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## **Development of JAEA Sorption Database (JAEA-SDB) : Update of Sorption/QA Data in FY2017**

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JAEA-Data/Code

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**Development of JAEA Sorption Database (JAEA-SDB) :**

**Update of Sorption/QA Data in FY2017**

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Sorption of radionuclides (RNs) in buffer materials (bentonites), rocks and cementitious materials is one of key processes in the safe geological disposal of radioactive waste, because migration of RNs in these barrier materials is expected to be retarded by sorption processes. It is therefore necessary to understand the sorption process and develop database compiling reliable data and mechanistic/predictive models, so that reliable parameters can be set under a variety of geochemical conditions relevant to performance assessment (PA). For this purpose, Japan Atomic Energy Agency (JAEA) has developed databases of sorption parameters in bentonites, rocks and cementitious materials. The sorption database (SDB) was firstly developed as an important basis for the H12 PA of high-level radioactive waste disposal, and has been provided through the Web. JAEA has been continuing to improve and update the SDB in view of potential future data needs, focusing on assuring the desired quality level and testing the usefulness of the databases for possible applications to PA-related parameter setting.

The present report focuses on updating of the sorption database (JAEA-SDB) as basis of integrated approach for PA-related distribution coefficient ( $K_d$ ) setting and mechanistic sorption model development. This includes an overview of database structure and contents.  $K_d$  data and their quality assurance (QA) results are updated by focusing the following systems as potential needs extracted from our recent activities on the  $K_d$  setting and mechanistic model development;

- i)  $K_d$  data for clay systems to develop and validate the mechanistic sorption model
- ii)  $K_d$  data for sedimentary rocks to enhance dataset covering wider ranges of geochemical conditions for  $K_d$  parameter setting
- iii)  $K_d$  data for cementitious materials to enhance dataset for  $K_d$  parameter setting

As a result, 4,256  $K_d$  data from 30 references were added, total number of  $K_d$  values in the JAEA-SDB reached about 63,000. The QA/classified  $K_d$  data reached about 69% for all  $K_d$  data in JAEA-SDB. The updated JAEA-SDB is expected to make it possible to give a basis for next-step PA-related  $K_d$  setting.

Keywords: Database, Sorption,  $K_d$ , Bentonite, Rock, Cementitious Materials, Parameter Setting, Geological Disposal

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<sup>※</sup> Inspection Development Company Ltd.

JAEA 収着データベース(JAEA-SDB)の開発：  
2017 年度における収着データ/信頼度情報の拡充

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(2017 年 12 月 21 日受理)

放射性廃棄物地層処分の性能評価において、放射性核種の緩衝材（ベントナイト）、岩石及びセメント系材料中での収着現象は、その移行遅延を支配する重要な現象の一つである。これら収着現象の理解、信頼性の高い収着データを集約したデータベース、並びに現象論的モデル/評価手法の開発が、性能評価において様々な地球化学条件を考慮して信頼性の高い核種移行パラメータ設定を行う上で重要となる。この目的のために、日本原子力研究開発機構では、ベントナイト、岩石及びセメント系材料を対象として、収着パラメータに関するデータベース開発を進めている。この収着データベース（SDB）は、第 2 次取りまとめを契機として最初のデータベースを整備し、ホームページでの公開を進めてきた。さらに、今後の性能評価におけるニーズへ対応するため、データベースに含まれるデータの信頼度評価、実際の地質環境に対するパラメータ設定におけるデータベース適用等に着目して、データベースの改良・更新を継続的に実施してきた。

今回、性能評価における収着分配係数（ $K_d$ ）設定のための統合的手法の構築の基礎として、収着データベース（JAEA-SDB）のデータ拡充を行った。本報告では、はじめに JAEA-SDB のデータベースの構造と内容の概要を確認したうえで、 $K_d$  設定や収着モデル開発の最近の取り組みにおいて抽出された課題として抽出された以下に示す 3 つの系に着目して実施した、 $K_d$  データと信頼度情報の拡充について報告する。

- i) 収着モデルを開発・確証するための粘土系の  $K_d$  データ
- ii) 幅広い地球化学条件に対応したデータセットを拡充するための堆積岩系の  $K_d$  データ
- iii) パラメータ設定に用いるデータセットを拡充するためのセメント系材料の  $K_d$  データ

今回の更新において、30 の文献から 4,256 件の  $K_d$  データとその信頼度情報が追加され、JAEA-SDB に含まれる  $K_d$  データは約 63,000 件となり、全データのうちの約 69%のデータに対して信頼度情報が付与されたこととなる。今回更新された JAEA-SDB によって、今後の性能評価における収着パラメータ設定に向けて、有効な基盤情報を提供するものと期待される。

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## 1. Introduction

Sorption of radionuclides (RNs) on buffer materials (bentonite), host rocks (rock matrix) and cementitious materials is one of key processes in the safe geological disposal of radioactive waste, because migration of RNs in these barrier materials is expected to be retarded by sorption processes. The magnitude of sorption of RNs on these barrier materials, expressed normally by a distribution coefficient ( $K_d$ ), depends critically on relevant geochemical conditions<sup>1-2)</sup>. It is therefore necessary to understand the detailed processes of sorption on these barrier materials under wide ranges of geochemical conditions, and to develop the database containing extensive compilation of sorption  $K_d$  data and the mechanistic/predictive model/database, so that reliable parameters can be set under a variety of geochemical conditions relevant to performance assessment (PA). Because of the conditional nature of sorption data,  $K_d$  values to be used in PA calculations need to correspond to the specific conditions that characterize the respective PA-setting. In addition, geochemical variability or uncertainty, and their effect on  $K_d$ , usually have to be considered for reference and alternative scenarios in PA, as discussed in NEA<sup>1)</sup>. Since it is not feasible to measure  $K_d$  values for all PA conditions, the use of existing sorption data obtained under generic experimental conditions and transferring such data to a range of PA-specific conditions is therefore a key challenge. The sorption database (SDB), containing large amount of sorption data for approximated, simplified, or generic systems, is used to  $K_d$  setting for PA conditions by taking into account any differences in substrate and geochemical conditions.

Japan Atomic Energy Agency (JAEA) has developed SDB, which were firstly developed as an important basis for the second progress report on high-level waste (H12 report)<sup>3-6)</sup>. JAEA has also developed the sorption database for the second progress report on trans-uranic (TRU) waste (TRU-2 report)<sup>7-9)</sup>. JAEA has been and is continuing to improve and update the SDB in view of potential future data needs, focusing on;

- 1) updating of sorption data<sup>10-14)</sup>
- 2) assuring the desired quality level for SDB<sup>12, 14-18)</sup>
- 3) testing and applying of the SDB to parameter-setting<sup>15-25)</sup>

The web-based sorption database system (JAEA-SDB) has been developed to utilize quality assuring procedure and to allow effective application for parameter setting<sup>26)</sup>(<https://migrationdb.jaea.go.jp/>).

The  $K_d$  setting approach is needed to apply for various rock types and geochemical conditions, and to evolve from site-generic to site-specific stages by considering site-specific information obtained in forthcoming site investigation stage. Such comprehensive  $K_d$  setting approach applicable for various conditions and situations was developed based on international state of the art knowledge by integrating three different methods as follows (Figure 1.1);

- 1) experimental data acquisition for specific/reference conditions
- 2) extraction and conversion from existing sorption and diffusion data through SDB
- 3) prediction by mechanistic sorption and diffusion model

This transfer can be done through expert judgment and semi-quantitative way, by considering difference in e.g. surface sites, speciations, competitive reactions, etc.<sup>1, 19-20, 23, 27-28)</sup>. The thermodynamic sorption model (TSM) makes it possible to estimate  $K_d$  variations directly, based on mechanistic understanding, as shown in NEA<sup>1)</sup>. JAEA has developed the integrated sorption/diffusion (ISD) database in combination with

thermodynamic sorption and diffusion model, and tested to explain the sorption and diffusion behavior of various RNs with a complex chemistry in compacted bentonites<sup>29-31)</sup>. JAEA has also tested these  $K_d$  setting approach for the derivation of  $K_d$  values and their uncertainties for rock matrix such as Horonobe mudstones and generic granites<sup>19-25)</sup>.

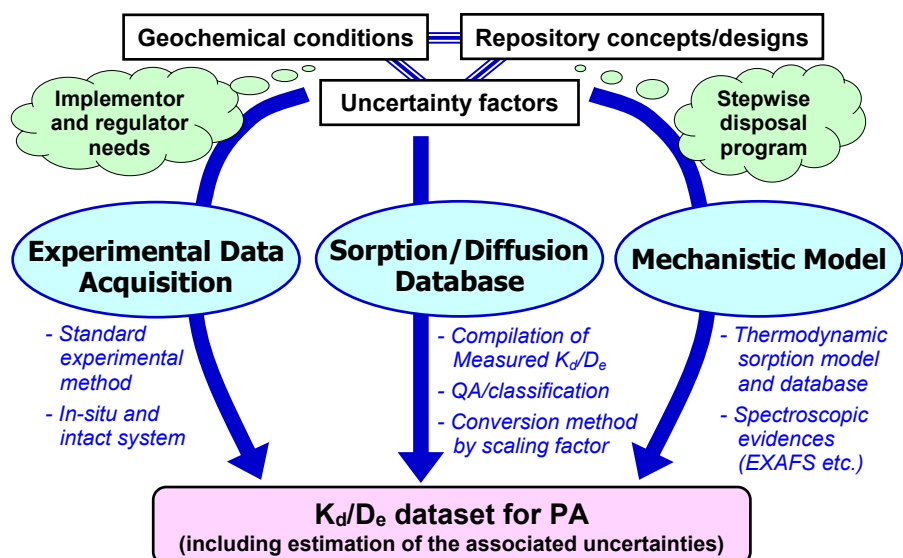


Figure 1.1 Integrated approach for sorption/diffusion parameter setting for PA

The present report focuses on updating of the JAEA-SDB as basis of integrated approach for PA-related  $K_d$  setting and mechanistic sorption model development. This includes an overview of database structure and contents.  $K_d$  data and their quality assurance (QA) results are updated by focusing the following systems as potential needs extracted from our recent activities on the  $K_d$  setting and mechanistic model development;

- $K_d$  data for clay systems to develop and validate the mechanistic sorption model
- $K_d$  data for sedimentary rocks to enhance dataset covering wider ranges of geochemical conditions for  $K_d$  parameter setting
- $K_d$  data for cementitious materials to enhance dataset for  $K_d$  parameter setting

## 2. System, functions and contents of JAEA-SDB

### 2.1 Overview and status of JAEA-SDB

The JAEA-SDB is a compilation of experimental  $K_d$  data for key RNs sorption on bentonite buffer, various rocks, cementitious materials and soils related to the radioactive waste disposal, determined by batch sorption experiments, including  $K_d$  values and associated experimental information. It is implemented in database software that allows quick searching/plotting of data as a function of selected key parameters. The contents, functions and systems are briefly summarized in Table 2.1. As pointed out in NEA sorption database project<sup>1)</sup>, the sorption database cannot be used blindly in PA-related  $K_d$  setting, without understanding and checking carefully the experimental details, because SDB includes a great variety of  $K_d$  obtained under various conditions and with different reliability levels. The JAEA-SDB has been therefore developed by focusing the following points, so that reliable and respective data relevant to PA conditions can be extracted from SDB in effective way;

- 1) detailed experimental conditions to understand and check the method and conditions (see 2.2)
- 2) QA/classification scheme to check the reliability (see 2.3)

Table 2.1 Summary of contents, functions, and systems of JAEA-SDB system and content

Contents/functions	Brief description for status
Number of $K_d$ values/references	$K_d$ ; 62,977 (4,909 was added in this update or revise*) Reference ; 724 (30 references were added in this update*)
Elements	78 elements; 1 <sup>st</sup> group (related to HLW disposal); Ac, Am, Bi, Cm, Cs, Nb, Ni, Np, Pa, Pb, Pd, Po, Pu, Ra, Sb, Se, Sm, Sn, Tc, Th, U, Zr 2 <sup>nd</sup> group; Ag, Ba, Ca, Ce, Cl, Co, Eu, Fe, I, Mn, Mo, Na, Nd, Ru, Sr, Zn Minor group; 40 elements
Solid phase	Bentonite (clay minerals); Rocks – 5 groups; Basaltic rock, granitic rock, mudstone, sandstone, tuff; Other minerals (Fe, Al-oxides/hydroxide, calcite, etc.); Cementitious materials (cement/concrete); Soils; Having special influence (grout, organic substance, etc.)
Search parameters	Element, solid phase group Detailed – Solid phase, water type, pH, Eh, ionic strength, temperature, liquid/solid ratio, contact time, initial concentration, separation method, atmosphere/redox condition
Graphing/data evaluation	$K_d$ plot as a function of ; pH, Eh, ionic strength, temperature, liquid/solid ratio, contact time, initial concentration; Grouping function to evaluate multi-parameter dependence; Statistical data evaluation; Grouping of $K_d$ data related to perturbations
QA/classification	QA information evaluated by QA guideline, and related evidences 43,538 $K_d$ (about 69% of total $K_d$ )* for key RNs have been evaluated.
Database systems	- Web application based database (since 2009) - Microsoft Access® database (since 2003/stand-alone/limited functions)

\*, Contents and functions updated or revised in this report.

## 2.2 Main data table and contents of JAEA-SDB

Main data table of JAEA-SDB contains  $K_d$  values and a large number of additional key information describing the experimental conditions and procedures pertinent to each  $K_d$  value associated, such as solid phase properties, solution composition and pH, RN redox state and initial concentration, liquid/solid ratio, and reference information, etc., as shown in Table 2.2. The hierarchical structure comprising of primary and detailed information is used to allow effective database operations.

Table 2.2 Main data table of JAEA-SDB (1/2)

Category	Parameters and notes recorded		Unit	Remarks
No.	Save No.		-	Number for managing data record
Elements	Element		-	Chemical symbol (basic search condition)
	Redox		-	Valency
Solid phase	Solid phase group		-	Solid phase group (basic search condition)
	Solid phase		-	Name of solid phase as rocks, clay minerals, minerals, etc.
	Detailed Info.	Specific surface area	m <sup>2</sup> /g	
		CEC	meq/100 g	Cation exchange capacity
		Chemical/mineral composition	-	
		Note	-	Particle size, source, name, conditions and methods for sample preparation, etc.
Liquid/solid ratio	Liquid/solid		mL/g	Liquid to solid ratio
	Detailed Info.	Liquid	mL	Amount of liquid phase
		Solid	g	Amount of solid phase
Liquid phase	Water type		-	Type and name of solution/groundwater
	Detailed Info.	Ca	ppm	Final or initial composition (concentration)
		Na	ppm	
		K	ppm	
		Mg	ppm	
		Cl	ppm	
		HCO <sub>3</sub>	ppm	HCO <sub>3</sub> <sup>-</sup> + CO <sub>3</sub> <sup>2-</sup>
		SO <sub>4</sub>	ppm	
		F	ppm	
		SiO <sub>2</sub>	ppm	
		Fe	ppm	
		NO <sub>3</sub>	ppm	
		ClO <sub>4</sub>	ppm	
		Ionic strength	mol/L	Calculated from each ion concentration
		DOC	ppm	Concentration of dissolved organic carbon
		Note	-	Details of type, name and preparation methods for test solution
	pH init		-	Initial pH
	pH end		-	Final pH
	Eh init		mV	Initial Eh
	Eh end		mV	Final Eh
Experimental condition	Atm/redox condition		-	Atmosphere, reducing agent, etc.
	C init		mol/L	Initial concentration of nuclide
	Temp		°C	
	Contact time		d	
	Separation		-	Solid-liquid separation method

Table 2.2 Main data table of JAEA-SDB (2/2)

Category	Parameters and notes recorded		Unit	Remarks
Distribution coefficient	$K_d$		$m^3/kg$	Distribution coefficient
	Detailed Info.	Error	$m^3/kg$	
		Type of information	-	Type of $K_d$ value reported, such as table, graph plot, etc.
	Replicates, n		-	Replicate numbers of experiments
Literature	Reference		-	Reference as source of data
	Detailed Info.	Author	-	
		Year	-	
		Title	-	
		Journal	-	
		Publisher	-	
		Vol	-	
		No	-	
		Page	-	
	Note		-	Additional information on related reference such as detailed report
Others	Additional Information		-	Additional explanation related to measurement of distribution coefficient

### 2.3 Scheme and criteria for QA/classification of $K_d$ in JAEA-SDB

As described in 2.1, it is important to assess the reliability of a wide variety of  $K_d$  data in SDB for PA-related  $K_d$  setting. The reliability of  $K_d$  values in the JAEA-SDB has been assessed using the following three main criteria;

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

- the documentation of each entry is detailed enough to allow further examination in the Criteria II.
- the reliability of  $K_d$  data input ; available in table format in comparison to graph format.

**Criteria II) Quality of reported data:**

- the appropriateness of the experimental conditions and procedures to produce reliable  $K_d$  data from a technical and scientific point of view.

**Criteria III) Consistency of data:**

- the examination of the level of internal consistency in SDB by comparing other  $K_d$  values in similar systems.

The QA/classification guideline describing details of each criteria and overall classification scheme is shown in Appendix<sup>15)</sup>, and is briefly summarized in Table 2.3.

In accordance with the guideline, Criteria I and key checkpoints II-b, II-c, II-d, II-h in Criteria II 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. The three Criteria I–III are evaluated separately, and the all results can be referred in JAEA-SDB<sup>12)</sup>. The JAEA-SDB uses the QA level (Class 1–6), classified in accordance with the total sum of points obtained for Criteria II, and the result of “unreliable” evaluation in Criteria I and II, as main reliability information. All results and evidences of Criteria I and II are also recorded in tabular form, and can be referred as PDF format in JAEA-SDB to keep the traceability. The results pertaining to Criteria III are discussed subsequently and illustrated in the form of plots of  $K_d$  vs. a relevant master variable (typically pH), and can be referred as PDF format in JAEA-SDB.

Table 2.3 Reliability information table of Sorption Database (JAEA-SDB)

QA-Criteria / checkpoints		Brief description	SDB parameters related	Rating	
Criteria I) Completeness of documentation and type of $K_d$ information:					
I-a.1	Completeness of information	Completeness of key parameter fields as screening for further classification	Key parameters as marked * below	Yes/No	
I-a.2	Information of units	Completeness of units for $K_d$ data, etc.	$K_d$ , same as above	Yes/No	
I-b	Type of $K_d$ information	Classification of level depending on table/figure, $K_d$ /%-sorbed, linear/log	Type of information	Class 1–6	
Criteria II) Quality of reported data:				Rating	Weighting factor
II-a	Solid phase	Sufficient characterization of solid phase ; major minerals, impurities, surface characteristic	Solid phase, specific surface area, CEC	A, B, C/D	×2
II-b*	Adjustment and control of pH*	Appropriate control of pH by acid-base and pH buffers	pH init, pH end	A, B, C, D	×8
II-c*	Redox conditions*	Appropriate control of redox condition, reducing agent	Atm/redox condition, redox	A/B, C/D	×8
II-d*	Final solution composition*	Composition from direct measurements of thermodynamic calculations	Solution composition	A/B, C/D	×8
II-e	Temperature	Control to keep constant temperature	Temp	A/B, C/D	×1
II-f	Liquid/solid ratio and particle size	Surface area of solid phase, weight of solid phase to avoid influence by vessel walls	Liquid/solid, specific surface area	A/B, C/D	×2
II-g	Sorption value	Appropriate experimental design to avoid sorption values near 0% and 100%	$K_d$ , liquid/solid	A, B, C/D	×2
II-h*	Initial RN concentration*	Confirmation of initial concentration setting less than solubility limit. (Calculation and experimental result under similar condition is applied.)	C init, solution composition, pH	A, B, C/D	×8
II-i*	Phase separation*	Appropriate phase separation method	Separation	A, B, C/D	×8
II-j*	Reaction time*	Confirmation for equilibrium by kinetic experiments, reasonably long reaction time	Contact time	A/B, C/D	×2
II-k	Agitation method	Appropriate agitation method	-	A/B, C/D	×1
II-l	RN loading	Appropriate RN loading to keep linear sorption, isotherm measurement	Liquid/solid, C init,	A, B, C/D	×2
II-m	Reaction vessels	Appropriate material for vessels, correction by blank tests, etc.	-	A, B, C/D	×1
II-n	Uncertainty estimates	Uncertainties based repeated experiments, error propagation	Error, replicates (n)	A, B, C, D	×2
II-o	Parameter variation	Systematic variations of key parameters	C init, pH init, pH end, liquid/solid	A, B, C, D	×8
Criteria III) Consistency of data:					
III	Evaluation of $K_d$ reliability from the perspective of consistency among data*. When there is clear mismatching with $K_d$ of another similar experimental condition and the reason is not explained, the case is classified as unreliable.		$K_d$	Reliable, unreliable	

\*, Indicates critical checkpoints with minimum requirements related with the judgment to be “unreliable”.

### 3. Updating of sorption data and its QA classification

#### 3.1 Selection of sorption data to be included in JAEA-SDB

As mentioned above, the sorption database plays important roles in PA-related  $K_d$  setting and mechanistic sorption model development. In this update, the references are therefore selected in relation to our recent activities on the mechanistic model/database development<sup>30-32)</sup> and PA-related  $K_d$  setting<sup>20-25)</sup>. Primary systems focused in this updating are key RNs in the three systems; i) clay systems, ii) sedimentary rocks, and iii) cementitious materials. Montmorillonite/bentonite, other clay minerals are targeted in relation to modeling and  $K_d$  setting for bentonite systems. Montmorillonite/bentonite is well researched clay minerals for RN sorption, and the sorption modeling such as TSM has been developed. Collecting reliable sorption data for these clay minerals lead to confirm the validity of the modeling. Sedimentary rocks are focused to enhance dataset covering a wider range of geochemical conditions and mineral compositions, etc. On the other hand, reports for RN sorption onto cementitious materials are scares compared with those for montmorillonite/bentonite and rocks. Therefore, expansion of reliable RN sorption data for cementitious materials is also needed.

Selected 30 references are listed as following, and these systems are summarized in Table 3.1. This updating is partly based on investigation of sorption data and QA evaluation for sedimentary rocks and cementitious materials as the collaborative research project between NUMO and JAEA<sup>33)</sup>.

Table 3.1 Overview of 30 references selected for updating the JAEA-SDB (1/4)

No.	Reference	Details of reference	Element	Solid phase	Solution type
1)	Aggarwal et al.(2000)	Aggarwal, S. , Angus, M. J. and Ketchen, J. : Sorption of radionuclides onto specific mineral phases present in repository cements, NSS/R312, AEA-DandR-0395 (2000).	Cl, Cs, I, Ni, Pu	HCP, CSH, ettringite, hydrotalcite/chloride	Concrete-equilibrated water, $\text{Ca(OH)}_2$ -saturated water
2)	Atkinson and Nickerson(1988)	Atkinson, A. and Nickerson, A. : Diffusion and sorption of cesium, strontium and iodine in water-saturated cement, Nuclear Technology, vol.81, pp.100-113 (1988).	Cs	HCP	$\text{Ca(OH)}_2$
3)	Bonhoure et al.(2003)	Bonhoure, I. , Wieland, E. , Scheidegger, A. M. , Ochs, M. and Kunz, D. : EXAFS study of Sn(IV) immobilization by hardened cement paste and calcium silicate hydrates, Environmental Science and Technology, vol.37, pp.2184-2191 (2003).	Sn	HCP	Artificial cement water
4)	Bradbury and Baeyens(2005)	Bradbury, M. H. and Baeyens, B. : Experimental and modelling investigations on Na-illite: Acid-base behaviour and the sorption of strontium, nickel, europium and uranyl, Nagra Technical Report, 04-02 (2005).	Eu, Ni, U	Illite	0.01 M-, 0.1 M-, 0.5 M- $\text{NaClO}_4$
5)	Ervanne et al.(2016)	Ervanne, H. , Hakanen, M. and Lehto, J. : Selenium sorption on clays in synthetic groundwaters representing crystalline bedrock conditions, Journal of Radioanalytical and Nuclear Chemistry, vol.307, pp.1365-1373 (2016).	Se	Illite, kaolinite	Synthetic groundwater
6)	Estes et al.(2012)	Estes, S. L. , Kaplan, D. I. and Powell, B. A. : Technetium sorption by cementitious materials under reducing conditions, Savannah River National Laboratory, SRNL-STI-2012-00596 (2012).	Tc	Cement, saltstone	Calcite-saturated solution
7)	Höglund et al.(1985)	Höglund, S. , Eliasson, L. , Allard, B. , Andersson, K. and Torstenfelt, B. : Sorption of some fission products and actinides in concrete systems, Materials Research Society Symposium Proceedings, vol.50, pp.683-690 (1985).	Am, Cs, I, Np, Pu, Th, U	Cement, concrete	Artificial porewater
8)	Holgersson(2009)	Holgersson, S. : Batch experiments of I, Cs, Sr, Ni, Eu, U and Np sorption onto soil from the Laxemar area, SKB report, P-09-29 (2009).	Cs, Eu, I, Ni, Np, Sr, U	Clay, gyttja, peat, sand, till	Naturel groundwater, synthetic groundwater
9)	Jan et al.(2014)	Jan, Y.-L. , Tsai, S.-C. and Li, Y.-Y. : Determination of sorption and diffusion parameters of Se(IV) on crushed granite, Journal of Radioanalytical and Nuclear Chemistry, vol.301, pp.365-371 (2014).	Se	Granite	Synthetic groundwater, synthetic seawater



Table 3.1 Overview of 30 references selected for updating the JAEA-SDB (2/4)

No.	Reference	Details of reference	Element	Solid phase	Solution type
10)	Jia and Lu(2014)	Jia, W. and Lu, S. : Effect of pH, foreign ions and temperature on radionickel sorption onto bentonite from Inner Mongolia, China, Journal of Radioanalytical and Nuclear Chemistry, vol.299, pp.1417-1426 (2014).	Ni	Na-bentonite	0.001 M-, 0.01 M-, 0.1 M-NaClO <sub>4</sub> , 0.01 M-KClO <sub>4</sub> , 0.01 M-NaCl, 0.01 M-NaNO <sub>3</sub>
11)	Li et al.(2016)	Li, S., Wang, X., Huang, Z., Du, L., Tan, Z., Fu, Y. and Wang, X. : Sorption and desorption of uranium(VI) on GMZ bentonite: effect of pH, ionic strength, foreign ions and humic substances, Journal of Radioanalytical and Nuclear Chemistry, vol.208, pp.877-886 (2016).	U	Bentonite, bentonite+humic acid	0.001 M-, 0.01 M-, 0.1 M-KCl, 0.01 M LiCl, 0.01 M-, 0.02 M-, 0.05 M-, 0.1 M-NaCl, 0.1 M-KCl+0.001 M-KH <sub>2</sub> PO <sub>4</sub> , 0.1 M-KCl+0.001 M-KHCO <sub>3</sub> , 0.1 M-KCl+0.001 M-KHSO <sub>4</sub> , distilled water
12)	Mace et al.(2007)	Mace, N., Landesman, C., Pointeau, I., Grambow, B. and Giffaut, E. : Characterisation of thermally altered cement pastes. Influence on selenite sorption, Advances in Cement Research, vol.19, No.4, pp.157-165 (2007).	Se	Cement	Not reported
13)	Missana et al.(2008)	Missana, T., Garcia-Gutierrez, M. and Alonso, U. : Sorption of strontium onto illite/smectite mixed clays, Physics and Chemistry of the Earth, vol.33, pp.S156-S162 (2008).	Sr	Smectite, illite	0.002 M-, 0.003 M-, 0.01 M-, 0.02 M-, 0.045 M, 0.05 M, 0.1 M-, 0.2 M-NaClO <sub>4</sub>
14)	Nagasaki et al.(2016)	Nagasaki, S., Saito, T. and Yang, T. T. : Sorption behavior of Np(V) on illite, shale and MX-80 in high ionic strength solutions, Journal of Radioanalytical and Nuclear Chemistry, vol.308, No.1, pp.143-153 (2016).	Np	Illite, shale	Brine
15)	Ochs and Talerico(2006)	Ochs, M. and Talerico, C. : Development of models and datasets for radionuclide retention by cementitious materials, Andra report, C.RP.0BMG.06.0001A (2006).	Se	HCP	Synthetic cement water
16)	Pointeau et al.(2004a)	Pointeau, I., Landesmann, C., Giffaut, E. and Reiller, P. : Reproducibility of the uptake of U(VI) onto degraded cement pastes and calcium silicate hydrate phase, Radiochimica Acta, vol.92, pp.645-650 (2004).	U	Cement, CSH, HCP	Concrete-equilibrated water, leached cement water

Table 3.1 Overview of 30 references selected for updating the JAEA-SDB (3/4)

No.	Reference	Details of reference	Element	Solid phase	Solution type
17)	Pointeau et al.(2004b)	Pointeau, I., Landesman, C., Coreau, N., Moisan, C. and Reiller, P. : Etude de la rétention chimique des radionucléides Cs(I), Am(III), Zr(IV), Pu(IV), Nb(V), U(VI) et Tc(VI) par les matériaux cimentaires dégradés, CEA report 2004, RT DPC/SECR 03-037 indice A (2004).	Am, Zr	HCP	HCP-equilibrated water
18)	Pointeau et al.(2006)	Pointeau, I., Hainos, D., Coreau, N. and Reiller, P. : Effect of organics on selenite uptake by cementitious materials, Waste Management, vol.26, pp.733-740 (2006).	Se	HCP	Cement water
19)	Pointeau et al.(2008)	Pointeau, I., Coreau, N. and Reiller, P. E. : Uptake of anionic radionuclides onto degraded cement pastes and competing effect of organic ligands, Radiochimica Acta, vol.96, pp.367-374 (2008).	C, Cl, I	HCP	HCP-equilibrated water
20)	Schmeide et al.(2014)	Schmeide, K., Gurtler, S., Muller, K., Steudtner, R., Joseph, C., Bok, F. and Brendler, V. : Interaction of U(VI) with Äspö diorite: A batch and in situ ATR FT-IR sorption study, Applied Geochemistry, vol.49, pp.116-125 (2014).	U	Diorite	0.1 M-NaClO <sub>4</sub> , groundwater
21)	Sugiyama et al.(2008)	Sugiyama, D., Chida, T. and Cowper, M. : Laser ablation microprobe inductively coupled plasma mass spectrometry study on diffusion of uranium into cement materials, Radiochimica Acta, vol.96, pp.747-752 (2008).	U	OPC, FAC	Cement-equilibrated solution
22)	Tits et al.(2004)	Tits, J., Wieland, E., Dobler, J.-P. and Kunz, D. : The uptake of strontium by calcium silicate hydrates under high pH conditions: an experimental approach to distinguish adsorption from co-precipitation processes, Material Research Society Symposium Proceedings, vol.807, pp.689-694 (2004).	Sr	CSH	Artificial cement porewater
23)	Tits et al.(2006)	Tits, J., Iijima, K., Wieland, E. and Kamei, G. : The uptake of radium by calcium silicate hydrates and hardened cement paste, Radiochimica Acta, vol.94, pp.637-643 (2006).	Ra	CSH, HCP	Artificial cement porewater, distilled water
24)	Tits et al.(2008)	Tits, J., Fujita, T., Tsukamoto, M. and Wieland, E. : Uranium(VI) uptake by synthetic calcium silicate hydrates, Materials Research Society Symposium Proceedings, vol.1107, pp.467-474 (2008).	U	CSH	Artificial cement pore water
25)	Vilks and Miller(2014)	Vilks, P. and Miller, N. H. : Sorption studies with sedimentary rock under saline conditions, NWMO TR-2013-22 (2014).	Cu, Li, Ni, Pb, U, Zr	Limestone, Na-bentonite, shale	Brine, dilute solution

Table 3.1 Overview of 30 references selected for updating the JAEA-SDB (4/4)

No.	Reference	Details of reference	Element	Solid phase	Solution type
26)	Vilks et al.(2011)	Vilks, P., Miller, N. H. and Felushko, K. : Sorption experiments in brine solutions with sedimentary rock and bentonite, NWMO TR-2011-11 (2011).	Cu, Eu, Ni, U	Limestone, Na-bentonite, shale	Na-Ca-Cl brine
27)	Wieland et al.(1998)	Wieland, E., Tits, J., Spieler, P. and Dobler, J. P. : Interaction of Eu(III) and Th(IV) with sulphate-resisting Portland cement, Materials Research Society Symposium Proceedings, vol.506, pp.573-578 (1998).	Th	HCP	Cement water
28)	Wieland et al.(2008)	Wieland, E., Tits, J., Kunz, D. and Dähn, R. : Strontium uptake by cementitious materials, Environmental Science and Technology, vol.42, pp.403-409 (2008).	Sr	HCP	Artificial cement water
29)	Wu et al.(2015)	Wu, M.-C., Lee, C.-P., Tsai, S.-C., Liu, C.-Y., Pan, C.-H., Tsai, T.-L., Wei, H.-J. and Men, L.-C. : Study on sorption and diffusion of Sr in crushed and intact basalt and granite investigated in through-diffusion experiments, Journal of Radioanalytical and Nuclear Chemistry, vol.304, pp.435-441 (2015).	Sr	Basalt, granite	Sr(NO <sub>3</sub> ) <sub>2</sub> solution
30)	Zuo et al.(2010)	Zuo, R., Teng, Y., Wang, J. and Hu, Q. : Factors influencing plutonium sorption in shale media, Radiochimica Acta, vol.98, pp.27-34 (2010).	Pu	Shale	Groundwater

### 3.2 QA evaluation on Criteria-I and -II

This section presents the QA/classification results for  $K_d$  data conducted in this update and revises. In addition to 30 references newly selected in this update (see 3.1), the  $K_d$  data for bentonite or clay minerals whose QA evaluation was not so far performed were additionally evaluated as shown in the following list (Table 3.2.1). When the QA evaluation is performed, several data are revised. The list of revised data is shown in the Table 3.2.2. The evaluation method is described in detail in the previous report<sup>12)</sup>. 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 Criteria III are discussed (in next section 3.3) subsequently and are illustrated in the form of plots of  $K_d$  vs. a relevant master variable (typically pH), where applicable. In accordance with the established classification guideline, Criteria I and checkpoints II-b, II-c, II-d, II-h were evaluated first. Classification and final numerical rating were only completed when an entry was evaluated as reliable based on these checkpoints. Otherwise, entries were labeled “unreliable” and were excluded from further evaluation. In this report, the QA results for only Am data newly selected for this update are presented as an illustration, although all QA results can be access in JAEA-SDB.

<b>Data table Am/1: REF: Höglund et al.(1985)</b>			
JAEA-SDB version 5 - DATA: Am/cementitious materials ; cement, #92572–92609			
GUIDELINE: Revision 4b (May 19, 2005)			
<b>Checkpoint*</b>		<b>Evaluation</b>	<b>Rating</b>
<b>I-a.1</b>	SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b>	SDB	All mandatory information is provided.	Yes
<b>I-b</b>	SDB	A log graph with $K_d$ values is provided in the reference.	Class 5
<b>II-a</b>	REF	The details of concrete components are given in other reference.	C/D
<b>II-b</b>	SDB	pH is indicated for range.	B
<b>II-c</b>	SDB	The atmosphere is controlled (CO <sub>2</sub> free).	A/B
<b>II-d</b>	SDB	<ul style="list-style-type: none"> <li>• #92572–92585, #92595–92609 : The final solution major composition is given.</li> <li>• #92586–92594 : The final solution major composition is not given.</li> </ul>	C/D Unreliable
<b>II-e</b>	SDB	The temperature is controlled.	A/B
<b>II-f</b>	SDB	The S:L ratio is given, but mass is not given.	C/D
<b>II-g</b>	REF	Based on the information given in the SDB, the following sorption value are calculated; <ul style="list-style-type: none"> <li>• #92580, #92582, #92584 : <math>2\% \leq</math> or <math>95\% &lt; 98</math></li> <li>• Other datapoints : <math>0\% \leq 2</math> or <math>98\% &lt; 100</math></li> </ul>	B C/D
<b>II-h</b>	SDB	Initial Am concentrations are low enough.	A
<b>II-i</b>	SDB	The separation method is a centrifugation.	B
<b>II-j</b>	SDB	This test has been carried out to confirm the effect of concentration on partition coefficients, not judged the equilibrium state.	C/D
<b>II-k</b>	REF	The information is not available.	C/D
<b>II-l</b>	REF	The information is not available.	C/D
<b>II-m</b>	REF	No information on the used experimental vessels is given.	C/D
<b>II-n</b>	REF	No error estimation is given.	D
<b>II-o</b>	SDB	The contact time dependence is investigated.	D

\*, SDB...Information from SDB system, REF...Information from original literature

<b>Data table Am/2: REF: Pointeau et al.(2004b)</b> JAEA-SDB version 5 - DATA: Am/cementitious materials ; HCP, #92936–92947 GUIDELINE: Revision 4b (May 19, 2005)		
<b>Checkpoint</b>	<b>Evaluation</b>	<b>Rating</b>
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A log graph with $K_d$ values is presented (Figure 7).	Class 5
<b>II-a</b> SDB	Details on the used concrete samples are given. Elaborate information on the chemical and physical properties is given in Appendix 1.	A
<b>II-b</b> SDB	A final pH is indicated for all data points.	A
<b>II-c</b> SDB	It is indicated that experiments have been carried out under $N_2$ atmosphere. Further details on how redox state has been controlled are given in Appendix 2.2.	A/B
<b>II-d</b> SDB	Initial solution composition is indicated. The final solution composition is not reported in detail.	C/D
<b>II-e</b> SDB	The temperature is controlled (Appendix 2) and reported for all data points.	A/B
<b>II-f</b> SDB	A liquid/solid ratio is indicated. More than 1000 mg of solid have been added to each vessel.	A/B
<b>II-g</b> REF	No direct information on the sorption value is given. Sorption value cannot be calculated as no initial RN concentration is specified (see II-h).	C/D
<b>II-h</b> SDB	The initial RN concentration is not reported (reportedly below solubility limit).	B
<b>II-i</b> SDB	One efficient centrifugation method is indicated. Only one separation method is used.	B
<b>II-j</b> SDB REF	Reaction times of 7–37 days are indicated. Demonstration of near-equilibrium is provided (page 24).	A/B
<b>II-k</b> REF	Agitation information is available (Appendix 2.1).	A/B
<b>II-l</b> REF	No information of initial Am concentration, or variation thereof, is provided, no isotherms is recorded.	C/D
<b>II-m</b> REF	The experiments have been carried out in polypropylene vessels. Sorption of Am to the vessel wall are found to be negligible (<4%).	A
<b>II-n</b> REF	Reported uncertainties are based on 3 replicate experiments and analyses.	A
<b>II-o</b> SDB	Various parameters (solid phase, pH, chemical parameters) are varied.	A

<b>Data table Am/3: REF: Allard et al.(1982)</b> JAEA-SDB version 5 - DATA: Am/bentonite (smectite) ; bentonite, #42577, #42578 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A table with log $K_d$ is provided.	Class 1
<b>II-a</b> SDB	The well-known Wyoming bentonite MX-80 is indicated as solid phase.	A
<b>II-b</b> SDB	Initial and final pH are indicated.	A
<b>II-c</b> SDB	It is indicated that the experiments have been conducted under ambient conditions.	A/B
REF	The oxidation state of Am is indicated as +III. III	
<b>II-d</b> SDB	A synthetic groundwater is indicated, only the total carbonate and salt content are known.	C/D
REF	Based on the available information, the final solution composition can be estimated approximately.	
<b>II-e</b> SDB	It is indicated that experiments have been done at 25°C.	A/B
<b>II-f</b> SDB	A L/S ratio of 100 mL/g is indicated.	A/B
REF	It is reported that 0.2 g of solid has been added to 20 mL of liquid. Assuming a BET (outer) surface area of ca. 35 m <sup>2</sup> /g, this would result in ca. 7 m <sup>2</sup> bentonite surface per 20 mL vessel.	
<b>II-g</b> REF	Based on the information provided in the SDB, the $K_d$ value can be calculated to correspond to %-sorbed values > 98%.	C/D
<b>II-h</b> SDB	Initial Am concentration $2.3 \times 10^{-9}$ and $2.9 \times 10^{-7}$ [M] is indicated.	A B
REF	The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated; • #42577 : significantly lower than the solubility • #42578 : more than a one-fifth of the solubility	
<b>II-i</b> SDB	It is indicated that phase separation has been done by centrifugation (27000g/1 h).	B
REF	No further information is available.	
<b>II-j</b> SDB	A contact time of 6 days is indicated.	A/B
REF	A range of reaction times (6 hours–6 weeks) is used, but only one dataset (for 6 days) is reported. It can only be assumed that the kinetic experiments showed that 6 days is a reasonable reaction time.	
<b>II-k</b> REF	No information is available. For the experimental technique, reference is made to a report that has not been available for the present evaluation. It is tentatively assumed that the kinetic experiments showed appropriate equilibration.	A/B
<b>II-l</b> REF	Only one L/S ratio is and two Am concentrations are indicated.	B
<b>II-m</b> REF	The experiments have been carried out in polypropylene vessels. No correction for sorption on vessel walls is done.	B
<b>II-n</b> SDB	It is indicated that error estimation is not available.	D
REF	No further information is available.	
<b>II-o</b> SDB	Initial Am concentration is varied.	C

<b>Data table Am/4: REF: JAERI(1995)</b> JAEA-SDB version 5 - DATA: Am/bentonite (smectite) ; Na-bentonite, Ca-bentonite, #41967, #41968 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	Information for pH, initial concentration and separation method is not provided.	No

<b>Data table Am/5: REF: JAERI(1995)</b> JAEA-SDB version 5 - DATA: Am/mudstone (sedimentary rocks) ; silt, #41999 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	Information for pH, initial concentration and separation method is not provided.	No

<b>Data table Am/6: REF: JAERI(1995)</b> JAEA-SDB version 5 - DATA: Am/sandstone ; sandstone, #42015 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	Information for pH, initial concentration and separation method is not provided.	No

<b>Data table Am/7: REF: JAERI(1995)</b> JAEA-SDB version 5 - DATA: Am/Tuff ; tuff, #42031 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	Information for pH, initial concentration and separation method is not provided.	No

<b>Data table Am/8: REF: Nagasaki et al.(1994b)</b> JAEA-SDB version 5 - DATA: Am/bentonite (smectite) ; bentonite, #53680–53697 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A figure with $K_d$ [ $\text{cm}^3/\text{g}$ ] is provided.	Class 3
<b>II-a</b> SDB REF	The solid used in experiments is a well-known Kunigel V1 (Na-bentonite). From other literatures, the mineralogical characterization, CEC and specific surface area can be supposed.	A
<b>II-b</b> SDB	The initial pH is reported.	C
<b>II-c</b> SDB REF	The atmospheric condition is not reported. Am(III) is not sensitive to redox condition.	A/B
<b>II-d</b> SDB REF	Sorption measurements are carried out in distilled water. The composition of the solution can be calculated by assuming equilibrium of distilled water and Na-bentonite.	C/D
<b>II-e</b> SDB	Information for temperature is not reported.	C/D
<b>II-f</b> SDB	A L/S ratio of 5–110 mL/g is indicated. The amount of solid and specific surface area is not reported.	C/D
<b>II-g</b> REF	Based on the information provided in the SDB; • #53687, #53697 : $5 < \% < 95$ • #53692–53696 : $95 \leq \% < 98$ • Other datapoints : $98 \leq \% < 100$	A B C/D
<b>II-h</b> SDB REF	Initial Am concentration $1.0 \times 10^{-9}$ [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated, initial Am concentration for all datapoints are significantly lower than the solubility.	A
<b>II-i</b> SDB REF	It is indicated that phase separation has been done by centrifugation, filtration (0.45 $\mu\text{m}$ ) and ultra-filtration (2 nm). In the case of phase separation by centrifugation, it is considered that the sorption is affected by colloids; • #53680–53685 : ultra-filtration (2 nm) • #53686–53697 : centrifugation or filtration (0.45 $\mu\text{m}$ )	A Unreliable
<b>II-j</b> SDB	The experiments have been performed for 2 weeks.	A/B
<b>II-k</b> REF	The agitation is not performed.	C/D
<b>II-l</b> REF	The initial Am concentration is not varied.	C/D
<b>II-m</b> REF	The material of experiment container is polypropylene. The effect of sorption on the container wall is not confirmed.	C/D
<b>II-n</b> SDB	The error estimation is performed in the figure by error bar. The replicate is not reported.	C
<b>II-o</b> SDB	The L/S ratio and the separation method are varied.	D



<b>Data table Am/9: REF: Nowak(1979)</b> JAEA-SDB version 5 - DATA: Am/bentonite (smectite) ; bentonite, #94246, #94247 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A table with $K_d$ [mL/g] is provided.	Class 1
<b>II-a</b> SDB	The solid used in experiments is a bentonite. The approximate composition and CEC are reported. The specific surface area is not reported.	A
<b>II-b</b> SDB	The final pH is reported.	A
<b>II-c</b> SDB REF	The atmospheric condition is not reported. Am(III) is not sensitive to redox condition.	A/B
<b>II-d</b> SDB REF	Sorption measurements are carried out in synthetic brine. The composition of the solution can be calculated by assuming equilibrium of brine and bentonite.	C/D
<b>II-e</b> SDB	The experiments are performed at room temperature.	A/B
<b>II-f</b> SDB REF	A L/S ratio of 40 mL/g is indicated. It is reported that 0.5 g of solid has been added to 20 mL of liquid. Assuming BET surface area of 3 m <sup>2</sup> /g, surface area of solid are smaller than 5 m <sup>2</sup> .	C/D
<b>II-g</b> REF	Based on the information provided in the SDB, sorption percentage of all datapoints are $98 \leq \% < 100$ .	C/D
<b>II-h</b> SDB REF	Initial Am concentration $5.0 \times 10^{-7}$ [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated, initial Am concentration for all datapoints is higher than solubility.	Unreliable
<b>II-i</b> SDB REF	It is indicated that phase separation has been done by centrifugation (12,000g/10 min) and filtration (0.8 μm). No further information is indicated.	C/D
<b>II-j</b> SDB	The experiments have been performed for 3 weeks.	A
<b>II-k</b> REF	The agitation method is stirring.	A/B
<b>II-l</b> REF	The initial Am concentration is not varied.	C/D
<b>II-m</b> REF	The material of experiment container is not reported. The blank test is performed to correct the results for losses of Am from solution.	A
<b>II-n</b> SDB	The error estimation is not performed. The replicate is duplicates.	A
<b>II-o</b> SDB	The parameter is not varied.	D

<b>Data table Am/10: REF: Nowak(1979)</b> JAEA-SDB version 5 - DATA: Am/other minerals ; clinoptilolite, #94252, #94253 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A table with $K_d$ [mL/g] is provided.	Class 1
<b>II-a</b> SDB	The solid used in experiments is a clinoptilolite. The chemical composition and CEC are reported. The specific surface area is not reported.	A
<b>II-b</b> SDB	The final pH is reported.	A
<b>II-c</b> SDB REF	The atmospheric condition is not reported. Am(III) is not sensitive to redox condition.	A/B
<b>II-d</b> SDB REF	Sorption measurements are carried out in synthetic brine. The composition of the solution can be calculated by assuming equilibrium of brine and clinoptilolite.	C/D
<b>II-e</b> SDB	The experiments are performed at room temperature.	A/B
<b>II-f</b> SDB REF	A L/S ratio of 40 mL/g is indicated. It is reported that 0.5 g of solid has been added to 20 mL of liquid. Assuming BET surface area of 3 m <sup>2</sup> /g, surface area of solid are smaller than 5 m <sup>2</sup> .	C/D
<b>II-g</b> REF	Based on the information provided in the SDB, sorption percentage of all datapoints are $98 \leq \% < 100$ .	C/D
<b>II-h</b> SDB REF	Initial Am concentration $5.0 \times 10^{-7}$ [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated, initial Am concentration for all datapoints are higher than the solubility.	Unreliable
<b>II-i</b> SDB REF	It is indicated that phase separation has been done by centrifugation (12,000g/10 min) and filtration (0.8 μm). No further information is indicated.	C/D
<b>II-j</b> SDB	The experiments have been performed for 3 weeks.	A
<b>II-k</b> REF	The agitation method is stirring.	A/B
<b>II-l</b> REF	The initial Am concentration is not varied.	C/D
<b>II-m</b> REF	The material of experiment container is not reported. The blank test has been performed to correct the results for losses of Am from solution.	A
<b>II-n</b> SDB	The error estimation is not performed. The replicate is duplicates.	A
<b>II-o</b> SDB	The parameter is not varied.	D

<b>Data table Am/11: REF: Nowak(1979)</b> JAEA-SDB version 5 - DATA: Am/sandstone ; sand/bentonite, sand/hectorite, #94248–94251 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A table with $K_d$ [mL/g] is provided.	Class 1
<b>II-a</b> SDB	The solid used in experiments is a mixed sand and bentonite or a mixed sand and hectorite. The chemical composition and CEC of each solid are reported. The specific surface area is not reported.	A
<b>II-b</b> SDB	The final pH is reported.	A
<b>II-c</b> SDB REF	The atmospheric condition is not reported. Am(III) is not sensitive to redox condition.	A/B
<b>II-d</b> SDB REF	Sorption measurements are carried out in synthetic brine. The composition of the solution can be calculated by assuming equilibrium of brine and solids.	C/D
<b>II-e</b> SDB	The experiments are performed at room temperature.	A/B
<b>II-f</b> SDB REF	A L/S ratio of 40 mL/g is indicated. It is reported that 0.5 g of solid has been added to 20 mL of liquid. Assuming BET surface area of 3 m <sup>2</sup> /g, surface area of solid are smaller than 5 m <sup>2</sup> .	C/D
<b>II-g</b> REF	Based on the information provided in the SDB, sorption percentage of all datapoints are $98 \leq \% < 100$ .	C/D
<b>II-h</b> SDB REF	Initial Am concentration $5.0 \times 10^{-7}$ [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated, initial Am concentration for all datapoints are higher than the solubility.	Unreliable
<b>II-i</b> SDB REF	It is indicated that phase separation has been done by centrifugation (12,000g/10 min) and filtration (0.8 μm). No further information is indicated.	C/D
<b>II-j</b> SDB	The experiments have been performed for 3 weeks.	A
<b>II-k</b> REF	The agitation method is stirring.	A/B
<b>II-l</b> REF	The initial Am concentration is not varied.	C/D
<b>II-m</b> REF	The material of experiment container is not reported. The blank test has been performed to correct the results for losses of Am from solution.	A
<b>II-n</b> SDB	The error estimation is not performed. The replicate is duplicates.	A
<b>II-o</b> SDB	The parameter is not varied.	D

<b>Data table Am/12: REF: Okajima et al.(1987)</b> JAEA-SDB version 5 - DATA: Am/bentonite (smectite) ; Kunigel V1, #61663–61665, #94280–94292 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A table with $K_d$ [mL/g] is provided; • #61663–61665 A figure adsorbed Am concentration is provided; • #94280–94292	Class 1 Class 6
<b>II-a</b> SDB	The solid used in experiments is a well-known Kunigel V1 (Na-bentonite). The chemical formula, specific surface area and CEC are reported.	A
<b>II-b</b> SDB	The initial and final pH are reported.	A
<b>II-c</b> SDB REF	The atmospheric condition is not reported. Am(III) is not sensitive to redox condition.	A/B
<b>II-d</b> SDB REF	Sorption measurements have been carried out in deionized water and synthetic groundwater. The composition for synthetic groundwater is reported. The composition of the solution can be calculated by assuming equilibrium of solution and Na-bentonite.	C/D
<b>II-e</b> SDB	Information for temperature is not indicated.	C/D
<b>II-f</b> SDB	A L/S ratio of 400 mL/g is indicated. It is reported that 0.05 g of solid has been added to 20 mL of liquid. Calculating BET surface area of 71 m <sup>2</sup> /g, surface area of solid are smaller than 5m <sup>2</sup> .	C/D
<b>II-g</b> REF	Based on the information provided in the SDB; • #61664, #94280–94284 : 98≤%<100 • #94286 : 95≤%<98 • Other datapoints : 5<%<95	C/D B A
<b>II-h</b> SDB REF	Initial Am concentration $3.1 \times 10^{-8}$ – $2.0 \times 10^{-6}$ [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated, initial Am concentration is significantly lower than the solubility.	A
<b>II-i</b> SDB REF	It is indicated that phase separation has been done by centrifugation (39,000 rpm/30 min). No further information is indicated.	C/D
<b>II-j</b> SDB	The experiments have been performed for 7 days.	A/B
<b>II-k</b> REF	It is indicated that samples have been agitated throughout the experiment.	A/B
<b>II-l</b> REF	The initial Am concentration is varied. Sorption isotherm is indicated.	A
<b>II-m</b> REF	Information for reaction container is not indicated.	C/D
<b>II-n</b> SDB	The error estimation is not performed. The replicate is not reported.	D
<b>II-o</b> SDB	The pH, ionic strength and initial Am concentration are varied.	A

<b>Data table Am/13: REF: Okajima et al.(1987)</b> JAEA-SDB version 5 - DATA: Am/soil ; loam#1, loam#2, #61674, #74677, #94293–94304 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A table with $K_d$ [mL/g] is provided; • #61674, #74677	Class 1
	A figure adsorbed Am concentration is provided; • #94293–94304	Class 6
<b>II-a</b> SDB	The solid used in experiments is Takadate loam and Hachinohe loam. The chemical formula, specific surface area and CEC are reported.	A
<b>II-b</b> SDB	The initial and final pH are reported.	A
<b>II-c</b> SDB REF	The atmospheric condition is not reported. Am(III) is not sensitive to redox condition.	A/B
<b>II-d</b> SDB REF	Sorption measurements have been carried out in deionized water. The composition of the solution can be calculated by assuming equilibrium of solution and solid.	C/D
<b>II-e</b> SDB	Information for temperature is not indicated.	C/D
<b>II-f</b> SDB	A L/S ratio of 400 mL/g is indicated. It is reported that 0.05 g of solid has been added to 20 mL of liquid. Calculating BET surface area; • #61674, #94293–94300 : surface area of solid are more than 5 m <sup>2</sup> (Takadate loam) • #74677, #94301–94304 : surface area of solid are smaller than 5 m <sup>2</sup> (Hachinohe loam)	A/B
		C/D
<b>II-g</b> REF	Based on the information provided in the SDB; • #94293 : 98≤%<100 • #61674, #94294, #94295 : 95≤%<98 • Other datapoints : 5<%<95	C/D B A
<b>II-h</b> SDB REF	Initial Am concentration $2.0 \times 10^{-9}$ – $1.4 \times 10^{-7}$ [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated, initial Am concentration is significantly lower than the solubility.	A
<b>II-i</b> SDB REF	It is indicated that phase separation has been done by centrifugation (39,000 rpm/30 min).	C/D
	No further information is indicated.	
<b>II-j</b> SDB	The experiments are performed for 7 days.	A/B
<b>II-k</b> REF	It is indicated that samples have been agitated throughout the experiment.	A/B
<b>II-l</b> REF	The initial Am concentration is varied. Sorption isotherm is indicated.	A
<b>II-m</b> REF	Information for reaction container is not indicated.	C/D
<b>II-n</b> SDB	The error estimation is not performed. The replicate is not reported.	D
<b>II-o</b> SDB	The pH and initial Am concentration are varied.	B

<b>Data table Am/14: REF: RWMC et al.(1989)</b> JAEA-SDB version 5 - DATA: Am/bentonite (smectite) ; bentonite, #61761, #67983 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Information for pH value and initial Am concentration are not provided.	No

<b>Data table Am/15: REF: RWMC et al.(1989)</b> JAEA-SDB version 5 - DATA: Am/cementitious materials ; cement paste, mortar, concrete, #49135–49155, #61758–61760 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Information for pH value and initial Am concentration are not provided.	No

<b>Data table Am/16: REF: RWMC et al.(1989)</b> JAEA-SDB version 5 - DATA: Am/sandstone ; sandstone, #67988, #67989 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Information for pH value and initial Am concentration are not provided.	No

<b>Data table Am/17: REF: RWMC et al.(1989)</b> JAEA-SDB version 5 - DATA: Am/soil ; soil, #67984, #67985 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Information for pH value and initial Am concentration are not provided.	No

<b>Data table Am/18: REF: RWMC et al.(1989)</b> JAEA-SDB version 5 - DATA: Am/tuff ; tuff, #67986, #67987 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Information for pH value and initial Am concentration are not provided.	No

<b>Data table Am/19: REF: Yu and Neretnieks(1997)</b> JAEA-SDB version 5 - DATA: Am/bentonite (smectite) ; bentonite, MX-80, #76464–76467 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	Information for separation method is not provided. The $K_d$ values are determined with a diffusion method and not with batch experiments.	No Unreliable

<b>Data table Am/20: REF: Allard et al.(1982)</b> JAEA-SDB version 5 - DATA: Am/other minerals ; SiO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub> , #42530–42535, #42579–42582, #63639, #63660–63668 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
<b>I-a.1</b> SDB	All mandatory fields are completed.	Yes
<b>I-a.2</b> SDB	All mandatory information is provided.	Yes
<b>I-b</b> SDB	A table with log K <sub>d</sub> is provided; • #42579 A figure with log K <sub>d</sub> is provided; • Other datapoints	Class 1 Class 6
<b>II-a</b> SDB REF	The solid used in experiments are SiO <sub>2</sub> and Al <sub>2</sub> O <sub>3</sub> . Particle size and CEC are reported. No further information is available.	B
<b>II-b</b> SDB	Initial pH is reported; • #42579 Final pH is reported; • Other datapoints	C A
<b>II-c</b> SDB REF	It is indicated that the experiments had been conducted under ambient conditions. The oxidation state of Am is indicated as +III.	A/B
<b>II-d</b> SDB REF	0.01 M NaClO <sub>4</sub> solution is indicated. Based on the available information, the final solution composition can be estimated approximately.	C/D
<b>II-e</b> SDB	It is indicated that experiments have been done at 25°C.	A/B
<b>II-f</b> SDB REF	A L/S ratio of 100 mL/g is indicated. It is reported that 0.2 g of solid has been added to 20 mL of liquid. Assuming a BET (outer) surface area of ca. 35 m <sup>2</sup> /g, this would result in ca. 7 m <sup>2</sup> bentonite surface per 20 mL vessel.	A/B
<b>II-g</b> REF	The following sorption values are calculated from K <sub>d</sub> and L/S ratios; • #42579, #63639, #63660, #63662, #63665, #63666 : 98≤%<100 • #42581, #42582, #63667 : 95≤%<98 • Others : 5<%<95	C/D B A
<b>II-h</b> SDB REF	Initial Am concentration 2.3×10 <sup>-9</sup> and 2.9×10 <sup>-7</sup> [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated; • #42579 : initial Am concentration is not reported. • #42580–42582, #63639, #63660–63662 : more than a one-fifth of the solubility • Other datapoints : significantly lower than the solubility	Unreliable B A
<b>II-i</b> SDB REF	It is indicated that phase separation was done by centrifugation (27000g/1 h). No further information is available.	B
<b>II-j</b> SDB REF	A contact time of 6 days is indicated. A range of reaction times (6 hours–6 weeks) is used, but only one dataset (for 6 days) is reported. It can only be assumed that the kinetic experiments showed that 6 days is a reasonable reaction time.	A/B
<b>II-k</b> REF	No information is available. For the experimental technique, reference is made to a report that has not been available for the present evaluation. It is tentatively assumed that the kinetic experiments showed appropriate equilibration.	A/B

<b>II-l</b>	REF	Only one L/S ratio is and two Am concentrations are indicated.	B
<b>II-m</b>	REF	The experiments have been carried out in polypropylene vessels. No correction for sorption on vessel walls is done.	B
<b>II-n</b>	SDB REF	It is indicated that error estimation is not available. No further information is available.	D
<b>II-o</b>	SDB	Initial Am concentration is varied.	C



Table 3.2.1 Overview of references additionally evaluated the QA (1/9)

Reference	Details of reference	Element	Solid phase	Solution type
Allard et al.(1982)	Allard, B., Olofsson, U., Torstenfelt, B., Kipatsi, H. and Andersson, K. : Sorption of actinides in well-defined oxidation states on geological media, Materials Research Society Symposium Proceedings, vol.11, pp.775-782 (1982).	Am, Np, Pa, Pu, Th, U	Al <sub>2</sub> O <sub>3</sub> , bentonite, SiO <sub>2</sub>	0.01 M-NaClO <sub>4</sub> , synthetic groundwater
Ames et al.(1981)	Ames, L. L., McGarrah, J. E. and Walker, B. A. : Basalt-radionuclide reactions: FY-1981 Annual Report, RHO-BW-CR-127 P (1981).	Am, Cs, Np, Pu, Ra, Se, Sr, U	Basalt, nontronite, smectite	0.0005 M-, 0.005 M-, 0.05 M-, 0.5 M-CaCl <sub>2</sub> , 0.001 M-, 0.01 M-, 0.1 M-, 0.1 M-NaCl, groundwater
Baeyens and Bradbury(1997)	Baeyens, B. and Bradbury, M. H. : A Mechanistic Description of Ni and Zn sorption on Na-montmorillonite Part I: Titration and sorption measurements, Journal of Contaminant Hydrology, vol.27, pp.199-222 (1997).	Mn, Ni, Zn	Na-SWy-1 montmorillonite	0.01 M-, 0.03 M-, 0.1 M-, 0.5 M-NaClO <sub>4</sub>
Baker et al.(1994)	Baker, S., McCrohon, R., Oliver, P. and Pilkington, N. J. : The sorption of niobium, tin, Iodine and chlorine onto Nirex reference vault backfill, Materials Research Society Symposium Proceedings, vol.333, pp.719-724 (1994).	Cl, I, Nb, Sn	Concrete	Cement water, saline water
Bascetin and Atun(2006)	Bascetin, E. and Atun, G. : Adsorption behavior of strontium on binary mineral mixtures of montmorillonite and kaolinite, Applied Radiation and Isotopes, vol.64, pp.957-964 (2006).	Sr	Kaolinite, montmorillonite	0.01 M-NaCl
Beall et al.(1979)	Beall, G. W., Kettle, B. H., Haire, R. G. and O Kelley, G. D. : Sorption behavior of trivalent actinides and rare earths on bentonite (clay minerals), Radioactive Waste in Geological Storage, ACS Symp. Series 100, pp.201-213 (1979).	Sm	Attapulgit, kaolinite, montmorillonite	0.19 M-, 0.375 M-, 0.75 M-, 1.5 M-, 3 M-NaCl
Benischek et al.(1992b)	Benischek, I., Hess, V. and Metzger, E. : Preliminary experiments for determining K <sub>d</sub> values for cesium and strontium as part of site selection part II., OEFZS-4631 (1992).	Cs, Sr	Austro deponal F, bentonite, calzonit, clay, montmorillonite, smectite	Cement solution
Berger(1992)	Berger, G. : Distribution of trace elements between clays and zeolites and aqueous solutions similar to sea water, Applied Geochemistry, Suppl. Issue, No.1 pp.193-203 (1992).	Sm	Smectite, zeolite	Seawater
Bradbury and Baeyens(1999)	Bradbury, M. H. and Baeyens, B. : Modelling the Sorption of Zn and Ni on Ca-montmorillonite, Geochimica et Cosmochimica Acta, vol.63, No.3/4, pp.325-336 (1999).	Ni, Zn	Ca-montmorillonite	0.0033 M-, 0.033 M-Ca(NO <sub>3</sub> ) <sub>2</sub>
Brandberg and Skagius(1991)	Brandberg, F. and Skagius, K. : Porosity, sorption and diffusivity data compiled for the SKB 91 study, SKB Technical Report, 91-16 (1991).	Nb	Bentonite	Groundwater

Table 3.2.1 Overview of references additionally evaluated the QA (2/9)

Reference	Details of reference	Element	Solid phase	Solution type
Brigatti et al.(1995)	Brigatti, M. F., Corradini, F., Franchini, G. C., Mazzoni, S., Medici, L. and Poppi, L. : Interaction between montmorillonite and pollutants from industrial waste-waters: exchange of $Zn^{2+}$ and $Pb^{2+}$ from aqueous solutions, Applied Clay Science, vol.9, pp.383-395 (1995).	Pb	Montmorillonite	Porewater
Brownsword et al.(2000)	Brownsword, M., Mihara, M. and Williams, S. J. : Sorption of uranium and plutonium on bentonite altered by highly alkaline water, Materials Research Society Symposium Proceedings, vol.608, pp.249-254 (2000).	Pu, U	Kunipia-F	Cement solution
Cornell and Aksoyoglu(1992)	Cornell, R. M. and Aksoyoglu, S. : Sorption of nickel on marl, Journal of Radioanalytical and Nuclear Chemistry, vol.164, No.6, pp.389-396 (1992).	Ni	Calcite, goethite, illite, kaolinite, montmorillonite, quartz	Groundwater
Dong et al.(2001)	Dong, W., Wang, X., Bian, X., Wang, A., Du, J. and Tao, Z. : Comparative study on sorption/desorption of radioeuropium on alumina, bentonite and red earth: effects of pH, ionic strength, fulvic acid, and iron oxides in red earth, Applied Radiation and Isotopes, vol.54, pp.603-610 (2001).	Eu	Alumina, bentonite, red earth, reddish soil, fulvic acid	0.1 M-, 0.3 M-CaCl <sub>2</sub> , 1 M-, 2.5 M-NaCl
Erdal et al.(1977)	Erdal, B. R., Wolfsberg, K., Vidale, R., Duffy, C. and Hoffman, D. C. : Laboratory measurements of radionuclide distribution between selected ground water and geologic media, Pacific Northwest Laboratory Report, PNL-SA-6957, pp.503-516 (1977).	Ba, Ce, Co, Cs, Eu, I, Mo, Nb, Ru, Sb, Sr, U	Alluvium, bentonite	Deionized water, groundwater
Eriksen and Jansson(1996)	Eriksen, T. E. and Jansson, M. : Diffusion of $I^-$ , $Cs^+$ and $Sr^{2+}$ in compacted bentonite -Anion exclusion and surface diffusion, SKB Technical Report, 96-16 (1996).	Cs, Sr	Bentonite	Groundwater
Farrah et al.(1980)	Farrah, H., Hatton, D. and Pickering, W. F. : The affinity of metal ions for clay surfaces, Chemical Geology, vol.28, pp.55-68 (1980).	Pb	Na-illite, Na-kaolinite, Na-montmorillonite	Metal nitrate solution
Farrah et al.(1980)	Farrah, H., Hatton, D. and Pickering, W. F. : The affinity of metal ions for clay surfaces, Chemical Geology, vol.28, pp.55-68 (1980).	Pb	Na-illite, Na-kaolinite, Na-montmorillonite	Metal nitrate solution
Hartmann et al.(2008)	Hartmann, E., Geckeis, H., Rabung, T., Luetzenkirchen, J. and Fanghaenel, T. : Sorption of radionuclides onto natural clay rocks, Radiochimica Acta, vol.96, pp.699-707 (2008).	Eu, U	Clay, Na-montmorillonite	0.1 M-NaClO <sub>4</sub>

Table 3.2.1 Overview of references additionally evaluated the QA (3/9)

Reference	Details of reference	Element	Solid phase	Solution type
Holland and Lee(1992)	Holland, T. R. and Lee, D. J. : Radionuclide getters in cement, Cement and Concrete Research, vol.22, pp.247-258 (1992).	Cs, I, Ra	Cement hydrate, cement paste, choy, clinoptilolite, ferric floe, fullers earth, heulandite, Minnoval-M, Minnoval -ZG, zeolite	Artificial pore water, cement water, lime water
Iijima et al.(2005)	Iijima, K., Tomura, T. and Masuda, T. : Sorption behavior of Cs onto bentonite colloid, Clays in Natural & Engineered Barriers for Radioactive Waste Confinement, pp.607-608 (2005).	Cs	Kunipia-F	0.0003 M-NaCl
Ikeda et al.(1995)	Ikeda, T., Ayama, T. and Chiba, T. : Study for sorption mechanism of radioactive nuclides in deep underground conditions (III), PNC Technical Report, PNC TJ1281 95-009 (1995) [in Japanese].	Sn	FeO(OH), montmorillonite	0.01 M-NaCl
JAERI(1995)	JAERI : Natural barrier safety proof examination at 1995 year (Phase II) report, The Japan Atomic Energy Research Institute (1995).	Am, C, Co, Cs, Sr	Ca-bentonite, Na-bentonite, sandstone, silt, till	Synthetic groundwater
Jan et al.(2006)	Jan, Y.-L., Tsai, S.-C., Jan, J.-C. and Hsu, C.-N. : Additivity of the distribution ratio of Cs and Se on bentonite/quartz sand mixture in seawater, Journal of Radioanalytical and Nuclear Chemistry, vol.267, pp.225-231 (2006).	Cs, Se	bentonite, quartz, bentonite/quartz	Synthetic seawater
Jedinakova-Krizova et al.(1998)	Jedinakova-Krizova, V., Jurcek, P. and Kohlickova, M. : Retardation of long-lived radionuclides on bentonites, Proceedings of the workshop on long-lived radionuclide chemistry in nuclear waste treatment Paris (France), OECD Publications 1998, pp.99-110 (1998).	Cs, Sr, Tc	Bentonite	Synthetic groundwater
Kanno et al.(1989)	Kanno, T., Wakamatsu, H., Hattia, M. and Miwa, K. : Static and Permeability sorption tests of buffer materials for geologic disposal for high-level wastes, Waste Processing, Transportation, Storage and Disposal, Technical Programs and Public Education, No.1, pp.647-651 (1989).	Ni	Bentonite	Simulated water
Kato et al.(1993)	Kato, H., Ueta, S., Yajima, T. and Akasaka, H. : Adsorption properties of cesium on vermiculite, 1993 Fall Meeting of the Atomic Energy Society of Japan, M18, p.656 (1993) [in Japanese].	Cs	Kunigel-VI, Kunipia-F, vermiculite	RI water
Kawachi and Kida(1990)	Kawachi, T. and Kida, D. : Adsorption property of unsaturated bentonite, Basic data associated with nuclear migration, pp.25-33 (1990).	Co, Cs, Sr	Bentonite	Not reported

Table 3.2.1 Overview of references additionally evaluated the QA (4/9)

Reference	Details of reference	Element	Solid phase	Solution type
Konishi et al.(1988)	Konishi, M., Yamamoto, K., Yanagi, T. and Okajima, Y.: Sorption behavior of cesium, strontium and americium ions on clay materials, Journal of Nuclear Science and Technology, vol.25, pp.929-933 (1988).	Am, Cs, Sr	Bentonite, loam	Deionized water, synthetic groundwater
Kozai et al.(1993)	Kozai, N., Ohnuki, T. and Muraoka, S.: Specific sorption of neptunium by smectite -Effect of calcium ion-, 1993 Fall Meeting of the Atomic Energy Society of Japan, M16, p.654 (1993) [in Japanese].	Np	Ca-bentonite, Na-bentonite	0.01 M-NaClO <sub>4</sub>
Kurosawa et al.(2004a)	Kurosawa, S., Ibaraki, M., Ueta, S., Yui, M. and Yoshikawa, H.: Effect of kinetic radionuclide sorption onto colloids for radionuclide transport in fractured rock, Experimental and Numerical Studies, Transactions of the Atomic Energy Society of Japan, vol.3, No.3, pp.249-256 (2004).	Cs	Kunipia-F, granodiorite	Bentonite solution
Liang and Sherriff(1993)	Liang, J.-J. and Sherriff, B. L.: Lead exchange into zeolite and bentonite (Clay minerals): a <sup>29</sup> Si, <sup>27</sup> Al, <sup>23</sup> Na solid-state NMR study, Geochimica et Cosmochimica Acta, vol.57, pp.3885-3894 (1993).	Pb	Mg-vermiculite, montmorillonite, Na-chabazite, Na-hectorite	0.01 M-Pb(NO <sub>3</sub> ) <sub>2</sub>
Lothenbach et al.(1997)	Lothenbach, B., Furrer, G. and Schulin, R.: Immobilization of Heavy Metals by Polynuclear Aluminium and Montmorillonite Compounds, Environmental Science and Technology, vol.31, pp.1452-1462 (1997).	Ni, Pb, Zn	Na-SWy-1 montmorillonite	0.033 M-Ba(ClO <sub>4</sub> ) <sub>2</sub> , 0.01 M-NaClO <sub>4</sub>
Maeda et al.(2003)	Maeda, T., Tanaka, T., Mukai, M., Ogawa, H., Yamaguchi, T., Munakata, M., Matsumoto, J., Kozai, N., Banba, T., Fan, Z., Cui, A., Gu, C., Zhao, Y. and Sun, Q.: Field tests on migration of TRU-nuclide, (II) Migration tests for engineered barrier materials in aerated soil, Transactions of the Atomic Energy Society of Japan, vol.2, No.3, pp.336-341 (2003).	Np, Pu, Sr	Cement paste, bentonite	Pure water
Molera and Eriksen(2002)	Molera, M. and Eriksen, T.: Diffusion of <sup>22</sup> Na <sup>+</sup> , <sup>85</sup> Sr <sup>2+</sup> , <sup>134</sup> Cs <sup>+</sup> and <sup>57</sup> Co <sup>2+</sup> in bentonite clay compacted to different densities: experiments and modeling, Radiochimica Acta, vol.90, pp.753-760 (2002).	Co, Cs, Na, Sr	MX-80	0.1 M-NaClO <sub>4</sub>
Murali and Mathur(1999)	Murali, M. S. and Mathur, J. M.: Sorption characteristics of caesium and strontium on back fill material, bentonite, Nuclear and Radiochemistry Symposium Mumbai (India), NUCAR 99, pp.315-316 (1999).	Cs, Sr	Bentonite	Natural groundwater

Table 3.2.1 Overview of references additionally evaluated the QA (5/9)

Reference	Details of reference	Element	Solid phase	Solution type
Muurinen et al.(1985)	Muurinen, A., Rantanen, J. and Penttilä-Hiltunen, P. : Diffusion mechanisms of strontium, cesium and cobalt in compacted sodium bentonite, Materials Research Society Symposium Proceedings, vol.50, pp.617-624 (1985).	Co, Cs, Sr	MX-80	0.001 M-, 0.003 M-, 0.02 M-, 0.2 M-, 0.6 M-, 1.2 M-NaCl, synthetic groundwater, synthetic groundwater+EDTA
Muurinen et al.(1987)	Muurinen, A., Penttilä-Hiltunen, P. and Rantanen, J. : Diffusion mechanisms of strontium and cesium in compacted sodium bentonite, Materials Research Society Symposium Proceedings, vol.84, pp.803-812 (1987).	Sr	MX-80	0.001 M-, 0.01 M-, 0.1 M-, 0.5 M-, 1 M-NaCl
Nagasaki et al.(1994b)	Nagasaki, S., Tanaka, S. and Suzuki, A. : Colloid formation of americium in bentonite, Journal of Nuclear Fuel Cycle and Environment, vol.1, No.1, pp.91-97 (1994).	Am	Na-bentonite	Distilled water
Nowak(1979)	Nowak, E. J. : Radionuclide sorption and migration studies of getters for backfill barriers, Technical report, Sandia National Laboratories, SAND79-1110 (1979).	Am, Cs, Eu, Pu, Sr, Tc	Bentonite, calcite, charcoal, clinoptilolite, hectorite, kaolin, montmorillonite, mordenite, sand/bentonite, sand/hectorite, soil, tuff	Saline solution
Ochs et al.(2002)	Ochs, M., Lothenbach, B. and Giffaut, E. : Uptake of oxo-anions by cements through solid-solution formation: Experimental evidence and modelling, Radiochimica Acta, vol.90, pp.639-646 (2002).	Cr, Se	Cement paste, ettringite	Porewater
Ohnuki and Kozai(1994)	Ohnuki, T. and Kozai, N. : Sorption characteristics of radioactive cesium and strontium on smectite, Radiochimica Acta, vol.66/67, pp.327-331 (1994).	Sr	Kunipia-F	0.01 M-NaAc
Ohnuki et al.(1992)	Ohnuki, T., Murakami, T., Sato, T. and Isobe, H. : Changes in sorption forms of radioactive cesium and strontium during smectite to illite alteration difference in sorption forms between dynamic and static conditions, Journal of the Atomic Energy Society of Japan, vol.34, No.12, pp.1139-1142 (1992).	Cs, Sr	Smectite	Chloride solution
Okajima et al.(1987)	Okajima, Y., Konishi, T., Yanagi, T. and Yamamoto, K. : The property as the backfilling material of various soils, Engineering barrier of land disposal, Atomic Energy Society of Japan, RWM-87009, pp.116-127 (1987).	Am, Cs, Sr	Kunigel-V1, loam, sand, zeolite	Deionized water, synthetic groundwater

Table 3.2.1 Overview of references additionally evaluated the QA (6/9)

Reference	Details of reference	Element	Solid phase	Solution type
Onodera et al.(1994)	Onodera, Y., Iwasaki, T., Hayashi, H., Torii, K., Mimura, H. and Akiba, K.: Sorption behavior of Cs on smectites, Journal of Nuclear Fuel Cycle and Environment, vol.1, No.1, pp.53-65 (1994).	Ca, Cs, Na, Sr	Smectite	0.005 M-CaCl <sub>2</sub> , 0.005 M-CsCl, 0.005 M-NaCl, 0.005 M-SrCl <sub>2</sub> , 0.1 M-NaNO <sub>3</sub>
Rancon(1988)	Rancon, D.: Comparative study of radioactive iodine behavior in soils under various experimental and natural conditions, Radiochimica Acta, vol.44/45, pp.187-193 (1988).	I	Attapulgite, bauxite, bentonite, cerusite, chalcopyrite, chrysocolla, clinoptilolite, galena, goethite, hematite, illite, kaolinite, laterite, limonite, quartz, sandy soil, sepiolite, siderite, vermiculite, zeolite	Not reported
Riebe et al.(2001)	Riebe, B., Bors, J. and Dultz, St.: Retardation capacity of organophilic bentonite for anionic fission products, Journal of Contaminant Hydrology, vol.47, pp.255-264 (2001).	I, Tc	MX-80	Groundwater, saline water
RWMC et al.(1989)	Radioactive Waste Management Center, Toshiba Corporation, JGC Corporation, Hitachi Ltd., Mitsubishi Materials Corporation, Mitsubishi Heavy Industries: About the distribution coefficients of some barrier materials (1989).	Am, C, Co, Cs, I, Nb, Ni, Pu, Sr, Tc	Bentonite, cement paste, concrete, mortar, sandstone, soil, tuff	0.1% sodium borate, 3.0% sodium borate, distilled water, enriched waste solution, synthetic groundwater
Sabodina et al.(2006a)	Sabodina, M. N., Kalmykov, S. N., Artemeva, K. A., Zakharova, E. V. and Sapozhnikov, Y. A.: Behavior of Cs, Np(V), Pu(IV), and U(VI) in pore water of bentonite, Radiochemistry, vol.48, No.5, pp.488-492 (2006).	Cs, Np, Pu, U	Na-bentonite	0.001 M-, 0.01 M-, 0.1 M-, 0.5 M-NaClO <sub>4</sub>
Sakamoto et al.(1988)	Sakamoto, Y., Konishi, M., Shirahashi, K., Senoo, M. and Moriyama, N.: Adsorption behavior of Np on soil and bentonite, 1988 Annual Meeting of the Atomic Energy Society of Japan, G46, p.46 (1988) [in Japanese].	Np	Bentonite, loam, sand	0.01 M-NaClO <sub>4</sub>
Salter et al.(1981)	Salter, P. F., Ames, L. L. and McGarrah, J. E.: Sorption of selected radionuclides on secondary minerals associated with the Columbia River Basalts, RHO-BWI-LD-43 (1981).	Am, Cs, I, Np, Pu, Ra, Se, Sr, Tc, U	Smectite	Groundwater
Salter(1982)	Salter, P. F.: Sorption behavior of selected radionuclides on potential backfill material, Rockwell Hanford Operations, RHO-BWI-TI-072 (1982).	Cs, Np, Sr, U	Bentonite	Synthetic groundwater



Table 3.2.1 Overview of references additionally evaluated the QA (7/9)

Reference	Details of reference	Element	Solid phase	Solution type
Sato et al.(1995)	Sato, H., Yu,i M. and Yoshikawa, H. : Diffusion behavior for Se and Zr in sodium-bentonite, Materials Research Society Symposium Proceedings, vol.353, pp.269-276 (1995).	Zr	Kunigel-V1	Equilibrated water
Sazarashi et al.(1994)	Sazarashi, M., Ikeda, Y., Kumagai, M., Seki, R. and Yoshikawa, H. : Adsorption behavior of iodide on natural and modified minerals, Journal of Nuclear Fuel Cycle and Environment, vol.1, No.1, pp.99-105 (1994).	Cl, I	Allophane, attapulgite, chalcopyrite, cinnabar, HgS reagent, M-cinnabar, montmorillonite	Test solution
Schulthess and Huang(1990)	Schulthess, C. P. and Huang, C. P. : Adsorption of heavy metals by silicon and aluminium oxide surfaces on Bentonite (Clay minerals), Soil Science Society of America Journal, vol.54, pp.679-688 (1990).	Cd, Ni, Pb, Zn	Al oxide, kaolinite, mordenite, Na-montmorillonite, Si oxide	0.01 M-NaClO <sub>4</sub>
Shade et al.(1984)	Shade, J. W., Ames, L. L. and McGarrah, J. E. : Actinide and technetium sorption on iron-silicate and dispersed clay collides, American Chemical Society, vol.246, pp.67-77 (1984).	Cs, Np, Pu, Sr, Tc, U	Iron silicate, Na-bentonite	HCl/NaOH
Sivaiah et al.(2005)	Sivaiah, M. V., Venkatesan, K. A., Sasidhar, P., Krishna, R. M. and Murthy, G. S. : Unusual extraction behaviour of crown ether when intercalated in bentonite, New Journal of Chemistry, vol.29, pp.564-569 (2005).	Cs, Sr	Na-bentonite	0.001 M-, 0.01 M-, 0.1 M-, 0.5 M-, 1 M-HNO <sub>3</sub>
Smith and Degueudre(1993)	Smith, P. A. and Degueudre, C. : Colloid-facilitated transport of radionuclides through fractured media, Journal of Contaminant Hydrology, vol.13, pp.143-166 (1993).	Bi, Pb, Po	Colloid, montmorillonite	Not reported
Srivastava et al.(1989)	Srivastava, S. K., Tyagi, R., Pant, N. and Pal, N. : Studies on the removal of some toxic metal ions: part II (removal of lead and cadmium by montmorillonite and kaolinite), Environmental Technology Letters, vol.10, pp.275-282 (1989).	Pb	H-kaolinite, H-montmorillonite	Porewater
Tachi et al.(2001)	Tachi, Y., Shibutani, T., Sato, H. and Yui, M. : Experimental and modeling studies on sorption and diffusion of radium in bentonite, Journal of Contaminant Hydrology, vol.47, pp.171-186 (2001).	Ra	Kunigel-V1, smectite	0.1 M-NaCl, distilled water
Tomura et al.(2001)	Tomura, T., Shibutani, T. and Kiramura, A. : Distribution coefficient of Np(IV) on smectite under carbonate conditions, 2001 Fall Meeting of the Atomic Energy Society of Japan, O25, p.903 (2001) [in Japanese].	Np	Kunipia-F	1 M-NaCl

Table 3.2.1 Overview of references additionally evaluated the QA (8/9)

Reference	Details of reference	Element	Solid phase	Solution type
Tripathi et al.(1993)	Tripathi, V. S., Siegel, M. D. and Kooner, Z. S. : Measurements of metal adsorption in oxide-clay mixtures: competitive-additivity among mixture components, Materials Research Society Symposium Proceedings, vol.294, pp.791-796 (1993).	Cu, Pb, Zn	Ca-montmorillonite, goethite, goethite+montmorillonite	0.1 M-NaNO <sub>3</sub>
Tsukamoto et al.(1995)	Tsukamoto, M., Ohe, T., Fujita, T., Hesbol, R. and Hermansson, H-P. : Diffusion of radionuclides in compacted bentonite: Results from combined glass dissolution and migration tests, Materials Research Society Symposium Proceedings, vol.353, pp.291-298 (1995).	Pu, Sb, U	Bentonite	Bentonite water
Ueta and Kuno(2004)	Ueta, S. and Kuno, Y. : Studies on data base management for nuclide migration and improvement of individual models, JNC Technical Report, TJ8400 2003-065 (2004).	Sr	Kunipia-F	Bentonite solution
Ulrich and Degueudre(1993)	Ulrich, H. J. and Degueudre, C. : The sorption of <sup>210</sup> Pb, <sup>210</sup> Bi and <sup>210</sup> Po on montmorillonite: a study with emphasis on reversibility aspects and on the radioactive decay of adsorbed nuclides, Radiochimica Acta, vol.62, pp.81-90 (1993).	Bi, Pb, Po	Na-bentonite	0.01 M-, 0.02 M-, 0.05 M-, 0.1 M-, 0.2 M-NaClO <sub>4</sub>
Vejsada et al.(2005)	Vejsada, J., Jelinek, E., Randa, Z., Hradil, D. and Prikryl, R. : Sorption of Cesium on smectite-rich clays from the Bohemian Massif (Czech Republic) and their mixtures with sand, Applied Radiation and Isotopes, vol.62, pp.91-96 (2005).	Cs	Bentonite, clay, sand	Synthetic groundwater
Vejsada(2006)	Vejsada, J. : The uncertainties associated with the application of batch technique for distribution coefficients determination -A case study of cesium adsorption on four different bentonites, Applied Radiation and Isotopes, vol.64, pp.1538-1548 (2006).	Cs	Ca-bentonite, Na-bentonite	Deionized water
Wanner et al.(1994)	Wanner, H., Wieland, E. and Albinsson, Y. : Project Caesium - An ion exchange model for the prediction of distribution coefficient of caesium in bentonite, SKB Technical Report, TR-94-10 (1994).	Cs	MX-80, sand/bentonite	0.025 M-, 0.25 M-CaCl <sub>2</sub> , 0.05 M-, 0.5 M-, 1 M-KCl, 0.05 M-, 0.5 M-, 1 M-MgCl <sub>2</sub> , 0.05 M-, 0.1 M-, 0.5 M-NaCl, 0.25 M-Ca(NO <sub>3</sub> ) <sub>2</sub> , Allard water, Äspö water
Wold and Eriksen(2000)	Wold, S. and Eriksen, T. E. : Diffusion of organic colloids in compacted bentonite. The influence of ionic strength on molecular size and transport capacity of the colloids, SKB Technical Report, TR-00-19, p.40 (2000).	Sr	MX-80, MX-80+humic acid	0.01 M-, 0.1 M-NaClO <sub>4</sub>



Table 3.2.1 Overview of references additionally evaluated the QA (9/9)

Reference	Details of reference	Element	Solid phase	Solution type
Wold and Pickering(1981)	Wold, J. and Pickering, W. F. : Influence of electrolytes on metal ion sorption by clays, Chemical Geology, vol.33, pp.91-99 (1981).	Pb	Montmorillonite, illite	0.05 M-Na <sub>2</sub> SO <sub>4</sub> , 0.25 M-NaCl, porewater
Yllera-de-Llano et al.(1998)	Yllera-de-Llano, A., Hernandez-Benitez, A. and Garcia-Gutierrez, M. : Cesium sorption studies on Spanish clay materials, Radiochimica Acta, vol.82, pp.275-278 (1998).	Cs	Montmorillonite, saponite	Groundwater
Yu and Neretnieks(1997)	Yu, J.-W. and Neretnieks, I. : Diffusion and sorption properties of radionuclides in compacted bentonite, SKB Technical Report, TR-97-12 (1997).	Am, Cs, I, Nb, Np, Pa, Pd, Pu, Ra, Se, Tc, Th, U, Zr	Bentonite, Ca-bentonite, Kunigel-V1, montmorillonite, MX-80, Na/Ca-montmorillonite, Na-montmorillonite	Groundwater, saline water, synthetic groundwater
Yu et al.(2006)	Yu, S. M., Ren, A. P., Chen, C. L., Chen, Y. X. and Wang, X. : Effect of pH, ionic strength and fulvic acid on the sorption and desorption of cobalt to bentonite, Applied Radiation and Isotopes, vol.64, pp.455-461 (2006).	Co	Bentonite, bentonite+fulvic acid	0.005 M-, 0.01 M-, 0.1 M-, 0.5 M-, 1 M-, 2 M-NaNO <sub>3</sub>
Zachara and McKinley(1993)	Zachara, J. M. and McKinley, J. P. : Influence of hydrolysis on the sorption of metal cations by smectites: Importance of edge coordination reactions, Aquatic Sciences, vol.55, No.4, pp.251-261 (1993).	Cd, U	Clay, smectite	0.01 M-, 0.1 M-NaClO <sub>4</sub>

The notation of reference is according to JAEA-SDB reference, considering relation with JAEA-SDB. QA-evaluated 74 references listed in Table 3.2-1 are not included in this reference list.

Table 3.2.2 Overview of references revised data

No.	Reference	Revised points
1)	Baker et al.(1994)	Solid phase group, liquid[mL], pH init, error[m <sup>3</sup> /kg]
2)	Bradbury and Baeyens(1999)	Addition of data
3)	Brownsword et al.(2000)	Liquid/solid[mL/g], liquid[mL], solid[g], temp[°C], C init[mol/L]
4)	Farrah et al.(1980)	Solid phase, liquid/solid[mL/g], liquid[mL], solid[g], water type
5)	Holland and Lee(1992)	Deletion of data, liquid[mL], solid[g], temp[°C], solution composition concentration, pH end
6)	Jan et al.(2006)	Addition of data
7)	Kato et al.(1993)	Addition of data, ionic strength[mol/L], C init[mol/L], separation
8)	Konishi et al.(1988)	Specific surface area[m <sup>2</sup> /g], CEC[meq/100 g]
9)	Kozai et al.(1993)	Water type, ionic strength[mol/L], contact time[d], separation
10)	Kurosawa et al.(2004a)	Addition of data, liquid/solid[mL/g], liquid[mL], solid[g], contact time[d], separation
11)	Liang and Sherriff(1993)	Water type, ionic strength[mol/L], pH init, contact time[d]
12)	Nagasaki et al.(1994b)	Contact time[d], separation
13)	Nowak(1979)	Addition of data
14)	Ochs et al.(2002)	Addition of data
15)	Okajima et al.(1987)	Addition of data, liquid/solid[mL/g], liquid[mL], solid[g], C init[mol/L], separation
16)	Sabodina et al.(2006a)	Addition of data, water type, separation
17)	Sakamoto et al.(1988)	Liquid[mL], solid[g], temp[°C], water type, pH end, C init[mol/L], contact time[d], separation
18)	Salter(1982)	Water type, solution composition concentration, ionic strength[mol/L], pH init
19)	Sazarashi et al.(1994)	Deletion of data, water type, separation
20)	Schulthess and Huang(1990)	Addition of data, liquid/solid[mL/g], liquid[mL], solid[g]
21)	Sivaiah et al.(2005)	Liquid/solid[mL/g], liquid[mL], solid[g], water type, ionic strength[mol/L], contact time[d], separation
22)	Tachi et al.(2001)	Solid phase, CEC[meq/100 g], solution composition concentration, ionic strength[mol/L], pH end, atm/redox condition, error[m <sup>3</sup> /kg]
23)	Tomura et al.(2001)	Addition of data, liquid[mL], solid[g], water type, contact time[d], separation
24)	Tripathi et al.(1993)	Addition of data
25)	Ulrich and Degueldre(1993)	Deletion of data, liquid/solid[mL/g], pH init, C init[mol/L], atm/redox condition
26)	Vejsada et al.(2005)	Solid phase group, solid phase, liquid[mL], solid[g], C init[mol/L], separation
27)	Vejsada(2006)	Addition of data, solid phase, liquid[mL], solid[g], ionic strength[mol/L], pH end, contact time[d], error[m <sup>3</sup> /kg]
28)	Wanner et al.(1994)	Deletion of data, solid phase, CEC[meq/100 g], liquid/solid[mL/g], pH end, C init[mol/L], contact time[d]
29)	Wold and Eriksen(2000)	Addition of data, liquid[mL], solid[g], pH init, pH end, contact time[d], separation, atm/redox condition
30)	Yllera-de-Llano et al.(1998)	Addition of data, solid phase, specific surface area[m <sup>2</sup> /g], CEC[meq/100 g], liquid[mL], solid[g], temp[°C], pH init, contact time[d], separation, atm/redox condition
31)	Yu et al.(2006)	Addition of data, specific surface area[m <sup>2</sup> /g], CEC[meq/100 g], pH end, contact time[d], separation

### 3.3 QA evaluation on Criteria III

Only the entries for data sets classified as reliable are being considered for Criteria III. All unreliable entries, or entries which their classification could not be completed in accordance with Criteria I and II are excluded.

As an example for bentonite, evaluation for nickel sorption is shown. Examples for cementitious materials, evaluation for thorium and uranium (VI) sorption are also shown as follows.

#### 3.3.1 Evaluation of data for nickel sorption onto bentonite (smectite)

Table 3.3.1 shows evaluated entries in this section; the respective data are shown in Figure 3.3.1.

Table 3.3.1 List of evaluated data for nickel sorption onto bentonite (smectite)

Reference	Data table	Solid phase
Baeyens and Bradbury(1997) <sup>34)</sup>	—	Montmorillonite
Chen and Dong(2013) <sup>35)</sup>	—	Montmorillonite
Lothenbach et al.(1997) <sup>36)</sup>	—	Montmorillonite
Tertre et al.(2005a) <sup>37)</sup>	—	Montmorillonite
Vilks and Miller(2014)	Ni/8	Bentonite
Vilks et al.(2011)	Ni/11	Bentonite

The pH dependence for nickel  $K_d$  values on bentonite (Na-Swy-1 montmorillonite, etc.) is shown in Figure 3.3.1. According to the data in JAEA-SDB, the  $K_d$  values tend to increase with pH ( $\text{pH} > 10$ ). The data for Brine SR-270 reported by Vilks and Miller(2014) is lower than other data due to the high ionic strength. The  $K_d$  values for brine are varied due to the difference of the reaction time. The data reported by Vilks et al.(2011) is obtained under relatively high ionic strength ( $> 0.2 \text{ M}$ ). These data are varied due to the difference of the initial RN concentration, ionic strength, liquid/solid ratio and reaction time.

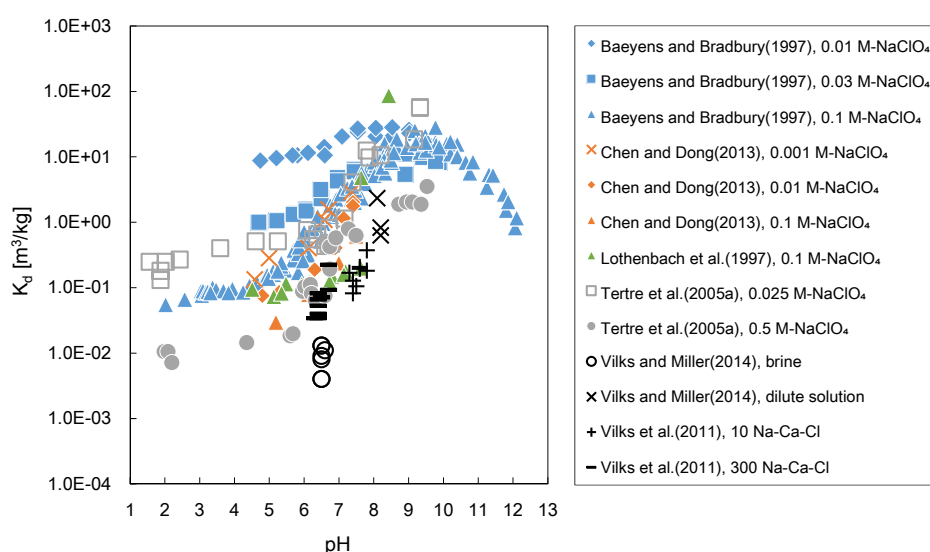


Figure 3.3.1 Overview of sorption data for nickel onto bentonite (smectite)

### 3.3.2 Evaluation of data for thorium sorption onto cementitious materials

Table 3.3.2 shows evaluated entries in this section; the respective data are shown in Figure 3.3.2.

Table 3.3.2 List of evaluated data for thorium sorption on cementitious materials

Reference	Data table	Solid phase
Albinsson et al.(1993) <sup>38)</sup>	—	FP concrete, M concrete, M paste
Cowper et al.(2006) <sup>39)</sup>	—	Cement hydrate
Sugiyama et al.(2000) <sup>40)</sup>	—	Cement paste
Sugiyama et al.(2003b) <sup>41)</sup>	—	Cement paste, cement hydrate
Höglund et al.(1985)	Th/1	Cement

The pH dependence for thorium  $K_d$  values on cementitious materials (cement paste, concrete, CSH, etc.) is shown in Figure 3.3.2. There is no obvious trend with data in JAEA-SDB. The solid used in Höglund et al.(1985) is the standard Portland cement. These  $K_d$  values are lower than other data.

Figure 3.3.2 Overview of sorption data for thorium onto cementitious materials

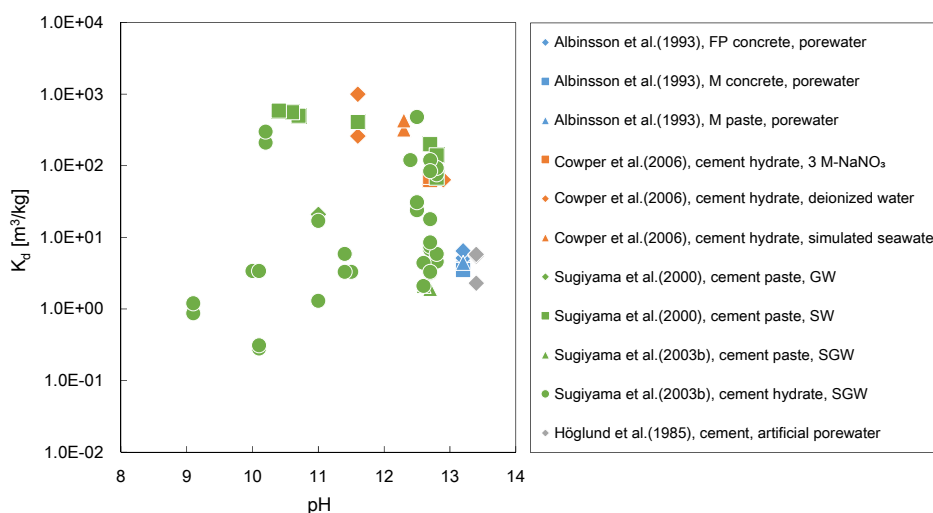


Figure 3.3.2 Overview of sorption data for thorium onto cementitious materials

### 3.3.3 Evaluation of data for uranium (VI) sorption onto cementitious materials

Table 3.3.3 shows evaluated entries in this section; the respective data are shown in Figure 3.3.3.

Table 3.3.3 List of evaluated data for uranium (IV) sorption on cementitious materials

Reference	Data table	Solid phase
Sugiyama et al. (2003b) <sup>41)</sup>	—	Cement hydrate
Zhao et al.(2000) <sup>42)</sup>	—	Concrete
Höglund et al.(1985)	U/8	Cement, concrete
Sugiyama et al.(2008)	U/10	OPC, FAC
Tits et al.(2008)	U/11	CSH

The pH dependence for uranium (VI)  $K_d$  values on cementitious materials (cement paste, concrete, CSH, etc.) is shown in Figure 3.3.3. There is no obvious trend with data in JAEA-SDB. The solid used in Höglund et al.(1985) are standard Portland cement and degraded concrete. These  $K_d$  values are consistent with other data. The data reported by Sugiyama et al.(2008) is varied due to the difference of the kinds of solid (OPC or FAC). The solid used in Tits et al.(2008) is the cement hydrates (CSH). The data are varied due to the difference of the reaction time and initial RN concentration.

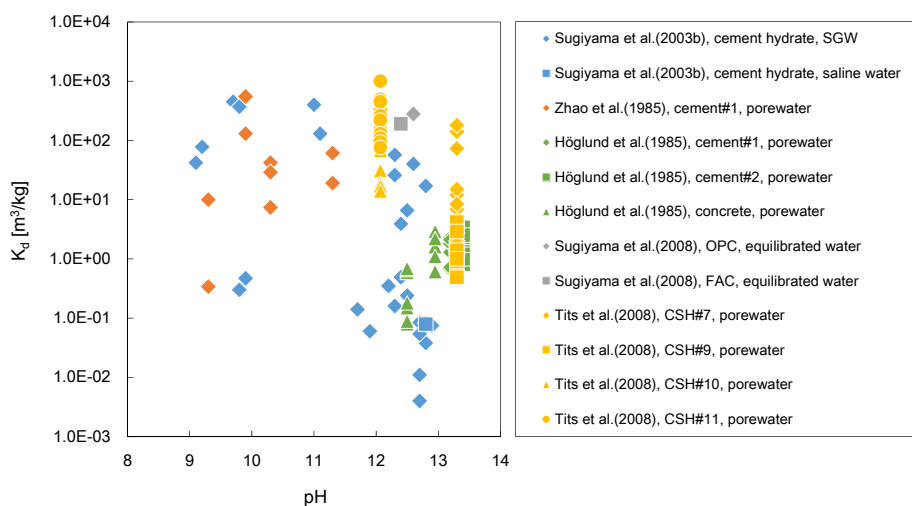


Figure 3.3.3 Overview of sorption data for uranium(VI) onto cementitious materials

#### 4. Conclusions

The present report focused on developing and updating of the sorption database (JAEA-SDB) as basis of integrated approach for PA-related  $K_d$  setting. This includes an updating of  $K_d$  data and QA classification, related to future  $K_d$ -setting and TSM development.

- $K_d$  data and their QA results are updated by focusing our recent activities on the  $K_d$  setting and mechanistic model development. As a result, 4,256  $K_d$  data from 30 references were added, total number of  $K_d$  values in the JAEA-SDB reached about 63,000. The QA/classified  $K_d$  data reached about 69% for all  $K_d$  data in JAEA-SDB.
- Further study is required to test the applicability of the JAEA-SDB and to improve their functions and contents by focusing on site-specific  $K_d$  setting including uncertainty assessment, and the combination with modeling approaches including integrated sorption-diffusion model.

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## Appendix

QA/classification guideline for JAEA-SDB  
(Ochs et al. 2007)

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## 1. Introduction, description of main criteria

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

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

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

### Criteria II — Quality of reported data

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

### Criteria III — Consistency of data:

While the previous two main criteria address the reliability of each  $K_d$  entry in the JAEA-SDB, criteria No. III requires an examination of the level of support that other  $K_d$  values in similar systems can lend to the entry under consideration. Any disagreement with data from related systems will have to be evaluated as well. It could be argued that this kind of data examination may be left to the user of the JAEA-SDB. However, the classification of data entries in the JAEA-SDB in terms of reliability adds an aspect of quality that is above that for a pure compilation, and users may expect that the listed  $K_d$  values passed some kind of check for internal consistency.

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

## 2. Description of checkpoints within each main criteria

### 2.1 General

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

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

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

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

- element
- solid phase
- solution composition
- atmosphere
- pH (or other information that allows to derive pH, e.g. portlandite equilibrium)
- pe/redox condition (only in case of redox-sensitive systems)
- method of pe control (only in case of redox sensitive systems and imposed reducing conditions)
- initial radionuclide (RN) concentration (except for RN that are not solubility controlled)
- method for phase separation
- type of experiment, if different from batch

→ In case of missing entries, the corresponding  $K_d$  is excluded from further evaluation and classified as unreliable (until remedied by operator). If all fields are completed, proceed to I-a.2.

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

- units

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

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

→ The following levels are distinguished:

class 1: table with  $K_d$  values given

class 2: table with % sorbed given

table with residual concentration given

class 3: linear graph  $K_d$

class 4: linear graph % sorbed

linear graph residual concentration

class 5: logarithmic graph  $K_d$

class 6: logarithmic graph % sorbed

logarithmic graph residual concentration

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

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

### II-a Solid phase (substrate)

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

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

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

1. It needs to be known whether a substrate consists of a single pure mineral phase, or whether it contains impurities or additional minerals. In general, some measure of site density per mass (e.g. CEC) needs to be known to properly design experiments, in particular with respect to achieving reasonable surface loading.
2. In case of simple substrates (pure minerals), no further information is necessary.

3. In case of complex substrates (i.e., where significant impurities are present, or where a substrate is composed of several minerals), and in particular in case of natural samples, detailed information on composition has to be provided in addition.
  4. In cases where sample treatment (such as crushing or sieving) had been performed, the respective information on particle size also needs to be provided (see II-f). Where any chemical treatments (e.g. acid washing to remove calcite; but also change of redox conditions in case of redox-sensitive substrates, see II-c) had been applied, the applied method and resulting mineralogy should be given as well.
  5. In case of many commercially available substrates (e.g., MX-80 or Kunigel-V1 bentonite; standard clay minerals from the Clay Minerals Society, such as SWy-1; Min-U-Sil SiO<sub>2</sub>, etc.) detailed solid phase information is widely known and can be retrieved from a large number of publications. Therefore, characterization of such solids is not required for each entry in the JAEA-SDB; i.e., level A or B can be reached even if such information is not reported. Note that this holds only when such solids have been used as received. Where washing procedures etc. have been applied, the procedures and resulting changes still need to be documented.
- Three levels of reliability:
- A) Major and minor mineralogy as well as surface characteristics are known.  
For example: The substrate is a single, well-defined mineral; or comprehensively characterized complex mineral assemblage. Either no sample treatment has been carried out, or it is described in detail and the result are documented.
  - B) Major mineralogy as well as surface characteristics are known.  
For example: The substrate is a single mineral that may contain impurities (such as a non-purified clay mineral) or a complex mineral assemblage where additional impurities could be present. Sample treatment may have led to minor changes in mineralogy.
  - C/D) Information on both major mineralogy or surface characteristics is lacking.  
For example: There is no information on CEC (or another measure of sorption capacity); or the substrate is a natural clay sample where it is not clear whether it is smectite, kaolinite, or illite; or a non-characterized soil or crushed rock. Sample treatment may have led to major changes in mineralogy that are not documented.

## II-b Adjustment and control of pH

One of the most important solution parameters controlling radionuclide(RN) sorption is pH. It needs to be known to interpret  $K_d$  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  $O_2$  (as a matter of fact, the latter may be the more common problem).

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

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

→ Two levels of reliability:

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

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



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

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

→ If a lower quality than required for level C/D is evident, the respective entry is excluded from further evaluation as unreliable. For example, cases where it has been attempted to achieve reducing conditions only by minimizing the level of O<sub>2</sub> (e.g., by performing experiments in a N<sub>2</sub> atmosphere) generally should be labeled "unreliable" (except where the oxidation state of a RN somehow has been confirmed, see description of level C/D). Also, if a strongly complexing reducing agent (such as many organic acids) is used at unspecified concentration levels, the respective entry is excluded from further evaluation as unreliable.

#### II-d Final solution composition

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

→ Two levels of reliability:

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

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

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

#### II-e Temperature

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

→ Two levels of reliability:

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

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

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

It is evaluated whether enough solid had been added to avoid a significant influence by the vessel walls (see II-m), and to ensure sample reproducibility and representativeness in case of complex substrates, especially in case of large grain sizes: It is estimated that in cases where

less than ca. 100 mg of solid (this value depends on grain size) has been added to each experimental vessel, sample reproducibility and representativeness becomes difficult to achieve in case of complex or crushed samples.

→ Two levels of reliability:

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

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

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

C/D) Any other than the above.

## II-g Sorption value

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

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

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

C/D) Any other than the above.

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

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

→ Three levels of reliability:

A) RN is not solubility limited, or initial [RN] was clearly (at least a factor of 5) below the solubility limit. Note that factor 5 does not take into account uncertainties in RN solubility; i.e., if the solubility of a given RN cannot be estimated with more certainty than e.g. 10<sup>-6</sup> to 10<sup>-8</sup> M, then initial [RN] has to be ≤ 2×10<sup>-9</sup> 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<sub>d</sub> value: For example: If the absence of artifacts has been demonstrated for some representative samples of a study by comparing an efficient and a standard method of phase separation, the rating A may be given to all datapoints of this study,

- even if they correspond to the standard method only.
- B) Only one, but efficient method (high-speed centrifugation, ultrafiltration) is used, and there is no evidence for artifacts such as colloid effects or significant sorption to the filter.
  - C/D) Only one general method (normal centrifugation, membrane filtration with nominal pore sizes of 0.01~0.45  $\mu\text{m}$ ) is used, and there is no evidence for artifacts such as colloid effects or significant sorption to the filter.
  - If no phase separation is used, or in case of obvious evidence for artifacts (colloid effect, adsorption on filter) the respective entry is excluded from further evaluation as unreliable.
- II-j Reaction time**
- Two levels of reliability:
  - A/B) Identical (similar) results are obtained with different reaction times, or some other demonstration of near-equilibrium is provided (e.g. separate kinetic experiments).
  - C/D) Only one, but reasonably long reaction time is used. What is “reasonably long” is highly dependent on the experimental system: In general, the time needed to reach equilibrium will increase with the complexity of the sorbing substrate and the strength of sorption. Sorption of Sr onto a pure clay mineral through ion exchange can be assumed to be complete within a day; sorption of a trivalent actinide onto a complex substrate may need several days to weeks for completion. In the absence of kinetic information, operator expert decisions will be required to assess this point. If possible, reaction times reported for similar systems included in the JAEA-SDB could be used to evaluate what is reasonably long. Further, even for the most simple systems a reaction time of 1 day is considered as minimum requirement.
  - If the requirement for level C/D is not met (i.e., if the reaction time cannot be assumed to be reasonably long), the respective entry is excluded from further evaluation as unreliable.
- II-k Agitation method**
- Two levels of reliability:
  - A/B) Appropriate agitation is required in all cases, except where enough kinetic information is provided to show that equilibrium has been reached. Shaking is the preferred method, as use of stir bars can lead to abrasion of samples. In case of simple and well crystallized substrates (such as Al-oxide) or of substrates with very small grain size that are easily suspended, stir bars can also be accepted.
  - C/D) Any other than the above.
- II-l RN loading**
- Ideal are values as a function of RN loading (i.e.,  $K_d$  values that form part of an isotherm), otherwise low loading is preferred. RN loading (e.g. in moles RN/kg substrate) refers to the amount of RN adsorbed in relation to the amount of different surface sites available. It is known from classical isotherms (e.g. Langmuir) that a linear sorption can only be assumed if sufficient unoccupied sites are present. In case of simple substrates (including some bentonites), the linear portion of an isotherm extends to fairly high RN loading. There are other cases where  $K_d$  depends significantly on RN loading over many orders of RN concentration.
- Three levels of reliability:
  - A) At least one isotherm has been determined (for a constant solution composition and L/S), and at least some experiments have been carried out using trace level RN concentration (i.e., at least some data are included within a linear sorption region).
  - B) No isotherm is available, but at least a limited variation of initial [RN] or L/S has been carried out, and some experiments have been carried out using trace level RN concentration (i.e., some data are included within a linear sorption region).
  - C/D) No variation as in A or B has been carried out.
- II-m Reaction vessels**
- High-density polyethylene (HDPE) or Teflon are preferred over normal PE, which is preferred over glass, which may lead to sorption of radionuclides by the vessel walls. Especially at high or very low pH, glass dissolution and release of dissolved or colloidal silica may also occur. On the other hand, glass is more gas-tight (especially than PE); if that is of experimental relevance.

Corrections for sorption on vessel walls should not be necessary if blank tests show that it can be neglected.

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

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

→ Three levels of reliability:

- A) An appropriate vessel has been used (taking into account sorption as well as tightness with respect to  $\text{CO}_2$  or  $\text{O}_2$ , 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,  $\text{pCO}_2$ , but also temperature, L/S, or grain size in case of crushed substrates), but not parameters that only help to determine the experimental framework (such as vessel type or reaction time). In particular, variation of key parameters allows improved detection of experimental problems and systematic errors. Especially the latter are not detected by repeating experiments under identical conditions. In the

application of this checkpoint, care has to be taken to take into account the characteristics of the particular system studied. For example, more parameter variation may be required to show clear trends in a complicated system in comparison to a simpler one. On the other hand, the pH and carbonate concentration in experiments with calcite are quite constrained by the solid itself, and only limited variations are possible.

→ Four levels of reliability:

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

## 2.4 Criteria III: Consistency of data

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

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

## 3. Overall classification

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

- The three criteria I-III are evaluated separately, the respective results are reported separately as well.
- Criteria I: The checkpoints under I-a are used in a yes/no screening fashion, entries not fulfilling I-a are labeled as unreliable and are not evaluated further.
- Criteria I-b is then used to assign classes 1-6 for documentation.
- Criteria II: a) The datasets that pass Criteria I are again classified according to a 6-level system, where classes 1-6 represent the highest and lowest levels of reliability. To ensure a minimum quality level, certain checkpoints are regarded as critical (marked with \* in Table 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 3.1 below.
- e) The total sum of points obtained for Criteria II is then used to indicate the level of reliability. With the present system, the maximum number of points would be 183, leading to an overall classification as follows (Table 3.2).

Table 3.1 Weighting of individual checkpoints under Criteria II.

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

\* indicates critical checkpoints with minimum requirements;  
**bold letters** indicate the checkpoints to be evaluated initially.

Table 3.2 Overall classes of reliability for Criteria II

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

- Criteria III: Criteria III is used to qualitatively assess consistency with other studies. In case of clear inconsistencies, an entry may be labeled as unreliable.
- Overall, the following classification system is used, with Criteria II as the main basis for assessing the reliability of entries in the JAEA-SDB (Table 3.3).

Table 3.3 The classification system

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



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

(a) 量濃度 (amount concentration) は臨床化学の分野では物質濃度 (substance concentration) ともよばれる。

(b) これらは無次元量あるいは次元 1 をもつ量であるが、そのことを表す単位記号である数字の 1 は通常は表記しない。

表 3. 固有の名称と記号で表されるSI組立単位

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

(a) SI接頭語は固有の名称と記号を持つ組立単位と組み合わせても使用できる。しかし接頭語を付した単位はもはやコヒーレントではない。

(b) ラジアンとステラジアンは数字の 1 に対する単位の特別な名称で、量についての情報をつたえるために使われる。実際には、使用する時には記号rad及びsrが用いられるが、習慣として組立単位としての記号である数字の 1 は明示されない。

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

(d) ヘルツは周期現象についてののみ、ベクレルは放射性核種の統計的過程についてののみ使用される。

(e) セルシウス度はケルビンの特別な名称で、セルシウス温度を表すために使用される。セルシウス度とケルビンの単位の大きさは同一である。したがって、温度差や温度間隔を表す数値はどちらの単位で表しても同じである。

(f) 放射性核種の放射能 (activity referred to a radionuclide) は、しばしば誤った用語で"radioactivity"と記される。

(g) 単位シーベルト (PV, 2002, 70, 205) についてはCIPM勧告2 (CI-2002) を参照。

表 4. 単位の中に固有の名称と記号を含むSI組立単位の例

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

表 5. SI 接頭語

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

表 6. SIに属さないが、SIと併用される単位

名称	記号	SI 単位による値
分	min	1 min=60 s
時	h	1 h=60 min=3600 s
日	d	1 d=24 h=86 400 s
度	°	1°=(π/180) rad
分	′	1′=(1/60)°=(π/10 800) rad
秒	″	1″=(1/60)′=(π/648 000) rad
ヘクタール	ha	1 ha=1 hm <sup>2</sup> =10 <sup>4</sup> m <sup>2</sup>
リットル	L, l	1 L=1 l=1 dm <sup>3</sup> =10 <sup>3</sup> cm <sup>3</sup> =10 <sup>-3</sup> m <sup>3</sup>
トン	t	1 t=10 <sup>3</sup> kg

表 7. SIに属さないが、SIと併用される単位で、SI単位で表される数値が実験的に得られるもの

名称	記号	SI 単位で表される数値
電子ボルト	eV	1 eV=1.602 176 53(14)×10 <sup>-19</sup> J
ダルトン	Da	1 Da=1.660 538 86(28)×10 <sup>-27</sup> kg
統一原子質量単位	u	1 u=1 Da
天文単位	ua	1 ua=1.495 978 706 91(6)×10 <sup>11</sup> m

表 8. SIに属さないが、SIと併用されるその他の単位

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

表 9. 固有の名称をもつCGS組立単位

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

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

表 10. SIに属さないその他の単位の例

名称	記号	SI 単位で表される数値
キュリー	Ci	1 Ci=3.7×10 <sup>10</sup> Bq
レントゲン	R	1 R=2.58×10 <sup>-4</sup> C/kg
ラド	rad	1 rad=1 cGy=10 <sup>-2</sup> Gy
レム	rem	1 rem=1 cSv=10 <sup>-2</sup> Sv
ガンマ	γ	1 γ=1 nT=10 <sup>-9</sup> T
フェルミ	f	1 フェルミ=1 fm=10 <sup>-15</sup> m
メートル系カラット		1 メートル系カラット=0.2 g=2×10 <sup>-4</sup> kg
トル	Torr	1 Torr=(101 325/760) Pa
標準大気圧	atm	1 atm=101 325 Pa
カロリ	cal	1 cal=4.1858 J (「15°C」カロリ), 4.1868 J (「IT」カロリ), 4.184 J (「熱化学」カロリ)
マイクロン	μ	1 μ=1 μm=10 <sup>-6</sup> m

