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Development of JAEA Sorption Database (JAEA-SDB) : Update of Data Evaluation Functions and Sorption/QA Data

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JAEA-Data/Code

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**Development of JAEA Sorption Database (JAEA-SDB) :
Update of Data Evaluation Functions and Sorption/QA Data**

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Sorption and diffusion of radionuclides in buffer materials (bentonite) and rocks are the key processes in the safe geological disposal of radioactive waste, because migration of radionuclides in this barrier is expected to be diffusion-controlled and retarded by sorption processes. It is therefore necessary to understand the sorption and diffusion processes 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 and diffusion parameters in buffer materials (bentonite) and rocks. These sorption and diffusion databases (SDB/DDB) were firstly developed as an important basis for the H12 PA of high-level radioactive waste disposal, and have been provided through the Web. JAEA has been continuing to improve and update the SDB/DDB 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 developing and updating of the sorption database (JAEA-SDB) as basis of integrated approach for PA-related K_d setting. This includes an overview of database structure, contents and functions including additional data evaluation function focusing on multi-parameter dependence, operating method, PA-related applications of the web-based JAEA-SDB. 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, 4,250 K_d data from 32 references are added, total K_d values in the JAEA-SDB are about 28,540. The QA/classified K_d data are about 39% for all K_d data in JAEA-SDB. The updated JAEA-SDB is expected to make it possible to obtain quick overview of the available data, and to have suitable access to the respective data for PA-related K_d setting in effective, traceable and transparent manner.

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

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JAEA 収着データベース(JAEA-SDB)の開発：
データ評価機能と収着データ/信頼度情報の拡充

日本原子力研究開発機構 地層処分研究開発部門
地層処分基盤研究開発ユニット

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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）及び岩石中での収着・拡散現象は、その移行遅延を支配する重要な現象である。これら収着・拡散現象の理解、信頼性の高い収着・拡散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うえで重要となる。

この目的のために、日本原子力研究開発機構では、緩衝材（ベントナイト）及び岩石を対象として、収着・拡散パラメータに関するデータベース開発を進めている。これら収着・拡散データベース（SDB/DDB）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の対応を念頭に、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注目して、データベースの改良・更新を継続的に実施してきた。

本報告は、性能評価における 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）の開発と更新の現状について報告する。はじめに JAEA-SDB の開発の現状として、データベースの構造、内容、今回拡充した複数のパラメータ依存性の評価手法を含む機能、さらには、操作方法並びに性能評価への適用法等の概要をまとめる。 K_d データと信頼度情報の更新については、 K_d 設定や現象論モデル開発との関連に着目して実施した。今回の更新において、32 の文献から 4,250 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 28,540 件となり、全体の約 39% 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、収着データベースから利用可能な関連データ群の速やかな抽出、 K_d 設定の際に参照すべきデータの適切な選定が、一層の効率性、追跡性、透明性をもって可能となると考えられる。

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1. Introduction

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

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

- 1) updating of sorption data (Suyama and Sasamoto, 2004; Saito et al., 2007) and diffusion data (Tochigi and Tachi, 2009, 2010)
- 2) assuring the desired quality level for SDB (Ochs et al., 2007; Saito et al., 2008; Ochs et al., 2010; Suyama et al., 2011) and DDB (Tochigi and Tachi, 2009)
- 3) testing and applying of the SDB to parameter-setting (Ochs et al., 2008).

The web-based sorption and diffusion database system (JAEA-SDB/DDB) has been developed to utilize quality assuring procedure and to allow effective application for parameter setting (Tachi et al., 2009; www/migrationdb.jaea.go.jp).

JAEA has developed the integrated approaches for site-specific K_d setting for PA calculations, as shown in Figure 1.1, can be made available by three different approaches;

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

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 (2005). It is not feasible to determine K_d value experimentally for all conditions to be considered in K_d setting in PA should be therefore based on the combination of above three approaches. The sorption database (SDB), containing large amount of sorption data for approximated, simplified, or generic systems, are used to K_d setting for PA conditions by taking into account any differences in substrate and geochemical conditions. This transfer can be done through expert judgment and semi-quantitative way, by considering difference in e.g. surface sites, speciations, competitive reactions, etc. (e.g., NEA, 2005; Ochs et al., 2008). The thermodynamic sorption model (TSM) makes it possible to estimate K_d variations directly, based on mechanistic understanding, as shown in NEA (2005). JAEA has developed the integrated sorption/diffusion (ISD) database in combination with thermodynamic sorption and diffusion model, and published first prototype model and database for bentonite system in FY2009 (Tachi et al., 2010).

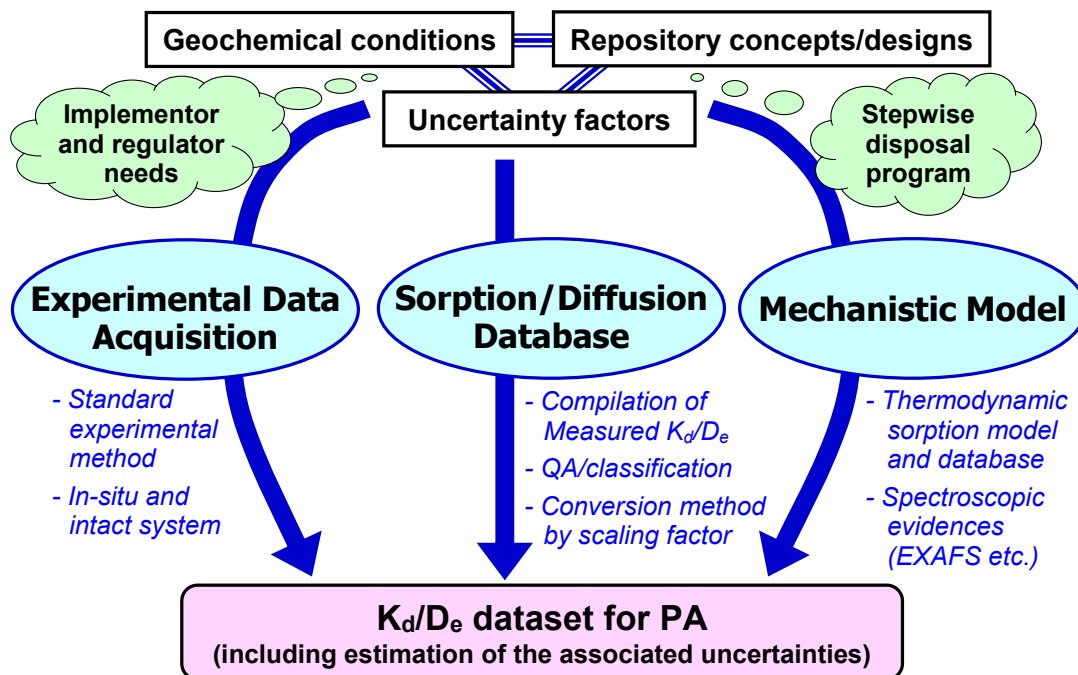


Figure 1.1 Integrated approach for sorption/diffusion parameter setting for PA

The present report focuses on developing and updating of the sorption database (JAEA-SDB) as basis of integrated approach shown in Figure 1.1. This includes an overview of basic functions, structures, applications of the web-based JAEA-SDB, including updated functions to effective data extractions (Chapter 2), updating of K_d data and QA classification, related to K_d-setting and TSM development (Chapter 3).

2. Overview of JAEA-SDB including updated functions and its PA-related applications

2.1 System, functions and contents of JAEA-SDB

2.1.1 Overview and status of JAEA-SDB

The JAEA-SDB is a compilation of original K_d data for key radionuclides sorption on bentonite buffer, rocks and cementitious materials 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 (Rüegger and Ticknor, 1992), 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 2.1.2)
- 2) QA/classification scheme to check the reliability (see 2.1.3 and 2.2.2)
- 3) data evaluation function to focusing on multi-parametric dependence of K_d (see 2.2.3)

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

Contents/functions	Brief description for status
Number of K_d values / references	K_d ; 28,540 (4,250 was added in this update*) Reference ; 350 (← 32 references were added in this update*)
Elements	37 elements; 1 st 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 nd group; Ag, Ba, Ca, Ce, Cl, Co, Eu, Fe, I, Mn, Mo, Na, Nd, Ru, Sr, Zn
Solid phase	Bentonite (clay minerals) Rocks – 5 group; Basaltic rock, Granitic rock, Mudstone, Sandstone, Tuff Other minerals (Fe, Al-oxides/hydroxide, calcite, etc.) Cementitious materials (cement / concrete)
Search parameters	Element, Solid phase group Detailed – solid phase, water type, pH, Eh, ionic strength, temperature, solid/liquid 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, solid/liquid ratio, contact time, initial concentration Grouping function to evaluate multi-parameter dependence*
QA/classification	QA information evaluated by QA guideline, and related evidences 10,990 K_d (about 39% of total K_d) for key RNs on Bentonite*, Mudstone, Granitic rock, Tuff have been evaluated
Database systems	- Web application based database (since 2009) - Microsoft Access based database (since 2003 / stand-alone / limited functions)

*; Contents and functions updated in this report.

2.1.2 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, radionuclide redox state and initial concentration, solid/liquid 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		-	valence
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 ² /g	
		CEC	meq/100g	Cation Exchange Capacity
		Chemical/mineral composition	-	as PDF file
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 ₃	ppm	HCO ₃ ⁻ + CO ₃ ²⁻
		SO ₄	ppm	
		F	ppm	
		SiO ₂	ppm	
		Fe	ppm	
		NO ₃	ppm	
		ClO ₄	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		degC	
	Contact time		day	
	Separation		-	Solid-liquid separation method

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

Category	Parameters and notes recorded		Unit	Remarks
Distributi- on coefficient	K _d		m ³ /kg	Distribution coefficient
	Detailed Info.	error	m ³ /kg	Error
		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

2.1.3 Scheme and criteria for QA/classification of K_d in JAEA-SDB

As discussed in 2.1.1, 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-I (Ochs et al., 2007), and is briefly summarized in Table 2.3.

According to 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, the all results can be referred in JAEA-SDB (Tachi et al., 2009). The JAEA-SDB uses the QA level (class I-VI), classified according to 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, can be referred as PDF format in JAEA-SDB to keep the traceability. The results pertaining to Criteria III are discussed subsequently and are illustrated in the form of plots of K_d vs. a relevant master variable (typically pH), 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	Temperature	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	solution/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 , solution/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	solution/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, solution/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'.

2.2 Methods of practical use of JAEA-SDB

2.2.1 Basic operating method of JAEA-SDB

The main objective of JAEA-SDB is to search of K_d data for related systems and to investigate K_d trends by plotting as a function of selected key parameters. These functions can be implemented in database software that allows quick searching/plotting of data as a wide variety of function of key parameters. Main functions and operating steps are i) searching, ii) viewing datasheet, iii) graph plotting, and iv) data download as follows;

1) Data searching

K_d data in JAEA-SDB can be searched by ‘elements’, ‘solid phase group’ and key parameters (experimental conditions) such as solid phase, solution type and pH/Eh, initial concentration of radionuclides, solid/liquid ratio, and separation method, etc., as shown in Figure 2.1 as the top page of JAEA-SDB.

The screenshot shows the main searching menu of the JAEA-SDB. The interface is titled "Japan Atomic Energy Agency Nuclide Migration Database Sorption Database". It includes several sections for data selection and search conditions:

- Buttons:** "Data Display", "Clear", "Graph Plot", "Japanese", and "Quit".
- Navigation:** "Top Page(data search)".
- Elements:** A grid of checkboxes for various elements. "Am" (Americium) is selected under the "Gr-1" group. Other elements include Ac, Bi, Cm, Cs, Nb, Ni, Np, Pa, Pb, Pd, Po, Pu, Ra, Sb, Se, Sm, Sn, Tc, Th, U, and Zr.
- Solid_Phase_Group:** A grid of checkboxes for different material types. "Bentonite (Clay minerals)" is selected. Other options include Basaltic rocks, Cementitious materials, Granitic rocks, Mudstone (Sedimentary rocks), Other minerals, Sandstone, and Tuff.
- Detailed Search Condition:** A section with a "Screen Update" button and several input fields:
 - Solid Phase:** A dropdown menu with options: BAS_MINER, BENTONITE, bentonite, bentonite/quartz(10:90), Ca-bentonite.
 - Water Type:** A dropdown menu with options: 0.01M CO3/0.01M Tris, 0.01M NaClO4, 0.06M NaCl, 0.10M NaCl, 0.1M NaClO4.
 - pH:** Two input fields with a minus sign between them.
 - Eh (mV):** Two input fields with a minus sign between them.
 - Ionic Strength (mol/L):** Two input fields with a minus sign between them.
 - Temperature (degC):** Two input fields with a minus sign between them.
 - Solution/Solid Ratio (mL/g):** Two input fields with a minus sign between them.
 - Contact Time (day):** Two input fields with a minus sign between them.
 - Initial Concentration (mol/L):** Two input fields with a minus sign between them.
- Separation Method:** Checkboxes for "Centrifugation", "filtration", "ultrafiltration", "unfiltration", and "others".
- Atmosphere/Redox Condition:** Checkboxes for "aerobic", "anaerobic", and "others".

Figure 2.1 Main searching menu / top page of JAEA-SDB

Number of K_d data and references for selected systems can be referred in ‘Data / Reference count table’ in main searching menu. Reference list as data source for selected systems can be viewed in the main menu, and can be directly accessed to dataset in concerned references by selecting checkbox (Figure 2.2).

The screenshot shows the 'Sorption Database' interface. At the top, there is a header with the Japan Atomic Energy Agency logo and the text 'Nuclide Migration Database' and 'Sorption Database'. Below the header are several buttons: 'Data Display', 'Clear', 'Graph Plot', 'Japanese', and 'Quit'. A link for 'Top Page(data search)' is also present.

The main content area is titled 'Data/Reference Count Table'. It features a 'Display Class Selection' dropdown menu set to 'Data Count'. Below this is a table with columns for different material classes and a row for the nuclide 'Am'.

	Basaltic rocks	Bentonite (Clay minerals)	Cementitious materials	Granitic rocks	Mudstone (Sedimentary rocks)	Other minerals	Sandstone	Tuff
Am	130	426	77	124	187	279	113	219

Below the count table is a section for 'Reference(Data Source)'. It includes a 'Clear' button, a 'Sort Key' field, and controls for 'Page No' (set to 1) and 'Data Count/page' (set to 50). The 'Hit Count' is displayed as 22.

Author	Reference	Year
Allard, B. and Beall, G.W.	<input type="checkbox"/> Allard and Beall(1979)	1979
Allard, B., Rydberg, J., Kipatsi, H. and Torstenfelt, B.	<input type="checkbox"/> Allard et al.(1979b)	1979
Ames, L. L., McGarragh, J. E. and Walker, B. A.	<input type="checkbox"/> Ames et al.(1981)	1981
Barney, G. S.	<input type="checkbox"/> Barney(1981)	1981
Baston, G. M. N., Berry, J. A., Brownword, M., Cowper, M. M., Haworth, A., Heath, T. G., Ilett, D. J., McCrohon, R., Tweed and C.J.	<input type="checkbox"/> Baston et al.(1998)	1998
Baston et al.	<input type="checkbox"/> Baston et al.(1999)	1999
Degueldre, C., Ulrich, H. J. and Silby, H.	<input type="checkbox"/> Degueldre et al.(1994)	1994
Fukumoto, M., Nishikawa, Y., Kagawa, A. and Kawamura, K.	<input type="checkbox"/> Fukumoto et al.(2000)	2000
Gorgeon, L.	<input type="checkbox"/> Gorgeon(1994)	1994
Higgo J. J. W., Rees L. V. C., Cronan D. S.	<input type="checkbox"/> Higgo et al.(1983)	1983
Ikeda, T. and Amaya, T.	<input type="checkbox"/> Ikeda and Amaya(1998)	1998
Konishi, M., Yamamoto, K., Yanagi, T. and Okajima, Y.	<input type="checkbox"/> Konishi et al.(1988)	1988
Morgan, R. D., Pryke, D. C. and Rees, J. H.	<input type="checkbox"/> Morgan et al.(1987)	1987
Morgan R. D., Pryke D. C. and Rees J. H. Rees	<input type="checkbox"/> Morgan et al.(1988)	1988

Figure 2.2 Data/reference counting table and reference list in top page of JAEA-SDB (Example for Am)

2) Viewing datasheet

K_d data and associated experimental methods and conditions can be viewed in table format for selected systems as shown in Figure 2.3. Detailed information for solid phase, solution/solid ratio, water type, K_d data and reference (green colored columns) can be displayed by sliding columns (indicated by red arrow from top to down in Figure 2.3). Some detailed information such as mineral/chemical compositions for solid phase can be checked via PDF file.

Japan Atomic Energy Agency
Sorption Database

Nuclide Migration Database

Top Page
Graph Plot
Download
Grouping Sheet
Reliability Info
Quit

Search Condition
Element: Am
Solid Phase Group: Bentonite (Clay minerals)

Page No: 1 Data Count/page: 50
Hit Count: 426

Save No.	Element	Charge	Solid Phase Group	Solid Phase	Solution/Solid(ml/g)	water type	pH init.	pH end	Eh init(mV)	Eh end(mV)	atm/radiox condit
42187	Am	□	Bentonite (Clay minerals)	kaolinite	67-100	groundwater	n.r.	7.21±0.5	n.r.	n.r.	oxidizing condition
42214	Am	□	Bentonite (Clay minerals)	montmorillonite	67-100	groundwater	n.r.	7.21±0.5	n.r.	n.r.	oxidizing condition
42253	Am	□	Bentonite (Clay minerals)	bentonite/quartz(0.90)	10-50	Aq1105	8.2	n.r.	n.r.	n.r.	aerobic condition
42254	Am	□	Bentonite (Clay minerals)	bentonite/quartz(0.90)	10-50	Aq293	8.2	n.r.	n.r.	n.r.	aerobic condition
42255	Am	□	Bentonite (Clay minerals)	bentonite/quartz(0.90)	10-50	Aq293	8.2	n.r.	n.r.	n.r.	aerobic condition
42256	Am	□	Bentonite (Clay minerals)	bentonite/quartz(0.90)	10-50	Aq1105	8.2	n.r.	n.r.	n.r.	aerobic condition
42257	Am	□	Bentonite (Clay minerals)	bentonite/quartz(0.90)	10-50	Aq293	8.2	n.r.	n.r.	n.r.	aerobic condition
42258	Am	□	Bentonite (Clay minerals)	bentonite/quartz(0.90)	10-50	Aq1105	8.2	n.r.	n.r.	n.r.	aerobic condition
42890	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	7.25	n.r.	n.r.	n.r.
42891	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	n.r.	n.r.	n.r.	n.r.
42892	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	7.2	n.r.	n.r.	n.r.
42893	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	n.r.	n.r.	n.r.	n.r.
42894	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	7.8	n.r.	n.r.	n.r.
42895	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	7.35	n.r.	n.r.	n.r.
42896	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	n.r.	n.r.	n.r.	n.r.
42897	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	n.r.	n.r.	n.r.	n.r.
42898	Am	□	Bentonite (Clay minerals)	smectite	n.r.	groundwater#1	n.r.	n.r.	n.r.	n.r.	n.r.
44467	Am	□	Bentonite (Clay minerals)	BAS_MINER	1.00E-09	room	7	c(4000 g/1h)	1.00E+01 - 1.59E+01	n.r.	Allard and Beall(1979)
44468	Am	□	Bentonite (Clay minerals)	BAS_MINER	<1.00E-08	25	7	c(7000rpm/50min)+H(2mm)	2.00E-01	n.r.	Allard et al(1979b)
44469	Am	□	Bentonite (Clay minerals)	BAS_MINER	<1.00E-08	65	7	c(7000rpm/50min)+H(2mm)	2.51E-01	n.r.	Allard et al(1979b)
44470	Am	□	Bentonite (Clay minerals)	BAS_MINER	<1.00E-08	25	7	c(7000rpm/50min)+H(2mm)	3.98E+00	n.r.	Allard et al(1979b)
44471	Am	□	Bentonite (Clay minerals)	BAS_MINER	<1.00E-08	25	180	c(7000rpm/50min)+H(2mm)	5.01E-01	n.r.	Allard et al(1979b)
44472	Am	□	Bentonite (Clay minerals)	BAS_MINER	<1.00E-08	25	180	c(7000rpm/50min)+H(2mm)	7.94E+00	n.r.	Allard et al(1979b)
44473	Am	□	Bentonite (Clay minerals)	BAS_MINER	2.06E-09	150	15	n.r.	1.30E-01	n.r.	Ames et al(1981)
44474	Am	□	Bentonite (Clay minerals)	BAS_MINER	2.06E-09	150	18	n.r.	1.38E-01	n.r.	Ames et al(1981)
44475	Am	□	Bentonite (Clay minerals)	BAS_MINER	2.06E-09	150	8	n.r.	1.37E-01	n.r.	Ames et al(1981)
44476	Am	□	Bentonite (Clay minerals)	BAS_MINER	2.06E-09	150	30	n.r.	1.44E-01	n.r.	Ames et al(1981)
44477	Am	□	Bentonite (Clay minerals)	BAS_MINER	2.06E-09	150	31	n.r.	1.47E-01	n.r.	Ames et al(1981)
44478	Am	□	Bentonite (Clay minerals)	BAS_MINER	2.06E-09	150	45	n.r.	1.51E-01	n.r.	Ames et al(1981)
					2.06E-09	150	4	n.r.	1.55E-01	n.r.	Ames et al(1981)
					2.06E-09	150	1	n.r.	1.58E-01	n.r.	Ames et al(1981)
					2.06E-09	150	11	n.r.	1.58E-01	n.r.	Ames et al(1981)
					2.06E-09	150	23	n.r.	1.71E-01	n.r.	Ames et al(1981)
					1.83E-12	n.r.	14	f(50angstrom)	1.20E-01	n.r.	Barney(1981)
					2.93E-11	n.r.	14	f(50angstrom)	3.57E-01	n.r.	Barney(1981)
					6.93E-12	n.r.	14	f(50angstrom)	5.90E-01	n.r.	Barney(1981)
					1.34E-11	n.r.	14	f(50angstrom)	6.30E-01	n.r.	Barney(1981)
					9.27E-12	n.r.	14	f(50angstrom)	7.30E-01	n.r.	Barney(1981)
					1.05E-11	n.r.	14	f(50angstrom)	8.30E-01	n.r.	Barney(1981)
					1.46E-11	n.r.	14	f(50angstrom)	1.19E+00	n.r.	Barney(1981)
					1.16E-11	n.r.	14	f(50angstrom)	1.17E+00	n.r.	Barney(1981)
					1.59E-11	n.r.	14	f(50angstrom)	1.27E+00	n.r.	Barney(1981)
					1.06E-11	n.r.	14	f(50angstrom)	1.28E+00	n.r.	Barney(1981)
					3.17E-11	n.r.	14	f(50angstrom)	1.39E+00	n.r.	Barney(1981)
					3.05E-11	n.r.	14	f(50angstrom)	1.44E+00	n.r.	Barney(1981)

Display of detailed information related to solid phase by sliding columns

Solid Phase	Specific Surface Area(m ² /g)	CEC(meq/100g)	note	Chemical/Mineral Composition
kaolinite	n.r.	n.r.	-	-
montmorillonite	n.r.	n.r.	-	-
bentonite/quartz(0.90)	n.r.	n.r.	bentonite : quartz = 10 : 90	-
bentonite/quartz(0.90)	n.r.	n.r.	bentonite : quartz = 10 : 90	-
bentonite/quartz(0.90)	n.r.	n.r.	bentonite : quartz = 10 : 90	-
bentonite/quartz(0.90)	n.r.	n.r.	bentonite : quartz = 10 : 90	-
bentonite/quartz(0.90)	n.r.	n.r.	bentonite : quartz = 10 : 90	-
smectite	n.r.	n.r.	smectite(Basalt secondary)	-
smectite	n.r.	n.r.	smectite(Basalt secondary)	s-12.pdf
smectite	n.r.	n.r.	smectite(Basalt secondary)	s-12.pdf
smectite	n.r.	n.r.	smectite(Basalt secondary)	s-12.pdf
smectite	n.r.	n.r.	smectite(Basalt secondary)	s-12.pdf
smectite	n.r.	n.r.	smectite(Basalt secondary)	s-12.pdf
smectite	n.r.	n.r.	smectite(Basalt secondary)	s-12.pdf
smectite	n.r.	n.r.	smectite(Basalt secondary)	s-12.pdf
BAS_MINER	640	75.6	Fraction Size (2microm). This is the secondary mineral sample obtained from a large vein in the Pomona basalt. Basalt fragments were removed from the clay vsp-filling. Color:blue-green, Major minerals:smectite clay	-
BAS_MINER	640	75.6	Fraction Size (2microm). This is the secondary mineral sample obtained from a large vein in the Pomona basalt. Basalt fragments were removed from the clay vsp-filling. Color:blue-green, Major minerals:smectite clay	-
DAG_MINER	646	75.6	Fraction Size (2microm). This is the secondary mineral sample obtained from a large vein in the Pomona basalt. Basalt fragments were removed from the clay vsp-filling. Color:blue-green, Major minerals:smectite clay	-
BAS_MINER	646	75.6	Fraction Size (2microm). This is the secondary mineral sample obtained from a large vein in the Pomona basalt. Basalt fragments were removed from the clay vsp-filling. Color:blue-green, Major minerals:smectite clay	-
DAG_MINER	646	75.6	Fraction Size (2microm). This is the secondary mineral sample obtained from a large vein in the Pomona basalt. Basalt fragments were removed from the clay vsp-filling. Color:blue-green, Major minerals:smectite clay	-

Chemical composition data as PDF file

basalt, smectite : Ames et al.(1981)
Characteristics of Rocks and Minerals Used in the Sorption Work

Oxide	Wt% Oxides			
	Untanum Basalt	Pomona Basalt	Flow E Basalt	Calined Smectite
SiO ₂	55.64	51.87	54.47	59.04
Al ₂ O ₃	13.62	15.02	14.37	8.78
Fe ₂ O ₃	2	2	2	12.77
TiO ₂	10.68	8.89	11.16	-
MnO	0.2	0.19	0.22	-
CaO	7.17	10.58	7.36	1.46
MgO	3.33	7.08	3.56	16.76
Na ₂ O	3.3	2.23	2.79	-
K ₂ O	1.62	0.39	1.58	0.93
TiO ₂	2.05	1.55	2.11	-
P ₂ O ₅	0.39	0.19	0.36	0.26
Total	100	100	100	100

Figure 2.3 Main data table of JAEA-SDB in a hierarchical data structure comprising primary and detailed information (Example for Am-bentonite system)

- 9 -

In addition to detailed datasheet, summary table (Figure 2.4) can be seen by selecting ‘grouping sheet’ to overview the existing data situation for the concerned system and to access to respective data sources.

Reference	Element	Solid Phase Group	Solid Phase	Solution	classified	Kd Data Count	Kd Data Minimum	Kd Data Maximum
Allard and Beall(1979)	Am	Bentonite (Clay minerals)	kaolinite	groundwater	class 3	1	12.925	12.925
			montmorillonite	groundwater	class 3	1	11.295	11.295
Allard et al.(1979b)	Am	Bentonite (Clay minerals)	bentonite/quartz(10:90)	Aq1105	class 4	3	1.58	7.94
				Aq293	class 3	3	0.2	0.501
Ames et al.(1981)	Am	Bentonite (Clay minerals)	smectite	groundwater#1	unreliable	10	0.133	0.171
Barney(1981)	Am	Bentonite (Clay minerals)	BAS_MINER	S_GW#1	unreliable	1	1.39	1.39
				S_GW#10	unreliable	1	1.13	1.13
				S_GW#11	unreliable	1	0.83	0.83
				S_GW#12	unreliable	1	1.47	1.47
				S_GW#13	unreliable	1	1.44	1.44
				S_GW#14	unreliable	1	0.53	0.53
				S_GW#15	unreliable	1	0.12	0.12
				S_GW#16	unreliable	1	0.357	0.357
				S_GW#17	unreliable	1	1.27	1.27
				S_GW#18	unreliable	1	0.63	0.63
				S_GW#19	unreliable	1	4.57	4.57
				S_GW#2	unreliable	1	1.28	1.28
				S_GW#20	unreliable	1	3.77	3.77
				S_GW#3	unreliable	1	1.47	1.47
				S_GW#4	unreliable	1	1.71	1.71
				S_GW#5	unreliable	1	1.17	1.17
				S_GW#6	unreliable	1	1.57	1.57
				S_GW#7	unreliable	1	2.27	2.27
				S_GW#8	unreliable	1	2.11	2.11
				S_GW#9	unreliable	1	0.73	0.73
Baston et al.(1998)	Am	Bentonite (Clay minerals)	Kunigel-V1	de-ionized water#4	class 2	6	12.0	110.0
Baston et al.(1999)	Am	Bentonite (Clay minerals)	bentonite	de-ionized water#4	class 2	6	12.0	110.0
Degeldre et al.(1994)	Am	Bentonite (Clay minerals)	illite	0.01 M CO3/0.01 M Tris	class 3	1	525.0	525.0
			montmorillonite	0.01 M CO3/0.01 M Tris	class 4	1	82.2	82.2
					class 3	2	26.9	139.0

Figure 2.4 Example of summary data table (Example for Am-bentonite system)

3) Graph plotting

The graph plotting is a central function in the JAEA-SDB to understand the K_d trends as functions of key parameters as shown in Figure 2.5. The graph can be displayed by selecting ‘Graph Plot’ in both main searching window and datasheet window. K_d graph can be plotted as pH, Eh, temperature, reaction time, initial concentration, solution / solid ratio and ionic strength, by selecting from pull-down menu. The K_d trends in each references and consistency between references can be discussed, as presented in the application to PA-related K_d setting (2.3.2) and QA results in Criteria-III (3.3). Histogram figure is also available to present the K_d distribution in wide range of conditions (Figure 2.6). Graph design can be customized, and copied and pasted as picture, and the dataset plotted in graph can be downloaded.

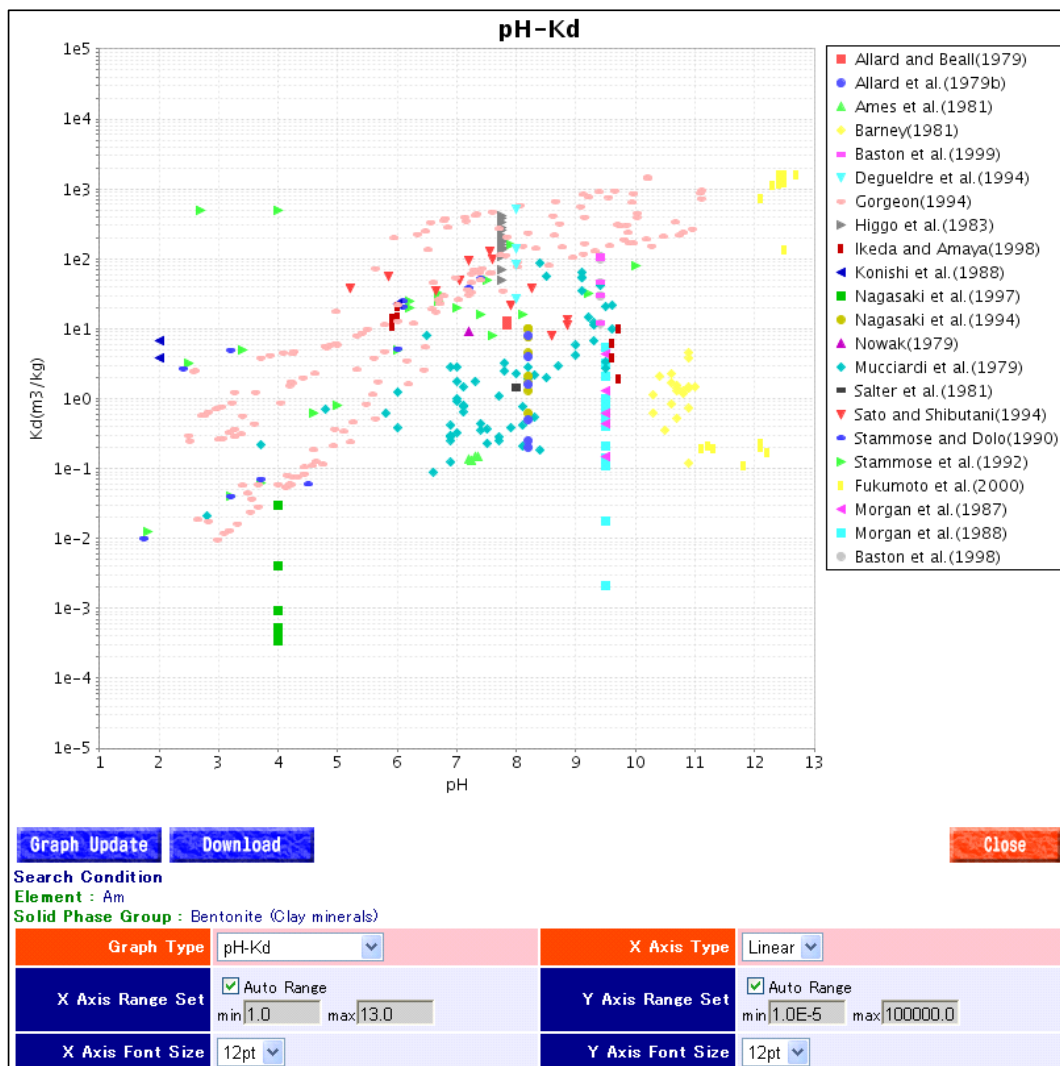


Figure 2.5 Graph viewing section in JAEA-SDB (Example for Am-bentonite system)

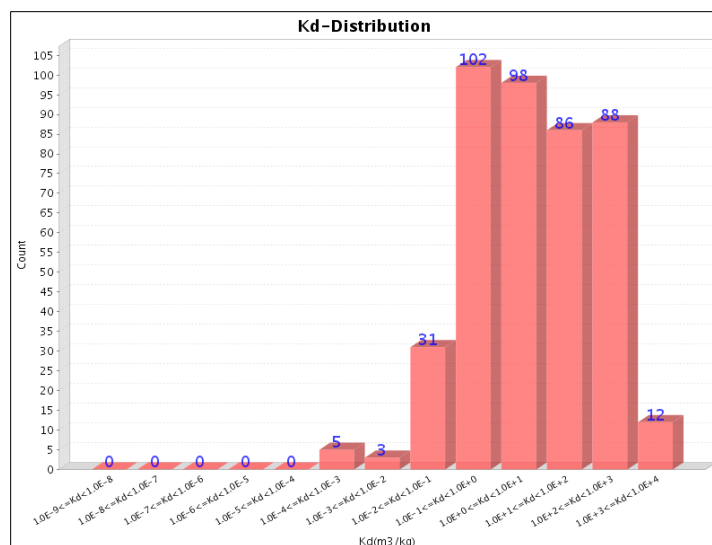


Figure 2.6 Histogram viewing in JAEA-SDB (Example for Am-bentonite system)

4) Data download

Searched K_d data and related all parameters and QA results can be downloaded in the download window (Figure 2.7). The data and parameters to be downloaded can be determined by selecting each checkbox. The download file is as text file format and can be opened by Microsoft Excel etc.

Japan Atomic Energy Agency
Nuclide Migration Database **Sorption Database**

Data Display **Download** **Quit**

Data Download

Main Data

<input checked="" type="checkbox"/> Save No	<input checked="" type="checkbox"/> Element	<input checked="" type="checkbox"/> Charge	<input checked="" type="checkbox"/> Solid Phase Group
<input checked="" type="checkbox"/> Solid Phase	<input checked="" type="checkbox"/> Solution/Solid	<input checked="" type="checkbox"/> Water type	<input checked="" type="checkbox"/> Ionic strength (mol/L)
<input checked="" type="checkbox"/> pH init	<input checked="" type="checkbox"/> pH end	<input checked="" type="checkbox"/> Eh init (mV)	<input checked="" type="checkbox"/> Eh end (mV)
<input checked="" type="checkbox"/> atm/redox condition	<input checked="" type="checkbox"/> C init (mol/L)	<input checked="" type="checkbox"/> temp (degC)	<input checked="" type="checkbox"/> Contact time (day)
<input checked="" type="checkbox"/> Separation	<input checked="" type="checkbox"/> Kd (m ³ /kg)	<input checked="" type="checkbox"/> replicates, n	<input checked="" type="checkbox"/> Reference
<input checked="" type="checkbox"/> additional/information	<input type="checkbox"/> Graph data(Kd (m ³ /kg), Temp (degC), pH, Time (day), Eh (mV), Cinit (mol/L), Solution/Solid (mL/g))		

Detailed info

Solid Phase(+Specific Surface Area (m²/g) + CEC (meq/100g) + note)

Solution/Solid (mL/g) (+Solution (mL) + Solid (g))

Water type(+Ca (ppm) + Na (ppm) + K (ppm) + Mg (ppm) + Cl (ppm) + HCO₃ (ppm) + SO₄ (ppm) + F (ppm) + SiO₂ (ppm) + Fe (ppm) + NO₃ (ppm) + ClO₄ (ppm) + Ionic strength (mol/L) + DOC (ppm) + note)

Kd (m³/kg) (+error + Data type)

Reference(+Author + Year + Title + Journal + Publisher + Vol + No + Page + Note)

Reliability info part of all fields, all fields

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Figure 2.7 Download window in JAEA-SDB

2.2.2 Functions and applications related to QA/classification information

The QA/classification results according to criteria I-III (see Table 2.3) can be seen by selecting ‘Reliability Info’ in datasheet window, as shown in Figure 2.8. Final QA results in criteria I-III are summarized in the first page as overview. Details of QA results for each checkpoints are displayed by changing ‘Display condition’. All results and evidences for criteria I and II, and reports for criteria-III can be seen as PDF format, as shown by red arrows in Figure 2.8.

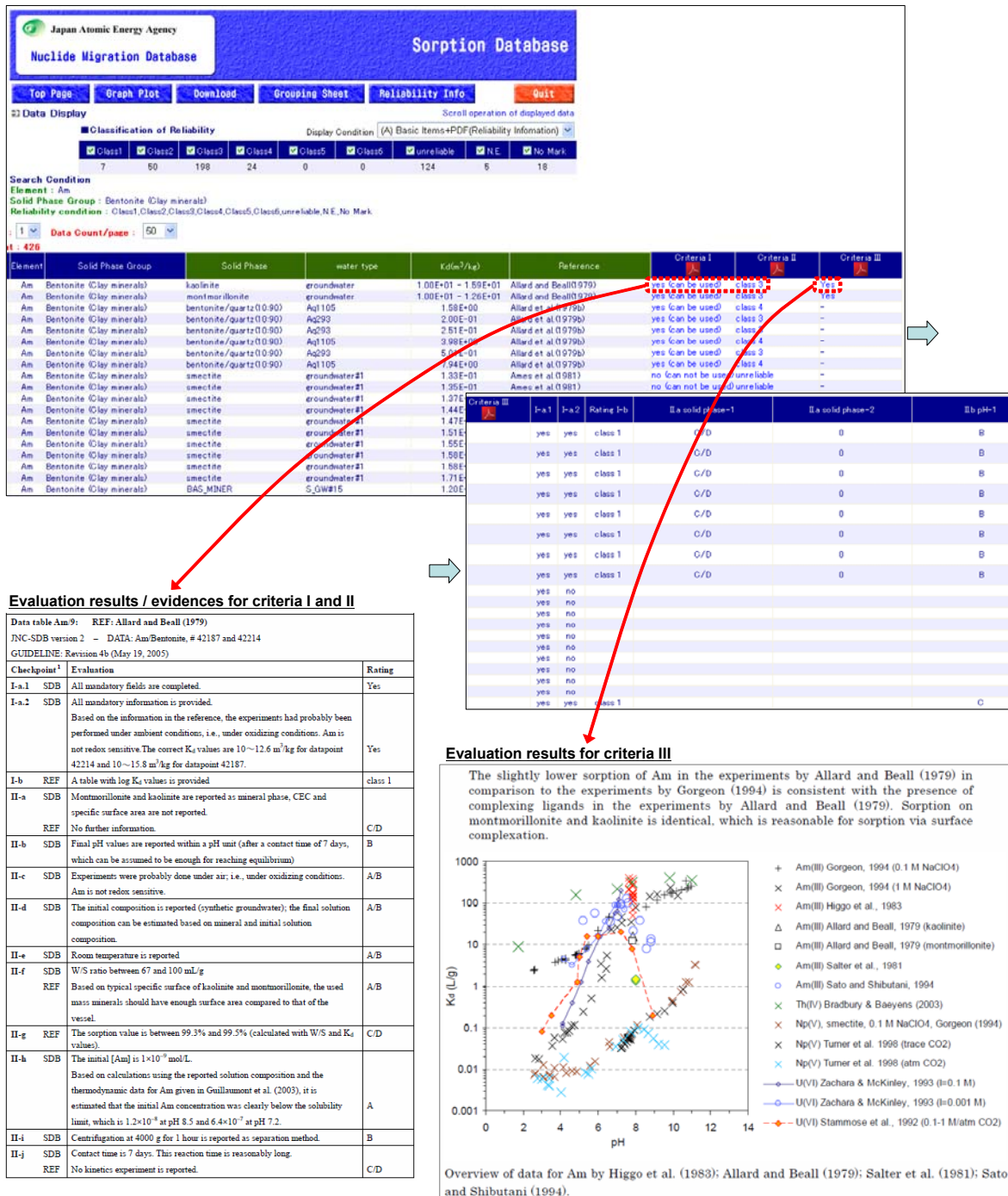


Figure 2.8 QA/classification results including evidences for criteria-I, II, III in JAESDB

In datasheet window, K_d data can be extracted in terms of reliability by using QA results, e.g., selecting reliable data (class 1-4) and excluding unreliable data, as shown in Figure 2.9. Graph can be plotted using QA-selected K_d data.

Japan Atomic Energy Agency Nuclide Migration Database Sorption Database

Buttons: Top Page, Graph Plot, Download, Grouping Sheet, Reliability Info, Quit

Data Display

Classification of Reliability: Display Condition (A) Basic Items+PDF(Reliability Information)

Class1
 Class2
 Class3
 Class4
 Class5
 Class6
 unreliable
 N.E
 No Mark

Counts: 7, 50, 198, 24, 0, 0, 124, 5, 18

Search Condition: Element: Am, Solid Phase Group: Bentonite (Clay minerals), Reliability condition: Class1,Class2,Class3,Class4,Class5,Class6

Data Count/page: 50

Element	Solid Phase Group	Solid Phase	water type	$K_d(m^3/kg)$	Reference	Criteria I	Criteria II	Criteria III
Am	Bentonite (Clay minerals)	kaolinite	groundwater	1.00E+01 ~ 1.59E+01	Allard and Beall(1979)	yes (can be used)	class 3	Yes
Am	Bentonite (Clay minerals)	montmorillonite	groundwater	1.00E+01 ~ 1.26E+01	Allard and Beall(1979)	yes (can be used)	class 3	Yes
Am	Bentonite (Clay minerals)	bentonite/quartz(10:90)	Aq1105	1.58E+00	Allard et al.(1979b)	yes (can be used)	class 4	-
Am	Bentonite (Clay minerals)	bentonite/quartz(10:90)	Aq293	2.00E-01	Allard et al.(1979b)	yes (can be used)	class 3	-
Am	Bentonite (Clay minerals)	bentonite/quartz(10:90)	Aq293	2.51E-01	Allard et al.(1979b)	yes (can be used)	class 3	-
Am	Bentonite (Clay minerals)	bentonite/quartz(10:90)	Aq1105	3.98E+00	Allard et al.(1979b)	yes (can be used)	class 4	-
Am	Bentonite (Clay minerals)	bentonite/quartz(10:90)	Aq293	5.01E-01	Allard et al.(1979b)	yes (can be used)	class 3	-
Am	Bentonite (Clay minerals)	bentonite/quartz(10:90)	Aq1105	7.94E+00	Allard et al.(1979b)	yes (can be used)	class 4	-
Am	Bentonite (Clay minerals)	bentonite	de-ionized water#4	1.00E+02	Bastion et al.(1999)	yes (can be used)	class 2	Yes
Am	Bentonite (Clay minerals)	bentonite	de-ionized water#4	1.10E+02	Bastion et al.(1999)	yes (can be used)	class 2	Yes
Am	Bentonite (Clay minerals)	bentonite	de-ionized water#4	1.20E+01	Bastion et al.(1999)	yes (can be used)	class 2	Yes
Am	Bentonite (Clay minerals)	bentonite	de-ionized water#4	3.00E+01	Bastion et al.(1999)	yes (can be used)	class 2	Yes
Am	Bentonite (Clay minerals)	bentonite	de-ionized water#4	3.00E+01	Bastion et al.(1999)	yes (can be used)	class 2	Yes
Am	Bentonite (Clay minerals)	bentonite	de-ionized water#4	4.60E+01	Bastion et al.(1999)	yes (can be used)	class 2	Yes
Am	Bentonite (Clay minerals)	illite	0.01 M CO3/0.01 M Tris	5.25E+02	Degueldre et al.(1994)	yes (can be used)	class 3	-
Am	Bentonite (Clay minerals)	illite	0.01 M CO3/0.01 M Tris	8.22E+01	Degueldre et al.(1994)	yes (can be used)	class 4	-
Am	Bentonite (Clay minerals)	montmorillonite	0.01 M CO3/0.01 M Tris	1.39E+02	Degueldre et al.(1994)	yes (can be used)	class 3	-
Am	Bentonite (Clay minerals)	montmorillonite	0.01 M CO3/0.01 M Tris	2.69E+01	Degueldre et al.(1994)	yes (can be used)	class 3	-
Am	Bentonite (Clay minerals)	Illite	1M NaClO4	1.05E+02	Gorgeon(1994)	yes (can be used)	class 3	Yes
Am	Bentonite (Clay minerals)	Illite	0.1M NaClO4	1.12E+02	Gorgeon(1994)	yes (can be used)	class 3	Yes
Am	Bentonite (Clay minerals)	Illite	1M NaClO4	1.15E+00	Gorgeon(1994)	yes (can be used)	class 3	Yes
Am	Bentonite (Clay minerals)	Illite	0.1M NaClO4	1.15E+02	Gorgeon(1994)	yes (can be used)	class 3	Yes
Am	Bentonite (Clay minerals)	Illite	1M NaClO4	1.20E+01	Gorgeon(1994)	yes (can be used)	class 3	Yes
Am	Bentonite (Clay minerals)	Illite	1M NaClO4	1.20E-02	Gorgeon(1994)	yes (can be used)	class 3	Yes
Am	Bentonite (Clay minerals)	Illite	0.1M NaClO4	1.22E+00	Gorgeon(1994)	yes (can be used)	class 3	Yes

Data extracting by using QA/classification results (class 1-6 in criteria II and unreliable in criteria I&II)

Graph plotting of K_d dataset extracted by QA/classification results

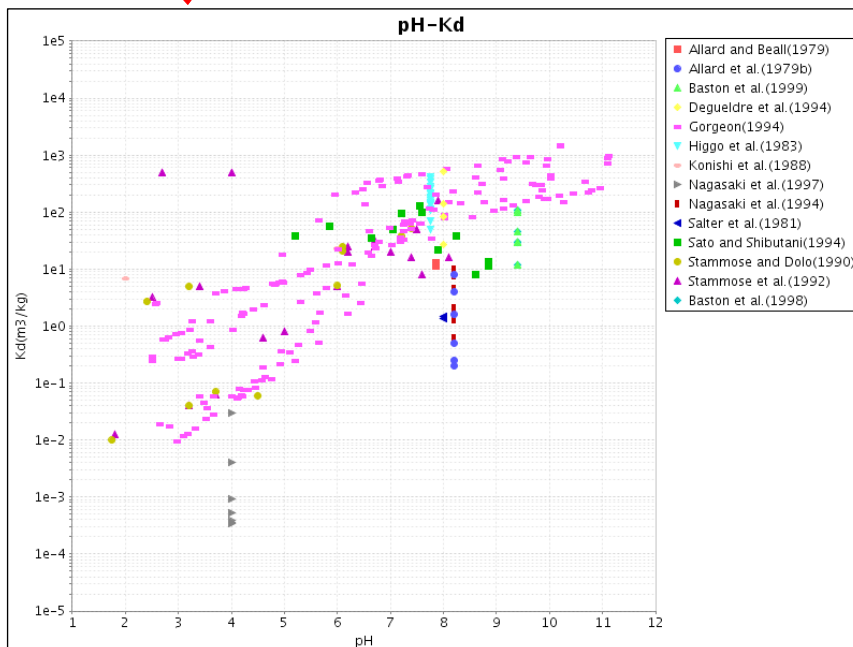


Figure 2.9 Data selection and graph plotting based on QA/classification results

2.2.3 Additional data evaluation function focusing on multi-parameter dependence

K_d data are conditional parameter, depending on various conditions such as pH, ionic strength, initial concentration of radionuclides, etc. K_d plotting as a function of pH usually shows a wide variation in K_d values as a result of various parameter dependence. PA-related K_d setting needs to access to the respective K_d data correspond to the specific PA conditions from a wide variety of K_d in the SDB. For this purpose, data evaluation function focusing on multi-parameter dependence was additionally introduced in the JAEA-SDB. As shown in Figure 2.10, K_d graph plots as a function of a parameter (e.g., pH) can be grouped by other parameters (e.g., ionic strength). This function makes it possible to investigate multi-parameter dependence between various key parameters.

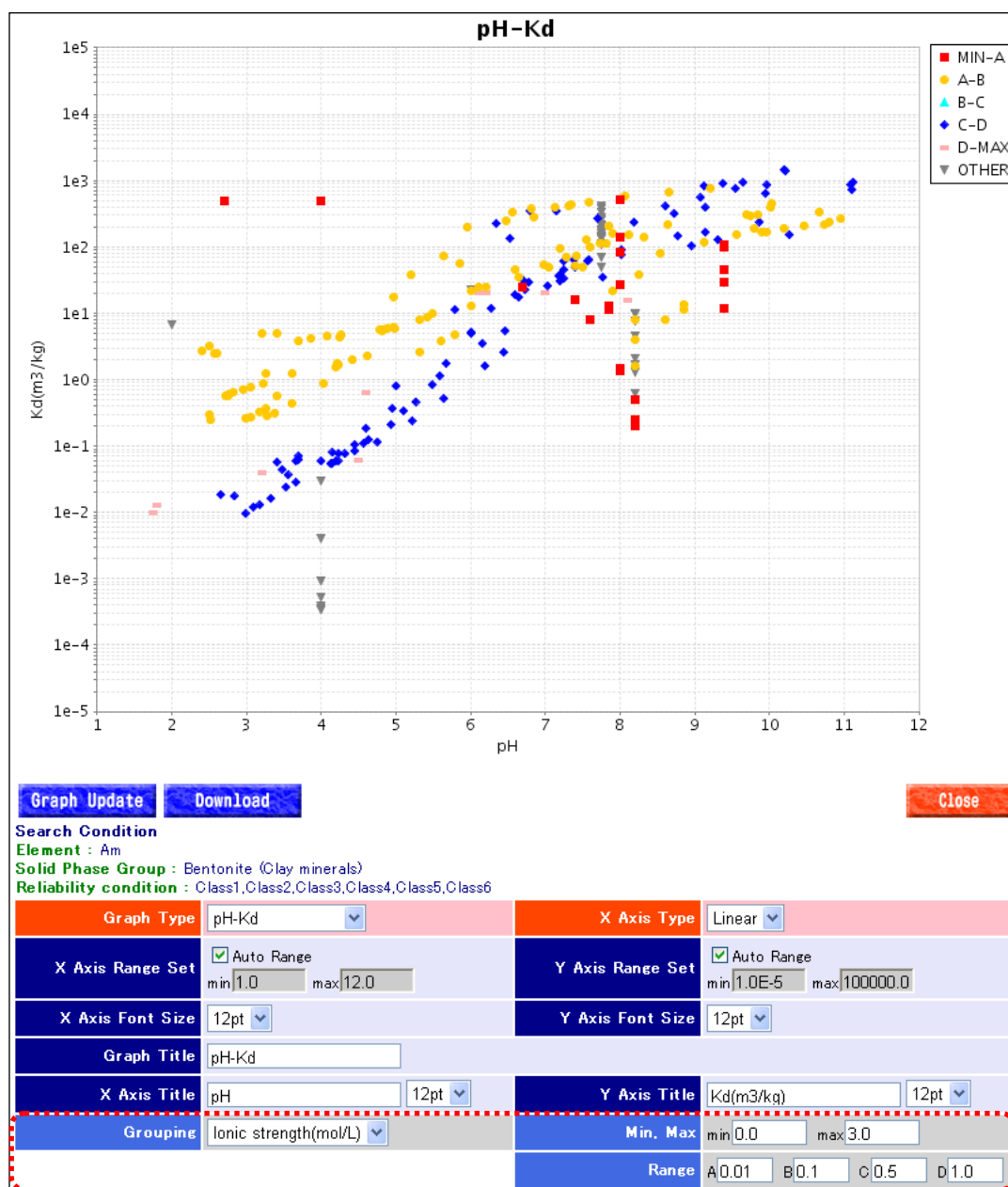


Figure 2.10 Additional data grouping function for viewing multi-parameter dependence

2.3 PA-related applications of JAEA-SDB

2.3.1 Overviews of PA-related K_d setting and roles of SDB

As presented in introduction (Figure 1.1), the development of integrated approaches for site-specific K_d setting for PA calculations is the goal of our project. Because of the conditional nature of sorption K_d values, geochemical variability or uncertainty, and their effect on K_d , usually have to be considered for reference and alternative scenarios in PA calculations. It is not feasible to determine K_d value experimentally for all conditions to be considered in K_d setting. A typical challenge is the relatively limited amount of site-specific data can be made available, due to experimental constraint and complexity of conditions. The sorption database (SDB), containing large amount of sorption data for approximated, simplified, or generic systems, are therefore expected to play a central role in PA-related K_d setting.

In this setting, key challenge is transferring sorption data from one set of conditions (experimental condition in SDB) to another (PA-related site-specific condition). This must take into account any differences in substrate (mineralogy, site density, etc.) and geochemical conditions (pH, ionic strength, etc.). This transfer can be done through the following methods (as presented in NEA (2005), and Figure 2.11):

- 1) qualitative expert judgment (e.g., H12 PA; JNC (1999))
- 2) semi-quantitative transfer by scaling method (e.g., Bradbury and Baeyens (2003), Ochs and Talerico (2004), Ochs et al.(2008))
- 3) fully quantitative transfer through the use of TSM (e.g., NEA, 2005; Tachi et al., 2010)

The application of the JAEA-SDB is illustrated in relation with these PA-related K_d setting in the following sections.

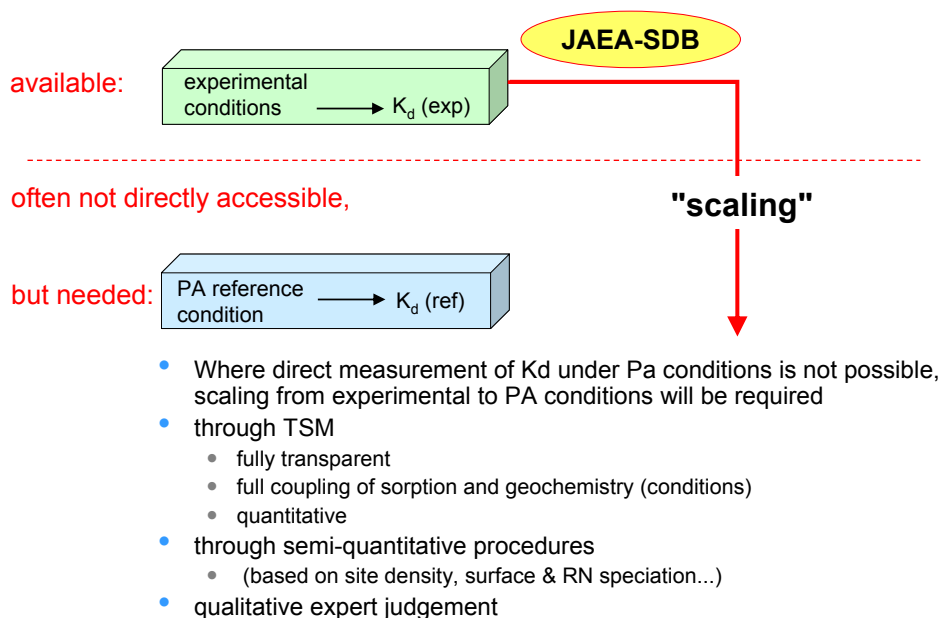


Figure 2.11 PA-related K_d setting approaches based on experimental data and scaling method (from NEA, 2005)

2.3.2 Illustrating application of the JAEA-SDB for PA-related K_d setting

The JAEA-SDB is applied and tested for PA-related K_d setting by using the data evaluation functions, shown in section 2.2.2 (QA/classification) and 2.2.3 (graph plotting for multi-parameter dependence). K_d setting for H12 PA calculation was selected as an example; K_d of Cs for granitic rock under FRHP groundwater (fresh reducing high-pH, pH; 8.5, ionic strength; 4mM, other details in JNC, 1999).

Step-1) Overview of K_d data for Cs-granitic rock systems:

All of K_d data for Cs on granitic rocks are firstly extracted from the JAEA-SDB as shown in Figure 2.12 (number of K_d data; 715).



Figure 2.12 Searched K_d data of Cs on granitic rocks in JAEA-SDB

Step-2) Data extraction by QA/classification results:

K_d data for Cs on granitic rocks are then extracted by excluding ‘unreliable data’ and ‘No mark (which can not be evaluated because of difficulties in access for data sources)’ based on the QA/classification results, as shown in Figure 2.13 (K_d data; 243).



Figure 2.13 K_d data of Cs on granitic rocks selected by QA/classification results in JAEA-SDB

Step-3) Data evaluation focusing on parameter dependence:

It is generally accepted that key parameters for Cs sorption are ionic strength and Cs concentration, K_d data for Cs on granitic rocks are therefore replotted as a function of ionic strength as shown in top of Figure 2.14. Although this graph shows a trend of decreasing K_d with increasing ionic strength, K_d variations at each pH are relatively large. K_d graph can be replotted, grouped by Cs concentration by additional data evaluation function (bottom of Figure 2.14). This figure represents that K_d variations at each pH are caused by difference in Cs concentration.

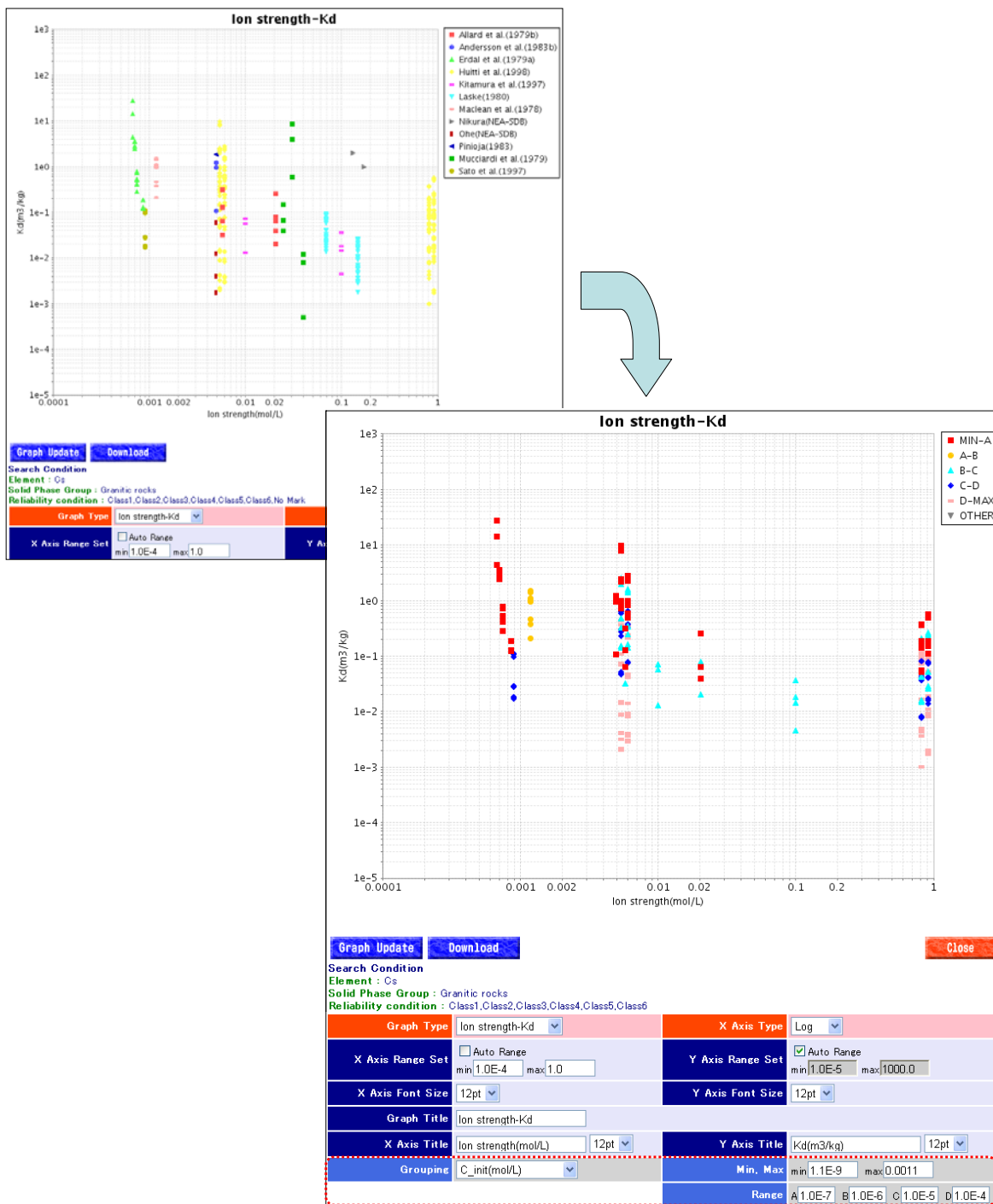


Figure 2.14 Single- and double-parameter dependence of Cs sorption on granitic rocks

Step-4) Extraction of respective data and K_d setting:

Based on the parameter dependences, respective K_d data are extracted using ‘detailed search function’ (pH; 7-10, ionic strength; 0.001-0.1M, initial Cs concentration; $< 1 \times 10^{-5} \text{M}$ are selected here) as shown in left in Figure 2.15. The K_d distribution can be viewed as histogram graph as right in Figure 2.15. The K_d value and its uncertainty range can be set as 0.001-0.5-10 (m^3/kg) based on the distribution. The conservative approach may be set to be 0.05 (m^3/kg), which is consistent with K_d value in H12 PA.

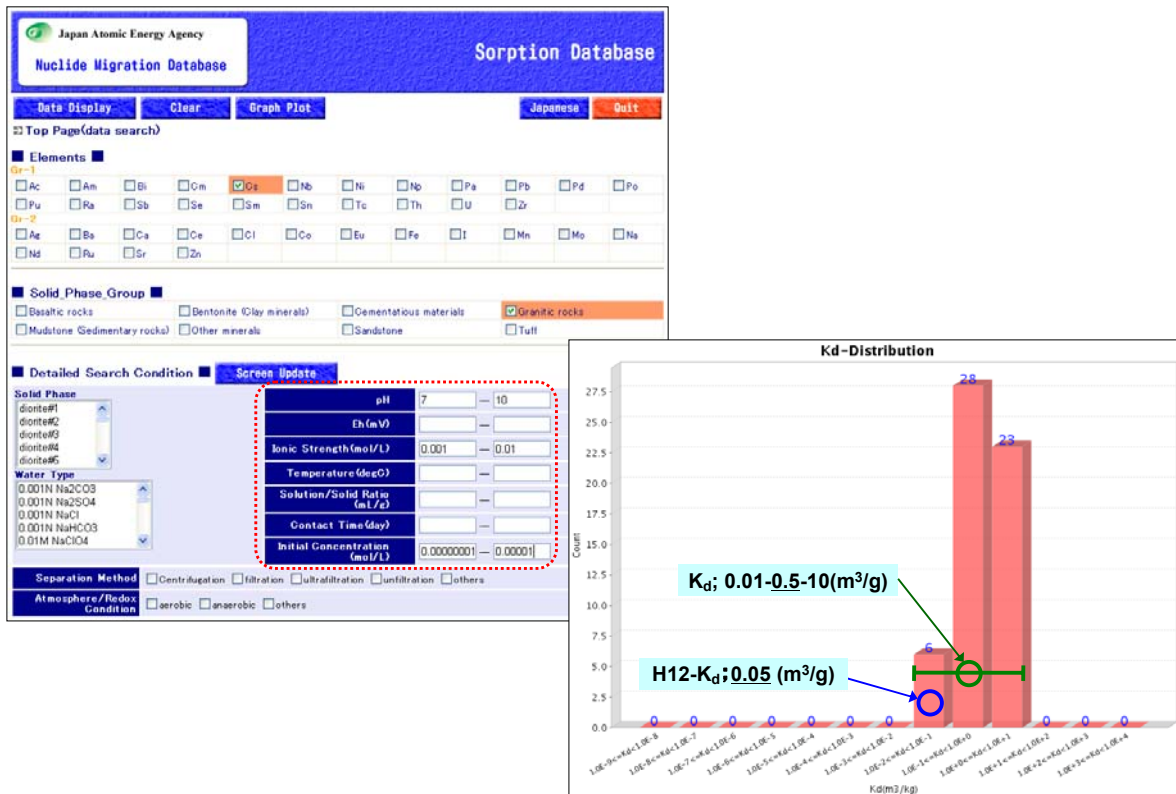


Figure 2.15 Extraction of respective K_d data and their distribution (Histogram)

2.3.3 Linkage with mechanistic sorption model/database development

As shown in section 2.3.1 (Figure 2.11), the thermodynamic sorption model (TSM) makes it possible to estimate K_d variations directly, based on mechanistic understanding. JAEA has developed the integrated sorption/diffusion (ISD) model and database (Tachi et al., 2010a; 2010b), in combination with JAEA-SDB/DDB compiling measured K_d and D_e/D_a values. The JAEA-SDB plays important roles in TSM development as shown focusing Np(V) sorption on bentonite/montmorillonite (Tachi et al., 2010a; 2010b) in the followings:

Step-1) Data selection for model parameterization:

To develop the model applicable to PA-related K_d setting, radionuclides sorption data should be selected by accounting for high quality, purified system, wide range of conditions. In case of Np(V) sorption on montmorillonite, two datasets by Turner et al. (1998) and Gorgeon (1994) can be selected, which covered a wide range of chemical conditions, pH, ionic strength and carbonate, and which had already been evaluated in the NEA sorption project (NEA, 2005).

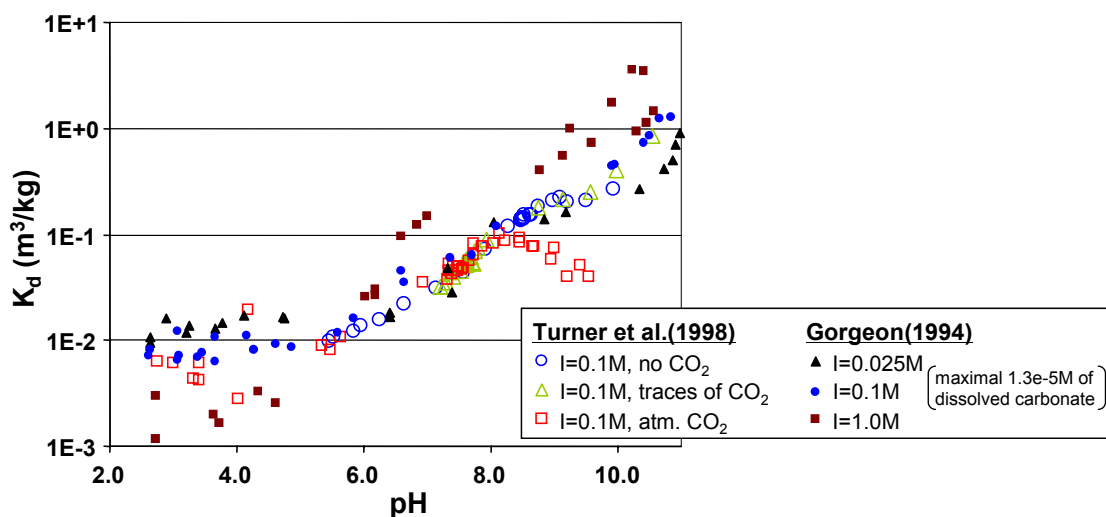


Figure 2.16 Data extraction for TSM parameterization (Np(V) sorption on montmorillonite)

Step-2) Model parameterization:

The thermodynamic sorption model parameters are then determined using selected dataset. Modeling results are shown as an example in Figure 2.17, which is based on a relatively simple model comprising 1-site surface complexation/diffuse layer model in combination with 1-site ion exchange model. The model can reproduce the Np(V) sorption data under a wide range of conditions, and uncertainty in TSM developed are also evaluated (Tachi et al., 2010a; Ochs et al., 2011).

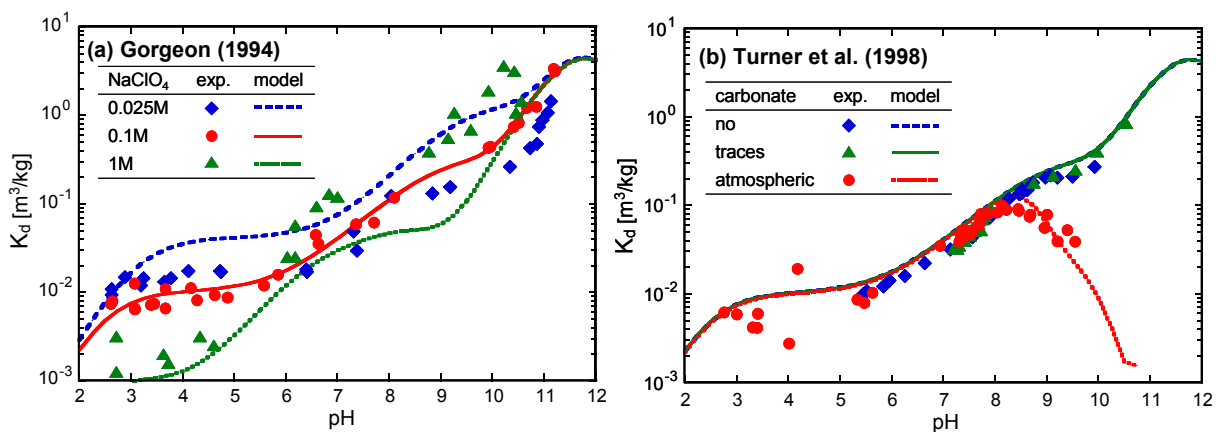


Figure 2.17 Modeled results for Np(V) sorption on montmorillonite

Step-3) Application and validation of the model to various systems:

After the model parameters are obtained, the final model needs to be tested to be applicable for various systems including complex bentonite system. Datasets for Np(V) sorption on bentonite and montmorillonite are extracted by considering QA results in JAEA-SDB as shown in top of Figure 2.18. These datasets shows a consistent trend of increasing K_d with pH increasing. Np(V) sorption datasets for bentonite (Kunigel-V1) reported by Ohe et al. (1993) are tested by coupling with porewater chemistry model as an example (bottom of Figure 2.18), indicating reasonable consistency in terms of dependence in pH and solid/liquid ratio. This model has been also tested for compacted system by coupling diffusion model (Tachi et al., 2010a; 2010b).

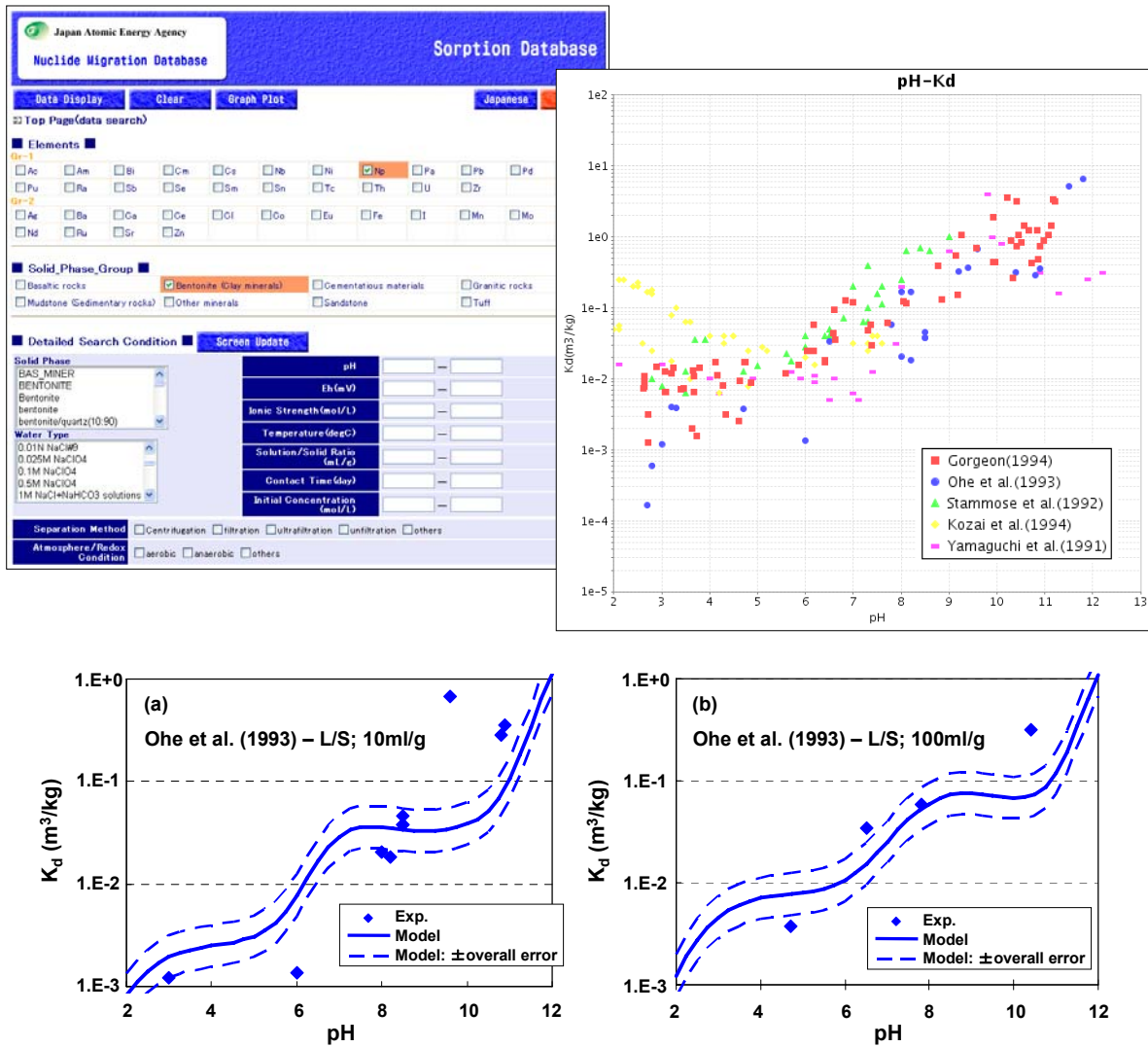


Figure 2.18 Np(V) sorption datasets extracted for model validation (Top) and tested results for bentonite system in Ohe et al. (1993)

3. Updating of sorption data and its QA classification

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

As presented in the section 2.3, 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 (Tachi et al., 2010a) and PA-related K_d setting for Horonobe URL conditions (Ochs et al., 2008). Primary systems focused in this updating are key radionuclides in i) montmorillonite/bentonite, ii) other clay minerals in relation to modeling and K_d setting for argillaceous rocks, and iii) Fe and Al oxide/hydroxide which are important for various rock systems. Selected 32 references are listed as following, and their systems are summarized in Table 3.1.

- 1) Baeyens, B. and Bradbury, M.H. : “A quantitative mechanistic description of Ni, Zn and Ca sorption on Na-montmorillonite, Part II: Sorption measurements”, PSI Bericht Nr. 95-11. Paul Scherrer Institute, Villigen, Switzerland (1995).
- 2) Balistrieri, L.S. and Chao, T.T. : “Selenium adsorption by goethite”, *Soil Sci. Soc. Am. J.*, vol.51, pp.1145 (1987).
- 3) Balistrieri, L.S. and Chao, T.T. : “Adsorption of selenium by amorphous iron oxyhydroxide and manganese Dioxide”, *Geochim. Cosmochim. Acta*, vol.54, p.739 (1990).
- 4) Bertetti, F., Pabalan, R. and Almedarez, M. : “Studies of neptunium(V) sorption behaviour on quartz, clinoptilolite, montmorillonite, and α -alumina”, In: Jenne, ed., *Adsorption of Metals by Geomedia – Variables, Mechanisms, and Model Applications*, Academic Press, New York, pp.131-148 (1998).
- 5) Bradbury, M. and Baeyens, B. : “Sorption of Eu on Na- and Ca-montmorillonites: experimental investigations and modelling with cation exchange and surface complexation”, *Geochim. Cosmochim. Acta*, vol.66, pp.2325-2334 (2002).
- 6) Bradbury M.H. and Baeyens, B. : “Near-field sorption data bases for compacted MX-80 bentonite for performance assessment of a high-level radioactive waste repository in Opalinus Clay host rock”, Nagra, Technical Report 02-18 (2003).
- 7) Bradbury, M.H. and Baeyens, B. : “Sorption modelling on illite Part I: Titration measurements and the sorption of Ni, Co, Eu and Sn”, *Geochim. Cosmochim. Acta*, vol. 73, pp. 990-1003 (2009).
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- 11) Girvin, D.C., Ames, L.L. , Schwab, A. P. and McGarrah, J. E. : “Neptunium adsorption on synthetic amorphous iron oxyhydroxide, *J. Colloid Interface Sci.*, vol.141, p.67 (1991).
- 12) Goldberg, S. and Glaubig, R.A. : “Anion sorption on a calcareous, montmorillonitic soil – Selenium”, *Soil, Sci. Soc. Am. J.*, vol.52, pp.954-957 (1988).
- 13) Ikhsan, J., Johnson, B.B. and Wells, J.D. : “A comparative study of the adsorption of transition metals on kaolinite”, *J. Colloid Interf. Sci.*, vol.217, pp.403-410 (1999).
- 14) Kohler, M., Wieland, E. and Leckie, J.O. : “Metal-ligand-surface interactions during sorption of uranyl and neptunyl on oxides and silicates”, In *Proceedings of the 7th International Symposium on Water-Rock Interaction*; Kharaka, Y.K. , Maest, A.S. , Eds.; Balkema: Rotterdam, The Netherlands, vol.1, pp.51-54

- (1992).
- 15) Korichi, S. and Bensmaili, A. : “Sorption of uranium(VI) on homoionic sodium smectite experimental study and surface complexation modeling”, *Journal of Hazardous Materials*, vol.169, pp.780-793 (2009).
 - 16) Lauber, M., Baeyens, B. and Bradbury, M.H. : “Physico-chemical characterisation and sorption measurements of Cs, Sr, Ni, Eu, Th, Sn and Se on Opalinus Clay from Mont Terri”, *Nagra Technical Report*, NTB 00-11 (2000).
 - 17) Marques Fernandes, M., Baeyens, B. and Bradbury, M.H. : “The influence of carbonate complexation on lanthanide/actinide sorption on montmorillonite”, *Radiochimica Acta*, vol.96, pp.691-697 (2008).
 - 18) Missana, T., Alonso, U. and García-Gutiérrez, M. : “Experimental study and modelling of selenite sorption onto illite and smectite clays”, *Journal of Colloid and Interface Science*, vol. 334, pp. 132-138 (2009a).
 - 19) Missana, T., Alonso, U., Garcia-Gutierrez, M., Albarran, N. and Lopez, T. : "Experimental study and modeling of uranium (VI) sorption onto a Spanish smectite", *Mater. Res. Soc. Symp. Proc.* vol.1124, pp.561-566 (2009b).
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 - 27) Staunton, S. and Robaud, M. : “Adsorption of ^{137}Cs on montmorillonite and illite: effect of charge compensating cation, ionic strength, concentration of Cs and fulvic acid”, *Clays and Clay Minerals*, vol.45, pp.251–260 (1997)
 - 28) Tertre, E., Berger, G., Castet, S., Loubet, M. and Giffaut, E. : “Experimental sorption of Ni^{2+} , Cs^+ and Ln^{3+} onto a montmorillonite up to 150 C”, *Geochimica et Cosmochimica Acta*, vol.69, No.21, pp.4937-4948 (2005).
 - 29) Turner, G.D., Zachara, J.M., McKinley, J.P. and Smith, S.C. : “Surface-charge properties and UO_2^{2+} adsorption of a subsurface smectite”, *Geochim. Cosmochim. Acta*, vol.60, pp.3399-3414 (1996).
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Table 3.1 Overview of 32 references selected for updating the JAEA-SDB (1/2)

No.	Reference	Element	Solid Phase	Solution Type
1)	Baeyens and Bradbury(1995)	Ca	Na-montmorillonite	0.01, 0.03, 0.1M-NaClO ₄
2)	Balistreri and Chao(1987)	Se	goethite	0.1M-KCl
3)	Balistreri and Chao(1990)	Se	Fe-oxyhydroxide, Mn-dioxide	0.1M-KCl
4)	Bertetti et al.(1998)	Np	quartz, clinoptilolite, α -alumina	0.01, 0.1M-NaNO ₃
5)	Bradbury and Baeyens(2002)	Eu	Ca-montmorillonite	0.066M-Ca(NO ₃) ₂
6)	Bradbury and Baeyens(2003)	Th, U	Na-montmorillonite (Swy-1)	0.01, 0.1, 1M-NaClO ₄ (Th -0.1, 1M; U-0.01, 0.1M)
7)	Bradbury and Baeyens (2009a)	Ni, Co, Eu, Sn	Na-illite (du Puy)	0.1M, 0.5M-NaClO ₄
8)	Bradbury and Baeyens (2009b)	Am, Th, Pa, U	Na-illite (du Puy)	0.1M-NaClO ₄
9)	de Preter et al. (1991)	Cs	Boom clay	0.015M-AgTU
10)	Ghosh et al.(1994)	Se	Alumina	0.1M-NaCl,
11)	Girvin et al.(1991)	Np	Fe ₂ O ₃ ·H ₂ O(am)	0.1M-NaNO ₃
12)	Goldberg and Glaubig(1988)	Se	Ca-montmorillonite, kaolinite, calcite, imperial soil	0.1M-NaCl
13)	Ikhsan et al.(1999)	Pb, Zn, Co	kaolinite	0.005M-KNO ₃
14)	Kohler et al.(1992)	Np	hematite, kaolinite	0.005-0.1M-NaClO ₄ , 0.1M-NaClO ₄ +EDTA
15)	Korichi and Bensmaili	U	Na-smectite	0.001-0.1M-NaNO ₃
16)	Lauber et al.(2000)	Cs, Sr, Ni, Eu, Th, Sn, Se	Opalinus Clay	SOPW(Synthetic Opalinus porewater)
17)	Marques Fernandes et al.(2008)	Eu	Na-montmorillonite (SWy-1)	0.1M-NaClO ₄ , (+NaHCO ₃ /Na ₂ CO ₃)
18)	Missana et al.(2009a)	Se	Na-smectite, Na-illite, 70%-smectite/30%-illite, 43%-smectite/57%-illite	0.001-0.5M-NaClO ₄
19)	Missana et al.(2009b)	U	Na-smectite	0.003, 0.01, 0.05, 0.1M-NaClO ₄
20)	Pabalan et al.(1993)	U	Na-clinoptilolite	U solution
21)	Pabalan and Turner(1997)	U	Na-SAz-1 montmorillonite	0.1M-NaNO ₃
22)	Prikryl et al.(1994)	U	α -Al ₂ O ₃	0.1M-NaNO ₃
23)	Prikryl et al.(2001)	U	quartz, clinoptilolite, Clin/Qtz	0.1M-NaNO ₃
24)	Rabung et al.(2005)	Eu, Cm	Ca-montmorillonite, Na-illite	0.066M-Ca(NO ₃) ₂ , 0.066M-Ca(ClO ₄) ₂ , 0.1M-NaClO ₄
25)	Sanchez et al.(1985)	Pu	goethite	0.03-0.3M-Na ₂ SO ₄ , 0.1-3M-NaNO ₃ (+DOC), 0.5-3M-NaCl
26)	Srivastave et al.(2005)	Pb, Zn	kaolinite	0.01M-NaNO ₃
27)	Staunton and Robaud(1997)	Cs	K-, Na-, Ca-montmorillonite, K-, Na-, Ca-illite,	2.5×10 ⁻⁵ -0.5M-CaCl ₂ , 5×10 ⁻⁵ -0.5M-KCl, 5×10 ⁻⁵ -0.5M-NaCl(+fulvic acid)

Table 3.1 Overview of 32 references selected for updating the JAEA-SDB (2/2)

No.	Reference	Element	Solid Phase	Solution Type
28)	Tertre et al.(2005)	Cs, Eu, Ni	Na- montmorillonite	0.025M, 0.5M-NaClO ₄
29)	Turner et al.(1996)	U	smectite, gibbsite, quartz	0.001 -0.1M-NaClO ₄ , 0.005-0.05M-Ca(ClO ₄) ₂
30)	Turner et al.(1998)	Np	Na-montmorillonite	0.1 -NaNO ₃
31)	Waite et al.(1994)	U	ferrhydrite	0.004-0.5M-NaNO ₃
32)	Zachara et al.(2002)	Cs	sediment	0.005-0.5M-Ca(NO ₃) ₂ , 0.005-7M NaNO ₃ , 0.01 - 1M-KNO ₃ ,0.015M-AgTU (+0.1M-KNO ₃)

3.2 QA evaluation on criteria I and II

This section presents the QA/classification results for K_d data selected in this update.

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

3.2.1 Cesium

Data table Cs/1: REF: de Preter et al. (1991)		
JAEA-SDB version 4.0 - DATA: Cs/Bentonite (Clay Minerals); Boom clay #67381~67396		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided. Atmosphere composition is not reported. Because Cs is not influenced by either redox condition or carbonate, this is accepted. The same holds for pH. For phase separation, see checkpoint II-i.	Yes
I-b REF	K_d values taken from a graph with linear axis.	class 3
II-a SDB	As solid phase, Boom Clay with a CEC of 33 [meq/100g] is indicated. Details of Boom Clay properties are reported elsewhere in the literature, including detailed mineralogy and surface properties.	A
REF	No sample treatment except grinding is indicated in the REF	
II-b SDB	It is indicated that no pH values are reported.	D
REF	No pH values are reported in the REF. Based on descriptions of experimental procedures in the underlying Ph.D thesis (de Preter, 1990), it can be concluded that pH was held at near-neutral values. Because Cs sorption on FES (or planar sites) is not influenced by small variations of pH, the data in the REF are considered reliable.	
II-c SDB	It is indicated that no information on redox conditions is reported. Cs sorption on Boom Clay is not redox-sensitive.	A/B
II-d SDB	Initial compositions of the 0.015M-AgTU(silver thiourea) and 0.01M-K contacting solutions are indicated. It can be assumed that the Boom Clay samples will contribute minor constituents to the solutions, but these are expected to be irrelevant in comparison to the high added K-concentrations. Thorough pre-equilibration is indicated in the REF.	C/D
II-e SDB	It is indicated that experiments had been performed at 25°C.	A/B
II-f SDB	It is indicated that the amount of solution and solid phase is not reported.	C/D
REF	No further information is available.	
II-g SDB	It is indicated that no solid/solution ratio is given in REF. From de Preter (1990), a solid/water ratio of 0.25 [g/L] can be taken. Based on this value, Cs sorption is in the range of 12~46% in all experiments.	A
II-h SDB	It is indicated that the initial Cs concentration is not reported. Cs is not solubility limited.	A
REF	If needed, initial Cs concentration could be estimated from the information that Cs additions lead to about 5% coverage of the FES capacity present in the experiments There are also isotherm data available, but it is not clear whether	

		these refer to the same S/W ratio as the other experiments.	
II-i	SDB REF	It is indicated, that no separation procedure is reported. It can be taken from de Preter (1990) that samples had been centrifuged for 20 min at 14,000 [rpm]. There is no particular evidence for artifacts (colloid effect).	C/D
II-j	SDB	A contact time of 1 day is indicated. This is considered to be reasonably long.	C/D
II-k	REF	No agitation method is indicated.	C/D
II-l	SDB REF	No variation in Cs or the L/S is indicated. Isotherm data are provided in the REF.	A
II-m	REF	No information about the reaction vessel is available. No correction for adsorption to vessel walls is mentioned. The REF briefly discusses other corrections (Cs sorption to planar and organic sites in Boom Clay).	C/D
II-n	REF	No error information reported.	D
II-o	REF	Both Cs as well as the solution composition (concentration of K- and AgTU-ions) has been varied systematically	A

Data table Cs/2: REF: Lauber et al. (2000)			
JAEA-SDB version 4.0 - DATA: Cs/Bentonite (Clay Minerals); Opalinus Clay #68072~68132			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Graphs with logarithmic K_d values are provided.	class 5
II-a	SDB	As solid phase Opalinus Clay (and CEC) is indicated. A detailed analysis of Opalinus Clay is available.	A
II-b	SDB REF	It is indicated that initial pH values are provided. The samples were pre-conditioned; therefore, it is assumed that initial and final pH is nearly identical. Further, the solution is well buffered.	A
II-c	SDB	It is indicated that experiments had been conducted under a nitrogen atmosphere. No addition of oxidizing or reducing agents is indicated. The experiments at pH 6.3 were carried out in a CO ₂ /N ₂ atmosphere. Cs is not redox sensitive.	A/B
II-d	SDB REF	It is indicated that experiments had been performed in synthetic porewater solution, composition is given. Final solution composition is not indicated. Clay samples were pre-conditioned. The composition of the conditioned solutions was determined.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25°C.	A/B
II-f	SDB REF	The solution/solid ratio is indicated. Actual solution volume and solid weight are not given. The Specific surface area of Opalinus Clay is reported as 33.3 [m ² /g]. Experiments were done in 40 [mL] centrifuge tubes. This results in about 8 [m ²] of sorbent surface per vial.	A/B
II-g	REF	The following sorption values were calculated from K_d and L/S ratios: • #68072~68094, #68098~68132 • #68095~68097	A B
II-h	SDB	Initial Cs concentrations of 3.2×10^{-7} [M] and 9.3×10^{-4} [M] are indicated for #68072~68097. Initial Cs concentrations of 3.2×10^{-7} ~ 9.3×10^{-4} [M] are indicated for #68078~68132. Cs is not solubility-limited.	A
II-i	SDB	Centrifugation (60 min at 95,000 [g]) is indicated.	B
II-j	SDB REF	Several contact times between about 4 hours and 8 months are indicated. It is estimated that sorption of Cs on Opalinus Clay is completed after 3 days. For Cs sorption, Figure 5 in the REF shows no significant deviation even at the shortest equilibration time used.	A/B
II-k	REF	End-over-end-shaker, continuous shaking.	A/B
II-l	REF	Sorption isotherm experiments were carried out, at high and low Cs concentration.	A
II-m	REF	Centrifuge tubes were used (material not specified). Wall sorption was not	A

		considered (experiments in similar systems had suggested only a small potential effect).	
II-n	REF	Error bars are provided for each K_d value. These are based partly on a few repeated experiments, partly on estimates of various experimental errors.	B
II-o	REF	It is indicated that Cs-concentration (isotherms), pH (solution composition) and sorption time were varied.	B

Data table Cs/3: REF: Staunton and Roubaud (1997)			
JAEA-SDB version 4.0 - DATA: Cs/Bentonite (Clay Minerals); K-, Ca-, Na-montmorillonite, K-, Ca-, Na-illite # 69332~69451			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB REF	Not all mandatory information is provided. Information about pH is missing. The missing information on pH can be roughly estimated from the information given in the REF. As Cs sorption does not depend on small variations of pH in the near-neutral pH range, the provided information is regarded as sufficient.	Yes
I-b	SDB	K_d is given in tabular form and as log graph: <ul style="list-style-type: none"> • #69332~69337 • #69338~69451 	class 1 class 5
II-a	SDB REF	The clay minerals montmorillonite and illite are indicated, including CEC and size fraction. The clay samples were made homoionic with either K, Na or Ca. No information on impurities is available.	B
II-b	SDB	It is indicated that no information about pH is provided. From the composition of the experimental systems (clay minerals plus neutral electrolyte solutions) it can be estimated that the solution pH was near neutral. In the case of Cs (which is sorbing via ion exchange), this is viewed as sufficient. Even in the experiments with added fulvic acid, where pH may be slightly lower, it is not expected that pH has an influence on Cs sorption.	D
II-c	SDB	It is indicated that no information about redox conditions is given. System is not redox-sensitive.	A/B
II-d	SDB	Initial solution composition is provided. The clays were homo-ionic (see II-a). The final solution composition can be estimated.	A/B
II-e	SDB	It is indicated that the temperature is 20°C.	A/B
II-f	SDB REF	A liquid/solid ratio of 1,000 [mL/g] is indicated (grain size was < 2 [μm]). The total amounts of clay material and solution volume are not available. Assuming 100 [mL]-vials and a BET surface area of about 30~50 [m ² /g] clay, each vial would contain 3~5 [m ²] of clay surface area.	C/D
II-g	SDB	Sorption values were calculated for all 120 data points. <ul style="list-style-type: none"> • #69332~69335, #69338~69373, #69376~69379, #69383~69387, #69389~69391, #69393~69397, #69400~69402, #69405, #69406, #69422~69441 • #69337, #69380~69382, #69398, #69399, #69404, #69417, #69418, #69421, #69446~69451 • Others 	A B C/D
II-h	SDB	Initial RN concentrations are indicated: Cs was added at trace levels. Cs is not solubility limited.	A
II-i	SDB REF	It is indicated that phase separation was performed by centrifugation (20,000 [g], 30 min.). It is reported that the completeness of phase separation was verified by preliminary trials.	B
II-j	SDB	A reaction time of 2 hours is indicated. The short reaction time was chosen deliberately and is considered to be sufficient for sorption by ion exchange. This is accepted.	C/D

II-k	REF	Samples were shaken end-over-end.	A/B
II-l	REF	Three adsorption isotherms are provided for each mineral.	A
II-m	REF	No information regarding reaction vessels is provided.	C/D
II-n	SDB	No information about uncertainty estimates is provided, except for the tabulated data:	
	REF	<ul style="list-style-type: none"> • #69332~69337: standard deviation from replicates • #69338~69451: no error information 	A D
II-o	SDB	Cs concentrations were varied.	
	REF	This was done in the form of isotherms at constant concentrations of a competing cation.	A

Data table Cs/4: REF: Tertre et al. (2005)

JAEA-SDB version 4.0 - DATA: Cs/Bentonite (Clay Minerals); Na-montmorillonite #69452~69562

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	It is indicated that K_d values are taken from graphs with a logarithmic axis.	class 5
II-a	SDB	As solid phases the MX-80 are indicated. A SSA of 24 [m ² /g] and a CEC of 87.5±2 [meq/100g] are reported, as well as the preparation procedure.	A
II-b	SDB	Final pH values are indicated.	A
	REF	pH values are adjusted using NaOH and HClO ₄ .	
II-c	SDB	It is indicated that experiments are conducted under air, no oxidizing or reducing agents are indicated. Cs in the oxidation state (I) is indicated. Cs is not redox sensitive.	A/B
II-d	SDB	Experiments had been performed in NaClO ₄ solution. Final solution composition is not indicated.	
	REF	Final elemental composition was calculated using the computer code CHESS. Chemical analysis was done by ICP-OES. The results are not included in the publication.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25, 40, 80 and 150°C.	A/B
II-f	SDB	The same amounts of solution (2 [mL]) and solid (5 [mg]) are indicated for all conditions.	
	REF	At 80°C, 17 [mg] of solid were reportedly used. For 150°C, the use of 200 [mL] clay-water suspension is reported, but it is not clear whether this refers to the clay stock suspension or the experimental suspension. Even in case of 17 [mg] clay added, less than 1 [m ²] of sorbent surface is added.	C/D
II-g	SDB	The %-sorbed can be calculated with K_d and L/S ratio:	
		<ul style="list-style-type: none"> • #69510, #69518, #69526, #69534 • #69480, #69501, #69508, #69517, #69520, #69523~69525, #69528, #69530, #69533, #69541, #69546, #69550, #69551, #69554, #69555 • Others 	C/D B A
II-h	SDB	An initial Cs concentration of 7.52×10^{-7} [M] is indicated.	
	REF	Cs is not solubility-limited.	A
II-i	SDB	Indicated are the following: centrifugation (2,000 [g]/30 min) at 25 and 40°C, filtration through 0.2 [μm] membranes at the higher temperatures.	A
II-j	SDB	A contact time of 3 days is indicated.	
	REF	7 days equilibration of solution and solid, 3 days reaction time of trace elements.	C/D
II-k	REF	The following is reported: 25/40°C: Shaking bank, 80°C: Shaken manually, 150°C: continuously shaken by rocking the set reactor and furnace.	A/B
II-l	REF	No variation in Cs or the L/S is reported, no isotherms are given.	C/D
II-m	REF	The following is reported: 25/40°C: Polycarbonate containers, 80°C: PTFE Savilex containers, 150°C: 300 [mL] PTFE hydrothermal reactor equipped with PTFE valves and tubing. Based on blank experiments and acid-washing of	A

		tube/container walls, wall sorption is estimated to be < 3% for Cs. No corrections are made.	
II-n	SDB	It is indicated that no error information is reported. For a number of selected data points (with the highest uncertainties), error bars are given which were derived from error propagation.	C
II-o	REF	Temperature, pH and ionic strength are varied.	B

Data table Cs/5: REF: Zachara et al.(2002)

JAEA-SDB version 4.0 - DATA: Cs/ Mudstone (Sedimentary rocks); sediment#1, sediment#2-1, sediment#2-2
#70399~70540, #71494~71513

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Log figures with K_d and sorption percent are given. •#70399~70491 •#70492~70540, #70494~71513	class 5 class 6
II-a	SDB	The solid samples were all derived from the Hanford formation, flood deposits of Pleistocene age. These were analyzed by X-ray diffraction (XRD) and optical microscopy. It is indicated that quartz is the dominant mineral with lesser amount of plagioclase and potassium feldspar, micas, chlorite, vermiculite, and smectite.	B
II-b	SDB REF	Final pH with a range was indicated. Reported pH range is over 1 pH unit. However, Cs is not pH sensitive. So, rating is to be a worst evaluation.	D
II-c	SDB REF	There is no information about redox condition. This experiment maybe performed under oxidizing condition. Cs is not redox sensitive.	A/B
II-d	SDB REF	Sorption experiment is performed using various solutions. Final solution composition is not reported. Concentration and composition of solution is known, and dominant mineral composition of solid sample is known. It is possible that final solution composition is estimated approximately.	A/B
II-e	SDB	A temperature was not reported.	C/D
II-f	SDB	Sorption experiment is performed with various liquid/solid ratios. Fraction size of solid samples are <63 μ m and 125~250 μ m. Surface area of solid sample is not reported.	C/D
II-g	SDB REF	Rating is done based on %-sorbed values calculated from the information given in the SDB.: •#70419, #70427, #70463, #70492, #70494, #70495 •#70399, #70407, #70417, #70418, #70426, #70442, #70449~70452, #70464~70467, #70482, #70491, #70498, #70535, #71512 •Others	C/D B A
II-h	SDB REF	Initial Cs concentration is reported $1.40 \times 10^{-9} \sim 1.05 \times 10^{-1}$ [M]. Cs is not solubility limited.	A
II-i	SDB	Separation method is centrifugation at 5,000 [ref] for 30 min.	C/D
II-j	SDB REF	It is indicated that contact time was 16 hours. There is a report that equilibrium was reached after about 10 min (Eriksen and Locklund,1987). Therefore, rating C/D is applied.	C/D
II-k	REF	The sample was shaken in 50-mL polycarbonate tubes at 80 rpm.	A/B
II-l	SDB	Initial Se concentration is varied. And sorption isotherm is presented.	A
II-m	REF	The experiments were carried out in 50-mL polycarbonate.	B
II-n	REF	No information is reported.	D
II-o	REF	The initial Cs concentration, solution composition, solution concentration and Liquid /Solid ratio were varied.	B

3.2.2 Nickel

Data table Ni/1: REF: Bradbury and Baeyens (2009a)		
JAEA-SDB version 4.0 - DATA: Ni/Bentonite (Clay Minerals); Na-illite, #70863~70953		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	Data are taken from a log graph with K_d values.	class 5
II-a SDB	Illite du Puy was conditioned to the homo-ionic Na-form with 1M-NaClO ₄ solution. XRD analysis showed the composition to be ~88 wt.% illite and ~12wt.% sanidine, a K-feldspar. The chemical composition is also shown in wt.%.	A
II-b SDB REF	It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 2 to 11 with NaOH or HNO ₃ . In the pH range 4–9, 5 types of buffers at a concentration of 2 mM in order to ensure pH stability (Separate measurements showed no significant influence of the buffers on sorption in the range of experimental conditions)	A
II-c SDB REF	Experiments were carried out in controlled N ₂ atmosphere glove boxes (CO ₂ <2 ppm, O ₂ <2 ppm). It is not used reducing agent. Ni is not sensitive to redox condition.	A/B
II-d SDB REF	0.1M and 0.5 M NaClO ₄ solution is indicated. Because purified Na-form illite is used under CO ₂ -free condition, the final solution composition is defined.	A/B
II-e SDB	Temperature is not reported. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f SDB	L/S value is indicated 1.8~2.3 [g/L] in 0.1M NaClO ₄ solution and 1.6 [g/L] in 0.5M NaClO ₄ solution, but volume of liquid and weight of solid is not reported.	C/D
II-g SDB	The sorption values were calculated from K_d and L/S ratios, the following rating is given: <ul style="list-style-type: none"> • #70887, #70890, #70909~70911, #70919 • #70865, #70883, #70884, #70886, #70888, #70891 ~ 70893, #70905, #70917, #70918, #70925, #70931, #70932, #70938 ~ 70940, #70945, #70946, #70952 • Others 	C/D B A
II-h SDB REF	An initial Ni-concentration is indicated 2×10^{-9} M in 0.1M NaClO ₄ solution and 7×10^{-9} M in 0.5M NaClO ₄ solution. Based on the thermodynamic calculations using JAEA TDB(100331c0.tdb), all data is given A.	A
II-i SDB	Centrifugation 1 hour at 108,800 [g] is indicated.	B
II-j SDB REF	A contact time of 3~84 days is indicated. Sorption equilibrium was reached at even if the least contact time 3 days.	A/B
II-k REF	It is indicated that samples were shaken end-over-end for at least 7 days.	A/B
II-l REF	Sorption isotherm experiments are not carried out.	C/D
II-m REF	Experimental vessel is 40-mL polypropylene centrifuge tube.	B
II-n SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o SDB	pH and ionic strength have been varied systematically.	A

Data table Ni/2: REF: Lauber et al. (2000)		
JAEA-SDB version 4.0 - DATA: Ni/Bentonite (Clay Minerals); Opalinus Clay #68145~68216		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes

I-b	SDB	Graphs with logarithmic K_d values are provided.	class 5
II-a	SDB	As solid phase Opalinus Clay (and CEC) is indicated. A detailed analysis of Opalinus Clay is available.	A
II-b	SDB REF	It is indicated that initial pH values is provided. The samples were pre-conditioned; therefore, it is assumed that initial and final pH is nearly identical. Further, the solution is well buffered.	A
II-c	SDB	It is indicated that experiments had been conducted under a nitrogen atmosphere. No addition of oxidizing or reducing agents is indicated. The experiments were carried out in a CO_2/N_2 atmosphere. Ni is not redox sensitive.	A/B
II-d	SDB REF	It is indicated that experiments had been performed in synthetic porewater solution, composition is given. Final solution composition is not indicated. Clay samples were pre-conditioned. The composition of the conditioned solutions was determined.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25°C.	A/B
II-f	SDB REF	The solution/solid ratio is indicated. Actual solution volume and solid weight are not given. The specific surface area of Opalinus Clay is reported as 33.3 [m ² /g]. Experiments were done in 40 [mL] centrifuge tubes. This results in about 8 [m ²] of sorbent surface per vial.	A/B
II-g	REF	The following sorption values were calculated from K_d and L/S ratios: <ul style="list-style-type: none"> • #68145, #68146, #68148, #68150, #68151, #68194~68200, #68203 • #68147, #68149, #68152, #68153, #68163, #68201, #68202, #68204~68211 • Others 	C/D B A
II-h	SDB REF	Initial Ni concentrations of 3.7×10^{-7} [M] and 9.2×10^{-4} [M] are indicated for #68145~68168. Initial Ni concentrations of $3.4 \times 10^{-7} \sim 8.6 \times 10^{-4}$ [M] are indicated for #68169~68216. Solubility calculation for Ni in the synthetic OPA porewaters at pH = 6.3 and 8 have been carried out, using the geochemical code MINEQL and thermodynamic database.	A
II-i	SDB	Centrifugation (60 min at 95,000[g]) is indicated.	B
II-j	SDB REF	Several contact times between about 7 and 220 days are indicated. At pH 6.3 and low Ni concentration, sorption is estimated to be complete after about 1 week. At high Ni concentration, sorption was observed to increase slightly within the experimental timeframe (up to 6 months). Fig. 9 in REF suggest stable concentrations after 20 days, and the following rating is given: <ul style="list-style-type: none"> • # 68145~68153, #68159~68162 • all other datapoints 	unreliable A/B
II-k	REF	End-over-end-shaker, continuous shaking.	A/B
II-l	REF	Sorption isotherm experiments were carried out, at high and low Ni concentration.	A
II-m	REF	Centrifuge tubes were used (material not specified). Wall sorption was not considered (experiments in similar systems had suggested only a small potential effect).	A
II-n	REF	Error bars are provided for each K_d value. These based on reported experiments, but it is not clear whether all experiments were reported.	B
II-o	SDB REF	It is indicated that Ni-concentration and reaction time was varied. Further data available in the REF concern a second set of solution composition.	B

Data table Ni/3: REF: Tertre et al. (2005)

JAEA-SDB version 4.0 - DATA: Ni/Bentonite (Clay Minerals); Na-montmorillonite #69563~69675

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes

I-b	REF	It is indicated that K_d values are taken from graphs with a logarithmic axis.	class 5
II-a	SDB	As solid phases the MX-80 are indicated. A SSA of 24 [m^2/g] and a CEC of 87.5 ± 2 [$\text{meq}/100\text{g}$] are reported, as well as the preparation procedure.	A
II-b	SDB REF	Final pH values are indicated. pH values are adjusted using NaOH and HClO_4 .	A
II-c	SDB	It is indicated that experiments are conducted under air, no oxidizing or reducing agents are indicated. Ni in the oxidation state (II) is indicated. Ni is not redox sensitive.	A/B
II-d	SDB REF	Experiments had been performed in NaClO_4 solution. Final solution composition is not indicated. Final elemental composition was calculated using the computer code CHESS. Chemical analysis was done by ICP-OES. The results are not included in the publication.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25, 40, 80 and 150°C .	A/B
II-f	SDB REF	The same amounts of solution (2 [mL]) and solid (5 [mg]) are indicated for all conditions. At 80°C , 17 [mg] of solid were reportedly used. For 150°C , the use of 200 [mL] clay-water suspension is reported, but it is not clear whether this refers to the clay stock suspension or the experimental suspension. Even in case of 17 [mg] clay added, less than 1 [m^2] of sorbent surface is added.	C/D
II-g	SDB	The %-sorbed can be calculated with K_d and L/S ratio: <ul style="list-style-type: none"> • #69584, #69592, #69593, #69603~69608, #69616~69619, #69623 • #69580~#69583, #69595, #69611, #69613, #69615, #69620~69622, #69624~69626, #69668, #69669 • Others 	C/D B A
II-h	SDB REF	An initial Ni concentration of 1.7×10^{-6} [M] is indicated. Based on speciation calculations using the SUPCRT92 database for different pH conditions, the initial Ni concentration is reported to be clearly below the solubility limit.	A
II-i	SDB	Indicated are the following: centrifugation (2,000 [g]/30min) at 25 and 40°C , filtration through 0.2 [μm] membranes at the higher temperatures.	A
II-j	SDB REF	A contact time of 3 days is indicated. 7 days equilibration of solution and solid, 3 days reaction time of trace elements.	C/D
II-k	REF	The following is reported: $25/40^\circ\text{C}$: Shaking bank, 80°C : Shaken manually, 150°C : continuously shaken by rocking the set reactor and furnace.	A/B
II-l	REF	No variation in Ni or the L/S is reported, no isotherms are given.	C/D
II-m	REF	The following is reported: $25/40^\circ\text{C}$: Polycarbonate containers, 80°C : PTFE Savilex containers, 150°C : 300 [mL] PTFE hydrothermal reactor equipped with PTFE valves and tubing. Based on blank experiments and acid-washing of tube/container walls, wall sorption is estimated to be $< 3\%$ for Ni. No corrections are made.	A
II-n	SDB	It is indicated that no error information is reported. For a number of selected data points (with the highest uncertainties), error bars are given which were derived from error propagation.	C
II-o	REF	Temperature, pH and ionic strength are varied.	B

3.2.3 Europium / Americium / Curium

Data table Eu/1: REF: Bradbury and Baeyens(2002)*		
JAEA-SDB version 4.0 - DATA: Eu/Bentonite (Clay minerals); Ca-montmorillonite #67322~67364		
GUIDELINE: Revision 4b (May 19, 2005)		
*REMARK: The preparatory experiments carried out before the sorption tests, and the methodology used for the sorption measurements themselves, are the same as those reported in Baeyens and Bradbury (1997) for Ni/Zn Sorption on Na-montmorillonite.		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	REF Data are taken from a log graph with K_d values.	class 5
II-a	SDB Montmorillonite used in the experiment is SWy-1 Na-montmorillonite. SWy-1 montmorillonite was conditioned to homo-ionic Na-form..	A
II-b	SDB pH was adjusted with HNO ₃ and NaOH. Final pH values are reported.	A
II-c	SDB This experiment is performed under N ₂ atmosphere. Eu is not sensitive to redox condition.	A/B
II-d	SDB The chemical composition (Na, K, Ca, Mg, Al, Fe and Si) of the 2 types of equilibrated solutions is reported.	A/B
II-e	SDB It is indicated that experiments had been performed at room temperature REF This can be assumed, but is not reported in the REF.	A/B
II-f	SDB A liquid/solid ratio of 1 [g/L] for Ca-montmorillonite and 1.5 [g/L] for REF Na-montmorillonite is reported.	A/B
II-g	SDB The following sorption values were calculated from K_d and L/S ratios: REF • #67324, #67325, #67329, #67331~67333, #67335, #67337, #67338, #67349 • #67334, #67336, #67340~67348 • Others	B A C/D
II-h	SDB Initial Eu is reported 9.5×10^{-9} and 1.3×10^{-7} [M]. REF This condition was chosen based on the thermodynamic calculations, indicated that the maximum initial Eu concentration used was at least one order of magnitude less than the solubility limit calculated for Eu(OH) ₃ (s).	A
II-i	SDB Separation method is centrifugation at 95,000 [g] for 1 hour.	B
II-j	SDB It is indicated that contact time was 4 days.	A/B
II-k	REF Samples were shaken.	A/B
II-l	SDB Initial Eu concentration is hardly varied.	C/D
II-m	REF The experiments were carried out in polypropylene centrifuge tube. Wall sorption effects are assessed.	B
II-n	REF The maximum absolute error calculated by considering the maximum error in each operation in batch sorption experiments at the highest and lowest sorption values, and on sets of repeat measurements, a realistic uncertainty in these measured sorption values was estimated to be a factor of 1.6.	D
II-o	REF The experiments are performed under different pH, Eu concentration, and type of montmorillonite (Ca-type and Na-type),.	B

Data table Eu/2: REF: Bradbury and Baeyens (2009a)		
JAEA-SDB version 4.0 - DATA: Eu/Bentonite (Clay Minerals); Na-illite, #70975~71002		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB Data are taken from a log graph with K_d values.	class 5
II-a	SDB Illite du Puy was conditioned to the homo-ionic Na-form with 1M-NaClO ₄ solution. XRD analysis showed the composition to be ~88 wt.% illite and ~12wt.% sanidine, a K-feldspar. The chemical composition is also shown in wt.%.	A

II-b	SDB REF	It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 2 to 11 with NaOH or HNO ₃ . In the pH range 4–9, 5 types of buffers at a concentration of 2 mM in order to ensure pH stability (Separate measurements showed no significant influence of the buffers on sorption in the range of experimental conditions)	A
II-c	SDB REF	Experiments were carried out in controlled N ₂ atmosphere glove boxes (CO ₂ <2 ppm, O ₂ <2 ppm). It is not used reducing agent. Eu is not sensitive to redox condition.	A/B
II-d	SDB REF	0.1M NaClO ₄ solution is indicated. Because purified Na-form illite is used under CO ₂ -free condition, the final solution composition is defined.	A/B
II-e	SDB	Temperature is not reported. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB	L/S value is indicated 0.6~1.6 [g/L], but volume of liquid and weight of solid is not reported.	C/D
II-g	SDB	The sorption values were calculated from K _d and L/S ratios, the following rating is given: • #70983, #70984 • #70975~70982 • Others	B A C/D
II-h	SDB REF	An initial Eu-concentration is indicated 3.9×10 ⁻⁹ M. Based on the thermodynamic calculations using JAEA-TDB(100331c0.tdb), all data is given A.	A
II-i	SDB	Centrifugation 1 hour at 108,800 [g] is indicated.	B
II-j	SDB REF	A contact time of 7 days is indicated. Because Ni and Sn are reached an equilibrium condition for 7 days, it is considered to reach an equilibrium condition for Eu.	A/B
II-k	REF	It is indicated that samples were shaken end-over-end for at least 7 days.	A/B
II-l	REF	Sorption isotherm experiments are not carried out.	C/D
II-m	REF	Experimental vessel is 40-mL polypropylene centrifuge tube.	B
II-n	SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o	SDB	pH has been varied systematically.	B

Data table Eu/3: REF: Marques Fernandes et al.(2008)			
JAEA-SDB version 4.0 - DATA: Eu/ Bentonite (Clay minerals); Na-Swy-1 montmorillonite #67397~67449			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	K _d values taken from a graph with log axis.	class 5
II-a	SDB REF	SWy-1 montmorillonite is used in this experiment. It was washed three times with 1M-NaClO ₄ to remove all soluble salts and/or sparingly soluble minerals such as calcite and to convert to the montmorillonite into the homo-ionic Na-form.	A
II-b	SDB REF	Final pH values are reported. In the case of fixed pH experiment and variable pH experiment, the total carbonate concentration was adjusted as a function of pH using NaHCO ₃ /Na ₂ CO ₃ solutions. The pH values of carbonate free experiments, and the experiments at varying pCO ₂ (closed systems), were buffered with MOPS, TRIS or CHES buffers at concentrations of 2×10 ⁻³ [M].	A
II-c	SDB REF	There is no information about redox condition. Eu(III) is not sensitive to redox condition.	A/B
II-d	SDB REF	Solution used in this experiment is 0.1M NaClO ₄ . The composition of final solution is not reported. Because purified Na-form montmorillonite is used under fixed pCO ₂ and	C/D

		variable pCO ₂ conditions, the final solution composition can be estimated.	
II-e	SDB	A temperature is not indicated. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB REF	A liquid/solid ratio of 1 [g/L] is reported. The weight of solid and the volume of solution are not reported. Particle size of solid is not indicated.	C/D
II-g	SDB REF	The sorption values were calculated from K _d and L/S ratios, the following rating is given: <ul style="list-style-type: none"> • #67415, #67417~67425, #67429~67434 • #67414, #67416, #67427, #67428, #67435~67437, #67443 • Others 	C/D B A
II-h	SDB REF	Initial Eu concentration is reported as 2.0×10 ⁻⁹ [M]. Initial Eu concentration is 9.5×10 ⁻⁹ had been compared with thermodynamic calculations using NEA-TDB for Am in REF. Then REF showed that any influence of the precipitation can be excluded.	A
II-i	SDB	The separations were centrifuged at 105,000 [g] (max) for one hour.	B
II-j	SDB REF	It is indicated that contact time was 7 days. In this experiment, Kinetic experiments performed for time periods between 2 and 60 days showed that equilibrium conditions were already reached after 2 days.	A/B
II-k	REF	Samples were shaken end-over-end.	A/B
II-l	SDB	Initial Eu concentrations are not varied.	C/D
II-m	REF	The experiments were carried out in polypropylene centrifuge tube. No correction for sorption on vessel walls is reported.	B
II-n	SDB REF	All experiments were carried out in triplicate. Error is not indicated. An error bar is indicated in figure.	A
II-o	REF	This experiment is performed as a function of pH and under different pCO ₂ systems.	B

Data table Eu/4: REF: Lauber et al. (2000)			
JAEA-SDB version 4.0 - DATA: Eu/Bentonite (Clay minerals); Opalinus Clay #68217~68278			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint	Evaluation	Rating	
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Graphs with logarithmic K _d values are provided.	class 5
II-a	SDB	As solid phase Opalinus Clay (and CEC) is indicated. A detailed analysis of Opalinus Clay is available.	A
II-b	SDB REF	It is indicated that initial pH values is provided. The samples were pre-conditioned; therefore, it is assumed that initial and final pH is nearly identical. Further, the solution is well buffered.	A
II-c	SDB	It is indicated that experiments had been conducted under a nitrogen atmosphere. No addition of oxidizing or reducing agents is indicated. The experiments were carried out in a CO ₂ /N ₂ atmosphere. Eu is not redox sensitive.	A/B
II-d	SDB REF	It is indicated that experiments had been performed in synthetic porewater solution, composition is given. Final solution composition is not indicated. Clay samples were pre-conditioned. The composition of the conditioned solutions was determined.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25°C.	A/B
II-f	SDB REF	The solution/solid ratio is indicated. Actual solution volume and solid weight are not given. The specific surface area of Opalinus Clay is reported as 33.3 [m ² /g]. Experiments were done in 40 [mL] centrifuge tubes. This results in about 8 [m ²] of sorbent surface per vial.	A/B
II-g	REF	The following sorption values were calculated from K _d and L/S ratios. For	

		#68238~68250 and #68266~68278, L/S is indicated the region of 180.51~420 [mL/g]. Because sorption value can not been calculated, these datapoints are evaluated as C/D. <ul style="list-style-type: none"> • #68218~68224, #68227~68237 • #68217 • Others 	B A C/D
II-h	SDB REF	Initial Eu concentrations of 4.7×10^{-9} [M] are indicated for #68217~68225. Initial Eu concentrations of $9.8 \times 10^{-9} \sim 7.1 \times 10^{-7}$ [M] are indicated for #68226~68278. Solubility calculation for Eu in the synthetic OPA porewaters at pH = 6.3 and 8 have been carried out, using the geochemical code MINEQL and thermodynamic database.	A
II-i	SDB	Centrifugation (60 min at 95,000 [g]) is indicated.	B
II-j	SDB	Several contact times between about 0.2 and 210 days are indicated. At pH 6.3, sorption is estimated to be complete after about 1 week. Therefore, the following rating is given: <ul style="list-style-type: none"> • datapoint #68217~68220 • all other datapoints 	unreliable A/B
II-k	REF	End-over-end-shaker, continuous shaking.	A/B
II-l	REF	Sorption isotherm experiments were carried out, at high and low Eu concentration.	A
II-m	REF	Centrifuge tubes were used (material not specified). Wall sorption was not considered (experiments in similar systems had suggested only a small potential effect).	A
II-n	REF	Error bars are provided for each K_d value. These are based partly on a few repeated experiments, partly on estimates of various experimental errors.	B
II-o	SDB REF	Indicated are experiments for a given set of conditions. Further data (isotherms, different solution composition) are available in the REF	B

Data table Eu/5: REF: Rabung et al.(2005)			
JAEA-SDB version 4.0 - DATA: Eu/Bentonite (Clay minerals); Ca-montmorillonite, Na-illite #68936~69004			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint	Evaluation	Rating	
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Graphs with logarithmic K_d values are provided.	class 5
II-a	SDB	Samples used in this experiment are Ca-montmorillonite and Na-illite. Ca-montmorillonite was conditioned from SWy-1 montmorillonite. Illite is collected in region of Le Puy-en-Velay (Haute-Loire), France. Their mineral compositions are not reported. Surface area and CEC are reported.	B
II-b	SDB	pH was adjusted with HClO ₄ /HNO ₃ or NaOH. Final pH values are reported.	A
II-c	SDB REF	This experiment was performed under Ar atmosphere for Ca-montmorillonite, under N ₂ atmosphere for Na-illite. Eu(III) is not redox sensitive.	A/B
II-d	REF	Solutions used are 0.066M Ca(NO ₃) ₂ , 0.066M Ca(ClO ₄) ₂ for Ca-montmorillonite. Solution used is 0.1M NaClO ₄ for Na-illite. The final solution composition can be estimated.	A/B
II-e	SDB	A temperature is reported 24±2°C.	A/B
II-f	REF	Solid /liquid ratios of 0.25, 1.8 [g/L] are reported. Particle size of solids is not indicated.	C/D
II-g	REF	The following sorption values were calculated from K_d and L/S ratios: <ul style="list-style-type: none"> • #68942~68945, #68967, #68969, #68983 • #68936~68941, #68963~68966, #68975~68982 • Others 	B A C/D
II-h	SDB	Initial Eu concentration is reported as 6.5×10^{-7} [M] for Ca-montmorillonite, 2.1×10^{-9} [M] for Na-illite.	A

	REF	This condition was chosen based on the thermodynamic calculations in Bradbury and Baeyens(2002), indicated that the maximum initial Eu concentration used was at least one order of magnitude less than the solubility limit calculated for Eu(OH) ₃ (s).	
II-i	REF	Separation method is centrifugation (35,000 [rpm], 30 min).	B
II-j	REF	It is indicated that contact time was 2 days.	C/D
II-k	REF	Information about an agitation method is not reported.	C/D
II-l	REF	No sorption isotherm and no variation of S/W ratio are reported. Sorption isotherm had been reported in Bradbury and Baeyens(2002).	C/D
II-m	REF	The experiments were carried out in polypropylene centrifuge tube. No correction for sorption on vessel walls is reported.	B
II-n	REF	Although the experiments were performed in triplicate, errors were not evaluated.	B
II-o	REF	Influences of pH, clay types (Ca-montmorillonite and Na-illite) were investigated.	B

Data table Eu/6: REF: Tertre et al. (2005)

JAEA-SDB version 4.0 - DATA: Eu/Bentonite (Clay minerals); Na-montmorillonite #69676~69783
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	It is indicated that K _d values are taken from graphs with a logarithmic axis.	class 5
II-a	SDB	As solid phases the MX-80 are indicated. A SSA of 24 [m ² /g] and a CEC of 87.5±2 [meq/100g] are reported, as well as the preparation procedure.	A
II-b	SDB REF	Final pH values are indicated. pH values are adjusted using NaOH and HClO ₄ .	A
II-c	SDB	It is indicated that experiments are conducted under air, no oxidizing or reducing agents are indicated. Eu in the oxidation state (III) is indicated. Eu is not redox sensitive.	A/B
II-d	SDB REF	Experiments had been performed in NaClO ₄ solution. Final solution composition is not indicated. Final elemental composition was calculated using the computer code CHESS. Chemical analysis was done by ICP-OES. The results are not included in the publication.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25, 40, 80 and 150°C.	A/B
II-f	SDB REF	The same amounts of solution (2 [mL]) and solid (5 [mg]) are indicated for all conditions. At 80°C, 17 [mg] of solid were reportedly used. For 150°C, the use of 200 [mL] clay-water suspension is reported, but it is not clear whether this refers to the clay stock suspension or the experimental suspension. Even in case of 17 [mg] clay added, less than 1 [m ²] of sorbent surface is added.	C/D
II-g	SDB	The %-sorbed can be calculated with K _d and L/S ratio: <ul style="list-style-type: none"> • #69676~69679, #69683, #69684, #69695, #69704~69706, #69730~69745, #69751~69753, #69759~69762, #69774 • #69680~69682, #69685, #69686, #69696, #69697, #69707, #69708, #69754~69757, #69775 • Others 	C/D B A
II-h	SDB REF	An initial Eu concentration of 6.58×10 ⁻⁷ is indicated. Based on speciation calculations using the SUPCRT92 database for different pH conditions, the initial Eu concentrations are reported to be clearly below the solubility limit. It is argued that final concentrations are much lower than the solubility limit, but it is not clearly discussed whether initial concentrations may have lead to precipitation. Based on the experimental solubility data given in Rai et al. (1999) and	

		Hummel et al. (2002), the following rating is applied: <ul style="list-style-type: none"> • #69693, #69694, #69703, 69716~69719, #69728, #69729, #69746~69750, #69772, #69773(pH≥8) • #69702, #69714, #69715, #69758, #69769~69771(pH 7.5~8) • datapoints corresponding to pH < 7.5 	Unreliable B A
II-i	SDB	Indicated are the following: centrifugation (2,000 [g]/30min) at 25 and 40°C, filtration through 0.2 [μm] membranes at the higher temperatures.	A
II-j	SDB REF	A contact time of 3 days is indicated. 7 days equilibration of solution and solid, 3 days reaction time of trace elements.	C/D
II-k	REF	The following is reported: 25/40°C: Shaking bank, 80°C: Shaken manually, 150°C: continuously shaken by rocking the set reactor and furnace.	A/B
II-l	REF	No variation in Eu or the L/S is reported, no isotherms are given.	C/D
II-m	REF	The following is reported: 25/40°C: Polycarbonate containers, 80°C: PTFE Savilex containers, 150°C: 300 [mL] PTFE hydrothermal reactor equipped with PTFE valves and tubing. Based on blank experiments and acid-washing of tube/container walls, wall sorption is estimated to be < 6% for Eu. No corrections are made.	A
II-n	SDB	It is indicated that no error information is reported. For a number of selected data points (with the highest uncertainties), error bars are given which were derived from error propagation.	C
II-o	REF	Temperature, pH and ionic strength are varied.	B

Data table Am/1: REF: Bradbury and Baeyens (2009b)

JAEA-SDB version 4.0 - DATA: Am/Bentonite (Clay Minerals); Na-illite, #71033~71110

GUIDELINE: Revision 4b (May 19, 2005)

REMARK : It is considered that this experiment procedure is a same with Bradbury and Baeyens (2009a).

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB Data are taken from a log graph with K_d values.	class 5
II-a	SDB Illite du Puy was conditioned to the homo-ionic Na-form with 1M-NaClO ₄ solution. XRD analysis showed the composition to be ~88 wt.% illite and ~12wt.% sanidine, a K-feldspar. The chemical composition is also shown in wt.%.	A
II-b	SDB REF It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 2 to 11 with NaOH or HNO ₃ . In the pH range 4-9, 5 types of buffers at a concentration of 2 mM in order to ensure pH stability (Separate measurements showed no significant influence of the buffers on sorption in the range of experimental conditions)	A
II-c	SDB REF Experiments were carried out in controlled N ₂ atmosphere glove boxes (CO ₂ <2 ppm, O ₂ <2 ppm). It is not used reducing agent. Am is not sensitive to redox condition.	A/B
II-d	SDB REF 0.1M NaClO ₄ solution is indicated. Because purified Na-form illite is used under CO ₂ -free condition, the final solution composition is defined.	A/B
II-e	SDB Temperature is not reported. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB L/S value is indicated 0.58 [g/L], but volume of liquid and weight of solid is not reported.	C/D
II-g	SDB The sorption values were calculated from K_d and L/S ratios, the following rating is given: <ul style="list-style-type: none"> • #71033~71036 • Others 	A C/D
II-h	SDB An initial Am-concentration is indicated 4×10^{-11} M.	A

	REF	Based on the thermodynamic calculations using JAEA TDB(100331c0.tdb), all data is given A.	
II-i	SDB	Centrifugation 1 hour at 108,800 [g] is indicated.	B
II-j	SDB REF	A contact time of 7 days is indicated. Based on the sorption kinetics measured for Ni and Sn in Bradbury and Baeyens (2009a), it is considered to reach an equilibrium condition for Am.	A/B
II-k	REF	It is indicated that samples were shaken end-over-end for at least 7 days.	A/B
II-l	REF	Sorption isotherm experiments are not carried out.	C/D
II-m	REF	Experimental vessel is 40-mL polypropylene centrifuge tube.	B
II-n	SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o	SDB	pH has been varied systematically.	A

Data table Cm/1: REF: Rabung et al.(2005)

JAEA-SDB version 4.0 - DATA: Cm/Bentonite (Clay minerals); Ca-montmorillonite, Na-illite #69005~69025
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Graphs with logarithmic K_d values are provided.	class 5
II-a	SDB	Samples used in this experiment are Ca-montmorillonite and Na-illite. Ca-montmorillonite was conditioned from SWy-1 montmorillonite. Illite is collected in region of Le Puy-en-Velay (Haute-Loire), France. Their mineral compositions are not reported. Surface area and CEC are reported.	B
II-b	SDB	pH was adjusted with $\text{HClO}_4/\text{HNO}_3$ or NaOH. Final pH values are reported.	A
II-c	SDB REF	This experiment was performed under Ar atmosphere for Ca-montmorillonite, under N_2 atmosphere for Na-illite. Cm(III) is not redox sensitive redox.	A/B
II-d	REF	Solution used is 0.066M $\text{Ca}(\text{ClO}_4)_2$ for Ca-montmorillonite. Solution used is 0.1M NaClO_4 for Na-illite. The final solution composition can be estimated.	A/B
II-e	SDB	A temperature is reported $24 \pm 2^\circ\text{C}$.	A/B
II-f	REF	A solid /liquid ratio of 0.25 [g/L] is reported. Particle size of solids is not indicated.	C/D
II-g	SDB REF	The following sorption values were calculated from K_d and L/S ratios: <ul style="list-style-type: none"> • #69017, #69024, #69025 • #69015, #69016 • Others 	C/D B A
II-h	SDB REF	Initial Cm is reported 2.5×10^{-7} [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Cm is more than initial concentration for pH<8. <ul style="list-style-type: none"> • #69014~69016 • Others 	unreliable A
II-i	REF	Separation method is centrifugation (35,000 [rpm], 30 min).	B
II-j	REF	It is indicated that contact time was 2 days.	C/D
II-k	REF	Information about an agitation method is not reported.	C/D
II-l	REF	No sorption isotherm and no variation of S/W ratio are reported.	C/D
II-m	REF	The experiments were carried out in polypropylene centrifuge tube. No correction for sorption on vessel walls is reported.	B
II-n	REF	Although the experiments were performed in triplicate, errors were not evaluated.	B
II-o	REF	Influences of pH, clay types (Ca-montmorillonite and Na-illite) were investigated.	B

3.2.4 Thorium

Data table Th/1: REF: Bradbury and Baeyens (2003)*		
JAEA-SDB version 4.0 - DATA: Th/Bentonite (Clay Minerals); Na-montmorillonite(Swy-1) #67365~67380 #70541~70546		
GUIDELINE: Revision 4b (May 19, 2005)		
*REMARK: This table is a revision of data table Th/4 in Saito et al.(2008); it entirely replaces the previous rating, which was carried out before the data had been entered in the JAEA-SDB. The rating for most checkpoints is identical to the previous rating. The underlying K_d data are read from graphs, and the numbers have slightly changed in comparison to Table Th/4.		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB Data are taken from a log graph with K_d values.	class 5
II-a	SDB Purified Na-SWy1montmorillonite with determined mineralogical composition and characteristics was used for the experiments.	A
II-b	SDB It is indicated that final pH-values were measured.	A
II-c	SDB Experiments were carried out in CO ₂ -free conditions (presumably in an inert atmosphere). Th is not redox-sensitive.	A/B
II-d	SDB 0.1 M and 1 M NaClO ₄ solution are indicated.	A/B
II-e	SDB Temperature is not reported in the REF. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB It is indicated that the amount solid added to reaction vessels is not known.	C/D
II-g	SDB The sorption values can be calculated from K_d and L/S ratios, the following rating is given: • #67365, #67366 • #67367~67369 • #67370~67380, #70541~70546	A B C/D
II-h	SDB An initial Th-concentration $<1 \times 10^{-9}$ [M] is indicated. Based on the experimental and thermodynamic data in Hummel et al. (2002), the following rating is given: • #67365~67371, #67380, #70541, #70542 • #67372~67379, #70543~70546	A B
II-i	SDB Centrifugation 60 min at 95,000 [g] is indicated.	B
II-j	SDB A contact time of 7 days is indicated.	C/D
II-k	REF No information available. Assumed is shaking end-over-end, based on Baeyens and Bradbury (1997).	A/B
II-l	REF No sorption isotherm experiments or variations of L/S are indicated.	C/D
II-m	REF No information is available.	C/D
II-n	SDB Error is indicated $\log K_d \pm 0.15$. REF An error of $\log K_d \pm 0.15$ is reported. Based on Baeyens and Bradbury (1997), it is assumed that this is derived based on error propagation estimates.	C
II-o	SDB pH has been varied systematically.	C

Data table Th/2: REF: Bradbury and Baeyens (2009b)		
JAEA-SDB version 4.0 - DATA: Th/Bentonite (Clay Minerals); Na-illite, #71111~71135		
GUIDELINE: Revision 4b (May 19, 2005)		
REMARK : It is considered that this experiment procedure is a same with Bradbury and Baeyens (2009a).		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB Data are taken from a log graph with K_d values.	class 5
II-a	SDB Illite du Puy was conditioned to the homo-ionic Na-form with 1M-NaClO ₄ solution. XRD analysis showed the composition to be ~88 wt.% illite and ~12wt.% sanidine, a K-feldspar. The chemical composition is also shown in	A

		wt. %.	
II-b	SDB REF	It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 2 to 11 with NaOH or HNO ₃ . In the pH range 4–9, 5 types of buffers at a concentration of 2 mM in order to ensure pH stability (Separate measurements showed no significant influence of the buffers on sorption in the range of experimental conditions)	A
II-c	SDB REF	Experiments were carried out in controlled N ₂ atmosphere glove boxes (CO ₂ <2 ppm, O ₂ <2 ppm). It is not used reducing agent. Th is not sensitive to redox condition.	A/B
II-d	SDB REF	0.1M NaClO ₄ solution is indicated. Because purified Na-form illite is used under CO ₂ -free condition, the final solution composition is defined.	A/B
II-e	SDB	Temperature is not reported. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB	L/S value is indicated 0.67 [g/L], but volume of liquid and weight of solid is not reported.	C/D
II-g	SDB	The sorption values were calculated from K _d and L/S ratios: All data is higher 98% sorption.	C/D
II-h	SDB REF	An initial Th-concentration is indicated $\sim 1 \times 10^{-11}$ M. Based on the thermodynamic calculations in JAEA-TDB(100331c0.tdb), all data is given A.	A
II-i	SDB	Centrifugation 1 hour at 108,800 [g] is indicated.	B
II-j	SDB REF	A contact time of 7 days is indicated. Based on the sorption kinetics measured for Ni and Sn in Bradbury and Baeyens (2009a), it is considered to reach an equilibrium condition for Th.	A/B
II-k	REF	It is indicated that samples were shaken end-over-end for at least 7 days.	A/B
II-l	REF	Sorption isotherm experiments are not carried out.	C/D
II-m	REF	Experimental vessel is 40-mL polypropylene centrifuge tube.	B
II-n	SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o	SDB	pH has been varied systematically.	B

Data table Th/3: REF: Lauber et al. (2000)			
JAEA-SDB version 4.0 - DATA: Th/Bentonite (Clay Minerals); Opalinus Clay #68279~68352			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Graphs with logarithmic K _d values are provided.	class 5
II-a	SDB	As solid phase Opalinus Clay (and CEC) is indicated. A detailed analysis of Opalinus Clay is available.	A
II-b	SDB REF	It is indicated that initial pH values is provided. The samples were pre-conditioned; therefore, it is assumed that initial and final pH is nearly identical. Further, the solution is well buffered.	A
II-c	SDB	It is indicated that experiments had been conducted under a nitrogen atmosphere. No addition of oxidizing or reducing agents is indicated. The experiments were carried out in a CO ₂ /N ₂ atmosphere. Th is not redox sensitive.	A/B
II-d	SDB REF	It is indicated that experiments had been performed in synthetic porewater solution, composition is given. Final solution composition is not indicated. Clay samples were pre-conditioned. The composition of the conditioned solutions was determined.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25°C.	A/B
II-f	SDB REF	The solution/solid ratio is indicated. Actual solution volume and solid weight are not given. The specific surface area of Opalinus Clay is reported as 33.3 [m ² /g]. Experiments were done in 40 [mL] centrifuge tubes. This results in about 8 [m ²]	A/B

		of sorbent surface per vial.	
II-g	REF	The following sorption values were calculated from K_d and L/S ratios. For #68306~68318 and #68338~68352, L/S is indicated the region of 180.51~420 [mL/g]. Because sorption value can not been calculated, these datapoints are evaluated as C/D. Adsorption % of other datapoints are >99%.	C/D
II-h	SDB REF	Initial Th concentrations of 6.7×10^{-11} M are indicated for #68279~68296. Initial Th concentrations of $3.8 \times 10^{-11} \sim 7.6 \times 10^{-7}$ [M] are indicated for #68297~68352. Solubility calculation for Th in the synthetic OPA porewaters at pH = 6.3 and 8 have been carried out, using the geochemical code MINEQL and thermodynamic database.	A
II-i	SDB	Centrifugation (60 min at 95,000 [g]) is indicated.	B
II-j	SDB REF	Several contact times between about 7 and 210 days are indicated. At pH 6.3 and low Th concentrations, sorption is estimated to be complete after about 1 day. Therefore, the following rating is given: • # 68279, #68280 • all other datapoints	unreliable A/B
II-k	REF	End-over-end-shaker, continuous shaking.	A/B
II-l	REF	Sorption isotherm experiments were carried out, at high and low Th concentration.	A
II-m	REF	Centrifuge tubes were used (material not specified). Wall sorption was not considered (experiments in similar systems had suggested only a small potential effect).	A
II-n	REF	Error bars are provided for each K_d value. These are based on repeated experiments, but it is not clear whether all experiments were repeated.	B
II-o	SDB REF	Indicated are experiments for a given set of conditions. Further data (isotherms, different solution composition) are available in the REF	B

3.2.5 Neptunium

Data table Np/1: REF: Bertetti et al.(1998)		
JAEA-SDB version 4.0 - DATA: Np/Other minerals; clinoptilolite, quartz, α -alumina #67140~67321		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	REF Log K_d from figure is given.	class 5
II-a	SDB Details of clinoptilolite can be found in Pabalan(1994), reported the results of ICP analysis.	A
II-b	SDB pH was adjusted with HNO ₃ , NaHCO ₃ and NaOH. Final pH values are reported.	A
II-c	SDB Information about Eh values is not given. Np(V) is indicated for all conditions	A/B
	REF Experiments were conducted under atmosphere and glove-box conditions.	
II-d	SDB Test solutions are 0.01M and 0.1MNaNO ₃ . Solids are clinoptilolite, quartz and α -alumina. The final solution composition can be estimated.	A/B
II-e	SDB Experiments were carried out at room temperature (20±2°C).	A/B
II-f	SDB A range of L/S ratio between 12.5 and 250 [mL/g] is reported.	
	REF 0.1~2.0 [g] solid were added to 25 [mL] solution. Surface area values of clinoptilolite, quartz and α -alumina are reported to be 10.1±0.3, 0.03±0.01 and 0.23±0.01 [m ² /g], respectively.	C/D
II-g	SDB The following sorption values were calculated from K_d and L/S ratios: • #67147, #67149, #67157, #67162~67166, #67181, #67202, #67204, #67208, #67222~67225, #67238~67243, #67255~67262, #67276, #67293, #67294, #67298, #67299, #67301, #67302, #67304, #67309~67318 • #67209, #67263~67272, #67277~67290, #67303, #67319~67321 • Others	B A C/D

II-h	SDB REF	Initial Np is reported 1.0×10^{-7} and 1.0×10^{-6} [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np is above 1.0×10^{-6} [M].	A
II-i	SDB	Separation method is carried out with a centrifugation.	C/D
II-j	SDB	It is indicated that contact time was 14 days.	A/B
II-k	REF	The experimental mixtures were agitated using gyratory shakers.	A/B
II-l	SDB	Initial Np concentration is hardly varied.	C/D
II-m	REF	The experiments were carried out in polycarbonate centrifuge tube. Additional tests were conducted to evaluate potential wall sorption, indicating wall sorption can be negligible.	A
II-n	REF	No information is reported.	D
II-o	REF	pH and L/S ratio were systematically varied.	A

Data table Np/2: REF: Girvin et al.(1991)			
JAEA-SDB version 4.0 - DATA: Np/Other minerals; Fe ₂ O ₃ ·H ₂ O(am) #67538~67581			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Linear graph % sorbed is given.	class 4
II-a	SDB	Samples used are synthetic Fe ₂ O ₃ ·H ₂ O amorphous.	A
II-b	SDB	pH was adjusted with 0.1M HNO ₃ and 0.1M NaOH. Final pH values are reported.	A
II-c	SDB	All experiments were carried out as Np(V) under aerobic condition.	A/B
II-d	SDB	Solution used is 0.1M NaNO ₃ , and solid is Fe ₂ O ₃ ·H ₂ O(am). Final solution compositions can be defined.	A/B
II-e	SDB	A temperature is 25°C.	A/B
II-f	SDB REF	A liquid/solid ratio of 177.72, 657.564 and 1777.2 [mL/g] is reported. It is considered that enough solid had been added to each vessel.	A/B
II-g	SDB REF	The following sorption values were scanned from figure: <ul style="list-style-type: none"> • #67538, #67542, #67543, #67545, #67554, #67560~67562, #67567, #67573, #67581 • #67544, #67553, #67555, #67559, #67566, #67572, #67574, #67580 • Others 	C/D B A
II-h	SDB REF	Initial [Np] is reported to be 4.5×10^{-13} , 4.7×10^{-12} , 4.5×10^{-11} [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np is more than the initial concentration.	A
II-i	SDB	Separation method is filtration with 180 nm pore.	B
II-j	SDB	It is indicated that contact time was 3~4 hours. The time required for Np(V) sorption to reach equilibrium was determined by kinetic measurements from 1h to 96h.	A/B
II-k	REF	No information is reported.	C/D
II-l	SDB	Initial Np concentrations were changed.	B
II-m	REF	The experiments were carried out in polyethylene tube. Sorption onto vessel walls was not investigated.	B
II-n	REF	No error information is reported.	D
II-o	REF	This experiment is performed different liquid/solid ratio, initial Np concentration, and pH.	A

Data table Np/3: REF: Kohler et al.(1992)		
JAEA-SDB version 4.0 - DATA: Np/Other minerals; hematite #67990~68040		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint ¹	Evaluation	Rating
I-a.1 SDB	Separation is not completed.	No
I-a.2 SDB	Separation information is not completed.	No

Data table Np/4: REF: Kohler et al.(1992)		
JAEA-SDB version 4.0 - DATA: Np/Bentonite (Clay minerals); kaolinite #68041~68071		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint ¹	Evaluation	Rating
I-a.1 SDB	Separation is not completed.	No
I-a.2 SDB	Separation information is not completed.	No

Data table Np/5: REF: Turner et al. (1998)		
JAEA-SDB version 4.0 - DATA: Np/Bentonite (Clay Minerals), Na-montmorillonite #70110~70195		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	K_d values are taken from linear graphs.	class 3
II-a SDB	As solid phase Na-montmorillonite is indicated, characterized by XRD. CEC has not been determined.	A
II-b SDB REF	Indicated are final pH values. The pH was adjusted using HNO_3 , NaHCO_3 and NaOH .	A
II-c SDB REF	It is indicated that Np is in the oxidation state +V. It is reported that experiments were carried out under atmospheric, oxidizing conditions (with varying CO_2 levels). The presence of Np(V) was confirmed by UV-VIS-NIR spectrometry.	A/B
II-d SDB	It is indicated that experiments had been performed in 0.1 M NaNO_3 solution. Because the clay was in the Na-form and carbonate levels are known, the final concentration of all major components of the solution are determined.	A/B
II-e SDB	It is indicated that experiments had been performed at $20 \pm 2^\circ\text{C}$.	A/B
II-f SDB	The amount of solution and solid used in the experiments is indicated. About 0.1 [g] clay were used in the experiments, corresponding to about 10 [m^2] surface area.	A/B
II-g SDB	The %-sorbed can be calculated with K_d and L/S ratio: <ul style="list-style-type: none"> • #70110~70112, #70159, #70160, #70163, #70166~70168 • #70161, #70162, #70164 • Others 	B C/D A
II-h SDB REF	Initial Np concentrations of 8.79×10^{-7} , 9.25×10^{-7} and 9.46×10^{-7} [M] are indicated. It is stated that Np concentration low enough to avoid precipitation was used for experiments. This is corroborated by the sorption model, which can describe Np concentrations without invoking precipitation. Based on the solubility data by Yamaguchi et al. (1991), the following rating is given: <ul style="list-style-type: none"> • #70158 • #70133, #70134, #70156, #70157, #70177 • all other datapoints 	C/D B A
II-i SDB	Centrifugation is indicated (20 min at 10,000 [rpm])	C/D
II-j SDB REF	A contact time of 14 days is indicated. Previous kinetic experiments suggested that sorption reactions are almost complete within 48h. Reverse and forward experiments (pH-change) gave nearly identical results.	A/B

II-k	REF	Gyratory shakers, continuous shaking is reported.	A/B
II-l	REF	No sorption isotherm experiments are reported, batch experiments at nearly identical Np concentrations and L/S ratios.	C/D
II-m	REF	50 [mL] polycarbonate Oak Ridge-type centrifuge tubes were used. Additional tests to determine potential losses of Np to container walls were conducted, losses were found to be negligible.	A
II-n	SDB REF	It is indicated that there is no error information reported. Error bars are given, which appear to reflect only analytical error (counting statistics).	C
II-o	REF	The pH has been varied at three pCO ₂ levels.	B

3.2.6 Uranium

Data table U/1: REF: Bradbury and Baeyens (2003)			
JAEA-SDB version 4.0 - DATA: U/Bentonite (Clay Minerals); Na-montmorillonite(Swy-1) #70547~70579			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Data are taken from a log graph with K _d values.	class 5
II-a	SDB	Purified Na-SWy1 montmorillonite with determined mineralogical composition and characteristics was used for the experiments.	A
II-b	SDB	It is indicated that final pH-values were measured.	A
II-c	SDB	Experiments were carried out in CO ₂ -free conditions (presumably in an inert atmosphere). It is indicated that U is U(VI) in the reference.	A/B
II-d	SDB	0.01M and 0.1 M NaClO ₄ solution is indicated.	A/B
II-e	SDB	Temperature is not reported in the REF. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB	It is indicated that the amount solid added to reaction vessels is not known.	C/D
II-g	SDB	The sorption values can be calculated from K _d and L/S ratios, the following rating is given: <ul style="list-style-type: none"> • #70547~70550, #70562~70566, #70579 • #70560, #70561, #70567~70569 • #70551~70559, #70570~70578 	A B C/D
II-h	SDB	An initial U-concentration 1.4×10^{-7} [M] is indicated. Based on the experimental and thermodynamic data in Hummel et al. (2002), All datapoints are given A	A
II-i	SDB	Centrifugation 60 min at 95,000 [g] is indicated.	B
II-j	SDB	A contact time of 7 days is indicated.	C/D
II-k	REF	No information available. Assumed is shaking end-over-end, based on Baeyens and Bradbury (1997).	A/B
II-l	REF	No sorption isotherm experiments or variations of L/S are indicated.	C/D
II-m	REF	No information is available.	C/D
II-n	SDB REF	Error is indicated $\log K_d \pm 0.15$. An error of $\log K_d \pm 0.15$ is reported. Based on Baeyens and Bradbury (1997), it is assumed that this is derived based on error propagation estimates.	C
II-o	SDB	pH has been varied systematically.	C

Data table U/2: REF: Bradbury and Baeyens (2009b)			
JAEA-SDB version 4.0 - DATA: U/Bentonite (Clay Minerals); Na-illite, #71136~71188			
GUIDELINE: Revision 4b (May 19, 2005)			
REMARK : It is considered that this experiment procedure is a same with Bradbury and Baeyens (2009a).			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes

I-b	SDB	Data are taken from a log graph with K_d values.	class 5
II-a	SDB	Illite du Puy was conditioned to the homo-ionic Na-form with 1M-NaClO ₄ solution. XRD analysis showed the composition to be ~88 wt.% illite and ~12wt.% sanidine, a K-feldspar. The chemical composition is also shown in wt.%.	A
II-b	SDB REF	It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 2 to 11 with NaOH or HNO ₃ . In the pH range 4–9, 5 types of buffers at a concentration of 2 mM in order to ensure pH stability (Separate measurements showed no significant influence of the buffers on sorption in the range of experimental conditions)	A
II-c	SDB REF	Experiments were carried out in controlled N ₂ atmosphere glove boxes (CO ₂ <2 ppm, O ₂ <2 ppm). It is not used reducing agent. It is indicated that redox state of U is VI.	A/B
II-d	SDB REF	0.1M NaClO ₄ solution is indicated. Because purified Na-form illite is used under CO ₂ -free condition, the final solution composition is defined.	A/B
II-e	SDB	Temperature is not reported. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB	L/S value is indicated 2.6 [g/L], but volume of liquid and weight of solid is not reported.	C/D
II-g	SDB	The sorption values were calculated from K_d and L/S ratios, the following rating is given: <ul style="list-style-type: none"> • #71136, #71137, #71146~71148, #71169, #71170 • #71138~71145, #71151~71157, #71171 • Others 	B A C/D
II-h	SDB REF	An initial U-concentration is indicated $\sim 1 \times 10^{-7}$ M. Based on thermodynamic calculations using JAEA-TDB_100331c0.tdb: <ul style="list-style-type: none"> • #71162, #71163, #71177, #71178, #71183~71185 • #71164, #71179~71182 • Other data 	B unreliable A
II-i	SDB	Centrifugation 1 hour at 108,800 [g] is indicated.	B
II-j	SDB REF	A contact time of 7 days is indicated. Based on the sorption kinetics measured for Ni and Sn in Bradbury and Baeyens (2009a), it is considered to reach an equilibrium condition for U.	A/B
II-k	REF	It is indicated that samples were shaken end-over-end for at least 7 days.	A/B
II-l	REF	Sorption isotherm experiments are not carried out.	C/D
II-m	REF	Experimental vessel is 40-mL polypropylene centrifuge tube.	B
II-n	SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o	SDB	pH has been varied systematically.	B

Data table U/3: REF: Korichi and Bensmaili (2009)		
JAEA-SDB version 4.0 - DATA: U/Bentonite (Clay Minerals); Na-smectite, #71230~71493		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB A linear graph with adsorbed % is provided.	class 6
II-a	SDB The purified smectite has been obtained from unpurified bentonite (from Maghnia, west of Algeria). Particles for purified Na-smectite with diameter less than 2 μ m were obtained by sedimentation and saturated with Na ⁺ washing with NaCl solution. A CEC of 80 meq/100g and a BET surface area of 56.6 m ² /g are reported.	B
II-b	SDB REF It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 3 to 10 with 0.1M NaOH	A

		or HNO ₃ .	
II-c	SDB	Experiments were carried out under aerobic condition. It is indicated that U is U(VI) in the reference.	A/B
II-d	SDB	0.001M, 0.01M and 0.1 M NaNO ₃ solutions are indicated.	A/B
II-e	SDB	Temperature is room temperature.	A/B
II-f	SDB	It is investigated the influence of solid to liquid ratio. S/L ratio was varied from 0.2 to 4 [g/L], while keeping the volume of the uranium solution constant (50mL). <ul style="list-style-type: none"> • #71270~71278, #71282~71290, #71294~71302, #71306~71314 • Others 	C/D A/B
II-g	SDB	The following sorption values were calculated from K _d and L/S ratios: <ul style="list-style-type: none"> • #71230, #71231, #71240~71242, #71251, #71278~71281, #71291~71293, #71324, #71357, #71439, #71456 • #71232, #71233, #71250, #71260, #71277, #71290, #71303~71305, #71315~71317, #71323, #71335, #71373, #71390, #71406 • Others 	C/D B A
II-h	SDB	An initial U-concentration $4.2 \times 10^{-6} \sim 8.4 \times 10^{-5}$ [M] is indicated. Based on the thermodynamic calculation using JAEA-TDB, all data is given A.	A
II-i	SDB	Separation method is indicated as centrifugation and filtration.	A
II-j	SDB	A contact time of 0.45 hours~1 day is indicated. According to the figure, data of less than 15 hours is not equilibrated. <ul style="list-style-type: none"> • #71234~71239, #71243~71248, #71252~71257, #71261~71266 • Others 	unreliable A/B
II-k	REF	It is indicated that batch studies were carried out by shaking.	A/B
II-l	REF	Experiments were carried out as a function of initial U concentration (4.2×10^{-6} , 2.1×10^{-5} , 4.2×10^{-6} , and 8.4×10^{-5}).	B
II-m	REF	Experimental vessel is 250 mL Erlenmeyer flask. But material of flask is not reported, but maybe it is glass.	C/D
II-n	SDB	Error is not indicated	C
II-o	SDB	Initial U concentration, contact time, S/L, pH and ionic strength have been varied systematically. And influence of humic acid was investigated.	A

Data table U/4: REF: Missana et al. (2009b)

JAEA-SDB version 4.0 - DATA: U/Bentonite (Clay Minerals); Na-smectite, #70750~70862
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB Data are taken from a log graph with K _d values and sorbed concentration. <ul style="list-style-type: none"> • #70750~70791, #70834~70862 • #70792~70833 	class 5 class 6
II-a	SDB The smectite used in these experiments (FEBEX bentonite) comes from the Spanish deposit of Cortijo de Archidona. This clay contains mainly smectite (93%), with quartz (2%), plagioclase (3%), cristobalite (2%), potassium feldspar, calcite and trydimite as accessory minerals. The FEBEX clay was purified and homoionized in Na-form.	A
II-b	SDB REF It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 3 to 11 with 0.1M NaOH or HCl.	A
II-c	SDB Experiments were carried out under N ₂ atmosphere in an anoxic glove box. It is indicated that U is U(VI) in the reference.	A/B
II-d	SDB 0.003M, 0.01M, 0.05M and 0.1 M NaClO ₄ solutions are indicated.	A/B
II-e	SDB Temperature is room temperature (22±2°C).	A/B
II-f	SDB It is indicated that the hydrodynamic diameter of bentonite particle is around	C/D

		300 [nm]. L/S value is indicated, but volume of liquid and weight of solid is not reported.	
II-g	SDB	The following sorption values were calculated from K_d and L/S ratios: <ul style="list-style-type: none"> • #70775~70779, #70788 • #70754, #70761, #70768, #70769, #70774, #70780, #70781, #70827 • Others 	C/D B A
II-h	SDB	An initial U-concentration 4.4×10^{-7} [M] for sorption edges experiment and 1.0×10^{-8} to $\times 10^{-3}$ [M] for sorption isotherms experiment is indicated. Based on the thermodynamic calculations using JAEA-TDB, all data is given A.	A
II-i	SDB	Centrifugation 30 min at 645,000 [g] is indicated.	B
II-j	SDB	A contact time of 7 days is indicated.	C/D
II-k	REF	It is indicated that samples were maintained in continuous stirring.	A/B
II-l	REF	Sorption isotherm experiments are carried out.	A
II-m	REF	Experimental vessel is 12.5 mL ultracentrifuge tubes. But material of tube is not reported.	C/D
II-n	SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o	SDB	pH, ionic strength and initial U concentration have been varied systematically.	A

Data table U/5: REF: Pabalan et al.(1993)

JAEA-SDB version 4.0 - DATA: U/Other minerals; Na-clinoptilolite #68435~68508

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB Separation is not completed.	No
I-a.2	SDB Separation information is not completed.	No

Data table U/6: REF: Pabalan and Turner(1997)

JAEA-SDB version 4.0 - DATA: U/ Bentonite (Clay minerals); Na-SAz-1 montmorillonite #68509~68632

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	REF Data are taken from a log graph with K_d values.	class 5
II-a	SDB Ca-montmorillonite (SAz-1) was converted to the Na-form by contacting it with 2M NaCl. REF SAz-1 montmorillonite is well known clay.	A
II-b	SDB pH was adjusted with HNO_3 and NaHCO_3 . Final pH values are reported.	A
II-c	SDB Eh values are not reported. This experiment was performed under atmospheric pCO_2 . U(VI) is indicated for all tests. REF	A/B
II-d	SDB Solution used is 0.1M NaNO_3 and solid is purified Na-montmorillonite. The final solution composition can be estimated.	A/B
II-e	SDB Information about a temperature is not reported.	C/D
II-f	REF A liquid/solid ratio is varied 0.025 to 3.5 [g/L]. Particle size of montmorillonite is $< 2 \mu\text{m}$.	A/B
II-g	SDB The following sorption values were calculated from K_d and L/S ratios: <ul style="list-style-type: none"> • #68522~68527, #68531, #68532, #68546~68550, #68552~68555, #68575~68577, #68579, #68580, #68604, #68607, #68629, #68631 • #68521, #68528~68530, #68533, #68544, #68551, #68556, #68574, #68578, #68605, #68606, #68608~68610, #68630, #68632 • Others 	C/D B A
II-h	SDB Initial U concentrations are reported as 2.0×10^{-7} and 2.0×10^{-6} [M]. REF Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of U(VI) is above 1.0×10^{-7} [M].	A
II-i	SDB Information about a separation method is not reported.	C/D

	REF	It is considered that separation method in these experiments is a centrifugation, because centrifuge tubes were used in the experiments and other literatures by same group such as Turner et al. (1998) involved centrifuging.	
II-j	SDB	It is indicated that contact time was 10 days.	C/D
II-k	REF	Samples were agitated using a gyratory shaker.	A/B
II-l	SDB REF	Initial U concentration is varied (2.0×10^{-7} and 2.0×10^{-6} [M]). However sorption isotherm is not indicated.	B
II-m	REF	The experiments were carried out in Teflon-FEP (fluorinated ethylene propylene) centrifuge tubes. It is investigated about sorption competition between the mineral and container surface.	A
II-n	REF	Error bar is shown in the figures.	D
II-o	REF	Influences of initial U concentration, pH, liquid/solution ratio were investigated.	A

Data table U/7: REF: Prikryl et al.(1994)

JAEA-SDB version 4.0 - DATA: U/Other minerals; α -Al₂O₃#1, α -Al₂O₃#2, α -Al₂O₃#3 #68633 ~ #68741
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Linear graphs with adsorbed % are provided.	class 4
II-a	SDB	Sample used in this experiment is α -Al ₂ O ₃ issued by NIST.	A
II-b	SDB	pH was adjusted with HNO ₃ and NaHCO ₃ . Final pH values are reported.	A
II-c	SDB REF	This experiment was performed under aerobic condition. U(VI) is indicated for all tests.	A/B
II-d	REF	Initial solution is 0.1M NaNO ₃ and solid is pure α -Al ₂ O ₃ . The final solution composition can be estimated.	A/B
II-e	SDB	A temperature is not reported.	C/D
II-f	REF	A liquid/solid ratio of 400 [mL/g] is reported. 0.1 [g] solid was added to 40 [mL] solution. Particle size of basalt was not indicated.	A/B
II-g	SDB REF	The following sorption values were calculated from K _d and L/S ratios: • #68669~68677, #68700~68705, #68720~68724, #68741 • #68678, #68694~68699, #68706, #68719, #68725~68727, #68740 • Others	C/D B A
II-h	SDB REF	Initial U concentration is reported as 4.0×10^{-9} [M]. Based on thermodynamic calculations with PHREEQC (database : JNC-TDB 011213c2.tdb), all data is given A.	A
II-i	REF	Separation method is centrifugation (13,000 [rpm], 20 min).	B
II-j	REF	Kinetics sorption experiments (0.1~14 days) were performed.	A/B
II-k	REF	The agitation method is by a gyratory shaker.	A/B
II-l	REF	Initial U concentration is not varied.	C/D
II-m	REF	Teflon FEP centrifuge tube was used. Blank experiments were performed.	A
II-n	REF	Although the experiments were performed in duplicate, errors were not evaluated.	B
II-o	REF	Influences of pH, reaction time and surface area of solid were investigated.	B

Data table U/8: REF: Prikryl et al.(2001)

JAEA-SDB version 4.0 - DATA: U/Other minerals; quartz, Clin/Qtz(0.035), Clin/Qtz(0.35), Clin/Qtz(0.7), clinoptilolite #68742~68935
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Graphs with logarithmic K _d values are provided.	class 5
II-a	SDB	Samples used in this experiment are quartz and clinoptilolite. They were mixed	A

		with mass ratios (clinoptilolite to quartz) of 0.035, 0.35 and 0.7. Their surface areas are reported.	
II-b	SDB	pH was adjusted with HNO ₃ , NaHCO ₃ or NaOH. Final pH values are reported.	A
II-c	SDB REF	This experiment was performed under atmospheric pCO ₂ and controlled atmosphere glove box. U(VI) is indicated for all experimental conditions.	A/B
II-d	SDB	Initial solution is 0.1M NaNO ₃ , and solids are pure clinoptilolite and quartz. The final solution composition can be estimated.	A/B
II-e	SDB	A temperature is room temperature (22±2°C).	A/B
II-f	SDB REF	A liquid/solid ratio of 20~50 [mL/g] is reported. 1.035~1.7 [g] solid were added to 35 [mL] solution. Particle size of solids is not indicated.	C/D
II-g	SDB REF	The following sorption values were calculated from K _d and L/S ratios: <ul style="list-style-type: none"> • #68742, #68743, #68761, #68763, #68799~68801, #68820, #68821, #68842~68844, #68911, #68913 • #68744, #68760, #68762, #68764, #68765, #68782~68784, #68798, #68819, #68845~68848, #68864, #68926, #68934, #68935 • Others 	C/D B A
II-h	SDB REF	Initial U concentration is reported as 1.92×10 ⁻⁷ ~2.1×10 ⁻⁷ [M]. Based on thermodynamic calculations with PHREEQC (database : JNC-TDB_011213c2.tdb), all data is given A.	A
II-i	SDB REF	Information about separation method is not reported. It is considered that separation method in these experiments is a centrifugation, because centrifuge tubes were used in the experiments and other literatures by same group such as Turner et al. (1998) involved centrifuging.	C/D
II-j	SDB	It is indicated that equilibration time is 10 days.	C/D
II-k	REF	The agitation method is by a gyratory shaker.	A/B
II-l	SDB	No sorption isotherm and no variation of S/W ratio are reported.	C/D
II-m	REF	The experiments were done in polycarbonate centrifuge tubes.	B
II-n	REF	No information is reported.	D
II-o	REF	Influences of pH, pCO ₂ and mixing of minerals were investigated.	B

Data table U/9: REF: Turner et al.(1996)

JAEA-SDB version 4.0 - DATA: U/ Bentonite (Clay minerals); smectite #69951~70022

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Linear graphs with adsorbed % are provided.	class 4
II-a	SDB	Smectite sample is conditioned from clay-sized material (<2 μm) isolated from a shale-derived regolith, which underlies the Kenoma silt loam in eastern Kansas. Clay-sized fractions were separated by sedimentation from Na ⁺ -saturated material that had been sieved to <2 mm. The clay isolate was concentrated by flocculation with NaClO ₄ and then dialyzed against deionized water. The clay isolate was then treated to remove small amounts of Fe oxides and organic matter. Chemical formula, surface area, mean particle size and CEC are reported.	A
II-b	SDB	pH was adjusted upward with 0.1M NaOH. Final pH values are reported.	A
II-c	SDB REF	The experiments were performed under N ₂ atmosphere. U(VI) is relevant for all experimental conditions.	A/B
II-d	SDB	Solutions used in this experiments are NaClO ₄ (0.001M, 0.01M, 0.1M) and Ca(ClO ₄) ₂ (0.005M and 0.05M). Solid is an isolated/purified smectite. The final solution composition can be estimated approximately.	A/B
II-e	SDB	A temperature was at 25°C.	A/B
II-f	SDB	A solid/liquid ratio of 1.5 [g/L] is reported.	A/B
II-g	SDB	The %-sorbed can be calculated with K _d and L/S ratio:	

REF		<ul style="list-style-type: none"> • #69974~69977, #69989~69992, #70002~70008, #70017~70022 • #69951~69954, #69960~69962, #69965~69972, #69981~69986, #69993~69999, #70009~70015 • Others 	C/D B A
II-h	SDB REF	Initial U concentration is reported as 8.5×10^{-6} [M]. Based on the thermodynamic calculations using JAEA-TDB(100331c0.tdb), all data is given A.	A
II-i	SDB	Separation method is a centrifugation (26,895 [g] for 30 min).	C/D
II-j	SDB	It is indicated that contact time was 1 day.	C/D
II-k	REF	No information about agitation method is reported.	C/D
II-l	SDB	Initial U concentration is not varied.	C/D
II-m	REF	Reaction vessel of this experiment is 50 [mL] polycarbonate centrifuge tube.	B
II-n	REF	This is carried out a duplicate experiment.	A
II-o	REF	pH and electrolyte concentration are varied.	A

Data table U/10: REF: Turner et al.(1996)

JAEA-SDB version 4.0 - DATA: U/ Other minerals; gibbsite, quartz #70023~70109

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Linear graphs with adsorbed % are provided.	class 4
II-a	SDB	Solids are gibbsite and quartz. It is considered that these solids are single pure minerals. Solids are measured surface area.	A
II-b	SDB	pH was adjusted. Final pH values are reported.	A
II-c	SDB REF	An atmosphere of this experiment is reported N ₂ condition. U(IV) is not sensitive to redox condition.	A/B
II-d	SDB	NaClO ₄ (0.001M, 0.1M) is used in this experiment. Solids are single pure minerals. So, it is possible to predicted final solution composition.	A/B
II-e	SDB	A temperature was carried out at 25°C.	A/B
II-f	SDB	A solid/liquid ratio of 0.013~5.74 [g/L] is reported.	A/B
II-g	SDB REF	The %-sorbed can be calculated with K _d and L/S ratio: <ul style="list-style-type: none"> • #70029~70039, #70046~70053, #70078, #70080~70082, #70092, #70098, #70099 • #70027, #70028, #70054, #70065, #70074~70076, #70079, #70083, #70093~70097 • Others 	C/D B A
II-h	SDB REF	Initial U is reported 8.5×10^{-6} [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), in the case of gibbsite, solubility of U is more than initial concentration at 3<pH<4. In the case of quartz, solubility of U is more than initial concentration at 3<pH<4 in 0.001M NaClO ₄ solution, and at 3<pH<5 in 0.1M NaClO ₄ solution. <ul style="list-style-type: none"> • #70066, #70067, #70083~70087 • Others 	A unreliable
II-i	SDB	Separation method is a centrifugation (26,895 [g] for 30 min).	C/D
II-j	SDB	It is indicated that contact time was 1 day.	C/D
II-k	REF	No information about agitation method is reported.	C/D
II-l	SDB	Initial U concentration is not varied.	C/D
II-m	REF	Reaction vessel of this experiment is 50 [mL] polycarbonate centrifuge tube.	B
II-n	REF	This is carried out a duplicate experiment.	A
II-o	REF	pH and electrolyte concentration are varied.	A

Data table U/11: REF: Waite et al.(1994)		
JAEA-SDB version 4.0 - DATA: U/ Other minerals; ferrihydrite #70196~70398		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	REF Linear graphs with adsorbed % are provided.	class 4
II-a	SDB Solid is ferrihydrite. Ferrihydrite is a microcrystalline hydrous Fe oxide that may exhibit a number of different crystalline phases with a stoichiometry near $\text{Fe}_2\text{O}_3 \cdot \text{H}_2\text{O}$.	A
II-b	SDB pH was adjusted. Final pH values are reported.	A
II-c	SDB The experiments were performed under atmospheric conditions, and in a glove box at an elevated partial pressure of carbon dioxide. The gas composition used in the glovebox was a 50:50 mixture of ordinary air with a 2% CO_2 / REF 98% N_2 special gas mixture,	A/B
II-d	SDB Solutions used is NaNO_3 (0.004M, 0.02M, 0.1M and 0.5M), and solid is pure ferrihydrite . The final solution composition can be estimated approximately.	A/B
II-e	SDB It is indicated that experiments had been performed at 25°C.	A/B
II-f	SDB A solid/liquid ratio is reported as total Fe concentration (10^{-3}M).	C/D
II-g	SDB REF The %-sorbed can be calculated with K_d and L/S ratio: <ul style="list-style-type: none"> • #70213, #70219, #70232, #70242~70247, #70255, #70283~70288, #70293, #700295, #70296, #70301~70305, #70322~ 70324, #70331, #70339, #70341, #70355, #70366~70372, #70380, #70382, #70383, #70389, #70390, #70394~70398 • #70220, #70225, #70241, #70248, #70256~70258, #70273, #70282, #70289, #70290, #70294, #70300, #70306, #70313, #70314, #70321, #70325~70328, #70340, #70342, #70348, #70349, #70354, #70356, #70365, #70373, #70381, #70384, #70387, #70391 • Others 	C/D B A
II-h	SDB REF Initial U concentration is reported as $1.0 \times 10^{-8} \sim 1.0 \times 10^{-4}$ [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), all data is given A.	A
II-i	SDB Separation method is a centrifugation.	C/D
II-j	SDB It is indicated that contact time was usually 2 days. And influence of reaction time is investigated.	A/B
II-k	REF No information about agitation method is reported.	C/D
II-l	SDB Initial U concentration is varied. However, sorption isotherm is not calculated.	B
II-m	REF Reaction vessel of this experiment is polypropylene centrifuge tube.	B
II-n	REF No information is reported.	D
II-o	REF This experiment is investigated an influence of reaction time, pH, initial U concentration, solid/solution ratio, pCO_2 concentration and electrolyte concentration.	A

3.2.7 Selenium

Data table Se/1: REF: Balistreri and Chao(1987)		
JAEA-SDB version 4.0 - DATA: Se/Other minerals; goethite #66924~67049		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	REF A linear graph with % sorbed is given.	class 4
II-a	SDB Goethite ($\alpha\text{-FeOOH}$) was synthetically prepared according to the procedure of Atkinson et al.(1967).	A
II-b	SDB pH was adjusted with 0.1M KOH and 0.1M HCl. Final pH is reported.	A

II-c	SDB REF	The experiments were conducted under normal atmospheric conditions. Preliminary experiments indicated that dissolved selenite and selenate in a 0.1M KCl solution did not change oxidation states over the 24-h time period of the experiments	A/B
II-d	SDB	Test solution is 0.1M KCl and Solid is synthetic goethite. Final solution composition can be defined.	A/B
II-e	SDB	Experiments were carried out at 22.5°C (room temperature) or 32.5°C(water bath).	A/B
II-f	SDB	A liquid/solid ratio of 3~300 [mg/L] is reported. Surface area of goethite is 49.2 [m ² /g].	A/B
II-g	SDB REF	The following sorption values were evaluated from figure: <ul style="list-style-type: none"> • #66924~66926, #66928~66930, #66932, #66933, #66959, #66970~66975, #66991~66998, #67002, #67011, #67020~67024, #67037~67039 • #66927, #66931, #66943, #66958, #66969, #66976, #66990, #66999, #67025, #67040~67042 • Others 	C/D B A
II-h	SDB REF	Initial [Se] is reported 0.02~5×10 ⁻⁵ [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Se is above initial [Se].	A
II-i	SDB	Separation method is centrifugation at 15,000 [g] for 10 min.	C/D
II-j	SDB	Contact time was 24 hour.	C/D
II-k	REF	The sample was periodically shaken to ensure mixing.	A/B
II-l	SDB	Initial Se concentration and L/S ratio were varied systematically.	B
II-m	REF	The experiments were carried out in Pyrex Erlenmeyer flasks.	C/D
II-n	REF	No information is reported.	D
II-o	REF	The initial Se concentration, pH and Liquid /Solid ratio is varied.	A

Data table Se/2: REF: Balistrieri and Chao(1990)			
JAEA-SDB version 4.0 - DATA: Se/Other minerals; Fe oxyhydroxide, Mn dioxide #67050~67139			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	A linear graph with % sorbed is given.	class 4
II-a	SDB	Amorphous iron oxyhydroxide was freshly prepared for each set of experiments according to the method of Davis and Leckie(1978) and Benjamin and Leckie(1981). Hydrous manganese dioxide was prepared according to the procedures given in the papers of Morgan and Stumm(1964) and Murray(1975).	A
II-b	SDB	pH was adjusted with 0.1M KOH and 0.1M HCl. Final pH is reported.	A
II-c	SDB REF	The experiments were conducted under normal atmospheric conditions. Preliminary experiments indicated that dissolved selenite and selenate in a 0.1M KCl solution did not change oxidation states over the 24-h time period of the experiments, as given in Balistrieri and Chao(1987)	A/B
II-d	SDB REF	A 0.1M KCl solution is indicated. Because pure minerals are used, the final solution composition is defined.	A/B
II-e	SDB	Experiments were carried out at 22.5°C (room temperature) or 32.5°C(water bath).	A/B
II-f	SDB	Liquid/solid ratios between - 300 [mg/L] is reported. Surface area of Fe oxyhydroxide and Mn dioxide is 600 and 290 [m ² /g], respectively.	A/B
II-g	SDB REF	The following sorption values were evaluated from figure: <ul style="list-style-type: none"> • #67057, #67058, #67068~67072, #67081~67085, #67092~67117, #67119, #67129 • #67056, #67067, #67118, #67127, #67128, #67130 • Others 	C/D B A

II-h	SDB REF	Initial Se is reported $6.5 \times 10^{-7} \sim 7.1 \times 10^{-7}$ [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Se is above initial [Se].	A
II-i	SDB	Separation method is filtration through 0.45 μm Millipore filters.	C/D
II-j	SDB	It is indicated that contact time was 24 hour.	C/D
II-k	REF	The sample was periodically shaken to ensure mixing.	A/B
II-l	SDB	Initial Se concentration and L/S ratio were varied systematically.	C/D
II-m	REF	The experiments were carried out in Pyrex Erlenmeyer flasks.	C/D
II-n	REF	No information is reported.	D
II-o	REF	pH and liquid/solid ratio were varied.	A

Data table Se/3: REF: Ghosh et al.(1994)			
JAEA-SDB version 4.0 - DATA: Se/Other minerals; Alumina #67450~67537			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Linear graph % sorbed is given.	class 4
II-a	SDB	Samples used in this experiment are 92% pure $\gamma\text{-Al}_2\text{O}_3$.	A
II-b	SDB	pH was adjusted with 1M HCl and 1M NaOH. Final pH values are reported.	A
II-c	SDB REF	No information about experimental atmosphere is indicated. Se(IV) and Se(VI) are analyzed by AAS and hydride reduction.	A/B
II-d	SDB	Solution used in this experiment is 0.1M NaCl. Solid is 92% pure $\gamma\text{-Al}_2\text{O}_3$. Final solution compositions can be defined.	A/B
II-e	SDB	A temperature is ambient temperature 20°C.	A/B
II-f	SDB	A solid/liquid ratio of 3.3 and 1 [g/L] is reported. No other information is indicated.	C/D
II-g	SDB REF	The sorption values were calculated from K_d and L/S ratios, the rating is given: <ul style="list-style-type: none"> • #67450, #67451, #67454, #67462, #67499~67503, #67523~67525 • #67456, #67459~67461, #67463, #67464, #67475, #67480, #67491~67493, #67498, #67505, #67518~67522, #67528, #67529, #67533, #67537 • Others 	C/D B A
II-h	SDB REF	Initial Se concentration is reported to be $1.27 \times 10^{-6} \sim 8.62 \times 10^{-4}$ [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Se is more than 1.42×10^{-4} [M].	A
II-i	SDB	Separation method is 0.45 μm filtration.	B
II-j	SDB	It is indicated that contact time was 2 days. It is confirmed that equilibrium can be reached from kinetic experiments.	A/B
II-k	REF	Agitation method is continuously shaken by the shaker.	A/B
II-l	SDB	Initial Se concentrations are varied.	B
II-m	REF	The experiments were carried out in glass bottles. Vessel wall sorption is not investigated.	C/D
II-n	REF	No error information is reported.	D
II-o	REF	This experiment is performed at different liquid/solid ratio, initial Se concentration, SO_4^{2-} concentration and pH.	A

Data table Se/4: REF: Goldberg and Glaubig(1988)			
JAEA-SDB version 4.0 - DATA: Se/Bentonite (Clay Minerals); Ca-montmorillonite #67582~67605, Kaolinite, #67606~67620			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes

I-b	SDB REF	It is indicated that adsorption values are taken from a figure. A linear graph with adsorbed values is provided.	class 4
II-a	SDB	Ca-montmorillonite and kaolinite are indicated as solid phases. Specific surface area is given, but no CEC or other characteristics. The specific materials are Ca-SAz-1 montmorillonite and KGa-2 kaolinite. The montmorillonite sample is reported to contain 27% clay, the kaolinite to contain 60% clay. The mineralogy of the remainder is not specified. Both materials were used without pretreatment.	B
II-b	SDB	pH values measured at the end of the experiments are indicated.	A
II-c	SDB REF	It is indicated that experiments with Se(IV) were performed under air. Se is redox sensitive, no oxidizing or reducing agents had been added to the reaction mixture. No oxidation or reduction has been observed under the used experimental conditions (oxidation state-specific analysis by hydride generation). Se(IV) is typically stable under ambient conditions.	A/B
II-d	SDB REF	It is indicated that experiments had been performed in 0.1 M NaCl solutions. Final solution composition is not indicated. In case of Ca-montmorillonite, kaolinite, the final solution composition can be estimated approximately.	C/D
II-e	SDB	It is indicated that experiments had been performed at 23±1°C.	A/B
II-f	SDB	The amounts of solution and solid are indicated as 30 [mL] and 1.2 [g], respectively. This corresponds to > 20 [m ²] sorbent surface area per vessel.	A/B
II-g	SDB	The following sorption values were calculated from K _d and L/S ratios: • #67582~67616 • #67617~67620	A B
II-h	SDB REF	Initial Se concentration is indicated as 1.9×10 ⁻⁵ [M]. Reportedly thermodynamic calculations showed that the experimental systems were orders of magnitude undersaturated with respect to Ca- and Fe-selenite.	A
II-i	SDB	Centrifugation (20 min at 10,000 [rpm]) is indicated.	C/D
II-j	SDB REF	A contact time of 2h is indicated. It is reported that independent experiments had shown this to be sufficient.	A/B
II-k	REF	Reciprocating shaker, continuous shaking.	A/B
II-l	REF	No sorption isotherm and no variation of L/S ratio are reported.	C/D
II-m	REF	Experiments were done in polypropylene centrifuge tubes. No correction for sorption on vessel walls was used.	B
II-n	REF	There is no error information reported.	D
II-o	REF	pH had been varied systematically.	C

Data table Se/5: REF: Goldberg and Glaubig(1988)

JAEA-SDB version 4.0 - DATA: Se/Other minerals; calcite #67621~67635

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB REF It is indicated that adsorption values are taken from a figure. A linear graph with adsorbed values is provided.	class 4
II-a	SDB The CaCO ₃ was identified as calcite using x-ray diffraction analysis. Specific surface area of the calcite was 12.1 [m ² /g].	A
II-b	SDB pH values measured at the end of the experiments are indicated.	A
II-c	SDB REF It is indicated that experiments with Se(IV) were performed under air. Se is redox sensitive, no oxidizing or reducing agents had been added to the reaction mixture. No oxidation or reduction has been observed under the used experimental conditions (oxidation state-specific analysis by hydride generation). Se(IV) is typically stable under ambient conditions.	A/B
II-d	SDB REF It is indicated that experiments had been performed in 0.1 M NaCl solutions. Final solution composition is not indicated. In case of calcite, the final solution composition can be estimated approximately.	C/D

II-e	SDB	It is indicated that experiments had been performed at 23±1°C.	A/B
II-f	SDB	The amounts of solution and solid are indicated as 30 [mL] and 1.2 [g], respectively. This corresponds to > 20 [m ²] sorbent surface area per vessel.	A/B
II-g	SDB	The following sorption values were calculated from K _d and L/S ratios: All data is 5%<sorption values<95%	A
II-h	SDB REF	Initial Se concentrations are indicated as 1.9×10 ⁻⁵ [M]. Reportedly thermodynamic calculations showed that the experimental systems were orders of magnitude undersaturated with respect to Ca- and Fe-selenite.	A
II-i	SDB	Centrifugation (20 min at 10,000 [rpm]) is indicated.	C/D
II-j	SDB REF	A contact time of 2h is indicated. It is reported that independent experiments had shown this to be sufficient.	A/B
II-k	REF	Reciprocating shaker, continuous shaking.	A/B
II-l	REF	No sorption isotherm and no variation of L/S ratio are reported.	C/D
II-m	REF	Experiments were done in polypropylene centrifuge tubes. No correction for sorption on vessel walls was used.	B
II-n	REF	There is no error information reported.	D
II-o	REF	pH had been varied systematically.	C

Data table Se/6: REF: Goldberg and Glaubig(1988)

JAEA-SDB version 4.0 - DATA: Se/Mudstone (Sedimentary rocks); imperial soil#1, imperial soil#2, imperial soil#3 #67636~67750

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB REF It is indicated that adsorption values are taken from a figure. A linear graph with adsorbed values is provided.	class 4
II-a	SDB The <2[mm] fraction of imperial soil was used. It contained 44% clay as determined using the hydrometer method. Specific surface area was found to be 36.1[m ² /g]. imperial soil#1 are untreated soil. imperial soil#2 are treated to remove calcite. imperial soil#3 are in the presence of arsenate.	C/D
II-b	SDB pH values measured at the end of the experiments are indicated.	A
II-c	SDB REF It is indicated that experiments with Se(IV) were performed under air. Se is redox sensitive, no oxidizing or reducing agents had been added to the reaction mixture. No oxidation or reduction has been observed under the used experimental conditions (oxidation state-specific analysis by hydride generation). Se(IV) is typically stable under ambient conditions.	A/B
II-d	SDB REF It is indicated that experiments had been performed in 0.1 M NaCl solutions. Final solution composition is not indicated. The final solution composition can be estimated approximately.	C/D
II-e	SDB It is indicated that experiments had been performed at 23±1°C.	A/B
II-f	SDB The amounts of solution and solid are indicated as 30 [mL] and 1.2 [g], respectively. This corresponds to > 20 [m ²] sorbent surface area per vessel.	A/B
II-g	SDB The following sorption values were calculated from K _d and L/S ratios: All data is 2%>sorption values	C/D
II-h	SDB REF Initial Se concentrations are indicated as 1.9×10 ⁻⁵ [M]. Reportedly thermodynamic calculations showed that the experimental systems were orders of magnitude undersaturated with respect to Ca- and Fe-selenite.	A
II-i	SDB Centrifugation (20 min at 10,000 [rpm]) is indicated.	C/D
II-j	SDB REF A contact time of 2h is indicated. It is reported that independent experiments had shown this to be sufficient.	A/B
II-k	REF Reciprocating shaker, continuous shaking.	A/B
II-l	REF No sorption isotherm and no variation of L/S ratio are reported.	C/D

II-m	REF	Experiments were done in polypropylene centrifuge tubes. No correction for sorption on vessel walls was used.	B
II-n	REF	There is no error information reported.	D
II-o	REF	pH had been varied systematically.	C

Data table Se/7: REF: Lauber et al. (2000)			
JAEA-SDB version 4.0 - DATA: Se/Bentonite (Clay Minerals); Opalinus Clay #68374~68434			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Graphs with logarithmic K_d values are provided.	class 5
II-a	SDB	As solid phase Opalinus Clay (and CEC) is indicated. A detailed analysis of Opalinus Clay is available.	A
II-b	SDB REF	It is indicated that initial pH values is provided. The samples were pre-conditioned; therefore, it is assumed that initial and final pH is nearly identical. Further, the solution is well buffered.	A
II-c	SDB REF	It is indicated that experiments had been conducted under a nitrogen atmosphere. No addition of oxidizing or reducing agents is indicated. The experiments at pH 6.3 were actually carried out in a CO ₂ /N ₂ atmosphere. Se is redox sensitive, it is indicated in the REF that Se(0) may be present in the system in addition to Se(IV) UNRELIABLE, NO FURTHER EVALUATION	unreliable

Data table Se/8: REF: Missana et al. (2009a)			
JAEA-SDB version 4.0 - DATA: Se/Bentonite (Clay Minerals); Na-smectite, Na-illite, 70%-smectite/30%-illite, 43%-smectite/57%-illite #70580~70749			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Graphs with K_d values are provided.	class 5
II-a	SDB	The smectite clay (FEBEX bentonite) mined at the Cortijo de Archidona(Spain), has a high smectite content(93%). Accessory minerals are: quartz , plagioclase, feldspar, calcite, and tridymite. Its CEC is 102 meq/100g and BET SA is 33 m ² /g. These natural clays were washed three times with 1M NaClO ₄ to eliminate all the soluble salts and to obtain the homoionic Na-form. The "as-received" illite (Illite du Puy) comes from the region of Le Puy-en-Velay (France); it contains 74% illite and kaolinite, 20% calcite and 5% quartz. After the purification and homoionisation process, this clay has a small percentage of kaolinite (7%) but high illite content (93%). Its CEC is 22.5 meq/100g and BET SA is 97 m ² /g..	A
II-b	SDB REF	It is indicated that final pH values is provided. Kinetic tests were carried out at pH 5~6. Sorption edges were measured by varying the pH of the suspensions from pH 3 to 11 with NaOH or HCl 0.1 or 1M. Sorption isotherms were obtained at a fixed pH.	A
II-c	SDB REF	It is indicated that experiments were carried out under atmospheric condition. It is indicated that valence of Se is +IV, calculating Se speciation.	A/B
II-d	SDB REF	It is indicated that experiments had been performed in 0.001~0.5M NaClO ₄ . Final solution composition is not indicated. The clays were homo-ionic (see II-a). The final solution composition can be estimated.	A/B
II-e	SDB	It is indicated that no temperature is given.	C/D
II-f	SDB	The solution/solid ratio is indicated. Actual solution volume and solid weight	A/B

	REF	are not given. The N ₂ -BET surface area of smectite and are 33[m ² /g] and 97[m ² /g], respectively.	
II-g	REF	The following sorption values were calculated from K _d and L/S ratios: <ul style="list-style-type: none"> • #70685, #70703 • #70596, #70597, #70599, #70613~70616, #70623~70625, #70668~70670, #70672, #70674, #70678~70684, #70686, #70688, #70690~70702, #70705~70709, #70717~70719, #70722~70725, #70727, #70730, #70731, #70734, #70735, #70740 • Others 	C/D B A
II-h	SDB REF	Initial Se concentrations for kinetic tests and sorption edge are 1×10 ⁻¹⁰ and 4×10 ⁻¹⁰ [M], respectively. Sorption isotherms are obtained by varying the radionuclide concentration 1×10 ⁻¹⁰ ~1×10 ⁻³ [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb); <ul style="list-style-type: none"> • #70669, #70724, #70725, #70735 • #70646, #70647, #70657, #70658, #70668, #70723, #70734 • Others 	unreliable B A
II-i	SDB	Centrifugation (30 min at 694,000 [g]) is indicated.	B
II-j	SDB	Kinetic tests indicated that K _d for both clays reaches a nearly constant value after 4 or 5 days. <ul style="list-style-type: none"> • #70624~70628, #70709~70711 • Others 	unreliable A/B
II-k	REF	Information about agitation method is not reported.	C/D
II-l	REF	Sorption isotherm experiments were carried out, at high and low Se concentration.	A
II-m	REF	Polyallomere Beckman Quick-Seal ultracentrifuge tubes were used (material not specified). Wall sorption was not considered (experiments in similar systems had suggested only a small potential effect).	A
II-n	REF	It is indicated that no error information is reported. For almost data points, error bars are given which were derived from error propagation.	C
II-o	REF	Ionic strength, contact time, pH and Se-concentration were varied.	A

3.2.8 Others

Data table Ca/1: REF: Baeyens and Bradbury(1995)			
JAEA-SDB version 4.0 - DATA: Ca/Bentonite (Clay minerals); Na-montmorillonite #66858~66923			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Log K _d from figure is given.	class 5
II-a	SDB REF	SWy-1 montmorillonite is used in this experiment. It was converted to homo-ionic Na-form with 1.0M NaClO ₄ . Mineralogical composition, CEC and BET surface area for SWy-1 Na-montmorillonite and conditioned Na-montmorillonite were reported.	A
II-b	SDB	pH was adjusted with NaOH and HNO ₃ . Final pH values are reported.	A
II-c	SDB	This experiment is performed under N ₂ atmosphere. Ca is not sensitive to redox condition.	A/B
II-d	SDB REF	A 0.1 M NaClO ₄ solution is indicated. Because highly purified Na-form montmorillonite is used under CO ₂ -free condition, the final solution composition is defined.	C/D
II-e	SDB	Temperature is not reported in the REF. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB	A solid/liquid ratio of 1.14 [g/L] is reported.	C/D

	REF	BET surface area of conditioned Na-montmorillonite is 35 [m ² /g].	
II-g	SDB REF	The following sorption values were calculated from K _d and L/S ratios: All data are within 5~95%.	A
II-h	SDB REF	Initial Ca concentration is reported as 1.14×10 ⁻⁶ [M]. This is estimated to be significantly below the solubility of Ca.	A
II-i	SDB	Separation method is centrifugation at 95,000 [g] for one hour.	C/D
II-j	SDB	Contact periods of 1, 3, 7 and 21 days are indicated.	C/D
II-k	REF	Agitation method is shaking end-over-end.	A/B
II-l	SDB	No sorption isotherm experiments or variations of S/L are indicated.	A
II-m	REF	Polypropylene centrifuge tube is used in the experiment. It is considered that the normal method of measuring wall sorption in blank experiments.	A
II-n	REF	Error is not reported. And it is not replicated.	D
II-o	REF	pH and electrolyte concentration has been varied systematically.	A

Data table Sr/1: REF: Lauber et al. (2000)			
JAEA-SDB version 4.0 - DATA: Sr/Bentonite (Clay Minerals); Opalinus Clay #68133~68144			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Table with logarithmic K _d values are provided.	class 2
II-a	SDB	As solid phase Opalinus Clay (and CEC) is indicated. A detailed analysis of Opalinus Clay is available.	A
II-b	SDB REF	It is indicated that initial pH values are provided. The samples were pre-conditioned; therefore, it is assumed that initial and final pH is nearly identical. Further, the solution is well buffered.	A
II-c	SDB	It is indicated that experiments had been conducted under a nitrogen atmosphere. No addition of oxidizing or reducing agents is indicated. The experiments at pH 6.3 were carried out in a CO ₂ /N ₂ atmosphere, pH 7.7 were carried out in a N ₂ atmosphere. Sr is not redox sensitive.	A/B
II-d	SDB REF	It is indicated that experiments had been performed in synthetic porewater solution, composition is given. Final solution composition is not indicated. Clay samples were pre-conditioned. The composition of the conditioned solutions was determined.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25°C.	A/B
II-f	SDB REF	The solution/solid ratio is indicated. Actual solution volume and solid weight are not given. The Specific surface area of Opalinus Clay is reported as 33.3 [m ² /g]. Experiments were done in 40 [mL] centrifuge tubes. This results in about 8 [m ²] of sorbent surface per vial.	A/B
II-g	REF	The following sorption values were calculated from K _d and L/S ratios. Adsorption % of all datapoints are 5~95%.	A
II-h	SDB REF	Initial Sr concentrations of 2.2×10 ⁻⁴ and 2.6×10 ⁻⁴ M are indicated. Measurements were carried out at fixed concentrations in the OPA porewaters which were determined via saturation with respect to the solid phase celestite (SrSO ₄). It cannot be excluded that the added Sr tracer was also taken up by isotopic exchange in addition to sorption. Conservatively, the data are therefore rated unreliable. NO FURTHER EVALUATION	unreliable

Data table Co/1: REF: Bradbury and Baeyens (2009a)			
JAEA-SDB version 4.0 - DATA: Co/Bentonite (Clay Minerals); Na-illite, #70954~70974			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes

I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Data are taken from a log graph with K_d values.	class 5
II-a	SDB	Illite du Puy was conditioned to the homo-ionic Na-form with 1M- NaClO_4 solution. XRD analysis showed the composition to be ~ 88 wt.% illite and ~ 12 wt.% sanidine, a K-feldspar. The chemical composition is also shown in wt.%.	A
II-b	SDB REF	It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 2 to 11 with NaOH or HNO_3 . In the pH range 4–9, 5 types of buffers at a concentration of 2 mM in order to ensure pH stability (Separate measurements showed no significant influence of the buffers on sorption in the range of experimental conditions)	A
II-c	SDB REF	Experiments were carried out in controlled N_2 atmosphere glove boxes ($\text{CO}_2 < 2$ ppm, $\text{O}_2 < 2$ ppm). It is not used reducing agent. Co is not sensitive to redox condition.	A/B
II-d	SDB REF	0.1M NaClO_4 solution is indicated. Because purified Na-form illite is used under CO_2 -free condition, the final solution composition is defined.	A/B
II-e	SDB	Temperature is not reported. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB	L/S value is indicated 1.6 [g/L], but volume of liquid and weight of solid is not reported.	C/D
II-g	SDB	The sorption values were calculated from K_d and L/S ratios, the following rating is given: <ul style="list-style-type: none"> • #70968, #70969 • #70970~70974 • Others 	B C/D A
II-h	SDB REF	An initial Co-concentration is indicated 1×10^{-10} M. Based on the thermodynamic calculations using JAEA TDB(100331c0.tdb), all data is given A.	A
II-i	SDB	Centrifugation 1 hour at 108,800 [g] is indicated.	B
II-j	SDB REF	A contact time of 7 days is indicated. Because Ni and Sn are reached an equilibrium condition for 7 days, it is considered to reach an equilibrium condition for Co.	A/B
II-k	REF	It is indicated that samples were shaken end-over-end for at least 7 days.	A/B
II-l	REF	Sorption isotherm experiments are not carried out.	C/D
II-m	REF	Experimental vessel is 40-mL polypropylene centrifuge tube.	B
II-n	SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o	SDB	pH has been varied systematically.	B

Data table Co/2: REF: Ikhsan et al.(1999)			
JAEA-SDB version 4.0 - DATA: Co/Bentonite (Clay minerals); kaolinite #67907~67946			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint	Evaluation		Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	A linear graph with adsorbed % and adsorbed concentration is provided.	class 4
II-a	SDB	It was indicated that XRD analysis showed a standard kaolinite pattern with no contaminant lines.	A
II-b	SDB	pH was adjusted with 0.1M HNO_3 and 0.1M KOH. Final pH values are reported.	A
II-c	SDB REF	It is investigated Co(II) sorption under N_2 atmosphere condition. Co(II) is not sensitive redox condition.	A/B
II-d	SDB	Solution used is 0.005M KNO_3 and solid is pure kaolinite. The final solution composition can be estimated approximately.	A/B
II-e	SDB	A temperature is 25°C.	A/B

II-f	SDB	A solid /liquid ratio of 6.789 [g/L] is reported. No other information is indicated.	C/D
II-g	SDB	The following sorption values were calculated from K_d and L/S ratios:	C/D
	REF	• #67907 • Others	A
II-h	SDB	Initial Co concentration is reported to be 1.0×10^{-4} [M]. It is assumed that solubility of Co is more than 1.0×10^{-4} [M] like Pb, Cu and Zn.	A
II-i	SDB	Separation method is used 0.2 μ m Poretics polycarbonate membrane filters.	B
II-j	SDB	It is indicated that equilibration time is 30 minutes.	C/D
II-k	REF	No information is reported.	C/D
II-l	SDB	Initial Co concentration is varied from 1.0×10^{-6} to 1.0×10^{-4} [M]. Sorption isotherm is determined.	A
II-m	REF	No information is reported.	C/D
II-n	REF	No error information is reported.	D
II-o	REF	pH and initial Co concentration are varied systematically.	A

Data table Zn/1: REF: Ikhsan et al.(1999)

JAEA-SDB version 4.0 - DATA: Zn/Bentonite (Clay minerals); kaolinite #67865~67906

UIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	A linear graph with adsorbed % and adsorbed concentration is provided.	class 4
II-a	SDB	It was indicated that XRD analysis showed a standard kaolinite pattern with no contaminant lines.	A
II-b	SDB	pH was adjusted with 0.1M HNO ₃ and 0.1M KOH. Final pH values are reported.	A
II-c	SDB REF	It is investigated Zn(II) sorption under N ₂ atmosphere condition. Zn(II) is not sensitive redox condition.	A/B
II-d	SDB	Solution used is 0.005M KNO ₃ and solid is pure kaolinite. The final solution composition can be estimated approximately.	A/B
II-e	SDB	A temperature is 25°C.	A/B
II-f	SDB	A solid /liquid ratio of 6.789 [g/L] is reported. No other information is indicated.	C/D
II-g	SDB	The following sorption values were calculated from K_d and L/S ratios:	C/D
	REF	• #67865, #67885, #67886 • #67883, #67884 • Others	B A
II-h	SDB REF	Initial Zn is reported 1.0×10^{-4} [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Zn is more than 1.0×10^{-4} [M].	A
II-i	SDB	Separation method is used 0.2 μ m Poretics polycarbonate membrane filters.	B
II-j	SDB	It is indicated that equilibration time is 30 minutes.	C/D
II-k	REF	No information is reported.	C/D
II-l	SDB	Initial Zn concentration is varied from 1.0×10^{-6} to 1.0×10^{-4} [M]. Sorption isotherm is determined.	A
II-m	REF	No information is reported.	C/D
II-n	REF	No error information is reported.	D
II-o	REF	pH and initial Zn concentration are varied systematically.	A

Data table Zn/2: REF: Srivastave et al.(2005)

JAEA-SDB version 4.0 - DATA: Zn/Bentonite (Clay minerals); kaolinite #69302~69331

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes

I-b	REF	Linear graphs with adsorbed % are provided.	class 4
II-a	SDB	Sample used in this experiment is acid-washed kaolinite supplied by Ajax Chemicals, without further treatment. The XRD pattern showed characteristic peaks of kaolinite, and no other mineral component was detected. The surface area is reported as 14.4 m ² /g, but CEC is not reported.	A
II-b	SDB	pH was adjusted by addition of 0.1 M HCl and 0.1M NaOH. Final pH values are reported.	A
II-c	SDB	The experiments were conducted under N ₂ atmosphere. Zn(II) is not redox sensitive.	A/B
II-d	SDB	Initial solution used is 0.01M NaNO ₃ and solid is pure kaolinite. The final solution composition can be estimated approximately.	A/B
II-e	SDB	A reaction temperature of 22±1°C is indicated.	A/B
II-f	SDB REF	A liquid/solid ratio of 6460 [mL/g] is reported (surface area concentration is 96.3 [m ² /L], surface area is 14.4 [m ² /g]). Particle size is not reported.	A/B
II-g	SDB REF	The following sorption values were calculated from K _d and L/S ratios: • # 69328~69331 • #69327 • Others	C/D B A
II-h	SDB REF	Initial Zn concentration is reported as 3.33×10 ⁻⁵ ~1.33×10 ⁻⁴ [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_050000c0.tdb): • #69311~69317, #69327~69331 • Others	unreliable A
II-i	SDB	Separation method is a centrifugation and filtration.	A
II-j	SDB REF	A contact time of 1 hour is indicated. It is considered to reach to equilibrium state. Sorption kinetics seems to be investigated, however data is not reported.	C/D
II-k	REF	It is not reported agitation method.	C/D
II-l	SDB REF	Initial Zn concentration is varied. An adsorption isotherm is presented.	A
II-m	REF	A borosilicate reaction vessel is used in the experiment. However, sorption on vessel is not evaluated.	C/D
II-n	REF	No information is reported.	D
II-o	REF	pH and initial Zn concentration were varied.	B

Data table Sn/1: REF: Bradbury and Baeyens (2009a)

JAEA-SDB version 4.0 - DATA: Sn/Bentonite (Clay Minerals); Na-illite, #71003~71032

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB Data are taken from a log graph with K _d values.	class 5
II-a	SDB Illite du Puy was conditioned to the homo-ionic Na-form with 1M-NaClO ₄ solution. XRD analysis showed the composition to be ~88 wt.% illite and ~12wt.% sanidine, a K-feldspar. The chemical composition is also shown in wt.%.	A
II-b	SDB REF It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 2 to 11 with NaOH or HNO ₃ . In the pH range 4-9, 5 types of buffers at a concentration of 2 mM in order to ensure pH stability (Separate measurements showed no significant influence of the buffers on sorption in the range of experimental conditions)	A
II-c	SDB REF Experiments were carried out in controlled N ₂ atmosphere glove boxes (CO ₂ <2 ppm, O ₂ <2 ppm). It is not used reducing agent. Sn is not sensitive to redox condition.	A/B
II-d	SDB 0.1M NaClO ₄ solution is indicated.	A/B

	REF	Because purified Na-form illite is used under CO ₂ -free condition, the final solution composition is defined.	
II-e	SDB	Temperature is not reported. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB	L/S value is indicated 1.1 [g/L], but volume of liquid and weight of solid is not reported.	C/D
II-g	SDB	The sorption values were calculated from K _d and L/S ratios, the following rating is given: • #71011, #71012, #71021, #71022, #71031, #71032 • Others	A C/D
II-h	SDB REF	An initial Sn-concentration is indicated 5×10 ⁻⁹ M. Based on the thermodynamic calculations using JAEA TDB(100331c0.tdb), all data is given A.	A
II-i	SDB	Centrifugation 1 hour at 108,800 [g] is indicated.	B
II-j	SDB REF	A contact time of 7~60 days is indicated. At the least contact time 7 days, it is considered to reach an equilibrium condition.	A/B
II-k	REF	It is indicated that samples were shaken end-over-end for at least 7 days.	A/B
II-l	REF	Sorption isotherm experiments are not carried out.	C/D
II-m	REF	Experimental vessel is 40-mL polypropylene centrifuge tube.	B
II-n	SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o	SDB	pH has been varied systematically.	B

Data table Sn/2: REF: Lauber et al. (2000)			
JAEA-SDB version 4.0 - DATA: Sn/Bentonite (Clay Minerals); Opalinus Clay #68353~68373			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Graphs with logarithmic K _d values are provided. • #68353~68367 Table with logarithmic K _d values are provided. • #68368~68373	class 5 class 2
II-a	SDB	As solid phase Opalinus Clay (and CEC) is indicated. A detailed analysis of Opalinus Clay is available.	A
II-b	SDB REF	It is indicated that initial pH values are provided. The samples were pre-conditioned; therefore, it is assumed that initial and final pH is nearly identical. Further, the solution is well buffered.	A
II-c	SDB	It is indicated that experiments had been conducted under a nitrogen atmosphere. No addition of oxidizing or reducing agents is indicated. The experiments were carried out in a CO ₂ /N ₂ and N ₂ atmosphere. This is not redox sensitive.	A/B
II-d	SDB REF	It is indicated that experiments had been performed in synthetic porewater solution, composition is given. Final solution composition is not indicated. Clay samples were pre-conditioned. The composition of the conditioned solutions was determined.	A/B
II-e	SDB	It is indicated that experiments had been performed at 25°C.	A/B
II-f	SDB REF	The solution/solid ratio is indicated. Actual solution volume and solid weight are not given. The specific surface area of Opalinus Clay is reported as 33.3 [m ² /g]. Experiments were done in 40 [mL] centrifuge tubes. This results in about 8 [m ²] of sorbent surface per vial.	A/B
II-g	REF	The following sorption values were calculated from K _d and L/S ratios. Adsorption % of all datapoints are >99%.	C/D

II-h	SDB REF	Initial Sn concentrations of 5.3×10^{-8} [M] are indicated. In this report, solubility studies of Sn(IV) by Amaya et al.(1997) show that the Sn solubility is in the range of ~ 3 to 6×10^{-8} [M] at pH = 6.3 The measured Sn concentration in the conditioned OPA Porewater is well range of the solubility of Sn(IV).	A
II-i	SDB	Centrifugation (60 min at 95,000 [g]) is indicated.	B
II-j	SDB	Contact times between 1~50 days are indicated. Equilibrium is reportedly established after about 1 week: • # 68353~68355 • all other datapoints	unreliable A/B
II-k	REF	End-over-end-shaker, continuous shaking.	A/B
II-l	REF	Sorption isotherm experiments were not carried out. Initial Sn concentration is not varied.	C/D
II-m	REF	Centrifuge tubes were used (material not specified). Wall sorption was not considered (experiments in similar systems had suggested only a small potential effect).	A
II-n	REF	Error bars are provided for each K_d value. These are based on repeated experiments, but it is not clear whether all experiments were repeated.	B
II-o	REF	Indicated are experiments for two sets of conditions and different equilibration times	B

Data table Pb/1: REF: Ikhsan et al.(1999)

JAEA-SDB version 4.0 - DATA: Pb/Bentonite (Clay minerals); kaolinite #67751~67812

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	REF A linear graph with adsorbed % and adsorbed concentration is provided.	class 4
II-a	SDB It was indicated that XRD analysis showed a standard kaolinite pattern with no contaminant lines.	A
II-b	SDB pH was adjusted with 0.1M HNO ₃ and 0.1M KOH. Final pH values are reported.	A
II-c	SDB It is investigated Pb(II) sorption under N ₂ atmosphere condition.	A/B
	REF Pb(II) is not sensitive redox condition.	
II-d	SDB Solution used is 0.005M KNO ₃ and solid is pure kaolinite. The final solution composition can be estimated approximately.	A/B
II-e	SDB A temperature is 25°C.	A/B
II-f	SDB A solid/liquid ratio of 6.789 [g/L] is reported. No other information is indicated.	C/D
II-g	SDB The following sorption values were calculated from K_d and L/S ratios: • #67751, #67785~67791	C/D
	REF • #67753, #67783, #67784 • Others	B A
II-h	SDB Initial Pb concentration is reported to be 1.0×10^{-4} [M].	A
	REF Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Pb is more than 1.0×10^{-4} [M].	
II-i	SDB Separation method is used 0.2 μ m Poretics polycarbonate membrane filters.	B
II-j	SDB It is indicated that equilibration time is 30 minutes.	C/D
II-k	REF No information for agitation is reported.	C/D
II-l	SDB Initial Pb concentration is varied from 1.0×10^{-6} to 1.0×10^{-4} [M]. Sorption isotherm is determined.	A
II-m	REF No information for vessel is reported.	C/D
II-n	REF No error information is reported.	D
II-o	REF pH and initial Pb concentration are varied systematically.	A

Data table Pb/2: REF: Srivastave et al.(2005)		
JAEA-SDB version 4.0 - DATA: Pb/Bentonite (Clay minerals); kaolinite #69277~69301		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	Linear graphs with adsorbed % are provided.	class 4
II-a SDB	Sample used in this experiment is acid-washed kaolinite supplied by Ajax Chemicals, without further treatment. The XRD pattern showed characteristic peaks of kaolinite, and no other mineral component was detected. The surface area is reported as 14.4 m ² /g, but CEC is not reported.	A
II-b SDB	pH was adjusted by addition of 0.1 M HCl and 0.1M NaOH. Final pH values are reported.	A
II-c SDB REF	The experiments were conducted under N ₂ atmosphere. Pb(II) is not redox sensitive.	A/B
II-d SDB	Initial solution used is 0.01M NaNO ₃ and solid is pure kaolinite. The final solution composition can be estimated approximately.	A/B
II-e SDB	A reaction temperature of 22±1°C is indicated.	A/B
II-f SDB REF	A liquid/solid ratio of 6460 [mL/g] is reported (surface area concentration is 96.3 [m ² /L], surface area is 14.4 [m ² /g]). Particle size is not reported.	A/B
II-g SDB REF	The following sorption values were calculated from K _d and L/S ratios: • # 69277, #69296~69301 • #69278 • Others	C/D B A
II-h SDB REF	Initial Pb concentration is reported as 3.33×10 ⁻⁵ ~1.33×10 ⁻⁴ [M]. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Pb is more than initial Pb concentration (3.33×10 ⁻⁵ M) at 3<pH<8.5.	A
II-i SDB	Separation method is a centrifugation and filtration.	A
II-j SDB REF	A contact time of 1hour is indicated. It is considered to reach to equilibrium state. Sorption kinetics seems to be investigated, however data is not reported.	C/D
II-k REF	It is not reported agitation method.	C/D
II-l SDB REF	Initial Pb concentration is varied. An adsorption isotherm is presented.	A
II-m REF	A borosilicate reaction vessel is used in the experiment. However, sorption on vessel is not evaluated.	C/D
II-n REF	No information is reported.	D
II-o REF	pH and initial Pb concentration were varied.	B

Data table Pa/1: REF: Bradbury and Baeyens (2009b)		
JAEA-SDB version 4.0 - DATA: Pa/Bentonite (Clay Minerals); Na-illite, #71189~71229		
GUIDELINE: Revision 4b (May 19, 2005)		
REMARK : It is considered that this experiment procedure is same with Bradbury and Baeyens (2009a).		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	Data are taken from a log graph with K _d values.	class 5
II-a SDB	Illite du Puy was conditioned to the homo-ionic Na-form with 1M-NaClO ₄ solution. XRD analysis showed the composition to be ~88 wt.% illite and ~12wt.% sanidine, a K-feldspar. The chemical composition is also shown in wt.%.	A
II-b SDB REF	It is indicated that final pH-values were measured. Sorption edges were carried out changing the pH from 2 to 11 with NaOH or	A

		HNO ₃ . In the pH range 4–9, 5 types of buffers at a concentration of 2 mM in order to ensure pH stability (Separate measurements showed no significant influence of the buffers on sorption in the range of experimental conditions)	
II-c	SDB REF	Experiments were carried out in controlled N ₂ atmosphere glove boxes (CO ₂ <2 ppm, O ₂ <2 ppm). It is not used reducing agent. Pa is not sensitive to redox condition.	A/B
II-d	SDB REF	0.1M NaClO ₄ solution is indicated. Because purified Na-form illite is used under CO ₂ -free condition, the final solution composition is defined.	A/B
II-e	SDB	Temperature is not reported. Room temperature can be assumed, but is not reported in the REF.	C/D
II-f	SDB	L/S value is indicated 0.67 [g/L], but volume of liquid and weight of solid is not reported.	C/D
II-g	SDB	The sorption values were calculated from K _d and L/S ratios, the following rating is given: • #71189, #71190, #71195, #71202~71205, #71207, #71213 • #71198~71201, #71220~71229 • Other data	A C/D B
II-h	SDB REF	An initial Pa-concentration is indicated <1×10 ⁻¹³ M. Based on the thermodynamic calculations using JAEA TDB(100331c0.tdb), all data is given A.	A
II-i	SDB	Centrifugation 1 hour at 108,800 [g] is indicated.	B
II-j	SDB REF	A contact time of 1 and 7 days is indicated. At the least contact time 1 day, it is considered to reach an equilibrium condition.	A/B
II-k	REF	It is indicated that samples were shaken end-over-end for at least 7 days.	A/B
II-l	REF	Sorption isotherm experiments are not carried out.	C/D
II-m	REF	Experimental vessel is 40-mL polypropylene centrifuge tube.	B
II-n	SDB REF	Error is not indicated An error bar is indicated in figure.	C
II-o	SDB	pH and contact time has been varied systematically.	B

Data table Pu/1: REF: Sanchez et al.(1985)			
JAEA-SDB version 4.0 - DATA: Pu/Other minerals; goethite #69026~69192			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	Figures with adsorbed % are given. • #69026~69174 Tables with adsorbed % are given. • #69175~69192	class 4 class 2
II-a	SDB	Sample used in this experiment is synthetic goethite (α-FeOOH), which was prepared using the method of Atkinson et al.(1967).	A
II-b	SDB	pH was adjusted with 0.1N HCl or 0.1N NaOH. Final pH values are reported.	A
II-c	SDB REF	No information on atmospheric and redox condition. It is reported that Pu exists as Pu(IV) or Pu(V), which are distinguished by the solvent extraction method.	A/B
II-d	SDB	Solutions used are three different electrolytes containing - 0.1M, 0.5M, 1M and 3M NaNO ₃ : 0.5M and 3M NaCl: and 0.03M, 0.15M and 0.3M Na ₂ SO ₄ . Solid is pure synthetic goethite. The final solution composition can be estimated.	A/B
II-e	SDB	A temperature is reported 20±2°C.	A/B
II-f	SDB	A solid /liquid ratio of 0.4 [g/L] is reported. Particle size of solids is not indicated.	C/D
II-g	SDB	The following sorption values were calculated from K _d and L/S ratios:	

	REF	<ul style="list-style-type: none"> • #69032~69037, #69044, #69045, #69050~69052, #69062, #69063, #69072, #69092, #69093, #69100, #69101, #69108~69110, #69116, #69132, #69133, #69146, #69151, #69152, #69165, #69179, #69181, #69183 • #69043, #69061, #69071, #69073~69075, #69082~69085, #69098, #69099, #69107, #69131, #69138, #69144, #69145, #69147, #69150, #69158~69160, #69175, #69177, #69180, #69184~69187, #69189~69192 • Others 	C/D B A
II-h	SDB REF	Initial Pu concentrations are reported as 1.0×10^{-10} and 1.0×10^{-11} [M]. Based on thermodynamic calculations with PHREEQC (database : JNC-TDB_011213c2.tdb), all data is given A.	A
II-i	SDB	Separation method is filtration (0.45 μm).	B
II-j	SDB	It is indicated that contact time was 1h~25 days. <ul style="list-style-type: none"> • #69026~69037, #69053~69072, #69100~69109, #69132~69138, #69146~69151, #69170~69192 : 1hour • Others : >1day 	unreliable A/B
II-k	REF	Information about an agitation method is not reported.	C/D
II-l	SDB	Initial Pu concentration is varied. However sorption isotherm is not calculated.	B
II-m	REF	The experiments were carried out in borosilicate glass vessels. It is performed a blank experiments.	A
II-n	REF	Error was reported for only sorption data as a function of ionic strength, presented in tabular form. <ul style="list-style-type: none"> • #69175~69192 : 1hour • Others : >1day 	C D
II-o	REF	pH, ionic strength, dissolved organic carbonate; carbonate alkalinity and reaction time are varied.	A

3.3 QA evaluation on criteria III

Only the entries for Ni, Eu/Am, Np, Th and Se for clay systems classified as reliable are being considered for criteria III. Entries for Cs are not included in this analysis because the final cation concentration would have to be estimated or calculated in most cases before a meaningful comparison can be done. In case of other radionuclides, not enough reliable data in the JAEA-SDB are available for an evaluation.

3.3.1 Evaluation of data for Ni

Both of the evaluated datasets were classified as reliable:

Reference	Data table	Solid phase(group/solids)
Lauber et al.(2000)	Ni/2	Bentonite(Clay minerals)/Opalinus Clay
Tertre et al.(2005)	Ni/3	Bentonite(Clay minerals)/ Na-montmorillonite

Figure 3.1 shows these datasets in comparison with Ni sorption data on Na- and Ca-forms of SWy-1 montmorillonite in the series of data by Bradbury and Baeyens. Tertre (2005) is consistent with SWy-1 datasets in terms of ionic strength dependence in low pH region and pH edges in pH 5-9, while it appears that the magnitude of K_d may be somewhat different between substrates. The variation of K_d data observed at two pH in Lauber et al. (2000) can be explained by the difference of Ni concentration and reaction time. The data by Lauber et al. (2000) is also consistent with other datasets in terms of trends vs. pH and in terms of magnitude, by comparing between data obtained under similar condition.

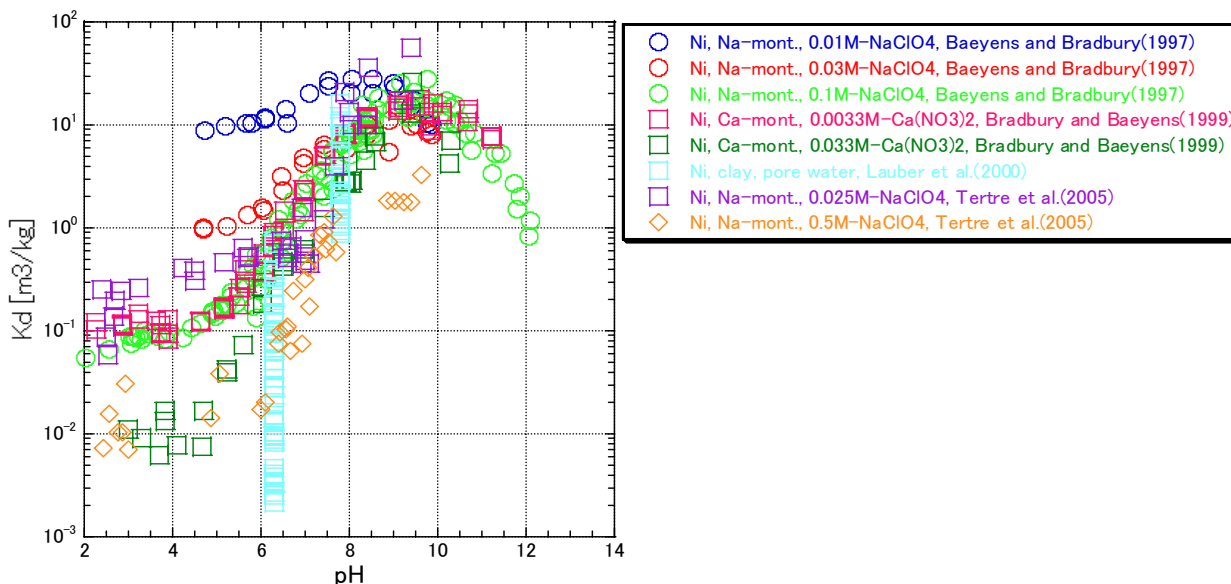


Figure 3.1 Overview of sorption data for Ni on Opalinus Clay (OPA) and smectite from MX-80. For comparison, several datasets for SWy-1 montmorillonite are also shown. (mont.: montmorillonite, SOPW1: synthetic OPA porewater)

3.3.2 Evaluation of data for Eu/Am

Evaluated datasets were classified as reliable:

Reference	Data table	Solid phase(group/solids)
Lauber et al.(2000)	Eu/3	Bentonite(Clay minerals)/Opalinus Clay
Marques Fernandes et al.(2008)	Eu/4	Bentonite(Clay minerals)/Na-Swy-1 montmorillonite
Rabung et al.(2005)	Eu/5	Bentonite(Clay minerals)/Ca-montmorillonite
Tertre et al.(2005)	Eu/6	Bentonite(Clay minerals)/Na-montmorillonite

An overview of the respective data and a comparison with other relevant datasets is given in Figure 3.2. Sorption K_d values of Eu and Am showed a fairly clear trend of increasing K_d with increasing pH. All datasets are consistent in terms of ionic strength dependence in low pH region and pH edges in pH 5-10, while it appears that the magnitude of K_d may be somewhat different between Na-montmorillonite and Ca-montmorillonite. Although K_d dataset for Ca-montmorillonite in Bradbury and Baeyens(2002) is obtained for relatively low electrolyte concentration (0.066M), their K_d values are lower in low pH region that those for Na-montmorillonite, reported by Fernandes et al. (2008) and Tertre et al.(2005). The variation of K_d data observed at two pH in Lauber et al. (2000) can be explained by the difference of Eu concentration. The data by Lauber et al. (2000) is also consistent with other datasets in terms of trends vs. pH and in terms of magnitude.

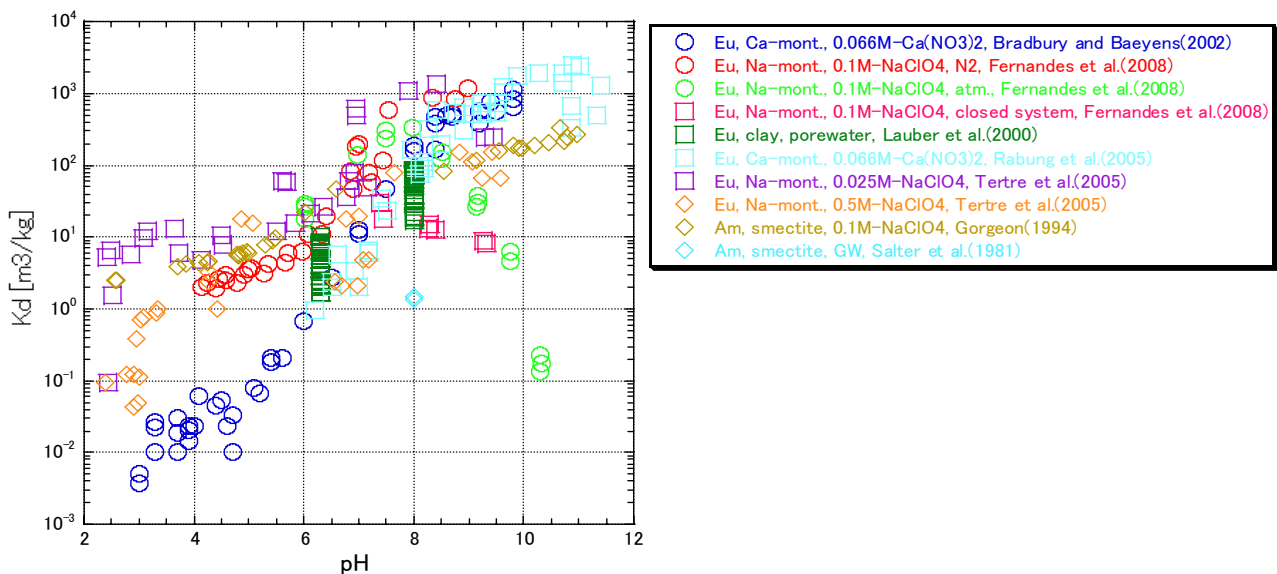


Figure 3.2 Overview of sorption data for Eu on montmorillonite. For comparison, sorption data for Am on montmorillonite are also shown. (mont.: montmorillonite, GW: groundwater)

3.3.3 Evaluation of data for Th

The reliable datasets are the following:

Reference	Data table	Solid phase(group/solids)
Bradbury and Baeyens (2003)	Th/1	Bentonite(Clay minerals)/ SWy-1 montmorillonite
Lauber et al. (2000)	Th/3	Bentonite(Clay minerals)/ Opalinus Clay

They are plotted in Figure 3.3:

- The data by Bradbury and Baeyens (2003a) on SWy-1 had been used as reference data in our earlier reports (Ochs et al., 2008). They are viewed as reflecting Th sorption on a pure montmorillonite in the absence of any other competitive cation or ligand.
- The data on OPA by Lauber et al. (2000) agree with additional data on the same material by Bradbury and Baeyens (2003b) and with data on MX-80 by Bradbury and Baeyens (2003a).

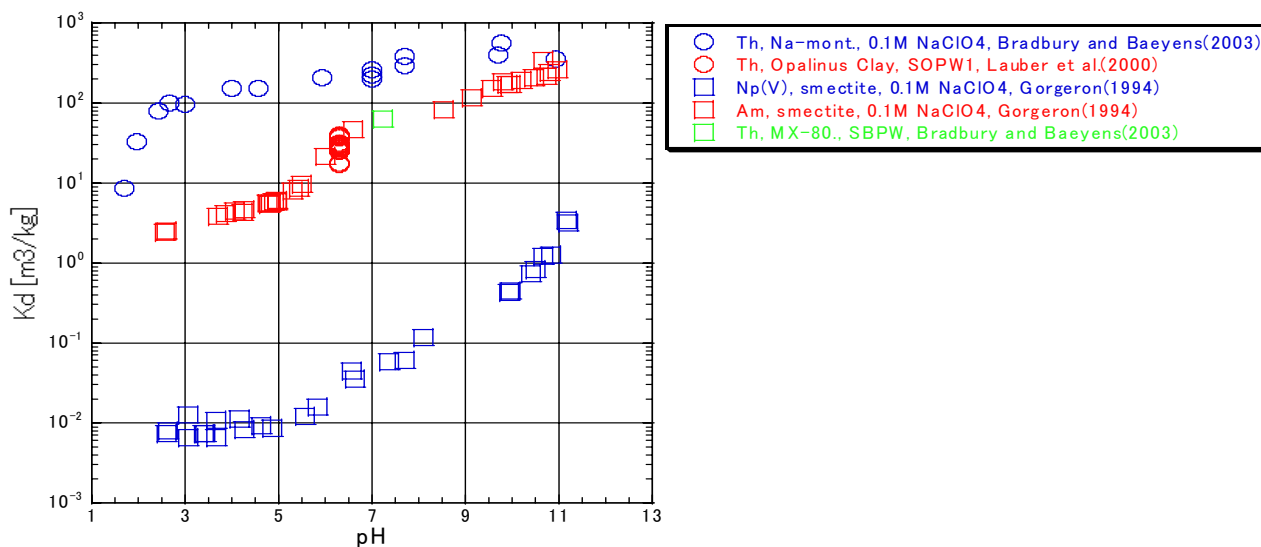


Figure 3.3 Overview of sorption data for Th on SWy-1, Opalinus Clay (OPA). For comparison, several other datasets for clays are also shown. Further, several reliable datasets for other actinides are included. (mont.: montmorillonite, SOPW1: synthetic OPA porewater, SBPW: synthetic bentonite porewater)

3.3.4 Evaluation of data for Np

Evaluated datasets were classified as reliable:

Reference	Data table	Solid phase(group/solids)
Turner et al.(1998)	Np/5	Bentonite(Clay minerals)/Na-montmorillonite

An overview of the respective data and a comparison with other relevant datasets is given in Figure 3.4. Turner et al. (1998) is the only K_d dataset in this SDB update, focused on Np sorption for clay minerals. K_d data trend in Turner et al. (1998) is consistent with Gorgeon(1994) and Stammose et al.(1992) in terms of ionic strength dependence in low pH region and pH edges in pH 5-10, while it appears that the magnitude of K_d may be somewhat different between literatures. K_d variation in low pH region can be explained by ionic strength effect, however it is difficult to explain the reason for K_d variation in higher pH region, excluding the case with high carbonate in Turner et al. (1998).

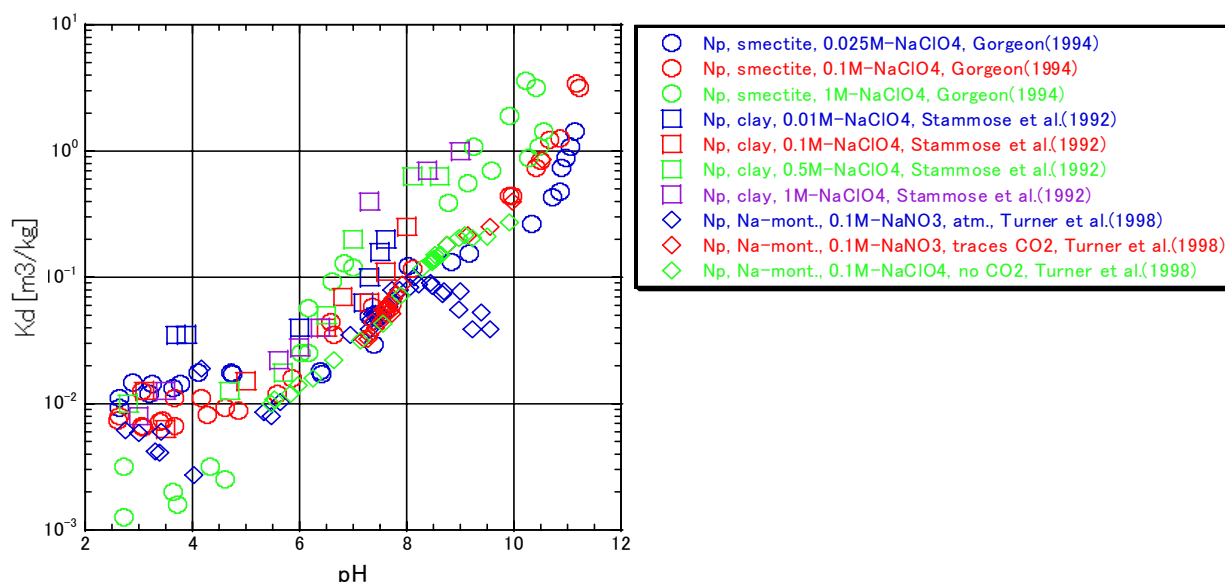


Figure 3.4 Overview of sorption data for Np(V) on montmorillonite. (mont. = montmorillonite)

3.3.5 Evaluation of data for Se

The following datasets are classified as reliable and are further evaluated below.

Reference	Data table	Solid phase(group/solids)
Goldberg and Glaubig (1988)	Se/4	Bentonite(Clay minerals)/ Ca-montmorillonite, kaolinite
Lauber et al. (2000)	Se/7	Bentonite(Clay minerals)/ Opalinus Clay
Missana et al.(2009a)	Se/8	Bentonite(Clay minerals)/ Na-smectite, Na-illite

An overview of Se(IV) sorption on clays (montmorillonite, bentonite and Opalinus clay) is given in Figure 3.5. Although K_d values lie in wide ranges (2 orders of magnitude), a fairly clear trend of decreasing K_d with increasing pH. This K_d variation can presumably be explained in part with the different contents of montmorillonite clay and minor constituents such as pyrite and calcite, which has a significant influence on selenite sorption (see Goldberg and Glaubig (1988), Boulton et al.(1998)). The variation of K_d data observed at pH around 6 in Lauber et al. (2000) can be explained by the difference of Se concentration.

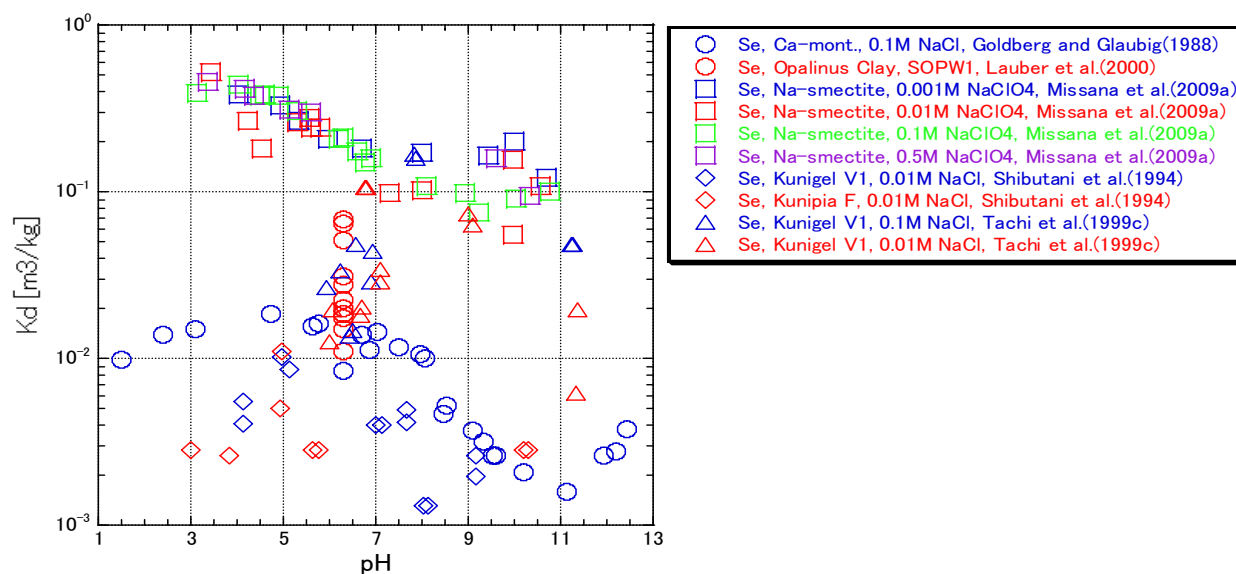


Figure 3.5 Overview of Se(IV) sorption on clays including montmorillonite, bentonite and Opalinus clay. (mont.: montmorillonite, SOPW1: synthetic OPA porewater)

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 overview of basic functions, structures, applications of the web-based JAEA-SDB, including updated functions to effective data extractions, updating of K_d data and QA classification, related to future K_d -setting and TSM development.

- Additional data evaluation function focusing on multi-parameter dependence is useful to extract K_d trends and respective data. The updated JAEA-SDB is expected to make it possible to obtain quick overview of the available data, and to have suitable access to the respective data for PA-related K_d setting in effective, traceable and transparent manner.
- K_d data in relation to our recent activities on the K_d setting and mechanistic model development, key RNs in i) montmorillonite/bentonite, ii) other clay minerals, and iii) Fe and Al oxide/hydroxide are introduced in the JAEA-SDB. Their QA/classification is also evaluated following the approach/guideline defined in our previous report. As a result, the 4,250 K_d data from 32 references are added, total K_d values in the JAEA-SDB are 28,540. The QA/classified K_d data are about 39% for all K_d data in JAEA-SDB.
- Further study would be continued 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 - I

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 SiO₂, etc.) detailed solid phase information is widely known and can be retrieved from a large number of publications. Therefore, characterization of such solids is not required for each entry in the 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 O₂ (as a matter of fact, the latter may be the more common problem).

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

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

→ Two levels of reliability:

A/B) Level A/B applies to entries in the 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-O₂ conditions with a subsequent confirmation of RN oxidation state). Evaluating the reliability of such measurements is likely to require an expert decision by the operator.

→ If a lower quality than required for level C/D is evident, the respective entry is excluded from further evaluation as unreliable. For example, cases where it has been attempted to achieve reducing conditions only by minimizing the level of O₂ (e.g., by performing experiments in a N₂ atmosphere) generally should be labeled "unreliable" (except where the oxidation state of a RN somehow has been confirmed, see description of level C/D). Also, if a strongly complexing reducing agent (such as

many organic acids) is used at unspecified concentration levels, the respective entry is excluded from further evaluation as unreliable.

II-d Final solution composition

Note that solution composition includes dissolved carbonate concentration, which may be controlled through, or expressed as $p\text{CO}_2$. 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) $[\text{surface area sorbent}] \gg [\text{surface area vessel}]$, i.e. that at least 5 m^2 of

sorbent surface had been added to each vessel, and to assume that
b) samples are reproducible and representative.

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

C/D) Any other than the above.

II-g Sorption value

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

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

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

C/D) Any other than the above.

II-h Initial RN concentration ([RN])

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

→ Three levels of reliability:

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

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

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

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

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

II-i Phase separation

Here, the appropriateness of phase separation is evaluated: Note that in cases where colloids or other artifacts are important, different phase separation methods will not lead to the same results. Identical or very similar results with different efficient methods are probably the best direct proof of absence of important colloid effects; hence such studies are rated A. Rating B

would be given for methods that can be presumed to remove colloids, but where no direct proof as in A is given.

→ Three levels of reliability:

A) Identical (very similar) results are obtained with different methods of phase separation, where at least one method needs to be efficient in terms of colloids removal (ultrafiltration or high-speed centrifugation). Accordingly, the best comparison would be between two efficient methods, such as ultrafiltration and high-speed centrifugation.

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

B) Only one, but efficient method (high-speed centrifugation, ultrafiltration) is used, and there is no evidence for artifacts such as colloid effects or significant sorption to the filter.

C/D) Only one general method (normal centrifugation, membrane filtration with nominal pore sizes of 0.01~0.45 μm) is used, and there is no evidence for artifacts such as colloid effects or significant sorption to the filter.

→ If no phase separation is used, or in case of obvious evidence for artifacts (colloid effect, adsorption on filter) the respective entry is excluded from further evaluation as unreliable.

II-j Reaction time

→ Two levels of reliability:

A/B) Identical (similar) results are obtained with different reaction times, or some other demonstration of near-equilibrium is provided (e.g. separate kinetic experiments).

C/D) Only one, but reasonably long reaction time is used. What is “reasonably long” is highly dependent on the experimental system: In general, the time needed to reach equilibrium will increase with the complexity of the sorbing substrate and the strength of sorption. Sorption of Sr onto a pure clay mineral through ion exchange can be assumed to be complete within a day; sorption of a trivalent actinide onto a complex substrate may need several days to weeks for completion. In the absence of kinetic information, operator expert decisions will be required to assess this point. If possible, reaction times reported for similar systems included in the 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-1 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 CO₂ or O₂, 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, pCO₂, 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 pCO₂ (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 pCO₂ (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 × 2
*II-b	pH	A-D × 8
*II-c	redox conditions	A/B-C/D × 8
*II-d	final solution composition	A/B-C/D × 8
II-e	temperature	A/B-C/D × 1
II-f	L/S, grain size	A/B-C/D × 2
II-g	sorption value	A-C/D × 2
*II-h	initial RN concentration	A-/CD × 8
*II-i	phase separation	A-C/D × 8
*II-j	reaction time	A/B-C/D × 2
II-k	agitation	A/B-C/D × 1
II-l	RN loading	A-C/D × 2
II-m	reaction vessel	A-C/D × 1
II-n	uncertainty estimates	A-D × 2
II-o	parameter variation	A-D × 8

* indicates critical checkpoints with minimum requirements;

bold letters indicate the checkpoints to be evaluated initially

Table 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 The classification system

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

Appendix - II

Summary tables for K_d classification

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Datapoint	Reference	I - Completeness of documentation and type of Kd												II - Technical and scientific quality of reported data												Rating II	Operator	Data	Classification Guideline
		Rating ⇒ I-a: Yes/No, I-b: class 1-6						Checkpoints ⇒ Level: A-D (numerical value: 3-0)/unreliable						Rating ⇒ class1-6/unreliable															
		I-a.1	I-a.2	Rating I-a	Rating I-b	II-a solid phase	II-b pH	II-c redox condition	II-d solution composition	II-e temperature	II-f S/W	II-g sorptive value	II-h initial [RN]	II-i phase separation	II-j reaction time	II-k agitation	II-l RN	II-m loading	II-n reaction vessels	II-o error estimates	parameter variation								
67381	de Preter et al.(1991)	Yes	Yes	yes (can be used)	class 3	A)	D)	A/B)	C/D)	A)	A)	C/D)	C/D)	C/D)	A)	C/D)	C/D)	D)	A)	class 3	M. Ochs, BMG	December 2009	Revision 4b (May 19, 2005)	Cs/1					
69377	Stauton and Roubaud(1997)	Yes	Yes	yes (can be used)	class 5	B)	D)	A/B)	A/B)	C/D)	A)	A)	B)	C/D)	A/B)	A)	C/D)	D)	A)	class 2	P.Bradsatsch/M.Ochs, BMG	December 2009	Revision 4b (May 19, 2005)	Cs/3					

Table with columns: Databoint, Reference, I-a-1, I-a-2, Rating, I-a, Rating I-a, Rating I-b, II-a, II-b, II-c, II-d, II-e, II-f, II-g, II-h, II-i, II-j, II-k, II-l, II-m, II-n, II-o, Rating II, comment/rating, Operator, Date, Classification Guideline.

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Table with columns: Dapoint, Reference, I-a.1, I-a.2, Rating, I-b, I-a, Rating I-b, II-a, II-b, II-c, II-d, II-e, II-f, II-g, II-h, II-i, II-j, II-k, II-l, II-m, II-n, II-o, Rating II, comment/rating, Operator, Data, Classification Guideline. The table lists numerous data points (70462-71513 and 70863-70881) with detailed technical specifications and consistency ratings.

Table with columns: Datepoint, Reference, I-a.1, I-a.2, Rating, Rating 1-a, Rating 1-b, II-a, II-b, II-c, II-d, II-e, II-f, II-g, II-h, II-i, II-j, II-k, II-l, II-m, II-n, II-o, Rating II, comment/rating, Operator, Data, Classification Guideline. The table contains 100 rows of data, each representing a specific datepoint and its associated technical and scientific quality parameters.

Datapoint	Reference	I - Completeness of documentation and type of Kd				II - Technical and scientific quality of reported data																			III - Consistency		Operator	Data	Classification Guideline																			
		Rating ⇒ I-a: Yes/No, I-b: class 1-6		Rating I-a		Rating I-b		II-a		II-b		II-c		II-d		II-e		II-f		II-g		II-h		II-i		II-j				II-k		II-l		II-m		II-n		II-o		Rating II		comment/rating						
		I-a.1	I-a.2	I-a.1	I-a.2	I-b.1	I-b.2	II-a	II-b	II-c	II-d	II-e	II-f	II-g	II-h	II-i	II-j	II-k	II-l	II-m	II-n	II-o	II-p	II-q	II-r	II-s				II-t	II-u	II-v	II-w	II-x	II-y	II-z	II-aa	II-ab	II-ac	II-ad	II-ae	II-af	II-ag	II-ah	II-ai			
70610	Missana et al.(2009a)	Yes	Yes	yes (can be used)	class 5	A)	A)	A/B)	A/B)	A/B)	C/D)	A/B)	A)	A)	A)	B)	A/B)	C/D)	A)	A)	C)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	A)	T.Suyama/Y.Tachi, JAEA	September 2009 Revision 4b (May 19, 2005)	Se/8

国際単位系 (SI)

表1. SI基本単位

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

表2. 基本単位を用いて表されるSI組立単位の例

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

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

表3. 固有の名称と記号で表されるSI組立単位

組立量	SI組立単位			
	名称	記号	他のSI単位による表し方	SI基本単位による表し方
平面角	ラジアン ^(b)	rad	1 ^(b)	m/m
立体角	ステラジアン ^(b)	sr ^(c)	1 ^(b)	m ² /m ²
周波数	ヘルツ ^(d)	Hz		s ⁻¹
力	ニュートン	N		m kg s ⁻²
圧力, 応力	パスカル	Pa	N/m ²	m ⁻¹ kg s ⁻²
エネルギー, 仕事, 熱量	ジュール	J	N m	m ² kg s ⁻²
仕事率, 工率, 放射束	ワット	W	J/s	m ² kg s ⁻³
電荷, 電気量	クーロン	C		s A
電位差 (電圧), 起電力	ボルト	V	W/A	m ² kg s ⁻³ A ⁻¹
静電容量	ファラド	F	C/V	m ² kg ⁻¹ s ⁴ A ²
電気抵抗	オーム	Ω	V/A	m ² kg s ⁻³ A ⁻²
コンダクタンス	ジーメン	S	A/V	m ² kg ⁻¹ s ³ A ²
磁束	ウエーバ	Wb	Vs	m ² kg s ⁻² A ⁻¹
磁束密度	テスラ	T	Wb/m ²	kg s ⁻² A ⁻¹
インダクタンス	ヘンリー	H	Wb/A	m ² kg s ⁻² A ⁻²
セルシウス温度	セルシウス度 ^(e)	°C		K
光照射度	ルーメン	lm	cd sr ^(c)	cd
放射線量	グレイ	Gy	J/kg	m ² s ⁻²
放射性核種の放射能 ^(f)	ベクレル ^(d)	Bq		s ⁻¹
吸収線量, 比エネルギー分与, カーマ	グレイ	Gy	J/kg	m ² s ⁻²
線量当量, 周辺線量当量, 方向性線量当量, 個人線量当量	シーベルト ^(g)	Sv	J/kg	m ² s ⁻²
酸素活性化	カタール	kat		s ⁻¹ 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み、ベクレルは放射性核種の統計的過程についてのみ使用される。
 (e) セルシウス度はケルビンの特別な名称で、セルシウス温度を表すために使用される。セルシウス度とケルビンの単位の大きさは同一である。したがって、温度差や温度間隔を表す数値はどちらの単位で表しても同じである。
 (f) 放射性核種の放射能 (activity referred to a radionuclide) は、しばしば誤った用語で"radioactivity"と記される。
 (g) 単位シーベルト (PV.2002.70,205) についてはCIPM勧告2 (CI-2002) を参照。

表4. 単位の中に固有の名称と記号を含むSI組立単位の例

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

表5. SI接頭語

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

表6. SIに属さないが、SIと併用される単位

名称	記号	SI単位による値
分	min	1 min=60s
時	h	1 h=60 min=3600 s
日	d	1 d=24 h=86 400 s
度	°	1°=(π/180) rad
分	'	1'=(1/60)°=(π/10800) rad
秒	"	1"=(1/60)'=(π/648000) rad
ヘクタール	ha	1 ha=1 hm ² =10 ⁴ m ²
リットル	L, l	1 L=1 dm ³ =10 ³ cm ³ =10 ⁻³ m ³
トン	t	1 t=10 ³ 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 ⁻¹⁹ J
ダルトン	Da	1 Da=1.660 538 86(28)×10 ⁻²⁷ 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 ¹¹ 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 ⁵ 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 ⁻¹⁰ m
海里	M	1 M=1852 m
バイン	b	1 b=100 fm ² =(10 ¹² cm) ² =10 ⁻²⁸ m ²
ノット	kn	1 kn=(1852/3600) m/s
ネーパ	Np	SI単位との数値的関係は、 対数量の定義に依存。
ベレル	B	
デジベル	dB	

表9. 固有の名称をもつCGS組立単位

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

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

表10. SIに属さないその他の単位の例

名称	記号	SI単位で表される数値
キュリー	Ci	1 Ci=3.7×10 ¹⁰ Bq
レントゲン	R	1 R=2.58×10 ⁻⁴ C/kg
ラド	rad	1 rad=1 cGy=10 ⁻² Gy
レム	rem	1 rem=1 cSv=10 ⁻² Sv
ガンマ	γ	1 γ=1 nT=10 ⁻⁹ T
フェルミ	f	1 フェルミ=1 fm=10 ⁻¹⁵ m
メートル系カラット		1メートル系カラット=200 mg=2×10 ⁻⁴ kg
トル	Torr	1 Torr=(101 325/760) Pa
標準大気圧	atm	1 atm=101 325 Pa
カロリ	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 ⁻⁶ m

