reported. Composition of water obtained in the field (groundwaters) is described in Erdal et al.(1979b): Los Alamos Scientific Laboratory report LA-7455-MS.	C/D
II-e SDB	A temperature of 32°C or room temperature is reported.	A/B
II-f SDB REF	Solution/solid ratios are not reported. The <75µm and 75-500µm fractions are used for the controlled- atmosphere studies. Several different particle-size fractions are used under atmospheric conditions.	C/D
II-g SDB	The sorption value cannot be calculated, because the Solution/solid ratios are lacking.	C/D
II-h SDB REF	The initial Cs concentration varied between 1.95×10^{-10} mol/L and 2.42×10^{-3} mol/L. Some initial [Cs] is not reported. However, Cs is not solubility limited.	A
II-i SDB	The membrane filtration with pore size of 0.45µm is used. -) Datapoints: 50065, 50067-50070, 50072, 50075-50078 No information is given about the separation method for some experiments. -) Datapoints: 50063, 50064, 50066, 50071, 50073, 50074	C/D unreliable
II-j SDB REF	It is indicated that contact time is 20.63 days, 21 days, 41.63 days or 91.63days for different datapoints. This reaction time is reasonably long. The kinetics of sorption is not tested. The K_d values on argillite increased slightly with time.	C/D
II-k REF	The batch sorption experiments are performed by shaking. It is indicated in Erdal et al.(1979b): Los Alamos Scientific Laboratory report LA-7455-MS.	A/B
II-l REF	A limited variation of initial Cs concentration has been used, including some experiments at trace concentrations.	B
II-m REF	The experiments are carried out in polyethylene centrifuge tubes. It is indicated in Erdal et al.(1979b): Los Alamos Scientific Laboratory report LA-7455-MS.	B
II-n SDB	Uncertainties are not reported.	D
II-o SDB	The initial pH, reaction time, initial Cs concentration and temperature are varied.	B

Data table Cs/4: REF: Duursma (1973) JNC-SDB version 2 – DATA: Cs /Mudstone, # 50310 – 50341 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 no information on phase separation is given. No further information is available.	No unreliable

Data table Cs/5: REF: Erdal et al. (1977) JNC-SDB version 2 – DATA: Cs /Mudstone, # 50648 – 50662 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 (the initial Cs concentration is not provided: see later comment at checkpoint II-h).	Yes
I-b SDB	Tables with K_d are given.	class 1
II-a SDB	Alluviums are reported as mineral phase (Hoffman et al., 1977: LA-6877-MS). CEC (10 to 17 meq/100 g) and surface area (6.11 to 20.2 m ² /g) are provided in table.	B
II-b SDB	Initial pH value and final pH range (from 8.3 to 8.7) are reported.	A
II-c SDB	It is reported that experiments are done under oxidizing conditions. Moreover, Cs is not a redox-sensitive element.	A/B
II-d REF	The initial composition of the groundwater is reported. The final solution composition is not reported, but can be estimated based on mineral and initial solution composition.	C/D
II-e SDB	A temperature of 20°C or 70°C is reported.	A/B
II-f SDB REF	Solution/solid ratio is 20mL/g. The used mass of 1g alluvium has a surface area of about 6 to 20m ² .	A/B
II-g SDB	The sorption value is between 99.26% and 99.81% (calculated with W/S and K_d values).	C/D
II-h SDB	Initial [Cs] is not reported. However, Cs is not solubility limited.	A
II-i SDB REF	The centrifugation is performed at 16000rpm for 1 hour. The supernatant is then centrifuged twice prior to measuring the Cs activity.	B
II-j SDB	A reaction time of between 2.8 days and 41.8 days is indicated.	

	REF	The kinetics of sorption is tested. No difference between 2.8 days and 41.8 days.	A/B
II-k	REF	Stirring is used as agitation method in reaction time.	C/D
II-l	REF	No isotherms, no variation of the Cs concentration is indicated.	C/D
II-m	REF	The reaction vessel is a polyethylene tube. No corrections for sorption on vessel walls are reported.	B
II-n	REF	No replicates and no error estimates are reported.	D
II-o	REF	No parameter variation.	D

Data table Cs/6: REF: Erdal et al. (1979b) JNC-SDB version 2 – DATA: Cs /Mudstone, # 50837 – 50858 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	Tables with K_d are given.	class 1
II-a SDB	Four different samples of the Eleana argillite are obtained from hole at the Nevada Test Site. The samples had all been wrapped in aluminum foil and waxed when they are originally taken. A petrographic description of the fractions is given in Table. CEC (8 meq/100 g to 14 meq/100 g) and Surface area (5.22 m ² /g to 12.5 m ² /g) are provided in table.	B
II-b SDB	Initial pH value and final pH are reported. -) Datapoints: 50839, 50842, 50843, 50846-50848 Final pH is reported. -) Datapoints: 50837, 50838, 50840, 50841, 50844, 50845, 50849-50858 After contact time of 56-60 days, it can be assumed to be enough for reaching equilibrium. However, pH is not a critical parameter for Cs.	A
II-c SDB	It is reported that experiments are done under aerobic conditions. Moreover, Cs is not a redox-sensitive element.	A/B
II-d REF	The initial composition of the groundwater is reported. The final solution composition is not reported, but can be estimated based on mineral and initial solution composition.	C/D
II-e SDB	A temperature of 22°C or 70°C is reported.	A/B
II-f SDB	Solution/solid ratio is 20mL/g.	A/B
REF	The used mass of 1g argillite has a surface area of about 5.22 to 12.5m ² .	

II-g	SDB	The %-sorbed can be calculated with K_d values and W/S ratio: -) Datapoint 50839: 97.45% -) Datapoints 50837, 50838, 50840-50858: between 98.01% and 99.5%	B C/D
II-h	SDB	Initial [Cs] is reported 1.4×10^{-9} M. Cs is not solubility limited.	A
II-i	REF	The centrifugation is performed at 16000rpm for one hour.	B
II-j	SDB	A reaction time of between 56 days and 60 days is indicated. This reaction time is reasonably long.	C/D
II-k	REF	The solid sample is dispersed with vigorous shaking, and the mixture is agitated gently for given time. The shaking rates are 200 oscillations per minute for the ambient temperature studies, and 80 oscillations per minute for the 70° C samples.	A/B
II-l	REF	No isotherms, no variation of the Cs concentration is indicated.	C/D
II-m	REF	The reaction vessel is a polyethylene tube. It is reported that cesium did not adsorb on the container walls.	A
II-n	REF	One replicate and no error estimates are reported.	D
II-o	REF	Only temperature is varied.	C

Data table Cs/7: REF: Erdal et al. (1979d)

JNC-SDB version 2 – DATA: Cs /Mudstone, # 50932 – 50934

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 (the initial Cs concentration is not provided: see later comment at point II-h).	Yes
I-b SDB	Tables with K_d are given.	class 1
II-a REF	Alluviums and Argillite are reported as mineral phase (Hoffman et al., 1977: LA-6877-MS). CEC and Surface area about alluviums are provided in table (Erdal et al., 1977). -)Datapoints: 50932, 50933 -)Datapoint: 50934	C/D B
II-b SDB REF	Neither initial nor final pH values are reported. There is no further information about pH conditions. However, pH is not a critical parameter for Cs.	D
II-c SDB REF	It is reported that experiments are done under atmosphere. Moreover, Cs is not a redox-sensitive element.	A/B

II-d	SDB	The initial composition of the groundwater is not reported.	
	REF	Composition of water obtained in the field (groundwaters) is described in Erdal et al. (1979b).	C/D
II-e	SDB	A temperature of 22°C or 70°C is reported.	A/B
II-f	SDB	Solution/solid ratio is 20mL/g.	A/B
	REF	The used mass of 1g alluvium has a surface area of about 6m ² to 20m ² .	
II-g	SDB	The sorption value is between 98.96% and 99.72% (calculated with W/S and K _d values).	C/D
II-h	SDB	Initial [Cs] is not reported.	
	REF	No further information. However, Cs is not solubility limited.	A
II-i	SDB	The centrifugation is performed at 16000rpm for one hour.	B
II-j	SDB	A reaction time of 7 days, 14 days, 28 days or 56 days is indicated.	
	REF	These reaction times are reasonably long.	C/D
II-k	REF	The sample is dispersed with vigorous shaking, and mixture is agitated gently for a given time. The shaking rates are 200 oscillations per minute for the ambient temperature studies, and 80 oscillations per minute for the 70° C samples.	A/B
II-l	REF	No isotherms, no variation of the Cs concentration is indicated.	C/D
II-m	REF	The reaction vessel is a polyethylene tube. It is reported that cesium did not adsorb on the container walls.	A
II-n	REF	No replicates and no error estimates are reported.	D
II-o	REF	Temperature and reaction time are varied.	B

Data table Cs/8: REF: Erdal (1980)

JNC-SDB version 2 – DATA: Cs /Mudstone, # 51200 – 51225

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 no information on final solution composition is given. No further information is available.	No unreliable

Data table Cs/9: REF: Fujikawa and Fukui (1997a) JNC-SDB version 2 – DATA: Cs /Mudstone, # 51763 – 51786 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 no information on Eh, separation method and final solution composition are given. No further information is available. The Eh is not a sensitive parameter for Cs, but the phase separation method and final solution composition are key points which are missing in the reference.	No unreliable

Data table Cs/10: REF: Higgo et al.(1987) JNC-SDB version 2 – DATA: Cs /Mudstone, # 53224 – 53248 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	Tables with K_d are given.	class 1
II-a SDB	Major and minor mineralogy is not known. Specific surface area and CEC are reported. It is not clear whether impurities are determined.	C/D
II-b SDB REF	Initial pH values are indicated. No use of any pH-buffer is reported.	C
II-c SDB	Experiments are carried out at aerobic condition. Cs is not redox sensitive.	A/B
II-d SDB REF	Seawater is indicated. The critical major components are approximately Known. Minor components may be unknown. Charge balance cannot be calculated, but seawater can be expected to be well poised.	C/D
II-e SDB	A temperature of 4°C is reported.	A/B
II-f SDB	Solution/solid ratios are not reported.	C/D
II-g SDB	The sorption value cannot be calculated, because the Solution/solid ratios are lacking.	C/D
II-h SDB	Initial [Cs] ranged from 3.4×10^{-9} M to 1.0×10^{-3} M. Cs is not solubility limited.	A
II-i SDB	The centrifugation (7000rpm / 90 min) and followed by filtration through 0.1 and 0.22µm Millipore filters is indicated.	C/D

II-j	SDB	A reaction time is 45days. This reaction time is reasonably long.	C/D
II-k	REF	Agitation is carried out by shaken at 120 strokes/min.	A/B
II-l	REF	The variation of initial Cs concentration is indicated.	B
II-m	REF	The quality of reaction vessel is not reported.	C/D
II-n	SDB	No replicates are reported. But error estimates are reported.	C
	REF	Uncertainties are based on error propagation, not on replicate measurements.	
II-o	REF	Initial Cs concentration is varied.	C

Data table Cs/11: REF: Konishi et al. (1988)

JNC-SDB version 2 – DATA: Cs / Mudstone, # 54009 – 54012

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 is provided.	class 1
II-a REF	The loam is reported as mineral's content. Takadate loam (CEC: 10-30 meq/100g and specific surface area 130cm ² /g) and Hachinohe loam (30-135 meq/100g and 60cm ² /g) are provided.	B
II-b SDB	Final pH value is reported (after a contact time of 7 days, which can be assumed to be enough for reaching equilibrium).	A
II-c SDB	Experiments are done under oxidizing conditions. Moreover, Cs is not a redox-sensitive element.	A/B
II-d SDB REF	The initial composition for datapoints 54009 and 54012 is reported (deionized water). The final solution composition can be estimated based on mineral and initial solution composition. The initial composition for datapoints 54010 and 54011 is not reported (synthetic groundwater). The composition of the synthetic water could be reported in Konishi et al.(1986). The final solution composition can be estimated based on mineral and initial solution composition.	C/D
II-e SDB	A room temperature is reported.	A/B
II-f SDB REF	A W/S ratio is not reported. No further information about W/S ratio.	C/D
II-g SDB	The sorption value cannot be evaluated, because of the lacking W/S ratio.	C/D
II-h SDB	The final Cs concentrations are between 5×10^{-7} - 1×10^{-3} mol/L. The initial	

		concentration is higher than the given equilibrium aqueous concentration, but cannot be estimated because no information is provided about the amount of loam used in the experiment. Since Cs is not solubility limited, the datapoints are classed as A.	A
II-i	SDB	Centrifugation at 39000g is reported as separation method.	B
II-j	SDB	Contact time is 7 days. This reaction time is reasonably long.	C/D
II-k	REF	There is no information about the agitation method. This information may be reported in Konishi et al.(1986).	C/D
II-l	REF	An isotherm has been measured (Experiment T-2 and H-2, Datapoints 54010, 54011). The lower points of the isotherm are in the linear sorption range.	A
II-m	REF	The material of the vessel is not reported.	C/D
II-n	SDB	No replicates and no error estimates are reported.	D
II-o	SDB	The pH value is varied (from 6.1 to 8.3).	C

Data table Cs/12: REF: Legoux et al. (1992)

JNC-SDB version 2 – DATA: Cs/Mudstone, # 55999 – 56002

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	Tables with K_d are given.	class 1
II-a SDB	The solid phase is indicated as soil (A, B, C and D). Mineralogical composition, specific surface area and cationic exchange capacity (CEC) are reported.	A
II-b SDB REF	Initial pH values and final pH values are reported. Variation of the equilibrium pH versus the initial pH of the solution is showed by the figure. The equilibrium pH of each of the samples is studied as a function of the initial pH of the reconstituted water.	A
II-c SDB REF	There is no information about Eh and redox conditions. Based on the information in the paper, experiments are done under air; i.e, under oxidizing conditions. Moreover, Cs is not a redox sensitive element.	A/B
II-d SDB	The final solution composition is reported.	A/B
II-e SDB	A temperature is not reported.	C/D

II-f	SDB	It is indicated that a W/S ratio of 10 mL/g had been used. The specific solid mass (1g) and solution volume (10mL) are reported.	
	REF	The soil mass of 1g has a surface area of 6.6-14.7m ² .	A/B
II-g	SDB	The sorption value is between 99.7% and 99.8% (calculated with W/S and K _d values).	C/D
II-h	SDB	2.0×10 ⁻⁷ M is indicated as initial Cs concentration. Cs is not solubility limited.	A
II-i	SDB	Centrifugation and ultrafiltration through 0.002μm and 0.025μm Millipore filters is reported. Centrifugation is done at 4000rpm prior to filtration.	A
II-j	SDB	Contact time is 2 days. This reaction time is reasonably long.	C/D
II-k	REF	Samples are agitated continuously.	A/B
II-l	SDB	No variation of W/S ratio and the initial Cs concentration is reported.	C/D
II-m	REF	The experiments are carried out in polypropylene vessels. It is reported that sorption to the vessel wall has been corrected for. No information about the correction procedure is available. It is assumed that the correction is based on the data obtained of a blank experiment.	C/D
II-n	SDB	The reported error represents the standard deviation of the average of at least	A
	REF	four experimental repetitions.	
II-o	SDB	No parameter variation is indicated.	D

Data table Cs/13: REF: Mackenzie et al. (1983)

JNC-SDB version 2 – DATA: Cs /Mudstone, # 56123 – 56142

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: it is indicated that no information on initial and final solution composition are given.	No
REF	Solid phase; LLM-marine sediment; LLL-lacustrine sediment are not reported about elemental analysis. No further information is available.	unreliable

Data table Cs/14: REF: Maclean et al. (1978) JNC-SDB version 2 – DATA: Cs /Mudstone, # 56183 – 56184 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	Tables with K_d are given.	class 1
II-a SDB	Conasauga shale is reported as mineral phase. CEC and surface area are not reported.	C/D
II-b SDB REF	Initial pH value is reported. Final pH value is not reported. There is no further information about pH conditions. However, pH is not a critical parameter for Cs.	C
II-c SDB REF	There is no information about Eh. It is reported that experiments are done under aerobic condition; i.e., under oxidizing conditions. Moreover, Cs is not a redox sensitive element.	A/B
II-d REF	The initial composition of the groundwater is reported. The final solution composition is not reported, but can be estimated based on mineral and initial solution composition.	C/D
II-e SDB	A temperature of 25°C is reported.	A/B
II-f SDB	A solution/solid ratio is 25mL/g. The used mass of 1 g shale is considered to have enough surface area.	A/B
II-g SDB	The sorption values are 99.6 % and 99.8% (calculated with W/S and K_d values).	C/D
II-h SDB REF	Initial [Cs] is reported 2.8×10^{-7} M. Cs is not solubility limited.	A
II-i SDB	Filtration through 0.10µm membranes is indicated	C/D
II-j SDB	A reaction time of 7 days is indicated. This reaction time is reasonably long.	C/D
II-k REF	Agitation of the 130 oscillations/min is used as method in reaction time.	A/B
II-l REF	No isotherms, no variation of the initial [Cs] is indicated.	C/D
II-m REF	The reaction vessel is a polycarbonate centrifuge tube. No corrections for sorption on vessel walls are reported.	B
II-n REF	Three replicates and error estimates are reported.	A
II-o REF	No parameter variation.	D

Data table Cs/15: REF: Mucciardi et al. (1979) JNC-SDB version 2 – DATA: Cs /Mudstone, # 57578 – 57589 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	Table with K_d values is provided.	class 1
II-a SDB	Argillaceous shale is reported as mineral phase. CEC and surface area are reported.	B
II-b SDB	Initial pH value and final pH value are reported.	A
II-c SDB	It is reported that experiments are done under air; i.e., under oxidizing conditions. Moreover, Cs is not redox sensitive.	A/B
II-d SDB REF	Only the initial composition is indicated (synthetic groundwater). It is assumed that the final solution composition can be estimated based on mineral and initial solution composition.	C/D
II-e SDB	Temperature of 20°C or 23.5°C is reported.	A/B
II-f SDB	Fraction size of shale is reported 300µm-850µm. Solution/solid ratio is 15mL/g. The used mass of 0.5g shale is considered to have enough surface area (~5m ²).	A/B
II-g REF	The %-sorbed can be calculated with K_d and W/S ratio: -) Datapoint 57578: 81.0% -) Datapoints 57579, 57580: 97.1% and 97.7% -) Datapoints 57581-57589: between 98.0% and 99.8% is sorbed	A B C/D
II-h SDB REF	Initial [Cs] is not reported. No information about initial [Cs] is reported. However, Cs is not solubility limited.	A
II-i SDB	Centrifugation (7000rpm for 20 minutes) is indicated.	C/D
II-j SDB	A reaction time of 3~ 30 days is indicated. This reaction time is reasonably long.	C/D
II-k REF	Agitation is carried out by shaking.	A/B
II-l REF	No isotherms, no variation of W/S ratio and no initial [Cs] have been performed.	C/D
II-m REF	The reaction vessel is a polycarbonate centrifuge tube.	B
II-n REF	Three replicates and error estimates in K_d are reported.	A
II-o REF	Two temperatures are used (20 and 23.5°C), two pH values (8.2 and 7) and four groundwaters; Eh (end) is varied.	B

Data table Cs/16: REF: Yamamoto et al. (1989) JNC-SDB version 2 – DATA: Cs /Mudstone, # 61762 – 61767 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: it is indicated that no information on Eh, separation method, reaction time and final solution composition are given.	No
REF	No further information is available. The Eh is not a sensitive parameter for Cs, but the phase separation method, contact time and final solution composition are key points which are missing in the reference.	unreliable

Data table Cs/17: REF: Rajec et al. (1998) JNC-SDB version 2 – DATA: Cs /Mudstone, # 62331 – 62350 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: it is indicated that no information on initial and final solution composition are given. Only one reaction time (2 hours) is reported.	No
REF	No further information is available. The final solution composition is a key point which is missing in the reference. The kinetics of sorption is not tested.	unreliable

Data table Cs/18: REF: Mollah and Ullah (1998) JNC-SDB version 2 – DATA: Cs /Mudstone, # 62474 – 62485 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	Table with K_d values is provided.	class 1
II-a SDB	Physical and chemical characteristics of the soils at the atomic energy research establishment campus in Bangladesh are reported. CEC is reported. Surface area is not reported.	B
REF		

II-b	SDB	Initial pH value and final pH value are indicated.	A
II-c	SDB	It is reported that experiments are done under air; i.e., under oxidizing conditions. Moreover, Cs is not redox sensitive.	A/B
II-d	SDB REF	Only initial characteristics are indicated (groundwater). It is assumed that the final solution composition can be estimated based on characteristics of the soils and initial solution composition.	C/D
II-e	SDB	A temperature of 25°C is reported.	A/B
II-f	SDB	Solution/solid ratio is 50mL/g. The used mass of 1g soil is considered to have enough surface area.	A/B
II-g	REF	The %-sorbed can be calculated with K_d and W/S ratio: between 96.2% and 97.7% is sorbed.	B
II-h	SDB REF	Initial [Cs] is reported 1.68×10^{-10} M. Cs is not solubility limited.	A
II-i	SDB	Centrifugation (5000rpm for 1 hour) is indicated.	C/D
II-j	SDB	A reaction time of 2 days is indicated. This reaction time is reasonably long.	C/D
II-k	REF	Agitation is carried out by shaking for 2 days.	A/B
II-l	REF	No isotherms, no variation of W/S ratio and no variation of initial [Cs] have been performed.	C/D
II-m	REF	The reaction vessel is a polypropylene centrifuge tube. Blank experiments showed that no sorption of Cs on the walls of the tubes.	A
II-n	REF	Three replicates estimates in K_d are reported. Error is not reported.	D
II-o	REF	No isotherm is recorded; no parameter variation.	D

Data table Cs/19: REF: Kamel and Ibrahim (1998)

JNC-SDB version 2 – DATA: Cs /Mudstone, # 62721 – 62736

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	Table with K_d values is provided.	class 1
II-a SDB REF	CEC is reported. Surface area is not reported. Mineralogical and chemical characteristics of compacted Egyptian soils are given in previous reference (Ibrahim and Kamel, 1998).	C/D
II-b SDB	Initial pH value and final pH value are indicated.	

	-) Datapoints 62731-62736 Initial pH value is indicated. The sorption of Cs is not strongly pH dependent.	A
	-) Datapoints 62721-62730	B
II-c SDB	It is reported that experiments are done under air; i.e., under oxidizing conditions. Moreover, Cs is not redox sensitive.	A/B
II-d SDB	Only initial physical and chemical characteristics are indicated (natural Ismailia canal water).	
REF	It is assumed that the final solution composition can be estimated based on characteristics of the soils and initial canal water solution composition.	C/D
II-e SDB	A temperature of 30°C is reported.	A/B
II-f SDB	Solution/solid ratio is 30mL/g. The used mass of 0.5g soil is considered to have enough surface area.	A/B
REF	The soil samples are crushed and grinded.	
II-g REF	The %-sorbed can be calculated with K_d and W/S ratio: -) Datapoints 62721-62736: between 12.2% and 87.8% is sorbed	A
II-h SDB	Initial [Cs] is reported from 1.0×10^{-4} M to 1.0×10^{-2} M.	
REF	Cs is not solubility limited.	A
II-i SDB	Centrifugation and filtered through 0.45µm is indicated; -) Datapoints 62721-62730	C/D
	Centrifugation is indicated; -) Datapoints 62731-62736	C/D
II-j SDB	A reaction time of 7 days is indicated. This reaction time is reasonably long.	C/D
II-k REF	Agitation is carried out by shaking for 7 days.	A/B
II-l REF	Variation of initial [Cs] has been performed.	B
II-m REF	The reaction vessel is a polyethylene bottle.	B
II-n REF	Replicates estimates in K_d are not reported. Error is not reported.	D
II-o REF	The pH and [Cs] are varied.	B

Data table Cs/20: REF: Strezov et al. (2000)

JNC-SDB version 2 – DATA: Cs /Mudstone, # 62772 – 62786

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	It is indicated that values are extracted from a graph (linear).	class 3
II-a	SDB REF	Mineral composition and chemical composition about the soil are reported. CEC and Surface area are not reported.	C/D
II-b	SDB	Initial pH values and final pH values are indicated. -) Datapoints 62777-62786 Initial pH values are indicated. -) Datapoints 62772-62776	A C
II-c	SDB	It is reported that experiments are done under air; i.e., under oxidizing conditions. Moreover, Cs is not redox sensitive.	A/B
II-d	SDB	The compositions of the groundwater before equilibration with the solid phase and after equilibration (the final solution composition) are given in table.	A/B
II-e	SDB	A temperature of 20°C is reported.	A/B
II-f	SDB REF	Solution/solid ratio is 30mL/g. The used mass of 0.3g soil is considered to have enough surface area. The geological formation is crushed and sieved into the fractions from 80µm to 400µm.	A/B
II-g	SDB	Based on the information given in the SDB, the %-sorbed values are between 33.3% and 92.3%.	A
II-h	SDB	Initial [Cs] is reported 1.0×10^{-6} M. Cs is not solubility limited.	A
II-i	SDB REF	Centrifugation at 6000rpm is indicated. No further information.	C/D
II-j	SDB	A reaction time of 0.2 day, 0.3 day and 0.4 day is indicated, which is not reached a steady-state. -) Datapoints 62772-62774 A reaction times of 6 days, 30 days and 48 days are indicated, which is reached a steady-state. Sorption kinetics of Cs on geological formation is showed in figure. -) Datapoints 62775-62786	unreliable A/B
II-k	REF	The samples are shaken for 1 month with groundwater for equilibration. The kinetics of Cs sorption is measured for a soil.	A/B
II-l	REF	The influence of Cs concentration on sorption on the geological media is investigated (sorption isotherm of Cs on geological formation).	B
II-m	REF	The measurements are performed in 50 mL polyethylene vials. Corrections for sorption on vials have not been performed.	B
II-n	REF	Each experiment is tripled. Error is not reported.	D
II-o	REF	An isotherm is reported. The pH is varied.	B

Data table Cs/21: REF: Ashida et al. (1999) JNC-SDB version 2 – DATA: Cs /Mudstone, # 62892 , 62896 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	It is indicated that values are extracted from a graph (log).	class 5
II-a REF	Mineral composition list about the mudstone (Miyagi prefecture Tomegun) is reported. Surface area is reported. CEC is not reported.	C/D
II-b SDB	Final pH value is indicated.	A
II-c SDB	It is reported that experiments are done under air; i.e., under oxidizing conditions. Moreover, Cs is not redox sensitive.	A/B
II-d SDB REF	0.01M-NaCl and 0.1M-NaCl are reported. It is assumed that the final solution composition can be estimated based on mineral composition of the mudstone and NaCl water.	C/D
II-e SDB	A temperature of 22°C is reported.	A/B
II-f SDB	Solution/solid ratio is 100mL/g. The used mass of mudstone is not reported.	C/D
II-g SDB	Based on the information given in the JNC-SDB, the %-sorbed values are between 39.4% and 44.4%.	A
II-h SDB REF	Initial [Cs] is reported 1.9×10^{-9} M. Cs is not solubility limited.	A
II-i SDB REF	Centrifugation at 10000rpm is indicated. No further information.	B
II-j SDB	A reaction time of 30 days is indicated, which is considered for enough to reached a steady-state.	A/B
II-k REF	The samples are shaken for 1 month with NaCl water for equilibration.	A/B
II-l REF	Neither [Cs] nor the W/S has been varied.	C/D
II-m REF	The measurements are performed in polyethylene vessels. Corrections for sorption on vessels have not been performed.	B
II-n REF	Each experiment is duplicated. Error is not reported.	D
II-o REF	No isotherm is recorded; no parameter variation.	D

Data table Cs/22: REF: Inoue and Morisawa (1975) JNC-SDB version 2 – DATA: Cs /Mudstone, # 63346 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 no information on Eh, separation method and reaction time are given. No further information is available. The Eh is not a sensitive parameter for Cs, but the phase separation method and contact time are key points which are missing in the reference.	No unreliable

Data table Cs/23: REF: Silva et al. (1979) JNC-SDB version 2 – DATA: Cs /Bentonite, # 65509 – 65658 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	Tables with K_d are given.	class 1
II-a SDB	The solid phase is reported as a montmorillonite #27(Belle Fourche clay). The chemical compositions of solid substrates are reported in the table. Major and minor mineralogy as well as surface characteristics are reported.	A
II-b SDB REF	Only initial pH values are reported. Just prior to the sorption measurements, the pH of the solutions are checked and readjusted if necessary.	B
II-c SDB	Experiments are performed under an argon filled, inert atmosphere box. Since the effect of dissolved CO_2 , i.e., HCO_3^- and CO_3^{2-} ions, it is decided to exclude CO_2 from the system. Cs is not a redox-sensitive element.	A/B
II-d SDB	A NaCl (0.002M, 0.01M, 0.1M and 1M) is reported as input solution. Initial chemical compositions of synthetic groundwater are reported in the additional file “solution composition” and had an ionic strength of 0.003M.	C/D
II-e SDB	A temperature of $26 \pm 2^\circ\text{C}$ is reported.	A/B
II-f SDB REF	A solution/solid ratio of 100 mL/g is reported. 1 g solid is added to 100 mL solution. The average particle size is 1.14 μm with 90% of the particle sizes in the range 0.5 – 2.0 μm . The BET (outer) surface areas are 18.1 m^2/g for a Belle Fourche Clay.	A/B

II-g	SDB	On a solution/solid ratio that may from 100 mL/g, sorption values between 5.3 - 98.3% sorbed can be calculated.	A B C/D
		<ul style="list-style-type: none"> Datapoints: 65510-65512, 65515-65517, 65520-65522, 65525-65527, 65530-65532, 65535-65537, 65540-65542, 65545-65547, 65550-65552, 65555-65557, 65560-65562, 65565-65567, 65570-65572, 65575-65577, 65580-65582, 65584-65587, 65590-65592, 65595-65597, 65600-65602, 65605-65607, 65609-65612, 65614-65617, 65620-65622, 65625-65627, 65630-65632, 65634-65647, 65650-65652, 65654-65657 Datapoints: 65509, 65513, 65514, 65518, 65519, 65523, 65524, 65528, 65529, 65533, 65534, 65538, 65539, 65543, 65544, 65549, 65553, 65554, 65558, 65559, 65563, 65564, 65568, 65569, 65573, 65574, 65578, 65579, 65583, 65588, 65589, 65593, 65594, 65598, 65599, 65603, 65604, 65608, 65613, 65618, 65619, 65623, 65624, 65628, 65629, 65633, 65648, 65649, 65653, 65658 Datapoints: 65548 	
II-h	SDB	Initial Cs concentrations are 0.93×10^{-3} , 1.00×10^{-4} , 1.00×10^{-5} , 1.01×10^{-7} and 1.04×10^{-9} M. Cs is not solubility limited.	A
II-i	SDB	Centrifuge for 3 minutes at 12000 rpm and membrane filtration with pore size of 0.2µm are used for phase separation.	B
II-j	SDB REF	It is reported that contact time is 2 days. The sorption of Cs as a function of time is investigated in separate experiments and no detectable increase in sorption is measured after 15 minutes.	A/B
II-k	REF	The solutions are agitated for 15 – 20 minutes. But the method is not specified.	C/D
II-l	SDB REF	A limited variation of initial Cs concentration has been used, including some experiments at trace concentrations. Cesium sorption isotherms using the sodium form of the Belle Fourche clay is obtained as a function of Cs concentration, pH and supporting electrolyte concentration in batch-type experiments.	A
II-m	REF	The experiments are carried out in polyethylene bottles. Corrections for sorption on vessel walls have not been performed.	B
II-n	SDB REF	Uncertainties in K _d are given for each K _d value. The assigned errors result from a consideration of errors associated with counting and sampling. Duplicates are run on only about 10% of the samples and agreements are within the estimated error. Cesium sorption isotherms are obtained.	B

II-o	SDB	Within the set of reliable experiments, Cs concentration (isotherm), pH and supporting electrolyte concentration are varied. The initial Cs concentrations ranged from 10^{-3} M to 10^{-9} M; pH values are 5, 6, 7, 8, 9 and 10; electrolyte solutions are (0.002M, 0.01M, 0.1M and 1M) NaCl and the simulated groundwater.	A
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3.1.5 Plutonium

Data table Pu/1: REF: Baston et al. (1998) JNC-SDB version 2 – DATA: Pu /Bentonite, # 65922 – 65927 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	Tables with K_d are given.	class 1
II-a SDB	The solid phase is indicated as Kunigel-V1.	A
REF	The surface area is $6.80 \text{ m}^2/\text{g}$. The concentration of sites $2.88 \times 10^{-2} \text{ mol dm}^{-3}$.	
II-b SDB	Final pH values are reported.	A
REF	No use of any pH-buffer is reported. The pH value is monitored every 7 days, the pH adjusted back to the appropriate value.	
II-c SDB	Experiments are performed under N_2 . The oxidation state of Pu is reported as +IV. Final Eh values are provided, as well as the reducing agent used ($\text{Na}_2\text{S}_2\text{O}_4$) at an initial concentration of $2.5 \times 10^{-3} \text{ M}$.	C/D
REF	O_2 levels are reportedly $<1 \text{ ppm}$. All solutions are de-oxygenated by bubbling an argon (96%) /hydrogen (4%) mixture through them before posting into the glovebox. The Eh value is monitored every 7 days, and when it increased towards -300mV more sodium hydrosulphite is added.	
II-d SDB	A NaCl, NaHCO_3 is reported as input solution; main solution compositions are indicated in the additional file “solution composition”.	A/B
REF	Samples are filtered using a 10000MWCO filter prior to analysis.	
II-e SDB	A temperature of 60°C is reported.	A/B
II-f SDB	It is indicated that a W/S ratio of 20 mL/g had been used, but that the specific solid mass and solution volume are not reported.	
	Assuming that the solution volume is $\geq 20 \text{ mL}$ would mean a corresponding solid mass of at least 1 g . This is accepted as reasonable.	A/B
II-g SDB	Based on the information provided in the JNC-SDB, all K_d values can be calculated to correspond to %-sorbed values $>99\%$.	C/D
II-h SDB	$4.3 \times 10^{-11} \text{ M}$ is indicated as initial Pu concentration.	
REF	Based on the experimental data shown for Th and Pu(III) in Rai et al.(1999), it is estimated that the initial Pu concentration is below the solubility limit, but possibly by less than a factor of 5.	B
	The solutions are pre-filtered ($45\mu\text{m}$) before being equilibrated with the solid.	

		Presumably, a possible Pu-precipitate would have been removed in this way.	
II-i	SDB	Filtration through 10000MWCO and 45µm membranes, as well as centrifugation at 1100g for 2.5 h is reported.	
	REF	Three methods of phase separation are used: 1) centrifugation at 1100 g for 2.5 h, 2) centrifugation at 1100 g for 2.5 h followed by filtration through 0.45 µm membranes, and 3) centrifugation at 1100 g for 2.5 h followed by filtration through 0.45 µm membranes and then by filtration through 10000 MWCO filters. It appears that the resulting K_d values are slightly dependent on the method of phase separation: surprisingly, the highest K_d is generally obtained with centrifugation alone, whereas filtration with 10000 MWCO membranes leads to the lowest values. However, the respective variation is of about the same magnitude as observed for different W/S. Therefore, it may be considered to be within the overall experimental uncertainties.	A
II-j	SDB	A reaction time of 122 days (four months) is reported. This reaction time is reasonably long.	C/D
II-k	REF	The experiments are gently agitated on a shaker table.	A/B
II-l	SDB	No variation of W/S ratio or no variation of the initial Pu concentration is reported.	C/D
II-m	REF	The experiments are carried out in polypropylene centrifuge tubes. And corrections for sorption on vessel walls have been performed.	A
II-n	SDB	It is indicated that each experiment is done in duplicate.	
	REF	Error estimates are given for each replicate, based on analytical uncertainties.	A
II-o	SDB	No relevant parameter variation is indicated.	D

3.1.6 Americium

Data table Am/1: REF: Barney and Anderson (1979) JNC-SDB version 2 – DATA: Am /Mudstone, # 44238 – 44243 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: it is indicated that no information on initial and final pH, final solution composition and atmosphere/ redox condition are given.	No
REF	No further information is available. Americium is not redox sensitive	unreliable

Data table Am/2: REF: Barney and Brown (1979) JNC-SDB version 2 – DATA: Am /Mudstone, # 44322 – 44324 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint ¹	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided: it is indicated that no information on initial and final pH, initial and final Eh, final solution composition, initial Am concentration and atmosphere/ redox condition are given.	No
REF	No further information is available. Americium is not redox sensitive	unreliable

Data table Am/3: REF: Baston et al. (1995b) JNC-SDB version 2 – DATA: Am /Mudstone, # 46664 – 46667 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint ¹	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	Tables with K_d are given.	class 1
II-a SDB REF	The solid phase is reported as cover soil at Rokkasho-Mura. Physico- chemical properties and specific surface of cover soil are not given.	C/D
II-b SDB	Initial and final pH values are reported.	A
II-c SDB	It is reported that experiments are done in nitrogen-atmosphere glove-boxes. Also, Am is not a redox-sensitive element.	A/B

II-d	SDB	The compositions of solutions (synthetic groundwater) used in experiments are reported.	A/B
II-e	SDB	A temperature is not reported.	C/D
II-f	SDB	Solution/solid ratios are reported for 50mL/g.	C/D
II-g	SDB	Based on the information given in the SDB, and on a solution/solid ratio of 50ml/g, sorption values between 99.77%- 99.88% sorbed can be calculated.	C/D
II-h	SDB REF	The initial Am concentrations are reported to be 4×10^{-11} M to 8×10^{-11} M. The exact initial Am concentration is not reported. Based on data from Rai et al. (1999), the solubility for Am at the highest pH of 8 is about 1×10^{-7} M. Therefore, the initial concentration is clearly below the solubility limit (the solution composition will not strongly influence the solubility of Am).	A
II-i	SDB	The membrane filtration with pore size of 0.45 μ m is used. -) Datapoints: 46664, 46666 Filtration with a 30000MWCO filter is reported as separation method. -) Datapoints: 46665, 46667	C/D B
II-j	SDB REF	It is indicated that contact time is not reported exactly. It is reported that one tube is analysed regularly to monitor the approach to a steady state concentration of radionuclide. The reaction time considered to be reasonably long.	C/D
II-k	REF	The batch sorption experiments are gently agitated continuously. But the agitation method is not specified.	C/D
II-l	REF	A limited variation of [Am] has been used, including some experiments at trace concentrations.	B
II-m	REF	The experiments are carried out in polypropylene centrifuge tubes. The sorption on vessel wall has been determined as lower than 0.5% than the actual value and thus corrections for sorption on vessel wall have not been performed.	A
II-n	SDB	Uncertainties are reported (n=3).	A
II-o	SDB	The phase separation and final pH are varied.	B

Data table Am/4: REF: Daniels et al.(1981) JNC-SDB version 2 – DATA: Am /Mudstone, # 50002 – 50025 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	Tables with K_d are given.	class 1
II-a SDB REF	The solid phase is reported as Eleana argillite. Additional Eleana argillite is crushed in the controlled-atmosphere boxes. Physico- chemical properties and specific surface are not given.	C/D
II-b SDB	Initial pH value and final pH value are reported.	A
II-c SDB	It is reported that experiments are done under atmosphere and controlled atmosphere. Also, Am is not a redox-sensitive element.	A/B
II-d SDB REF	The final composition of the solution is not reported. Composition of water obtained in the field (groundwaters) is described in Erdal et al.(1979b): Los Alamos Scientific Laboratory report LA-7455-MS.	C/D
II-e SDB	A temperature of 32°C or 22°C is reported.	A/B
II-f SDB	Solution/solid ratios are not reported.	C/D
II-g SDB	The sorption value cannot be calculated, because the Solution/solid ratios are lacking.	C/D
II-h SDB REF	The initial Am concentrations are 1.4×10^{-7} mol/L and 4.6×10^{-8} mol/L. Based on data from Rai et al. (1999), the solubility for Am at the highest pH of 8 is about 1×10^{-7} M. Therefore, the initial concentration of 4.6×10^{-8} mol/L is below the solubility limit (the solution composition will not strongly influence the solubility of Am). And the initial concentration of 1.4×10^{-7} mol/L is to close to the saturation concentration. Therefore following rating is given: -) Datapoints: 50004, 50005, 50007, 50008, 50011, 50012, 50015, 50017, 50020-50022, 50024 -) Datapoints: 50002, 50003, 50006, 50009, 50010, 50013, 50014, 50016, 50018, 50019, 50023, 50025	B unreliable
II-i SDB	Centrifugation and filtration are indicated. But there is no information about the concrete method.	C/D
II-j SDB REF	It is indicated that contact time is 20.7 days, 21.9 days, 41.6 days, 42.8days, 83.7days or 83.8days for different datapoints. These reaction times are reasonably long. The kinetics of sorption is not tested.	C/D

II-k	REF	The batch sorption experiments are performed by shaking. It is indicated in Erdal et al.(1979b): Los Alamos Scientific Laboratory report LA-7455-MS.	A/B
II-l	REF	No isotherm is performed.	C/D
II-m	REF	The experiments are carried out in polyethylene centrifuge tubes. It is indicated in Erdal et al.(1979b): Los Alamos Scientific Laboratory report LA-7455-MS.	B
II-n	SDB	Uncertainties are not reported.	D
II-o	SDB	The initial pH, reaction time and temperature are varied.	B

Data table Am/5: REF: Erdal (1980)

JNC-SDB version 2 – DATA: Am /Mudstone, # 50977 – 51062

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: it is indicated that no information on initial and final pH (# 50977 – 51000), initial and final Eh, final solution composition and atmosphere/ redox condition are given.	No
REF	No further information is available. Americium is not redox sensitive.	unreliable

Data table Am/6: REF: Higgo et al.(1987)

JNC-SDB version 2 – DATA: Am /Mudstone, # 53185 – 53223

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	Tables with K_d are given.	class 1
II-a SDB	Major and minor mineralogy is not known. Specific surface area and CEC are reported. It is not clear whether impurities are determined.	C/D
II-b SDB	Initial pH values are indicated.	C
REF	No use of any pH-buffer is reported.	
II-c SDB	Experiments are carried out at aerobic condition. Americium is not redox sensitive.	A/B
II-d SDB	Seawater is indicated.	

REF	The critical major components are approximately Known. Minor components may be unknown. Charge balance cannot be calculated, but seawater can be expected to be well poised.	C/D
II-e SDB	A temperature of 4°C is reported.	A/B
II-f SDB	Solution/solid ratios ranged from 1.69mL/g to 25000mL/g.	C/D
REF	Liquid volumes are reported 50mL.	
II-g SDB	The sorption value is between 98.64% and 99.99% (calculated with W/S and K_d values).	C/D
II-h SDB	Initial [Am] ranged from 6.24×10^{-10} M to 1.19×10^{-9} M. Based on the data in Rai et al. (1999), it is estimated that initial [Am] is below the respective solubility limit, but maybe by a factor <5.	B
II-i SDB	The centrifugation (7000rpm / 90 min) and followed by filtration through 0.1 and 0.22µm Millipore filters is indicated.	C/D
II-j SDB	A reaction time ranged from 23 days to 74days. This reaction time is reasonably long.	C/D
II-k REF	Agitation is carried out by shaken at 120 strokes/min.	A/B
II-l REF	No substantial variation of initial Am concentration is indicated.	C/D
II-m REF	The quality of reaction vessel is not reported.	C/D
II-n SDB	No replicates are reported. But error estimates are reported.	C
REF	Uncertainties are based on error propagation, not on replicate measurements.	
II-o REF	Solution/solid ratio and reaction time are varied.	B

Data table Am/7: REF: Kim et al.(1994)

JNC-SDB version 2 – DATA: Am /Mudstone, # 53965 – 53966

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: it is indicated that no information about phase separation is given.	No
REF	No further information is available.	unreliable

Data table Am/8: REF: Konishi et al. (1988) JNC-SDB version 2 – DATA: Am / Mudstone, # 54003 – 54004 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 is provided.	class 1
II-a REF	The loam is reported as mineral's content. Takadate loam (CEC: 10~ 30 meq/100g and specific surface area 130cm ² /g) and Hachinohe loam (30~ 135 meq/100g and 60cm ² /g) are provided (Konishi et al.1986).	B
II-b SDB	Final pH value is reported (after a contact time of 7 days, which can be assumed to be enough for reaching equilibrium).	A
II-c SDB REF	Experiments are done under oxidizing conditions. Moreover, Am is not a redox-sensitive element.	A/B
II-d SDB REF	The initial composition is reported (deionized water). The final solution composition can be estimated based on mineral and initial solution composition.	C/D
II-e SDB	A room temperature is reported.	A/B
II-f SDB REF	A W/S ratio is not reported. No further information about W/S ratio.	C/D
II-g SDB	The sorption value cannot be evaluated, because of the lacking W/S ratio.	C/D
II-h SDB REF	The final Am concentrations are between 2×10^{-9} - 9×10^{-9} mol/L. Based on the data in Rai et al. (1999), it is estimated that initial [Am] is below the respective solubility limit, but maybe by a factor <5.	B
II-i SDB	Centrifugation at 39000g is reported as separation method.	B
II-j SDB	Contact time is 7 days. This reaction time is reasonably long.	C/D
II-k REF	There is no information about the agitation method.	C/D
II-l REF	No isotherms and no variation of W/S ratio have been performed.	C/D
II-m REF	The material of the vessel is not reported.	C/D
II-n SDB	The replicate is reported to one. No error estimates are reported.	D
II-o SDB	Two pH values are varied (6.0 to 6.5).	C

Data table Am/9: REF:Legoux et al.(1992) JNC-SDB version 2 – DATA: Am /Mudstone, # 55991 – 55994 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	Tables with K_d are given.	class 1
II-a SDB	Four soils with known mineral composition are indicated. CEC value and specific surface area are reported.	A
II-b SDB REF	Initial and final pH values are indicated. No use of any pH-buffer is reported.	A
II-c SDB REF	It is indicated that no redox conditions are reported. There is no information about Eh. Experiments are carried out with Am (III). No reducing agents are added to the experiment and no inert gas atmosphere is reported. Therefore it is assumed that the experiment is conducted under ambient conditions. Moreover, Am is not redox-sensitive element.	A/B
II-d REF	The final solution composition is reported.	A/B
II-e SDB	A temperature is not reported.	C/D
II-f SDB	Solution/solid ratio is 10mL/g. The used mass of 1g soil (A, B, C, D) has a surface area of about 6.6 to 14.7m ² .	A/B
II-g SDB	The sorption value is between 99.93% and 99.94% (calculated with W/S and K_d values).	C/D
II-h SDB REF	Initial [Am] is 1.3×10^{-7} M. Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the initial [Am] are below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Am).	B
II-i SDB	The centrifugation is performed at 4000rpm followed by ultrafiltration through 0.025 and 0.002μm Millipore filters is indicated.	A
II-j SDB	A reaction time of 2 days is indicated. This reaction time is reasonably long.	C/D
II-k REF	Samples are agitated continuously.	A/B
II-l REF	No isotherms, no variation of the Am concentration is indicated.	C/D
II-m REF	The experiments are carried out in polypropylene vessels. It is reported sorption to the vessel wall has been corrected for. No information about the correction procedure is available. It is assumed that the correction is based on the data obtained of a blank experiment.	C/D

II-n	REF	The reported error represents the standard deviation of the average of at least four experimental repetitions.	A
II-o	REF	No parameter variation is indicated.	D

Data table Am/10: REF: Tanaka et al. (1996)

JNC-SDB version 2 – DATA: Am /Mudstone, # 60389 – 60394

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: it is indicated that no information on initial and final Eh, final solution composition and atmosphere/ redox condition are given.	No
REF	No further information is available. Americium is not redox sensitive.	unreliable

Data table Am/11: REF: Tanaka and Muraoka (1999)

JNC-SDB version 2 – DATA: Am /Mudstone, # 62326-62328

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 REF	It is indicated that K_d values are scanned from a graphical presentation. The K_d –axis is in logarithmic form.	class 5
II-a SDB	The solid phases are reddish soil, yellowish soil and ando soil. It is reported CEC (reddish soil: 8.7 meq/100g, yellowish soil: 5.2meq/100g, ando soil: 17.2 meq/100g). Specific surface area is not reported. Physico-chemical properties of the sedimentary samples are reported.	A
II-b SDB	The initial and final pH values are given.	A
II-c SDB	It is reported that experiments are done under air; i.e., under oxidizing conditions. Experiments are carried out with Am (III). Also, Am is not a redox-sensitive element.	A/B
II-d REF	Physico-chemical properties of the equilibrated solution are reported.	A/B
II-e SDB	Temperatures of 25°C by using a water jacket are reported.	A/B
II-f SDB	Solution/solid ratios are 20mL/g.	

REF	Solid masses of 0.5g are added to a liquid volume of 10 mL. The used mass minerals may be considered enough surface area compared to that of the vessel.	A/B
II-g SDB	Based on the information given in the JNC-SDB, all sorption values are calculated to >99.8% sorbed.	C/D
II-h SDB REF	An initial [Am] of 3.27×10^{-7} M is indicated. Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the experiments are considered to be below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Am).	B
II-i SDB	The phase separation is carried out by Millipore filters of 0.45 μ m pore diameter.	C/D
II-j SDB	A reaction time of 7 days is indicated. This reaction time is reasonably long.	C/D
II-k REF	The sample is gently agitated on a shaker at 60 rpm for 7 days.	A/B
II-l REF	No variation is indicated for either W/S or [Am].	C/D
II-m REF	The material of the vessel is not reported.	C/D
II-n REF	Error of K_d is not reported. No replicated are performed.	D
II-o REF	No parameter variation is indicated.	D

Data table Am/12: REF: Tanaka and Muraoka (1998)

JNC-SDB version 2 – DATA: Am /Mudstone, # 62367 - 62369

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	Tables with K_d are given.	class 1
II-a SDB	CEC and chemical composition are reported about the ando soil, yellowish soil and reddish soil.	B
REF	Humic substance and humic acid are reported. Surface area are not reported.	
II-b SDB	Initial pH values and final pH values (as range < 1 pH unit) are reported.	B
II-c SDB	It is reported that experiments are done under air; i.e., under oxidizing conditions. Also, Am is not a redox-sensitive element.	A/B
II-d SDB	Physico-chemical properties of the equilibrated solution are reported.	A/B
II-e SDB	A temperature of 25°C is reported.	A/B

II-f	SDB	Solution/solid ratio is 20mL/g.	A/B
	REF	The used mass of 0.5g soil is added to liquid volumes (de-ionized water) of 10mL. It is assume that enough solid had been added to each vessel.	
II-g	SDB	The sorption values are >99.64 % (calculated with W/S and K_d values).	C/D
II-h	SDB	An initial [Am] of 3.27×10^{-7} M is indicated.	
	REF	Based on thermodynamic calculations with PHREEQC (database: JNC-TDB_011213c2), the experiments are considered to be below the solubility limit (but it is not clear by how much, due to the uncertainty in initial concentration as well as in solubility data for Am).	B
II-i	SDB	The 5000MWCO filters are used for phase separation.	B
II-j	SDB	A reaction time of 7 days is indicated.	
	REF	Identical (similar) results are obtained with different reaction times (>48 hours).	A/B
II-k	REF	The sample is shaking for 7 days.	A/B
II-l	REF	No isotherms, no variation of the Am concentration is indicated.	C/D
II-m	REF	The reaction vessel is made from teflon. Corrections for sorption on vessel walls are not mentions.	B
II-n	SDB	Error of K_d is not reported. And no replicated are performed.	D
II-o	REF	No parameter variation is indicated.	D

Data table Am/13: REF: Tanaka et al. (1999)

JNC-SDB version 2 – DATA: Am /Mudstone, # 62810 - 62814

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: it is indicated that no information on phase separation is given.	No
REF	No further information is available.	unreliable

Data table Am/14: REF: Baston et al., (1998) JNC-SDB version 2 – DATA: Am /Bentonite, # 65940 – 65945 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	Tables with K_d are given.	class 1
II-a SDB REF	The solid phase is indicated as Kunigel-V1. The surface area is $6.80\text{m}^2/\text{g}$. The concentration of sites $2.88 \times 10^{-2} \text{ mol dm}^{-3}$.	A
II-b SDB REF	Final pH values are reported. No use of any pH-buffer is reported. The pH value is monitored every 7 days, the pH adjusted back to the appropriate value.	A
II-c SDB REF	Experiments are performed under N_2 . The oxidation state of Am is reported as III. Final Eh values are provided, as well as the reducing agent used ($\text{Na}_2\text{S}_2\text{O}_4$) at an initial concentration of $2.5 \times 10^{-3} \text{ M}$. O ₂ levels are reportedly <1 ppm. All solutions are de-oxygenated by bubbling an argon(96%) /hydrogen(4%) mixture through them before posting into the glovebox. Also, Am is not a redox sensitive element.	A/B
II-d SDB REF	A NaCl, NaHCO_3 is reported as input solution; main solution compositions are indicated in the additional file “solution composition”. Samples are filtered using a 10000MWCO filter prior to analysis.	A/B
II-e SDB	A temperature of 60°C is reported.	A/B
II-f SDB	It is indicated that W/S ratio of 20 mL/g had been used, but that the specific solid mass and solution volume are not reported. Assuming that the solution volume is $\geq 20 \text{ mL}$ would mean a corresponding solid mass of at least 1 g. This is accepted as reasonable.	A/B
II-g SDB	Based on the information provided in the JNC-SDB, all K_d values can be calculated to correspond to %-sorbed values >99%.	C/D
II-h SDB	$1.2 \times 10^{-10} \text{ M}$ is indicated as initial Am concentration. Based on the data in Rai et al.(1999), as well as on speciation calculations using the thermodynamic data in Guillaumont et al.(2003), it is estimated that the initial Am concentration is below the respective solubility limit, but possibly by less than a factor of 5.	B
II-i SDB REF	Filtration through 10000MWCO and $45\mu\text{m}$ membranes, as well as centrifugation at 1100g for 2.5 h is reported. Three methods of phase separation are used: 1) centrifugation at 1100 g for 2.5	A

		h, 2) centrifugation at 1100 g for 2.5 h followed by filtration through 0.45 μm membranes, and 3) centrifugation at 1100 g for 2.5 h followed by filtration through 0.45 μm membranes and then by filtration through 10000 MWCO filters. It appears that the resulting K_d values are slightly dependent on the method of phase separation: surprisingly, the highest K_d is generally obtained with centrifugation alone, whereas filtration with 10000 MWCO membranes leads to the lowest values. However, the respective variation is of about the same magnitude as observed for different W/S. Therefore, it may be considered to be within the overall experimental uncertainties.	
II-j	SDB	A reaction time of 122 days (four months) is reported. This reaction time is reasonably long.	C/D
II-k	REF	The experiments are gently agitated on a shaker table.	A/B
II-l	SDB	No variation of W/S ratio or of the initial Am concentration is reported.	C/D
II-m	REF	The experiments are carried out in polypropylene centrifuge tubes. And corrections for sorption on vessel walls have been performed.	A
II-n	SDB REF	It is indicated that each experiment is done in duplicate. Error estimates are given for each replicate, based on analytical uncertainties.	A
II-o	SDB	No relevant parameter variation is indicated.	D

3.2 Criterion III

3.2.1 Examination of data in the JNC-SDB: Thorium

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

Reference	Solid phase (group/solids)
Lieser et al. (1990)	mudstone / glacial sediment
Legoux et al. (1992)	mudstone / soil
Östhols (1995)	other minerals / SiO ₂
Bradbury & Baeyens (2003)	Bentonite / SWy-1 montmorillonite

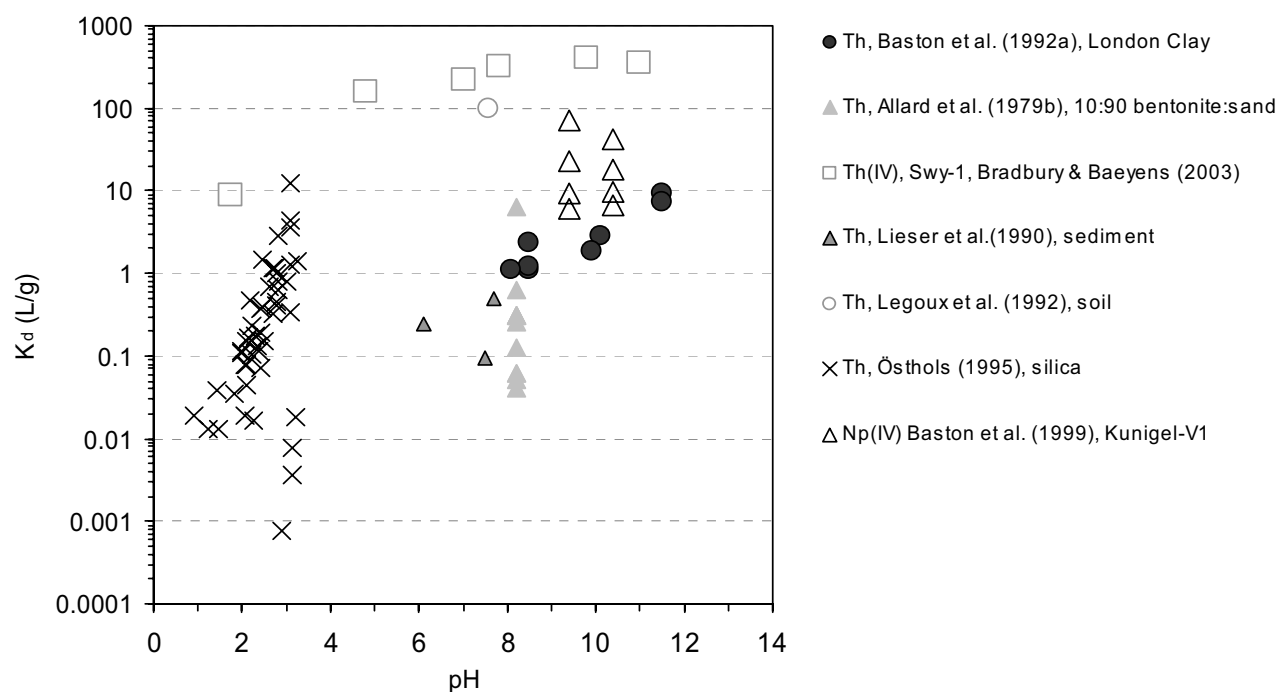


Figure 3.2.1 Overview of sorption data for Th on relevant substrates. The data by Baston et al. (1992a) refer to experiments with cement water in the absence of gluconate or degradation products, obtained after filtration through 30000 MWCO membranes. Relevant data for Np(IV) by Baston et al (1999) are also shown.

In comparison with the K_d -values obtained by Bradbury and Baeyens (2003) on pure montmorillonite (Swy-1), relatively low sorption of Th has been observed by both Allard et al. (1979) and Baston et al. (1992a), as well as Lieser et al. (1990). In all these cases, solution chemistry had been relatively complex, 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.

The data by Östhols appear to be consistent with the data by Bradbury and Baeyens (2003), considering that Th is expected to sorb on edge (i.e., oxide-type) surfaces and considering the hydrolysis behavior of Th at low-intermediate pH.

The datapoint by Legoux et al. (1992) appears to be consistent with the data by Bradbury and Baeyens (2003). On the other hand, the value measured by Legoux et al. (1992) is surprisingly high, considering the low CEC (3 meq/100 g) and the relatively complex solution chemistry in their experiments.

4. Summary

The QA/classification of selected entries (1,056 K_d values) in the JNC-SDB, especially of K_d values for mudstone systems to use in the K_d -derivation exercise for Horonobe rocks, was done following the classification guideline defined in our previous report.

Based on the results of the second application of classification guideline to K_d data for mudstone systems in the chapter 3, and the results of the application study of the JNC-SDB to K_d -setting in Horonobe rocks, 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, these approaches should be repeatedly tested through the application to various rocks and geochemical conditions.

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Appendix

Summary tables for K_d classification

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N.C. = not conclusive, N.E. = not evaluated, m.i. = missing information																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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A.m		I - Completeness of documentation and type of K _c				II - Technical and scientific quality of reported data																		III - Consistency		Operator	Date	Classification Guideline				
Rating ▼ I-a: yearNo, I-b: class 1-4		Checkpoints ▼ level: A-D (numerical value: 3-0) / unreliable Rating ▼ class 1-4 / unreliable																														
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II.a solid phase	II.b pH	II.c redox conditions	II.d solution composition	II.e temperature	II.f S/W	II.g sorption value	II.h initial [RN]	II.i phase separation	II.j reaction time	II.k agitation	II.l RN loading	II.m reaction vessels	II.n error estimates	II.o parameter variation	Rating II	comment/rating										
																					total value	class										
44238	Barney and Anderson (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
44239	Barney and Anderson (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
44240	Barney and Anderson (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
44241	Barney and Anderson (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
44242	Barney and Anderson (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
44243	Barney and Anderson (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
44322	Barney and Brown (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
44323	Barney and Brown (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
44324	Barney and Brown (1979)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
46684	Baston et al. (1995b)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	A/B	3	C/D	0	C/D	0	A	3	B	2	A	3	A	3	B	2	125	class 2	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
46685	Baston et al. (1995b)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	A/B	3	C/D	0	C/D	0	A	3	B	2	C/D	0	C/D	0	B	2	141	class 2	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
46686	Baston et al. (1995b)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	A/B	3	C/D	0	C/D	0	A	3	C/D	0	C/D	0	C/D	0	B	2	125	class 2	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
46687	Baston et al. (1995b)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	A/B	3	C/D	0	C/D	0	A	3	B	2	C/D	0	C/D	0	B	2	141	class 2	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50002	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50003	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50004	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50005	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50006	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50007	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50008	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50009	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50010	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50011	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50012	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50013	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50014	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50015	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50016	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50017	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50018	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50019	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50020	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50021	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50022	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50023	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50024	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	B	2	C/D	0	C/D	0	B	2	88	class 4	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50025	Daniels (1981)	yes	yes	yes (can be used)	class 1	C/D	0	A	3	A/B	3	C/D	0	A/B	3	C/D	0	C/D	0	unreliable									unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)
50977	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50978	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50979	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50980	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50981	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50982	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50983	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50984	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50985	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50986	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50987	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50988	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50989	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50990	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50991	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50992	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50993	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50994	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50995	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50996	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50997	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							
50998	Erdal (1980)	yes	no	no (can not be used)																		unreliable	Y. Saito(JAEA)	October 2007	Revision 4b (May 19, 2005)							

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[illegible]

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
物質の量	モル	mol
光度	カンデラ	cd

表2. 基本単位を用いて表されるSI組立単位の例

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

表5. SI 接頭語

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

表3. 固有の名称とその独自の記号で表されるSI組立単位

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

- (a) ラジアン及びステラジアンの使用は、同じ次元であっても異なった性質をもった量を区別するときの組立単位の表し方として利点がある。組立単位を形作るときいくつかの用例は表4に示されている。
- (b) 実際には、使用する時には記号rad及びsrが用いられるが、習慣として組立単位としての記号“1”は明示されない。
- (c) 測光学では、ステラジアンの名称と記号srを単位の表し方の中にそのまま維持している。
- (d) この単位は、例としてミリセルシウス度m℃のようにSI接頭語を伴って用いても良い。

表4. 単位の中に固有の名称とその独自の記号を含むSI組立単位の例

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

表6. 国際単位系と併用されるが国際単位系に属さない単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1 h=60 min=3600 s
日	d	1 d=24 h=86400 s
度	°	1°=(π/180) rad
分	′	1′=(1/60)°=(π/10800) rad
秒	″	1″=(1/60)′=(π/648000) rad
リットル	l, L	1 l=1 dm ³ =10 ⁻³ m ³
トン	t	1 t=10 ³ kg
ネーパ	Np	1 Np=1
ベル	B	1 B=(1/2) ln10 (Np)

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

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

表8. 国際単位系に属さないが国際単位系と併用されるその他の単位

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

表9. 固有の名称を含むCGS組立単位

名称	記号	SI 単位であらわされる数値
エルグ	erg	1 erg=10 ⁻⁷ J
ダイン	dyn	1 dyn=10 ⁻⁵ N
ボアズ	B	1 B=1 dyn・s/cm ² =0.1 Pa・s
ストークス	St	1 St=1 cm ² /s=10 ⁻⁴ m ² /s
ガウス	G	1 G ≐10 ⁻⁴ T
エルステッド	Oe	1 Oe ≐ (1000/4π) A/m
マクスウェル	Mx	1 Mx ≐10 ⁻⁸ Wb
スチルブ	sb	1 sb =1 cd/cm ² =10 ⁴ cd/m ²
ホト	ph	1 ph=10 ⁴ lx
ガリ	Gal	1 Gal =1 cm/s ² =10 ⁻² m/s ²

表10. 国際単位に属さないその他の単位の例

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

