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Development of JAEA Sorption Database (JAEA-SDB) : Update of Sorption/QA Data in FY2015

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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 these barrier materials is expected to be diffusion-controlled and retarded by sorption processes. It is therefore necessary to understand the sorption and diffusion processes and develop databases 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 bentonites 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 improving and updating of the sorption database (JAEA-SDB) as basis of integrated approach for PA-related K_d setting and mechanistic sorption model development. This includes an overview of database structure, contents and functions including additional data evaluation function focusing on statistical data evaluation and grouping of data related to potential perturbations. 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, 11,206 K_d data from 83 references were added, total number of K_d values in the JAEA-SDB reached about 58,000. The QA/classified K_d data reached about 60% 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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※ Collaborating Engineer

JAEA-Data/Code 2015-028

JAEA 収着データベース(JAEA-SDB)の開発：2015 年度における収着データ/信頼度情報の拡充

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（2015 年 12 月 18 日受理）

放射性廃棄物地層処分の性能評価において，放射性核種の緩衝材（ベントナイト）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上で重要となる。

この目的のために，日本原子力研究開発機構では，ベントナイト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着目して，データベースの改良・更新を継続的に実施してきた。

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）の改良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と内容，今回拡充した統計評価や擾乱影響に関するデータの分類を含む機能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，83 の文献から 11,206 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 58,000 件となり，全データのうちの約 60%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 parameters1),2). 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 database (SDB), which were firstly developed as an important basis for the H12 performance assessment3),4). JAEA has been and is continuing to improve and update the SDB in view of potential future data needs, focusing on;

1) updating of sorption data5)-8)

2) assuring the desired quality level for SDB7),9)-12)

3) testing and applying of the SDB to parameter-setting13)-17).

The web-based sorption database system (JAEA-SDB) has been developed to utilize quality assuring procedure and to allow effective application for parameter setting18)(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 NEA1). Since it is not feasible to measure K_d values for all PA conditions, the use of existing sorption data obtained under generic experimental conditions and transferring such data to a range of PA-specific conditions is therefore a key challenge. The sorption database (SDB), containing large amount of sorption data for approximated, simplified, or generic systems, 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.1),13),14),17),19),20). The thermodynamic sorption model (TSM) makes it possible to estimate K_d variations directly, based on mechanistic understanding, as shown in NEA1). JAEA has developed the integrated sorption/diffusion (ISD) database in combination with thermodynamic sorption and diffusion model, and tested to explain the sorption and diffusion behavior of various radionuclides with a complex chemistry in compacted bentonites21)-23). JAEA has also tested these K_d setting approach for the derivation of K_d values and their uncertainties for rock matrix such as Horonobe mudstones and generic granites[13)-17)].

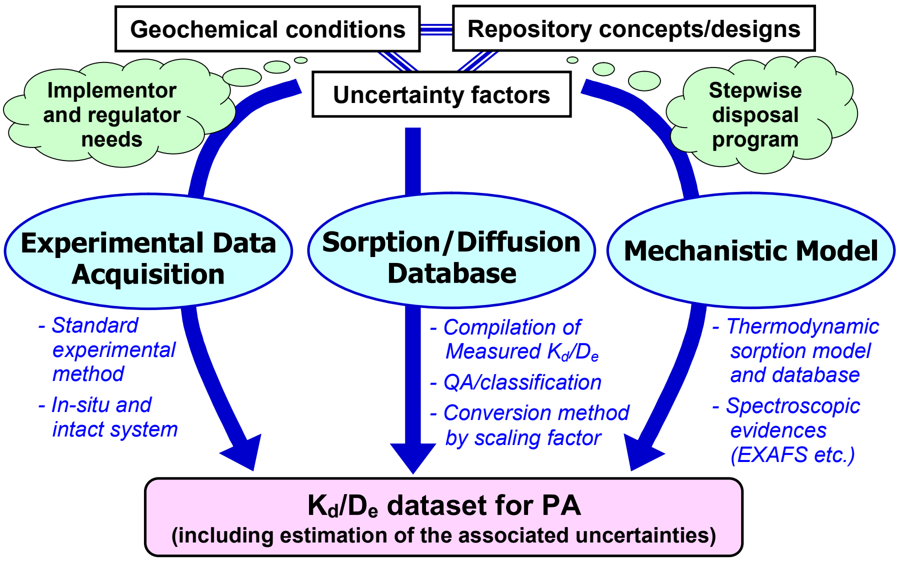


Figure 1.1 Integrated approach for sorption/diffusion parameter setting for PA

The present report focuses on updating of the sorption database (JAEA-SDB) as basis of integrated K_d setting approach shown in Figure 1.1. This includes an overview of basic functions and structures of the web-based JAEA-SDB, including updated functions to effective data evaluation (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 and additional data evaluation functions

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, various rocks, cementitious materials and soils related to the radioactive waste disposal, determined by batch sorption experiments, including K_d values and associated experimental information. It is implemented in database software that allows quick searching/plotting of data as a function of selected key parameters. The contents, functions and systems are briefly summarized in Table 2.1. As pointed out in NEA sorption database project$^{1)}$, 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)
3) database functions to focusing on multi-parametric and statistical evaluation of K_d (see 2.2.1)

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

Contents/functions	Brief description for status
Number of K_d values / references	**K_d ; 57,875 (11,206 was added in this update*)** **Reference ; 699 (83 references were added in this update*)**
Elements	78 elements; 1st 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 2nd group; Ag, Ba, Ca, Ce, Cl, Co, Eu, Fe, I, Mn, Mo, Na, Nd, Ru, Sr, Zn Minor group; 40 elements
Solid phase	Bentonite (clay minerals); Rocks – 5 group; Basaltic rock, Granitic rock, Mudstone, Sandstone, Tuff; Other minerals (Fe, Al-oxides/hydroxide, calcite, etc.); Cementitious materials (cement / concrete); Soils; **Having special influence (grout, organic substance etc.)***
Search parameters	Element, Solid phase group Detailed – solid phase, water type, pH, Eh, ionic strength, Temperature, 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; **Statistical data evaluation*; Grouping of K_d data related to perturbations***
QA/classification	**QA information evaluated by QA guideline, and related evidences** **34,421 K_d (about 60% 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® 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 of
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	mm	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
Distribution 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 described 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[9)], 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[7)]. 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 Additional functions for data evaluation

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 shown in details in the previous report7). In addition to data evaluating functions developed until the previous update7), two functions were added;

i) Function of statistical data evaluation to support PA-related K_d and uncertainty setting

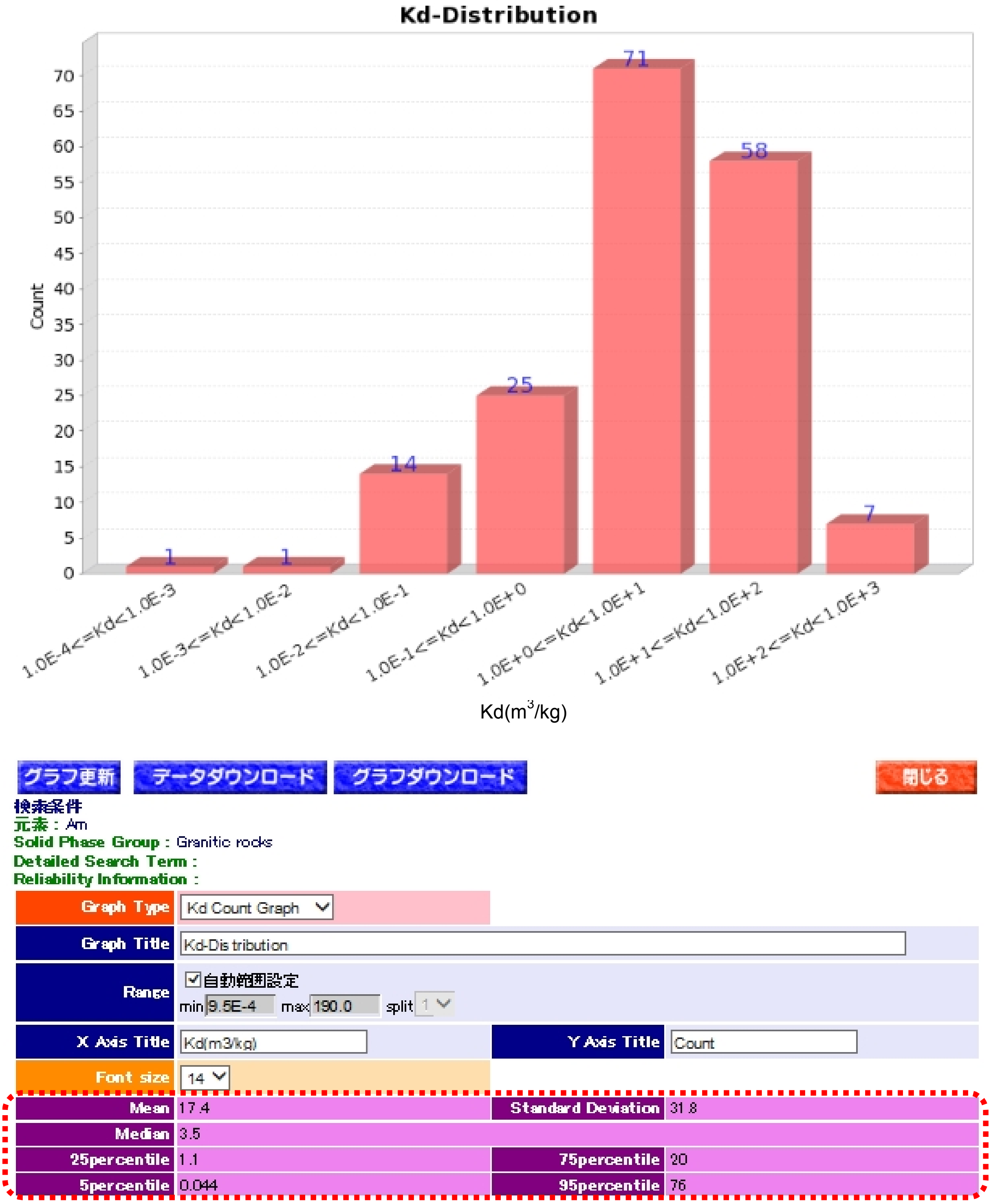
ii) Function of grouping for K_d data related to the potential perturbations.

2.2.1 Function of statistical data evaluation

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.

The JAEA-SDB has been applied and tested for PA-related K_d setting by using the data evaluation functions including QA/classification and multi-parameter dependence, etc (as shown in the previous report7)). K_d data are conditional parameter, depending on various conditions such as pH, ionic strength, initial concentration of radionuclides, etc. K_d data in JAEA-SDB can be searched by ‘elements’, ‘solid phase group’ and key parameters such as pH/Eh, ionic strength and initial concentration of radionuclides, solid/liquid ratio, and then can be extracted based on QA/classification results according to Criteria I-III. K_d plotting as a function of geochemical condition such as 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. The data evaluation function focusing on multi-parameter dependence makes it possible to extract such dataset by investigating multi-parameter dependence between various key parameters7). The K_d distribution can be finally confirmed as histogram graph, and the K_d values and their uncertainty range need to be set for the performance assessment.

In the derivation of the K_d values and their uncertainty range, it is important to select appropriate statistical treatments by considering K_d distributions. For this purpose, functions of statistical data evaluation were additionally introduced to JAEA-SDB. Two types of representative treatments for K_d setting were selected and introduced based on previous PA-related parameter setting and related discussions for uncertainty treatment24)-26): i) median values and 95/5 percentiles, ii) log mean values and standard deviations. As shown in Figure 2.1, these statistical treatments can support the setting of the K_d values and their uncertainty range.



検索条件
元素： Am
Solid Phase Group : Granitic rocks
Detailed Search Term :
Reliability Information :

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Graph Title	Kd-Distribution		
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X Axis Title	Kd(m3/kg)	**Y Axis Title**	Count
Font size	14		
Mean	17.4	**Standard Deviation**	31.8
Median	3.5		
25percentile	1.1	**75percentile**	20
5percentile	0.044	**95percentile**	76

Figure 2.1　Additional functions of statistical data evaluation

2.2.2 Function of grouping for K_d data related to the potential perturbations

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 has been introduced in the JAEA-SDB7). This function makes it possible to investigate multi-parameter dependence between various key parameters.

In addition to the analysis of K_d variations corresponding to geochemical conditions, the effect of coexisting competitive ligands must be considered in developing and using the sorption database. Natural and synthetic organics can cause significant effects on sorption of radionuclides. Natural groundwaters typically contain dissolved organic substances such as humic and fulvic acids. As synthetic organic and inorganic ligands27), low-molecular-weight organics (e.g., EDTA) resulted in degradation of organic materials, and isosaccharinic acid resulted in degradation of cellulose, as well as concrete admixtures (e.g., water reducers and superplasticizers)28) are taken into account as potential perturbations. Possible impacts of these perturbations on radionuclides sorption have been considered and quantified as reduction factors29). For this purpose, the function for grouping the K_d data related to the potential perturbations as shown in Figure 2.2.

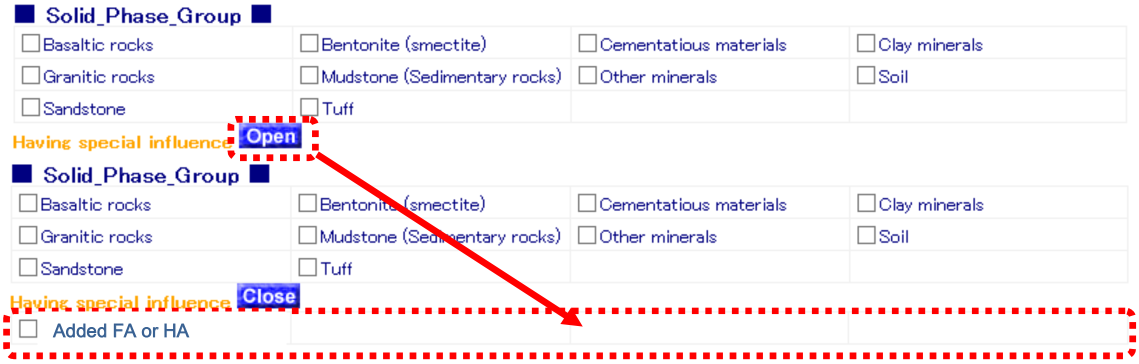

Figure 2.2 Additional functions of grouping for K_d data related to the potential perturbations

3. Updating of sorption data and its QA classification

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

As above mentioned, 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[22),23)] and PA-related K_d setting[14)-17)]. 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 and granitic rocks, and iii) new data for various barrier materials such as cement from the published literature. Selected 83 references are listed as following, and their systems are summarized in Table 3.1.

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (1/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
1)	Adeleye et al.(1994)	Adeleye, S. A. , Clay, P. G. and Oladipo, M. O. A. : Sorption of cesium, strontium and europium ions on clay minerals, Journal of Materials Science, vol.29, pp.954-958 (1994).	Cs, Eu, Sr	Na-montmorillonite, kaolinite, Na-kaolinite, Ca-montmorillonite, Ca-kaolinite	distilled water
2)	Akyil et al.(1998)	Akyil, S. , Aslani, M. A. A. and Aytas, S. : Distribution of uranium on zeolite X and investigation of thermodynamic parameters for this system, Journal of Alloys and Compounds, vol.271/273, pp.769-776 (1998).	U	zeolite	U solution
3)	Andersson et al.(2008)	Andersson, M. , Ervanne, H. , Glaus, M. A. , Holgersson, S. , Karttunen, P. , Laine, H. , Lothenbach, B. , Puigdomenech, I. , Schwyn, B. , Snellman, M. , Ueda, H. , Vuorio, M. , Wieland, E. and Yamamoto, T. : Development of Methodology for Evaluation of Long-term Safely Aspects of Organic Cement Paste Components, POSIVA Working Report, 2008-28 (2008).	Eu, Ni, Th	granite, granite_incl.SP, cement paste_incl.SP	artificial cement paste pore water, grout leaching Olkiluoto Saline Water, Olkiluoto Saline Water, grout leaching water
4)	Atun and Bodur(2002)	Atun, G. and Bodur, N. : Retention of Cs on zeolite, bentonite and their mixtures, Journal of Radioanalytical and Nuclear Chemistry, vol.253, No.2, pp.275-279 (2002).	Cs	bentonite, zeolite	0.0005M, 0.005M, 0.05M, 0.5M, 1M NaCl
5)	Bortun et al.(1998)	Bortun, A. I. , Bortun, L. N. , Khainakov, S. A. and Clearfield, A. : Ion exchange properties of the sodium phlogopite and biotite, Solvent Extraction and Ion Exchange, vol.16, No.4, pp.1067-1090 (1998).	Ba, Ca, Cd, Co, Cs, Cu, Hg, K, Li, Mg, Pb, Rb, Sr, Zn	Na-biotite, Na-phlogopite	0.0005M-1M $NaNO_3$, 0.01M-1M $CaCl_2$, 0.01M-0.5M HNO_3, 1-3M NaOH, $BaCl_2$, $CaCl_2$, $CdCl_2$, $CoCl_2$, CsCl, $CuCl_2$, $HgCl_2$, KCl, LiCl, $MgCl_2$, $PbCl_2$, RbCl, $SrCl_2$, $ZnCl_2$, groundwater, 1M $NaNO_3$+ (0.001M-1M)NaOH
6)	Bradbury and Baeyens(2006)	Bradbury, M. H. and Baeyens, B. : Modelling sorption data for the actinides Am(III), Np(V) and Pa(V) on montmorillonite, Radiochimica Acta, vol.94, pp.619-625 (2006).	Am, Eu, Np, Pa	Ca-montmorillonite, Na-montmorillonite	0.01M, 0.1M $NaClO_4$, 0.066M $CaCl_2$

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (2/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
7)	Bradbury and Baeyens(2011)	Bradbury, M. H. and Baeyens, B. : Physico-Chemical Characterisation Data and Sorption Measurements of Cs, Ni, Eu, Th, U, Cl, I and Se on MX-80 Bentonite, PSI Report, PSI Bericht Nr. 11-05 (2011).	Cs, Eu, I, Ni, Se, Th, U	MX-80	Porewater
8)	Chen and Dong(2013)	Chen, L. and Dong, Y. : Sorption of ^{63}Ni(II) to montmorillonite as a function of pH, ionic strength, foreign ions and humic substances, Journal of Radioanalytical and Nuclear Chemistry, vol.295, pp.2117-2123 (2013).	Ni	montmorillonite, montmorillonite+HA	0.001M-0.1M $NaClO_4$, 0.01M $KClO_4$, 0.01M $LiClO_4$, 0.01M NaCl, 0.01M $NaNO_3$
9)	Del Nero et al.(1997)	Del Nero, M. , Made, B. , Bontems, G. and Clement, A. : Adsorption of neptunium(V) on hydrargillite, Radiochimica Acta, vol.76, pp.219-228 (1997).	Np	hydrargillite	0.001M-0.1M $NaClO_4$
10)	Del Nero et al.(1998)	Del Nero, M. , Ben Said, K. , Made, B. , Clement, A. and Bontems, G. : Effect of pH and carbonate concentration in solution on the sorption of neptunium(V) by hydrargillite: Application of the non-electrostatic model, Radiochimica Acta, vol.81, pp.133-141 (1998).	Np	hydrargillite	0.1M $NaClO_4$, 0.1M $NaClO_4$+$NaHCO_3$
11)	Dong et al.(2011)	Dong, Y. , Liu, Z. and Li, Y. : Effect of pH, ionic strength, foreign ions and humic substance on Th(IV) sorption to GMZ bentonite studied by batch experiments, Journal of Radioanalytical and Nuclear Chemistry, vol.289, pp.257-265 (2011).	Th	GMZ bentonite, Na-bentonite	0.001M-0.1M $NaNO_3$, 0.01M NaCl, 0.01M KNO_3, 0.01M $LiNO_3$
12)	El-Rahman et al.(2006)	El-Rahman, K. M. A. , El-Kamash, A. M. , El-Sourougy, M. R. and Abdel-Moniem, N. M. : Thermodynamic modeling for the removal of Cs^+, Sr^{2+}, Ca^{2+} and Mg^{2+} ions from aqueous waste solutions using zeolite A, Journal of Radioanalytical and Nuclear Chemistry, vol.268, No.2, pp.221-230 (2006).	Ca, Cs, Mg, Sr	zeolite	Ca, Cs, Mg, Sr solution
13)	Ewart et al.(1991)	Ewart, F. , Greenfield, B. F. , Haworth, A. , Rosevear, A. and William, S. J. : The effects of organics in SFR on sorption coefficients, SKB PROGRESS REPORT SFR91-01 (1991).	Pu	OPC/BFS, OPC/BFS/limestone, OPC/BFS/limestone_incl.SP, OPC/PFA, OPC/PFA_incl.SP, SRPC/limestone, SRPC/limestone_incl.SP	leaching OPC:PFA cement blocks, leaching Solid

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (3/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
14)	Fairhurst et al.(1995)	Fairhurst, A. J. , Warwick, P. and Richardson, S. : The effect of pH on europium-mineral interactions in the presence of humic acid, Radiochimica Acta, vol.69, pp.103-111 (1995).	Eu	bentonite, kaolin, montmorillonite, quartz	0.05M $NaClO_4$
15)	Filipska and Stamberg(2006)	Filipska, H. and Stamberg, K. : Sorption of Cs(I) and Sr(II) on a mixture of bentonite and magnetite using SCM + IExM: A parametric study, Journal of Radioanalytical and Nuclear Chemistry, vol.270, No.3, pp.531-542 (2006).	Cs, Sr	bentonite, magnetite	0.001M-0.5M $NaNO_3$
16)	Frasca et al.(2014)	Frasca, B. , Savoye, S. , Wittebroodt, C. , Leupin, O. X. and Michelot, J.-L. : Comparative study of Se oxyanions retention on three argillaceous rocks: Upper Toarcian (Tournemire, France), Black Shales (Tournemire, France) and Opalinus Clay (Mont Terri, Switzerland), Journal of Environmental Radioactivity, vol.127, pp.133-140 (2014).	Se	Black Shales, OPA, Upper Toarcian	Porewater
17)	Galambos et al.(2012)	Galambos, M. , Magula, M. , Dano, M. , Osacky, M. , Rosskopfova, O. and Rajec, P. : Comparative study of cesium adsorption on dioctahedral and trioctahedral smectite, Journal of Radioanalytical and Nuclear Chemistry, vol.293, pp.829-837 (2012).	Cs	montmorillonite, saponite, hectorite	CsCl
18)	Gao et al.(2015)	Gao, Y. , Shao, Z. and Xiao, Z. : U(VI) sorption on illite: effect of pH, ionic strength, humic acid and temperature, Journal of Radioanalytical and Nuclear Chemistry, vol.303, pp.867-876 (2015).	U	illite	0.001M-0.1M $NaNO_3$
19)	Ghayaza et al.(2011)	Ghayaza, M. , Le Forestier, L. , Muller, F. , Tournassat, C. and Beny, J.-M. : Pb(II) and Zn(II) adsorption onto Na- and Ca-montmorillonite in acetic acid/acetate medium: Experimental approach and geochemical modeling, Journal of Colloid and Interface Science, vol.361, pp.238-246 (2011).	Pb, Zn	Ca-, Na-montmorillonite	0.02M $CaCl_2$, 0.04M NaCl
20)	Glaus and Van Loon(2004)	Glaus, M. A. and Van Loon, L. R. : A generic procedure for the assessment of the effect of concrete admixtures on the retention behaviour of cement for radionuclides: Concept and case studies, PSI Bericht 04-02, Paul Scherrer Institute (2004).	Eu, Ni, Th	cement paste_incl.SP	Artificial cement pore water

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (4/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
21)	Godelitsas et al.(1996)	Godelitsas, A. , Misaelides, P. , Filippidis, A. , Charistos, D. and Anousis, I. : Uranium sorption from aqueous solutions on sodium-form of HEU-type zeolite crystals, Journal of Radioanalytical and Nuclear Chemistry, vol.208, No.2, pp.393-402 (1996).	U	Na-zeolite	U solution
22)	Grutter et al.(1992)	Grutter, A. , von Gunten, H. R. and Rossler, E. : Sorption of barium on unconsolidated glaciofluvial deposits and clay minerals, Radiochimica Acta, vol.58/59, pp.259-265 (1992).	Ba	chlorite, glaciofluvial minerals, illite, montmorillonite	synthetic groundwater
23)	Grutter et al.(1994a)	Grutter, A. , von Gunte, H. R. , Rossler, E. and Keil, R. : Sorption of Nickel and Cobalt on a Size-Fraction of Unconsolidated Glaciofluvial Deposits and on Clay Minerals, Radiochimica Acta, vol.65, pp.181-187 (1994).	Ba, Co, Cs, Ni, Sr	Glaciofluvial minerals, montmorillonite, illite, SiO_2 powder	synthetic groundwater
24)	Grutter et al.(1994b)	Grutter, A. , von Gunte, H. R. , Rossler, E. and Keil, R. : Sorption of Strontium on Unconsolidated Glaciofluvial Deposits and on Clay Minerals; Mutual Interference of Cesium, Strontium and Barium, Radiochimica Acta, vol.64, pp.247-252 (1994).	Ba, Cs, Sr	Glaciofluvial minerals, chlorite, illite, montmorillonite	synthetic groundwater
25)	Gu and Evans(2007)	Gu, X. and Evans, L. J. : Modelling the adsorption of Cd(II), Cu(II), Ni(II), Pb(II), and Zn(II) onto Fithian illite, Journal of Colloid and Interface Science, vol.307, pp.317-325 (2007).	Cd, Cu, Ni, Pb, Zn	illite	0.001M-0.1M $NaNO_3$
26)	Guo et al.(2009)	Guo, Z. , Xu, J. , Shi, K. , Tang, Y. , Wu, W. and Tao, Z. : Eu(III) adsorption/desorption on Na-bentonite: Experimental and modeling studies, Colloids and Surfaces A: Physicochemical and Engineering Aspects, vol.339, pp.126-133 (2009).	Eu	Na-bentonite	0.1M NaCl
27)	Hou et al.(2015)	Hou, Z. , Shi, K. , Wang, X. , Ye, Y. , Guo, Z. and Wu, W. : Investigation of Se(IV) sorption on Na-kaolinite: batch experiments and modeling, Journal of Radioanalytical and Nuclear Chemistry, vol.303, pp.25-31 (2015).	Se	Na-kaolinite	0.001M-0.1M NaCl
28)	Hsi and Langmuir(1985)	Hsi, C.-K. D. and Langmuir, D. : Adsorption of uranyl onto ferric oxyhydroxides: Application of the surface complexation site-binding model, Geochimica et Cosmochimica Acta, vol.49, pp.1931-1941 (1985).	U	$Fe(OH)_3$(am), goethite, hematite	0.1M $NaNO_3$

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (5/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
29)	Huitti et al.(1996)	Huitti, T. , Hakanen, M. and Lindberg, A. : Sorption of cesium, radium, protactinium, uranium, neptunium and plutonium on rapakivi granite, POSIVA report, POSIVA-96-23 (1996).	Ba, Cs, Np, Pa, Pu, U	granite	Groundwater
30)	Iida et al.(2011)	Iida, Y. , Tanaka, T. , Yamaguchi, T. and Nakayama, S. : Sorption behavior of selenium(-II) on rocks under reducing conditions, Journal of Nuclear Science and Technology, vol.48, No.2, pp.279-291 (2011).	Se	albite, biotite, calcite, chlorite, goethite, granodiorite, montmorillonite, pyrite, quartz, sandy mudstone, tuffaceous sandstone	0.05M, 0.5M NaCl, groundwater
31)	Iida et al.(2014)	Iida, Y. , Yamaguchi, T. and Tanaka, T. : Sorption behavior hydroselenide (HSe^-) onto iron-containing minerals, Journal of Nuclear Science and Technology, vol.51, No.3, pp.305-322 (2014).	Se	biotite, ferrous oxide, goethite, magnetite	0.01M-1M NaCl
32)	Jan et al.(2014)	Jan, Y.-L. , Tsai, S.-S. and Li, Y.-Y. : Determination of sorption and diffusion parameters of Se(IV) on crushed granite, Journal of Radioanalytical and Nuclear Chemistry, vol.301, pp.365-371 (2014).	Se	granite	GW, SW
33)	Jin et al.(2014)	Jin, Q. , Wang, G. , Ge, M. , Chen, Z. , Wu, W. and Guo, Z. : The adsorption of Eu(III) and Am(III) on Beishan granite: XPS, EPMA, batch and modeling study, Applied Geochemistry, vol.47, pp.17-24 (2014).	Am, Eu	granite	0.033M $CaCl_2$, 0.1M NaCl, synthetic groundwater
34)	Kasar et al.(2014)	Kasar, S. , Kumar, S. , Kar, A. , Bajpai, R. K. , Kaushik, C. P. and Tomar, B. S. : Retention behaviour of Cs(I), Sr(II), Tc(VII) and Np(V) on smectite-rich clay, Journal of Radioanalytical and Nuclear Chemistry, vol.300, pp.71-75 (2014).	Cs, Np, Sr, Tc	clay	0.01M-1M NaCl
35)	Kohler et al.(1999)	Kohler, M. , Honeyman, B. D. and Leckie, J. O. : Neptunium(V) sorption on hematite (α-Fe_2O_3) in aqueous suspension: The effect of CO_2, Radiochimica Acta, vol.85, pp.33-48 (1999).	Np	goethite, hematite, quartz	0.005M-0.1M $NaClO_4$
36)	Kohlickova and Jedinakova-Krizove(1998)	Kohlickova, M. and Jedinakova-Krizove, V. : Effect of pH and Eh on the sorption of selected radionuclides, Journal of Radioanalytical and Nuclear Chemistry, vol.229, No.1-2, pp.43-48 (1998).	Cs, I, Sr, Tc	bentonite	synthetic groundwater

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (6/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
37)	Kulmala and Hakanen(1995)	Kulmala, S. and Hakanen, M. : Sorption of alkaline-earth elements Sr, Ba and Ra from groundwater on rocks from TVO investigation areas, Nuclear Waste Commission of Finnish Power Companies, YJT-95-03 (1995).	Ba, Ra, Sr	granite, mica gneiss, tonalite	fresh groundwater, saline groundwater
38)	Kulmala et al.(1996)	Kulmala, S. , Hakanen, M. and Lindberg, A. : Sorption of protactinium on rocks in groundwaters from Posiva investigation sites, POSIVA-96-18 (1996)	Pa	granite, mica gneiss, tonalite	Groundwater
39)	Kumar et al.(2013)	Kumar, S. , Pente, A. S. , Bajpai, R. K. , Kaushik, C. P. and Tomar, B. S. : Americium sorption on smectite-rich natural clay from granitic groundwater, Applied Geochemistry, vol.35, pp.28-34 (2013).	Am, Eu	Na-clay, Ca-clay, natural clay, montmorillonite	0.01M-0.1M NaCl, 0.0335M $CaCl_2$, 0.035M Na_2SO_4, 0.1M $NaNO_3$, groundwater
40)	Kunimaru et al.(2012)	Kunimaru, T. , Morikawa, K. , Tachi, Y. , Kuno, Y. , Hosoya, S. , Shimoda, S. , Kato, H. , Nakazawa, T. , Ikuse, H. and Kubota, M. : Measurements of Sorption, Diffusion and Pore Physicality for Granite Sample, JAEA Technical Report, JAEA-Data/Code 2012-013 (2012), 96p.	Cs, Sr	granite-fracture, granite-Intact	0.5M NaCl, groundwater
41)	Kyllonen et al.(2008)	Kyllonen, J. , Hakanen, M. and Lindberg, A. : Sorption of Cesium on Olkiluoto Mica Gneiss and Granodiorite in Saline Groundwater; Retardation of Cesium Transport in Rock Fracture Columns, POSIVA, Working Report 2008-62 (2008).	Cs	biotite	0.1M $CaCl_2$, 0.1M KCl, 0.1M NaCl
42)	Lee et al.(2006)	Lee, C.-P. , Lan, P.-L. , Jan, Y.-L. , Wei, Y.-Y. , Teng, S.-P. and Hsu, C.-N. : Sorption of cesium on granite under aerobic and anaerobic conditions, Radiochimica Acta, vol.94, pp.679-682 (2006).	Cs	granite	SGW
43)	Lee et al.(2007)	Lee, C.-P. , Jan, Y.-L. , Lan, P.-L. , Wei, Y.-Y. , Teng, S.-P. and Hsu, C.-N. : Anaerobic and aerobic sorption of cesium and selenium on mudrock, Journal of Radioanalytical and Nuclear Chemistry, vol.274, No.1, pp.145-151 (2007).	Cs, Se	mudstone	SGW
44)	Lee et al.(2012)	Lee, C.-P. , Wu, M.-C. , Tsai, T.-L. , Wei, H.-J. , Men, L.-C. and Lin, T.-Y. : Comparative study on retardation behavior of Cs in crushed and intact rocks: two potential repository host rocks in the Taiwan area, Journal of Radioanalytical and Nuclear Chemistry, vol.293, pp.579-586 (2012).	Cs	basalt, granite	de-ionized water

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (7/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
45)	Lee et al.(2013a)	Lee, C.-P. , Liu, C.-Y. , Wu, M.-C. , Pan, C.-H. , Tsai, T.-L. , Wei, H.-J. and Men, L.-C. : Simulation of a 2-site Langmuir model for characterizing the sorption capacity of Cs and Se in crushed mudrock under various ionic strength effects, Journal of Radioanalytical and Nuclear Chemistry, vol.296, pp.1119-1125 (2013).	Cs, Se	mudstone	groundwater, seawater
46)	Lee et al.(2013b)	Lee, C.-P. , Liu, C.-Y. , Wu, M.-C. , Pan, C.-H. , Tsai, T.-L. , Lin, T.-Y. , Wei, H.-J. and Men, L.-C. : Application of non-linear heterogeneity-based isotherm models for characterizing sorption of Cs and Se on mudrocks, Journal of Radioanalytical and Nuclear Chemistry, vol.298, pp.749-754 (2013).	Cs, Se	mudstone	Seawater
47)	Lee(1973)	Lee, S. H. : Studies on the Sorption and Fixation of Cesium by Vermiculite, Journal of the Korean Nuclear Society, vol.5, No.4, pp.310-320 (1973).	Cs	K-vermiculite, Natural-vermiculite, Na-vermiculite	0.3M $NaNO_3$
48)	Lujaniene et al.(2010)	Lujaniene, G. , Benes, P. , Stamberg, K. , Sapolaite, J. , Vopalka, D. , Radziute, E. and Seiglo, T. : Effect of natural clay components on sorption of Cs, Pu and Am by the clay, Journal of Radioanalytical and Nuclear Chemistry, vol.286, pp.353-359 (2010).	Am, Cs, Pu	clay, goethite, hematite, magnetite	0.01M, 0.1M $NaNO_3$
49)	Maes and Cremers(1986)	Maes, A. and Cremers, A. : Europium sorption on a clay sediment: Sulphate and ionic strength effects, Environmental Sciences, pp.103-110 (1986).	Eu	Mg-clay, Mg-montmorillonite, Na-clay, Na-montmorillonite	0.1N-0.4M $Mg(NO_3)_2$+$MgSO_4$, 0.1N-0.4N $NaNO_3$+Na_2SO_4
50)	Marques Fernandes et al.(2012)	Marques Fernandes, M. , Baeyens, B. , Dahn, R. , Scheinost, A. C. and Bradbury, M. H. : U(VI) sorption on montmorillonite in the absence and presence of carbonate: A macroscopic and microscopic study, Geochimica et Cosmochimica Acta, vol.93, pp.262-277 (2012).	U	Swy-1 montmorillonite	0.1M $NaClO_4$
51)	Marques Fernandes et al.(2015)	Marques Fernandes, M. , Ver, N. and Baeyens, B. : Predicting the uptake of Cs, Co, Ni, Eu, Th and U on argillaceous rocks using sorption models for illite, Applied Geochemistry, vol.59, pp.189-199 (2015).	Co, Cs, Eu, Ni, Th, U	clay, illite	0.1M $NaClO_4$, synthetic porewater

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (8/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
52)	Missana et al.(2013)	Missana, T. , Benedicto, A. , Garcia-Gutierrez, M. and Alonso, U. : Modeling cesium retention onto Na-, K- and Ca-smectite: Effects of ionic strength, exchange and competing cations on the determination of selectivity coefficients, Geochimica et Cosmochimica Acta, vol.128, pp.266-277 (2014).	Cs	Ca-, K-, Na-smectite	0.001M-1M $NaClO_4$, 0.03M-0.1M $CaCl_2$, 0.01M-0.1M KCl
53)	Missana et al.(2014)	Missana, T. , Garcia-Gutierrez, M. , Benedicto, A. , Ayora, C. and De-Pourcq, K. : Modeling of Cs adsorption in natural mixed-clay and the effects of ion competition, Applied Geochemistry, vol.49, pp.95-102 (2014).	Cs	Ca-, K-, Na-, NH_4-illite, Ca-, K-, Na-, NH_4-kaolinite, RC clay, SJ clay	0.1M $CaCl_2$, 0.1M KCl, 0.1M NH_4Cl, 0.1M, 0.5M NaCl, natural saline water
54)	Muurinen and Tournassat(2011)	Muurinen, A. and Tournassat, C. : Sorption and Diffusion of Fe(II) in Bentonite -Sorption Studies-, POSIVA, Working Report 2011-09 (2011).	Fe	MX-80, smectite	0.05M, 0.3M NaCl
55)	Muurinen et al.(2014)	Muurinen, A. , Tournassat, C. , Hadi, J. , Greneche, J.-M. : Sorption and diffusion of Fe(II) in bentonite, Working Reports contain information on work in progress or pending completion, Working Report 2014-04 (2014).	Fe	MX-80, smectite	0.05M, 0.3M NaCl
56)	Nakata et al.(2000)	Nakata, K. , Nagasaki, S. , Tanaka, S. , Sakamoto, Y. , Tanaka, T. and Ogawa, H. : Sorption and reduction of neptunium(V) on the surface of iron oxides, Radiochimica Acta, vol.90, pp.665-669 (2002).	Np	magnetite, hematite	0.1M $NaNO_3$
57)	Nakata et al.(2002)	Nakata, K. , Nagasaki, S. , Tanaka, S. , Sakamoto, Y. , Tanaka, T. and Ogawa, H. : Sorption and desorption kinetics of Np(V) on magnetite and hematite, Radiochimica Acta, vol.88, pp.453-457 (2000).	Np	magnetite, hematite	0.1M $NaNO_3$
58)	Nebelung and Brendler(2010)	Nebelung, C. and Brendler, V. : U(VI) sorption on granite: prediction and experiments, Radiochimica Acta, vol.98, pp.621-625 (2010).	U	granite	0.1M $NaClO_4$
59)	Norden et al.(1994)	Norden, M. , Ephraim, J. H. and Allard, B. : The influence of a fulvic acid on the adsorption of europium and strontium by alumina and quartz: Effects of pH and ionic strength, Radiochimica Acta, vol.65, pp.265-270 (1994).	Eu, Sr	alumina, quartz	0.01M, 0.1M $NaClO_4$
60)	Olin et al.(2006)	Olin, M. , Puukko, E. , Puhakka, E. , Lehikoinen, J. , Lindberg, A. and Hakane, M. : Sorption of nickel on biotite, The Technical Research Centre of Finland(VTT), VTT-R-08046-06 (2006).	Ni	biotite	0.05M, 0.5M $NaClO_4$

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (9/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
61)	Pabalan et al.(1998)	Pabalan, R. T. , Turner, D. R. , Bertetti, F. P. and Prikryl, J. D. : Uranium(VI) sorption onto selected mineral surfaces: Key Geochemical Parameters. Chapter 3., Adsorption of Metals by Geomedia, Academic Press, San Diego, California, E. Jenne, ed., pp.99-130 (1998).	U	alumina, Na-clinoptilolite, Na-montmorillonite, quartz	0.1M, 1M $NaNO_3$
62)	Papelis(2001)	Papelis, C. : Cation and anion sorption on granite from the Project Shoal Test Area, near Fallon, Nevada, USA, Advances in Environmental Research, vol.5, pp.151-166 (2001).	Cr, Cs, Pb, Se	granite	0.01M-1M $NaNO_3$, H-2 GW, HC-4 GW, HS-1GW
63)	Sabodina et al.(2006b)	Sabodina, M. N. , Kalmykov, S. N. , Sapozhnikov, Yu. A. and Zakharova, E. V. : Neptunium, Plutonium and ^{137}Cs Sorption by Bentonite Clays and Their Speciation in Pore Waters, Journal of Radioanalytical and Nuclear Chemistry, vol.270, No.2, pp.349-355 (2006).	Cs, Np, Pu	bentonite	0.001M-0.1M $NaClO_4$
64)	Schultz and Grundl(2004)	Schultz, C. and Grundl, T. : pH dependence of ferrous sorption onto two smectite clays, Chemosphere, vol.57, pp.1301-1306 (2004).	Fe	Wyoming montmorillonite, SWa-1 montmorillonite	deoxygenated water
65)	Shi et al.(2014)	Shi, K. , Ye, Y. , Guo, N. , Guo, Z. and Wu, W. : Evaluation of Se(IV) removal from aqueous solution by GMZ Na-bentonite: batch experiment and modeling studies, Journal of Radioanalytical and Nuclear Chemistry, vol.299, pp.583-589 (2014).	Eu, Se	Na-bentonite	0.1M NaCl
66)	Shimoda et al.(2014)	Shimoda, S. , Nakazawa, T. , Kato, H. , Tachi, Y. and Seida, Y. : The effect of alkaline alteration on sorption properties of sedimentary rock, Material Research Society Symposium Proceedings, vol.1665, pp.179-184 (2014).	Cs, Ni, Th	mudstone	synthetic groundwater
67)	Soltermann et al.(2013)	Soltermann, D. , Marques Fernandes, M. , Baeyens, B. , Dahn, R. , Miehe-Brendle, J. , Wehrli, B. and Bradbury, M. H. : Fe(II) Sorption on a Synthetic Montmorillonite. A Combined Macroscopic and Spectroscopic Study, Environmental Science and Technology, vol.47, pp.6978-6986 (2013).	Fe	Na-montmorillonite	0.1M, 0.3M $NaClO_4$

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (10/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
68)	Songsheng et al.(2012)	Songsheng, L. , Hua, X. , Mingming, W. , Xiaoping, S. and Qiong, L. : Sorption of Eu(III) onto Gaomiaozi bentonite by batch technique as a function of pH, ionic strength, and humic acid, Journal of Radioanalytical and Nuclear Chemistry, vol.292, pp.889-895 (2012).	Eu	Na-bentonite	0.001M-0.05M $NaClO_4$
69)	Tachi and Yotsuji(2014)	Tachi, Y. and Yotsuji, K. : Diffusion and sorption of Cs+, Na+, I- and HTO in compacted sodium montmorillonite as a function of porewater salinity: Integrated sorption and diffusion model, Geochimica et Cosmochimica Acta, vol.132, pp.75-93 (2014).	Cs	Na-bentonite	CsCl solution
70)	Tachi et al.(2009)	Tachi, Y. , Seida, Y. , Doi, R. , Xia, X. and Yui, M. : Sorption and diffusion of Cs in Horonobe-URL's sedimentary rock: Comparison and model prediction of retardation parameters from sorption and diffusion experiments, Materials Research Society Symposium Proceedings, vol.1124, pp.573-579 (2009).	Cs	mudstone	synthetic groundwater
71)	Tachi et al.(2011)	Tachi, Y. , Yotsuji, K. , Seida, Y. and Yui, M. : Diffusion and Sorption of Cs^+, I^- and HTO in Samples of the Argillaceous Wakkanai Formation from the Horonobe URL, Japan: Clay-based Modeling Approach, Geochimica et Cosmochimica Acta, vol.75, pp.6742-6759 (2011).	Cs	mudstone	GW
72)	Tachi et al.(2015)	Tachi, Y. , Ebina, T. , Takeda, C. , Saito, T. , Takahashi, H. , Ohuchi, Y. and Martin, A. J. : Matrix diffusion and sorption of Cs^+, Na^+, I^- and HTO in granodiorite: Laboratory-scale results and their extrapolation to the in situ condition, Journal of Contaminant Hydrology, vol.179, pp.10-24 (2015).	Cs, Na	granodiorite	synthetic groundwater
73)	Tsukamoto and Ohe(1993)	Tsukamoto M. and Ohe, T. : Effects of biotite distribution on cesium diffusion in granite, Chemical Geology, vol.107, pp.29-46 (1993).	Cs	granite	CsCl
74)	Ugur and Turhan(2011)	Ugur, F. A. and Turhan, S. : Experimental investigation of radiocesium sorption on ceramic clay using a batch method, Journal of Radioanalytical and Nuclear Chemistry, vol.288, pp.347-350 (2011).	Cs	clay	CsCl
75)	Van Loon et al.(2009)	Van Loon, L. R. , Baeyens, B. and Bradbury, M. H. : The sorption behaviour of caesium on Opalinus Clay: A comparison between intact and crushed material, Applied Geochemistry, vol.24, pp.999-1004 (2009).	Cs	clay	pore water

Table 3.1 Overview of 83 references selected for updating the JAEA-SDB (11/11)

No.	Reference	Details of reference	Element	Solid Phase	Solution Type
76)	Wahlberg and Fishman(1962)	Wahlberg, J. S. and Fishman, M. J. : Adsorption of Cesium on Clay Minerals, Geological Survey Bulletin 1140-A, United State Government Printing Office, Washington: 1962 (1962).	Cs	Ca-, K-, Mg, Na-halloysite, Ca-, K-, Mg, Na-kaolinite, K-, Na-illite, Ca-, K-, Mg, Na-montmorillonite	0.002M-0.2M KCl, 0.002M-0.2M NaCl, 0.002N-0.2N $CaCl_2$, 0.002N-0.2N $MgCl_2$
77)	Wahlberg et al.(1965)	Wahlberg, J. S. , Baker, J. H. , Vernon, R. W. and Dewar, R. S. : Exchange Adsorption of Strontium on Clay Minerals, Geological Survey Bulletin 1140-C, United State Government Printing Office, Washington: 1965 (1995).	Sr	Ca-, K-, Mg-, Na-illite, Ca-, K-, Mg-, Na-kaolinite, Ca-, K-, Mg-, Na-montmorillonite	0.00007M-0.007M $MgCl_2$, 0.001M-0.1M $CaCl_2$, 0.01M-0.2M KCl, 0.01M-0.2M NaCl
78)	Yan et al.(2011)	Yan, L. , Qiaohui, F. and Wangsuo, W. : Sorption of Th(IV) on goethite: effects of pH, ionic strength, FA and phosphate, Journal of Radioanalytical and Nuclear Chemistry, vol.289, pp.865-871 (2011).	Th	goethite	0.01M-0.5M NaCl, 0.1M $NaNO_3$
79)	Yang et al.(2010)	Yang, Z. , Huang, L. , Guo, Z. , Montavon, G. and Wu, W. : Temperature effect on U(VI) sorption onto Na-bentonite, Radiochimica Acta, vol.98, No.12, pp.785-791 (2010).	U	Na-bentonite	0.1M NaCl
80)	Yildiz et al.(2011)	Yildiz, B. , Erten, H. N. and Kis, M. : The sorption behavior Cs^+ ion on clay minerals and zeolite in radioactive waste management: sorption kinetics and thermodynamics, Journal of Radioanalytical and Nuclear Chemistry, vol.288, pp.475-483 (2011).	Cs	bentonite, kaolinite, zeolite	Groundwater
81)	Zazzi et al.(2012)	Zazzi, A. , Jakobsson, A.-M. and Wold, S. : Ni(II) sorption on natural chlorite, Applied Geochemistry, vol.27, pp.1189-1183 (2012).	Ni	chlorite	0.01M-0.5M $NaClO_4$
82)	Zazzi(2009)	Zazzi, A. : Chlorite: Geochemical properties, Dissolution kinetics and Ni(II) sorption, Ph. D thesis, Dept. of Chemistry, KTH Chemical Science and Engineering (2009).	Ni	chlorite	0.01M-0.5M $NaClO_4$
83)	Zhang et al.(2010)	Zhang, H. , Yu, X. , Chen, L. , Jing, Y. and Ge, Z. : Study of ^{63}Ni adsorption on NKF-6 zeolite, Journal of Environmental Radioactivity, vol.101, pp.1061-1069 (2010).	Ni	zeolite	0.001M-0.1M $NaClO_4$, 0.01M NaCl, 0.01M $NaNO_3$, 0.01M $LiClO_4$, 0.01M $KClO_4$

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

Newly added 83 references for JAEA-SDB listed in Table 3.1 are not included in this reference list.

3.2 QA evaluation on Criteria-I and -II

This section presents the QA/classification results for K_d data conducted in this update. In addition to 83 references newly selected in this update (see 3.1), the K_d data for granitic rocks that QA evaluation was not so far performed were additionally evaluated as shown in the following list (Table 3.2). The evaluation method is described in detail in the previous report7). For transparency and ease of presentation, all results of Criteria I and II are presented in tabular form, using the format of the following table throughout. The results pertaining Criteria III are discussed (in next section 3.3) subsequently and are illustrated in the form of plots of K_d vs. a relevant master variable (typically pH), where applicable. 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. In this report, the QA results for only Am are presented as an illustration, although all QA results can be access in JAEA-SDB.

Data table Am/1 : REF: Barney and Brown(1979)
JAEA-SDB version 5 - DATA: Am/Basaltic rocks; basalt#1, basalt#2, basalt#3, #32535～32537, #44376～44406
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	All mandatory information is provided.	Yes
I-b SDB	K_d values are provided in [mL/g] and equilibrated solution concentration from figure; ・#32535～32537 ・#44376～44406	 class 1 class 4
II-a REF	It is indicated mineral composition, chemical composition, surface are and CEC for basalts used in the experiments.	A
II-b SDB REF	Final pH value is given. The synthetic groundwater used in the experiment was conditioned with 295mg/L $NaHCO_3$. The pH was reported to be constant for each groundwater over the 154 days.	A
II-c SDB REF	Experiments had been performed under aerobic condition. Am is not a redox sensitive element.	A/B
II-d SDB	The concentrations of major ions (Na, Ca, K, Mg, Si) in the final synthetic groundwater are given as figure. And initial groundwater before equilibrated with solid; ・#44376～44406 ・#32535～32537	 A/B C/D
II-e SDB	A temperature was carried out at room temperature (23±2°C).	A/B
II-f SDB REF	A L/S ratio of 6mL/g is indicated. 2g solid were added to 30mL solution. Particle size of basalt was given “0.3 to 0.9mm”.	A/B
II-g SDB	Based on the information given in the SDB, sorption values can be calculated; ・#32535, #44391～44400 (5～95%) ・#44387～44389, #44404 (96～98%) ・Others (>98%)	 A B C/D

II-h SDB REF	An initial Am concentration 1.37×10^{-8} [M] is indicated. Based on the experimental and thermodynamic data in JAEA TDB, rating B is applied.	B
II-i SDB	A phase separation method was carried out by centrifugation for groundwater-B14 and filtration for groundwater-B.	C/D
II-j SDB	It is indicated that contact time was 14 days. In this experiment, kinetics sorption reaction was studied. Am concentration was indicated as a function of reaction time with figure.	A/B
II-k REF	The samples were shaken. Kinetics information was indicated.	A/B
II-l REF	No variation in L/S or initial Am concentration is indicated.	C/D
II-mREF	The experiments were carried out in polycarbonate centrifuge tube. No correction for sorption on vessel walls is reported.	B
II-n SDB	No error information is available.	D
II-o SDB	Changed parameters were reaction time and solid type (flesh solid and weathered solid).	D

Data table Am/2 : REF: Mucciardi et al. (1979)
JAEA-SDB version 5 - DATA: Am/Other minerals; albite, anorthite, augite, biotite, enstatite,
hornblende, microcline, quartz, #57381～57425, #58235～58298
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	It is indicated that no information is available regarding the initial RN concentration.	No unreliable

Data table Am/3 : REF: Shimooka et al. (1985)
JAEA-SDB version 5 - DATA: Am/Basaltic rocks; basalt, andesite, #69901, #69902, #69909, #69910
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	The experiment is not performed by a batch technique (Column dynamic circulation experiment).	No

Data table Am/4 : REF: Shimooka et al. (1985)
JAEA-SDB version 5 - DATA: Am/Granitic rocks; granite, granodiorite,
#69917, #69918, #69925, #69926
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	The experiment is not performed by a batch technique (Column dynamic circulation experiment).	No

Data table Am/5 : REF: Shimooka et al. (1985)
JAEA-SDB version 5 - DATA: Am/Other minerals; rhyolite, #69933, #69934
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	The experiment is not performed by a batch technique (Column dynamic circulation experiment).	No

Data table : Am/6 : REF: Barney and Anderson(1979)
JAEA-SDB version 5 - DATA: Am/Basaltic rocks; basalt#1, basalt#2, #44207～44212
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	Information for pH is not provided.	No

Data table : Am/7 : REF: Nakayama et al.(1986)
JAEA-SDB version 5 - DATA: Am/Other minerals; quartz, #56807～56815
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	All mandatory information is provided.	Yes
I-b SDB	A table with K_d values is given.	class 1
II-a REF	As solid phase, Myoken quartz is indicated. Mineral composition is not reported. Mesh size of quartz sample is indicated. Major and minor mineralogy are not reported.	C/D
II-b SDB REF	Final pH values are indicated. Approximate pH values are reported (e.g. pH ～7).	B
II-c SDB REF	It is indicated that experiments had been performed under aerobic conditions. Eh values are not reported. Am is not redox sensitive. The oxidation state of Am is not reported. It is reported that Am(III) was used for the experiments.	A/B
II-d SDB REF	As water type distilled water is indicated. Final solution compositions are not given. Since information about mineral composition including impurities is lacking as well, it is impossible to estimate the final solution composition.	unreliable

Data table Am/8: REF: Murali and Mathur (2002)
JAEA-SDB version 5 - DATA: Am/Bentonite (Clay Minerals); bentonite, #79794～79801
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	Information of initial Am concentration is not provided.	No

Data table Am/9: REF: Lujaniene et al.(2010)
JAEA-SDB version 5 - DATA: Am/Clay minerals; clay#1, #83179～83198
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	All mandatory information is provided.	Yes
I-b SDB	The adsorption [%] is taken from a figure.	class 6
II-a REF	The solid used this experiments is Triassic clay. The chemical composition and surface coatings of clay are reported. There is not the further information.	C/D
II-b REF	The pH values are adjusted with HNO_3 or NaOH.	A
II-c SDB REF	The experimental condition is not reported. Am(III) is not sensitive to redox condition.	A/B
II-d SDB REF	Sorption measurements are carried out in 0.01M and 0.1M $NaNO_3$ solution. However, the composition of solution equilibrated with solid after experiments are not indicated.	C/D

II-e SDB	The experiments are performed at 25°C.	A/B
II-f SDB	The solid/liquid ratio is reported. However, the volume of liquid and the mass of solid are not reported.	C/D
II-g REF	The following sorption values were calculated from K_d and L/S ratios; ･#83180, #83187 (95≤%<98) ･Others (5%～95%)	 B A
II-h SDB REF	An initial Am-concentration 3.0×10^{-11} [M] is indicated. The solubility calculation is performed using JAEA TDB (100331c1.tdb). The solubility based on these value are evaluated, an initial Am concentration of all data points are lower than the calculated solubility.	A
II-i SDB	It is indicated that phase separation is carried out by centrifugation at 10,000～20,000g.	C/D
II-j SDB REF	The experiments are performed for 2 days. It is not confirmed whether the experiment condition is reached to the equilibrium.	C/D
II-k REF	It is indicated that suspensions are shaken for time sufficient for establishment of sorption equilibrium.	A/B
II-l REF	The initial concentration of Am has not been varied.	C/D
II-m REF	The experimental vessel is a polypropylene bottle. Adsorption losses of the radionuclides from solutions to polypropylene bottle walls varied from 0.1 to 1% of the total radionuclide present and decreased with an increase of the sorption time. They are taken into account in calculations.	A
II-n SDB	The error estimate and the replication are not indicated.	D
II-o SDB	The pH value and ionic strength of solution have been varied.	B

Data table Am/10: REF: Lujaniene et al.(2010)
JAEA-SDB version 5 - DATA: Am/Other minerals; goethite, hematite, magnetite, #83199～83231
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	The adsorption [%] is taken from a figure.	class 6
II-a SDB REF	The solid used this experiments is the synthetic iron oxides (goethite, hematite and magnetite). There is not the further information.	C/D
II-b REF	The pH values are adjusted with HNO_3 or NaOH.	A
II-c SDB REF	The experimental condition is not reported. Am(III) is not sensitive to redox condition.	A/B
II-d SDB REF	Sorption measurements are carried out in 0.1M $NaNO_3$ solution. However, the composition of solution equilibrated with solid after experiments are not indicated.	C/D
II-e SDB	The experiments are performed at 25°C.	A/B
II-f SDB	The solid/liquid ratio is reported. However, the volume of liquid and the mass of solid are not reported.	C/D
II-g REF	The following sorption values were calculated from K_d and L/S ratios; ･#83220, #83226, #83228, #83229, #83231 (98≤%<100) ･#83203, #83216～83219, #83223～83225, #83227, #83230 (95≤%<98) ･Others (5%～95%)	 C/D B A
II-h SDB REF	An initial Am-concentration 3.0×10^{-11} [M] is indicated. The solubility calculation is performed using JAEA TDB (100331c1.tdb). The solubility based on these value are evaluated, an initial Am concentration of all data points are lower than the calculated solubility.	A

II-i SDB	It is indicated that phase separation is carried out by centrifugation at 10,000～20,000g.	C/D
II-j SDB REF	The experiments are performed for 2 days. It is not confirmed whether the experiment condition is reached to the equilibrium.	C/D
II-k REF	It is indicated that suspensions are shaken for time sufficient for establishment of sorption equilibrium.	A/B
II-l REF	The initial concentration of Am has not been varied.	C/D
II-m REF	The experimental vessel is a polypropylene bottle. Adsorption losses of the radionuclides from solutions to polypropylene bottle walls varied from 0.1 to 1% of the total radionuclide present and decreased with an increase of the sorption time. They are taken into account in calculations.	A
II-n SDB	The error estimate and the replication are not indicated.	D
II-o SDB	The pH value has been varied.	C

Data table Am/11: REF: Kumar et al.(2013)
JAEA-SDB version 5 - DATA: Am/Clay minerals; Na-clay, Ca-clay, #87947～88008
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	The K_d [mL/g] is taken from a log figure.	class 5
II-a REF	The solids used the experiments are Na-clay and Ca-clay. The CEC values, surface area and chemical composition are reported.	A
II-b REF	The pH is adjusted with NaOH or HCl solution.	A
II-c SDB REF	All experiments are performed under N_2 atmosphere condition. Am (III) is not sensitive to redox condition.	A/B
II-d SDB REF	Sorption measurements are carried out in 0.01M, 0.05M and0.1M NaCl solution, 0.1M $NaNO_3$ solution, 0.035M Na_2SO_4 solution, and 0.0335M $CaCl_2$ solution. The composition of solution after experiments is not indicated.	C/D
II-e SDB	All experiments are conducted at room temperature (25±2°C).	A/B
II-f SDB REF	The mass of solid are not reported. It cannot be judged whether surface area of solid is larger than surface area of reaction vessel.	C/D
II-g REF	The following sorption values were calculated from K_d and L/S ratios; ・#87955～87959, #87969～87973, #87979～87982, #87998～88001 : $0<\%\leq 2$ or $98\leq\%<100$ ・#87954, #87966～87968, #87974～87978, #87983～87989, #87997, #88004 : $2<\%\leq 5$ or $95\leq\%<98$ ・Other datapoints : $5<\%<95$	C/D B A
II-h SDB REF	An initial Am-concentration 6.0×10^{-9} [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated; ・#87973 : Higher than solubility ・#87958, #87959, #88001 : Higher than one-fifth of solubility ・Other datapoints : Lower than solubility.	unreliable B A
II-i SDB	It is indicated that phase separation is carried out by centrifugation (16,500rpm/45min).	C/D
II-j SDB REF	The reaction time is 48 hours. The reaction time is decided, based on a preliminary kinetic experiment.	A/B
II-k REF	Information for the agitation method is not reported.	C/D
II-l REF	Initial Am concentration is not varied.	C/D

II-m REF	The experimental vessels are polypropylene tubes. It is indicated that the wall sorption is found to be negligible (～2% at higher pH values).	A
II-n REF	It is indicated that an uncertainty is ±0.2 log units in the log K_d values at lower pH values, while it increases with pH to ±0.5 log units at the highest pH values.	C
II-o SDB	The pH value and ionic strength have been varied.	B

Data table Am/12: REF: Jin et al.(2014)
JAEA-SDB version 5 - DATA: Am/Granitic rocks; granite, granite+FA(2mg/L), granite+FA(10mg/L), granite+FA(20mg/L), #88210～88279
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	The K_d [mL/g] is taken from figure; ・#88210～88235, #88248～88279 The adsorption quantity is taken from a figure; ・#88236～88247	class 5 class 6
II-a REF	The solid used the experiments is Beishan granite. The CEC values and surface area are reported. The main mineral composition is not reported.	C/D
II-b REF	The pH is adjusted with NaOH or HCl solution.	A
II-c SDB REF	All experiments are performed under N_2 atmosphere condition. Am(III) is not sensitive to redox condition.	A/B
II-d SDB REF	Sorption measurements are carried out in 0.1M NaCl and 0.03M $CaCl_2$. The composition of solution after experiments is not indicated.	C/D
II-e SDB	All experiments are conducted at ambient temperature (22±2°C).	A/B
II-f SDB REF	The mass of solid are not reported. It cannot be judged whether surface area of solid is larger than surface area of reaction vessel.	C/D
II-g REF	The following sorption values were calculated from K_d and L/S ratios; ・#88271～88273 : 0<%≤2 or 98≤%<100 ・#88218～88220, #88222, #88223, #88235, #88270, #88274～88276 : 2<%≤5 or 95≤%<98 ・Other datapoints : 5<%<95	C/D B A
II-h SDB REF	An initial Am-concentration 5.0×10^{-10}～1.0×10^{-3} [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated; ・#88223, #88235 : Higher than solubility ・#88222, #88234, #88247, #88258, #88267, #88279 : Higher than one-fifth of solubility ・Other datapoints : Lower than solubility	unreliable B A
II-i SDB	It is indicated that phase separation is carried out by centrifugation (18,000g/30min).	C/D
II-j SDB REF	The reaction time is 5 days. Prior experiments indicated that adsorption equilibrium can be reached within 5 days.	A/B
II-k REF	The agitation method is a shaking.	A/B
II-l REF	The sorption isotherm is indicated.	A
II-m REF	The experimental vessels are polypropylene tubes.	A
II-n REF	The error is not estimated. Also, the number of replicate is not reported.	D
II-o SDB	The initial Am concentration and pH have been varied.	B

Data table Am/13: REF: Bradbury and Baeyens(2006)
JAEA-SDB version 5 - DATA: Am/Bentonite (smectite); Na-montmorillonite, Ca-montmorillonite,
#89328～89371
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	**Evaluation**	**Rating**
I-a.1SDB	All mandatory fields are completed.	Yes
I-a.2SDB	All mandatory information is provided.	Yes
I-b SDB	The log R_d [L/kg] is taken from figure.	class 6
II-a SDB	The solid used this experiments is purified SWy-1 montmorillonite. The CEC value and mineral composition are reported. The surface area isn’t reported.	B
II-b SDB REF	The final pH is reported. The pH values are adjusted with MES, MOPS or TRIS.	A
II-c SDB REF	The experiments are performed under inert atmosphere condition. Am(III) is not sensitive to redox condition.	A/B
II-d SDB REF	Sorption measurements are carried out in 0.1M $NaClO_4$ or 0.066M $CaCl_2$. The composition of solutions after experiment is not reported.	C/D
II-e SDB	The experimental temperature is not reported.	C/D
II-f SDB REF	The mass of solid and specific surface area is not reported. It cannot be judged whether the surface of solid is larger than the surface area of vessel wall.	C/D
II-g REF	The following sorption values were calculated from K_d and L/S ratios; ・#89339～89352, #89366～89371 : $0<\%\leq 2$ or $98\leq\%<100$ ・#89334, #89337, #89338 : $2<\%\leq 5$ or $95\leq\%<98$ ・Other datapoints : $5<\%<95$	C/D B A
II-h SDB REF	Initial Am concentration 1.5×10^{-10} or 6.2×10^{-8} [M] is indicated. The solubility calculation is performed using JAEA TDB (140331c0.tdb). The solubility based on this value is evaluated; ・#89368～89371 : Higher than solubility ・#89366, #89367 : Higher than a one-fifth of solubility ・Other datapoints : Lower than solubility	unreliable B A
II-i SDB	It is indicated that separation method is a centrifuge (105,000g/1hour).	C/D
II-j SDB REF	The reaction time is reported for 7 days. The kinetic experiments are not performed. However, it is considered that the experimental condition reaches to the equilibrium.	A/B
II-k REF	The agitation method is a shaking.	A/B
II-l REF	The initial Am concentration has not been varied.	C/D
II-mREF	The experimental vessel is a polyethylene centrifuge tube.	B
II-n REF	The error estimate is carried out with error bars in the figure. Experiments are normally carried out in triplicate.	A
II-o SDB	The pH has been varied.	C

Table 3.2 Overview of references additionally evaluated the QA (1/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Akiba and Hashimoto(1990)	Akiba, K. and Hashimoto, H. : Distribution Coefficient of Strontium on Variety of Minerals and Rocks, Journal of Nuclear Science and Technology, vol.27, No.3, pp.275-297 (1990).	Sr	albite, andesite, chlorite, epidote, forsterite, granite, grossularite, hedenbergite, hornblende, K-feldspar, limestone, microcline, plagiorhyolite, propylite, quartz, sandstone, shale, tuff	Sr solution
Akiba et al.(1986)	Akiba, K. , Hashimoto, H. , Okuno, T. and Yabe, I. : Ion exchange capacity of rock and distribution coefficient of cesium, Natural barrier of land disposal, RWM-86006, pp.1-11 (1986).	Cs	albite, andesite, basalt, biotite, granite, K-feldspar, limestone, quartz, sandstone, tuff	RI water
Akiba et al.(1989)	Akiba, K. , Hashimoto, H. and Kanno, T. : Distribution Coefficient of Cesium and Cation Exchange Capacity of Minerals and Rocks, Journal of Nuclear Science and Technology, vol.26, No.12, pp.1130-1135 (1989).	Cs	albite, andesite, basalt, biotite, chlorite, forsterite, granite, grossularite, hornblende, K-feldspar, limestone, plagio rhyolite, quartz, sandstone, shale, tuff	distilled water
Allard et al.(1978)	Allard, B., Kipatsi, H. and Torstenfelt, B. : Sorption of long-lived radionuclides on clays and rocks, part 2, KBS Technical Report 98, in Swedish (Abstract in English) (1978).	Am, Np, Pu, Ra, Th, Zr	bentonite, granite	groundwater
Allard et al.(1979a)	Allard, B. , Kigatsi, H. and Torstenfelt, B. : Technetium: Reduction and Sorption in Granitic Bedrock, Radiochemical and Radioanalytical Letters, vol.37, No.4/5, pp.223-230 (1979).	Tc	granite, biotite, magnetite	groundwater
Allard et al.(1979b)	Allard, B. , Rydberg, J. , Kipatsi, H. and Torstenfelt, B. : Disposal of Radioactive Waste in Granitic Bedrock, American Chemical Society, No.4, pp.47-73 (1979).	Am, Ce, Cs, Eu, I, Nd, Np, Pu, Ra, Sr, Tc, Th, U, Zr	bentonite/quartz, biotite, chlorite, granite, hornblende, magnetite	Aq1105, Aq293
Allard et al.(1981)	Allard, B. , Torstenfelt, B. and Andersson, K. : Sorption studies of $H^{14}CO_3^-$ on some geologic media and concrete., Scientific basis for nuclear waste management, vol.3, pp.465-472 (1981).	C	bentonite/quartz, calcite, cement paste, clayish moraine, concrete, granite, Na-montmorillonite, sandy moraine	Artificial ground water

Table 3.2 Overview of references additionally evaluated the QA (2/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Amaya et al.(1995)	Amaya, T. , Kobayashi, W. and Suzuki, K. : Absorption Study of the Tc(IV) on Rocks and Minerals under Simulated Geological Conditions, Materials Research Society Symposium Proceedings, vol.353, pp.1005-1012 (1995).	Tc	granite, biotite, K-feldspar, plagiclase, quartz, tuff	underground water
Andersson et al.(1983b)	Andersson, K. , Torstenfelt, B. and Allard, B. : Sorption of Radionuclides in Geologic Systems, SKB-KBS Technical Report, No.83-63 (1983).	Cs, I, Sr, Tc	apatite, attapulgite, bentonite, biotite, calcite, chalcopyrite, chlorite, cinnabar, corundum, $Cu(OH)_2$, diabase, dolomite, epidote, $Fe(OH)_3$, fluorite, galena, gneiss, granite, gypsum, halloysite, hematite, hornblende, illite, kaolinite, laumontite, limonite, magnetite, microcline, montmorillonite, muscovite, olivine, orthoclase, $Pb(OH)_2$, plagioclase, prehnite, pyrite, quartz, serpentine, stilbite	0.1M NaCl, 4M NaCl, artificial groundwater, groundwater
Andre et al.(2006)	Andre, M. , Malmstroem, M. E. and Neretnieks, I. : Determining sorption coefficients in intact rock using an electrical potential gradient as a driving force for migration, Materials Research Society Symposium Proceedings, vol.932, pp.975-982 (2006).	Cs	granite	distilled water
Ashida et al.(1999)	Ashida, T. , Shibutani, T, Sato, H. , Tachi, Y. , Kitamura, A. and Kawamura, K. : Nuclide Migration Study in the QUALITY -Data Acquisitions for the Second Progress Report-, JNC Technical Report, JNC TN8400 99-083 (1999), 63p.	Cm, Cs, Np, Pb	basalt, bentonite, granodiorite, mudstone, sandstone, smectite, tuff	0.01M-1M NaCl
Baik et al.(2003)	Baik, M. H. , Hyun, S. P. and Hahn, P. S. : Surface and bulk sorption of uranium(VI) onto granite rock, Journal of Radioanalytical and Nuclear Chemistry, vol.256, pp.11-18 (2003).	U	granite	0.01M NaClO4
Barney and Anderson(1979)	Barney, G. S. and Anderson, P. D. : The Kinetics and Reversibility of Radionuclide Sorption Reactions with Rocks- Progress Report for Fiscal Year 1978, PNL Report, PNL-SA-7352, pp.163-218 (1979).	Am, Cs, Np, Pu, Sr	argillite, basalt, granite	groundwater
Barney and Brown(1979)	Barney, G. S. and Brown, G. E. : The Kinetics and Reversibility of Radionuclide Sorption Reactions with Rocks, RHO-ST-29, pp.261-315 (1979).	Am, Cs, Np, Pu, Sr	argillite, basalt, granite	groundwater

Table 3.2 Overview of references additionally evaluated the QA (3/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Baston et al.(1992b)	Baston, G. M. N. , Berry, J. A. , Littleboy, A. K. and Pilkington, N. J. : Sorption of Activation Products on London Clay and Dungeness Aquifer Gravel, Radiochimica Acta, vol.58/59, pp.225-233 (1992).	Co, Eu, Nb, Ni, Sm	clay, gravel, mudrock	clay water, groundwater, porewater
Baston et al.(1993)	Baston, G. M. N., Berry, J. A. and Linklater, C. M. : Factors influencing the sorption of radium onto geological materials, Analytical Proceedings, vol.30, pp.194-195 (1993).	Ra	mudrock, tuff	porewater, cement water
Baston et al.(1995a)	Baston, G. M. N. , Berry, J. A. , Brownsword, M. , Cowper, M. M. , Heath, T. G. and Tweed, C. J. : The Sorption of Uranium and Technetium on Bentonite, Tuff and Granodiorite, Materials Research Society Symposium Proceedings, vol.353, pp.989-996 (1995).	Tc, U	granodiorite, Kunigel V1, tuff	de-ionized water, sea water
Baston et al.(1997)	Baston, G. M. N. , Berry, J. A. , Brownsword, M. , Heath, T. G. , Ilett, D. J. , Tweed, C. J. and Yui, M. : The Effect of Temperature on the Sorption of Technetium, Uranium, Neptunium and Curium on Bentonite, Tuff and Granodiorite, Materials Research Society Symposium Proceedings, vol.465, pp.805-812 (1997).	Cm, Np, Tc, U	granodiorite, Kunigel V1, tuff	de-ionized water
Baston et al.(1998)	Baston, G. M. N. , Berry, J. A. , Brownword, M. , Cowper, M. M. , Haworth, A. , Heath, T. G. , Ilett, D. J. , McCrohon, R. and Tweed C. J. : Sorption Studies of Radioelements on Geological Materials, AEAT-3142(Revised), AEA Technology plc (1998).	Am, Po, Pu	granodiorite, Kunigel V1, tuff	de-ionized water
Baston et al.(2000)	Baston, G. M. N. , Berry, J. A. , Brownsword, M. , Ilett, D. J. , Linklater, C. M. , Tweed, C. J. and Yui, M. : Effect of Carbonate Concentration on the Sorption of Plutonium onto Geological Materials, Materials Research Society Symposium Proceedings, vol.608, pp.293-298 (2000).	Pu	basalt, mudstone, sandstone	de-ionized water, seawater
Benischek et al.(1992a)	Benischek, I. , Hess, V. and Metzker, E. : Preliminary Experiments for Measuring Kd Values for Cesium and Strontium. To Be Used in Site Evaluations, OEFZS−4623 (1992).	Cs, Sr	granitegneiss, granodiorite, mylonite	cement water, in-situ water
Berry et al.(1990a)	Berry, J. A. , Bond, K. A. , Brownsword, M. , Ferguson, D. R. , Green, A. and Littleboy, A. K. : Radionuclide Sorption on Generic Rock Types, Nirex safety Series Report, NSS/R182 (1990).	Ni, Np, Pb, U	clay, granite, mudstone, sandstone, shale	synthetic water
Berry et al.(2007)	Berry, J. A. , Yui, M. and Kitamura, A. : Sorption Studies of Radioelements on Geological Materials, JAEA Technical Report, JAEA-Research 2007-074 (2007), 87p.	Ac, Am, Cm, Np, Pa, Po, Pu, Tc, U	bentonite, granodiorite, Kunigel V1, tuff	de-ionized water, seawater

Table 3.2 Overview of references additionally evaluated the QA (4/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Bortun et al.(1998)	Bortun, A. I. , Bortun, L. N. , Khainakov, S. A. and Clearfield, A. : Ion exchange properties of the sodium phlogopite and biotite, Solvent Extraction and Ion Exchange, vol.16, No.4, pp.1067-1090 (1998).	Ca, Cs, K, Li, Mg, Rb, Sr	Na-phlogopite, Na-biotite	RI solution
Bunatova(1998)	Bunatova, V. : Interactions of radionuclide with hard rock, NATO Advanced Study Institute on Actinide and the Environment; Maleme, Charles Univ., CZE, pp.313-316 (1998).	Cs, I, Sr	granite	groundwater
Byegard et al.(1998)	Byegard, J. , Johansson, H. , Skaalberg, M. and Tullborg, E. L. : The Interaction of Sorbing and Non-Sorbing Tracers with Different Aspo Rock Types. Sorption and Diffusion Experiments in the Laboratory Scale, SKB Technical Report, TR-98-18 (1998).	Ba, Cs, Rb, Sr	biotite, diorite, granite, mylonite	synthetic groundwater
Byegard et al.(2005)	Byegard, J. , Gustavsson, E. , Tullborg, E.-L. and Berglund, S. : Bedrock transport properties Preliminary site description Simpevarp subarea - version 1.2, SKB Technical Report, R-05-05 (2005).	Cs, Sr	diorite, granite	groundwater
Cho et al.(1997)	Cho, Y. H. , Park, C. K. and Hahn, P. S. : Studies on the sorption characteristics of 90Sr onto Granite and Tuff, Journal of the Korean Nuclear Society, No.29, pp.393-398 (1997).	Co, Cs, Sr	granite, tuff	groundwater
Daniels(1981)	Daniels, W. R. : Laboratory Studies of Radionuclide Distributions between Selected Groundwaters and Geologic Media: October, 1979-September, 1980., Los Alamos National Laboratory Report, LA-8586-PR (1981).	Am, Ce, Cs, Pu, Sr, Tc	argillite, granite	groundwater
Doi et al.(2007)	Doi, R. , Xia, X. , Shibata, M. , Kitamura, A. and Yoshikawa, H. : Investigation of the Applicability of the Model Based on the Ion Exchange Reaction for the Cesium Sorption onto Horonobe Sedimentary Rocks, JAEA Technical Report, JAEA-Research 2007-007 (2007), 21p.	Cs	mudstone, shale	distilled water, synthetic groundwater
Dong et al.(2001)	Dong, W. , Wang, X. , Bian, X. , Wang, A. , Du, J. and Tao, Z. Y. : Comparative study on sorption/desorption of radioeuropium on alumina, bentonite and red earth: effects of pH, ionic strength, fulvic acid, and iron oxides in red earth, Applied Radiation and Isotopes, vol.54, pp.603-610 (2001).	Eu	alumina, alumina+FA, bentonite, bentonite+FA, red earth, red earth+FA, reddish soil	0.1M-0.3M $CaCl_2$, 1M-2.5M NaCl
El-Naggar et al.(2000)	El-Naggar, H. A. , Ezz El-Din, M. R. and Sheha, R. R. : Speciation of Neptunium Migration in under Groundwater, Journal of Radioanalytical and Nuclear Chemistry, vol.246, pp.493-504 (2000).	Np	basalt, sand, shale, silt	synthetic groundwater

Table 3.2 Overview of references additionally evaluated the QA (5/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Erdal(1980)	Erdal, B. R. : Ladratory Studies of Radionuclide Distributions Between Selected Groundwaters and Geologic Media, LA-8088-PR (1980).	Am, Ba, Ce, Cs, Eu, Pu, Sr, U	aquifer, aquitard, argillite, granite, tuff	groundwater, brine,
Erdal et al.(1979a)	Erdal, B. R. , Aguilar, R. D. , Bayhurst, B. P. , Daniels, W. R. , Duffy, C. J. , Lawrence, F. O. , Maestas, S. , Oliver, P. Q. and Wolfsberg, K. : Sorption-Desorption Studies on Granite, LA-7456-MS (1979).	Am, Ba, Ce, Cs, Eu, Pu, Sr, Tc, U	granite	groundwater
Erdal et al.(1979b)	Erdal, B. R. , Aguilar, R. D. , Bayhurst, B. P. , Oliver, P. Q. and Wolfsberg, K. : Sorption-Desorption Studies on Argillite, LA-7455-MS (1979).	Ba, Ce, Cs, Eu, Sr, Tc	argillite	synthetic groundwater
Eriksen and Locklund(1987)	Eriksen, T. E. and Locklund, B. : Radionuclide Sorption on Granitic Drill Core Material, SKB Technical Report, No.87-22 (1987).	Cs, Eu, Sr	granite	groundwater
Eriksen and Locklund(1989)	Eriksen, T. E. and Locklund, B. : Radionuclide Sorption on Crushed and Intact Granitic Rock Volume and Surface Effects, SKB Technical Report, No.89-25 (1989).	Cs, Eu, Sr	granite	groundwater
Francis and Bondietti(1979)	Francis, C. W. and Bondietti, E. A. : Sorption-Desorption of Long-Lived Radionuclide Species on Geologic Media, ANNUAL REPORT October 1, pp.81-133 (1979).	Np, Pu, Tc, U	basalt, dolomite, granite, gypsum, shale	2M NaCl, deionized water, groundwater
Fujikawa and Fukui(1997)	Fujikawa, Y. and Fukui, M. : Radionuclide Sorption to Rocks and Minerals: Effects of pH and Inorganic Anions. Part 2. Sorption and Speciation of Selenium, Radiochimica Acta, vol.76, pp.163-172 (1997).	Co, Cs, Mn, Se, Sr	calcite, chert, granodiorite, hematite, magnetite, shale	0.001N-0.1N Na_2CO_3, 0.001N-0.1N Na_2SO_4, 0.001N-0.1N NaCl, 0.001N-0.1N $NaHCO_3$
Higgo et al.(1987)	Higgo J. J. W. , Rees L. V. C. , Coles, T. G. and Cronan, D. S. : Distribution of Radionuclides through Deep-Sea Sediments, DOE-RW-87053 (1987).	Am, Cs, Np, Pu	sediment	seawater
Holgersson et al.(1998a)	Holgersson, S. , Albinsson, Y. , Allard, B. , Boren, H. , Pavasars, I. and Engkvist, I. : Effects of gluco-isosaccharinate on Cs, Ni, Pm, and Th sorption onto, and diffusion into cement, Radiochimica Acta, vol.82, pp.393-398 (1998).	Cs, Ni, Pm, Th	cement paste	Artificial water
Holtta et al.(1997)	Holtta, P. , Siitari-Kauppi, M. , Huihuri, P. , Lindberg, A. and Hautojarvi, A. : The effect of specific surface area on radionuclide sorption on crushed crystalline rock, Materials Research Society Symposium Proceedings, vol.465, pp.789-796 (1997).	Sr	mica gneiss, tonalite	groundwater

Table 3.2 Overview of references additionally evaluated the QA (6/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Holtta et al.(1998)	Holtta, P. , Siitari-Kauppi, M. , Lindberg, A. and Hautojarvl, A. : Na, Ca and Sr retardation on crushed crystalline rock, Radiochimica Acta, vol.82, pp.279-285 (1998).	Ca, Na, Sr	mica gneiss, tonalite	groundwater
Hsu et al.(2002)	Hsu, C.-N. , Wei, Y.-Y. , Chuang, J.-T. , Tseng, C.-L. , Yang, J.-Y. , Ke, C.-H. , Cheng, H.-P. and Teng, S.-P. : Sorption of several safety relevant radionuclides on granite and diorite - a potential repository host rock in the Taiwan area, Radiochimica Acta, vol.90, pp.659-664 (2002).	Co, Cs, Sr, U	granite, diorite	distilled water, synthetic groundwater
Huitti et al.(2000)	Huitti, T. , Hakanen, M. and Lindberg, A. : Sorption and desorption of cesium on rapakivi granite and its minerals, POSIVA 2000-03 (2000).	Cs	biotite, chlorite, dolomite, granite, hornblende, kaolinite, K-feldspar, plagioclase, quartz	groundwater, saline water
Igarashi et al.(1992)	Igarashi, T. , Mahara, Y. , Okamura, M. and Ashikawa, N. : Relation between distribution coefficient of radioactive strontium and solid-liquid distribution ratio of background stable strontium, Radioisotopes, vol.41, pp.350-356 (1992).	Sr	diorite, sand	groundwater
Igarashi et al.(1998)	Igarashi, T. , Mahara, Y. , Ashikawa, N. and Okamura, M. : Evaluation of Radioactive Strontium Distribution Coefficient by Analyzing Background Stable Strontium, Journal of Nuclear Science and Technology, vol.35, pp.190-197 (1998).	Sr	granite, sand, shale	groundwater, spring water
Ikada and Amaya(1998)	Ikeda, T. and Amaya, T. : Model Development of Chemical Evolution in Repository Vol.II Acquisition of Nuclide Migration Data in Near-Field, PNC Technical Report, PNC TJ 1281 98-003 (1998).	Am, Nb, Pb, Sb	bentonite, granodiorite, tuff	0.001M NaCl, distilled water, seawater
Ito and Kanno(1988)	Ito, K. and Kanno, T. : Sorption Behavior of Carrier - Free Technetium-95m on Minerals, Rocks and Backfill Materials under both Oxidizing and Reducing Conditions, Journal of Nuclear Science and Technology, vol.25, No.6, pp.534-539 (1988).	Tc	active carbon, albite, alumina gel, andesite, basalt, bentonite, biotite, chlorite, epidote, forsterite, granite, grossularite, hedenbergite, hornblende, limestone, microcline, muscovite, plagiorhyolite, quartz, sandstone, shale, tuff	0.016M $NaNO_3$+0.1M $NaBH_4$, 0.16M $NaNO_3$, 0.16M $NaNO_3$+0.1M $NaBH_4$, 0.66M $NaNO_3$+0.1M $NaBH_4$, 1.16M $NaNO_3$+0.1M $NaBH_4$
Jan et al.(2007)	Jan, Y.-L. , Wang, T.-H. , Hsu, C.-N. et al. : Evaluating adsorption ability of granite to radioselenium by chemical sequential extraction, Journal of Radioanalytical and Nuclear Chemistry, vol.273, pp.299-306 (2007).	Se	granite	de-ionized water, groundwater, seawater

Table 3.2 Overview of references additionally evaluated the QA (7/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
JGC Corporation(1991)	JGC Corporation : Analytical Code Development and Data Set Preparation for Near Field Analysis(Vol. 3), PNC Technical Report, PNC TJ1281 91-005(3) (1991).	Ni, Tc	basalt, bentonite, granodiorite, mudstone, tuff	distilled water, seawater
Johansson et al.(1997)	Johansson, H. , Byegard, J. , Skarnemark, G. and Skalberg, M. : Matrix diffusion of some alkali- and alkaline earth-metals in granitic rock, Materials Research Society Symposium Proceedings, vol.465, pp.871-878 (1997).	Ca, Na, Sr	granite, aspodiorite	groundwater
Johansson et al.(1998)	Johansson, H. , Siitari-Kauppi, M. , Skalberg, M. and Tullborg, E.-L. : Diffusion Pathways in Crystalline Rocks -Examples from Äspö-diorite and fine-grained Granite, Journal of Contaminant Hydrology, vol.35, pp.41-53 (1998).	Ba, Cs	granite, diorite	groundwater
Kato et al.(2001)	Kato, K. , Amano, O. , Tanaka, S. , Noshita, K. , Yoshida, T. and Tsukamoto, M. : Systematic Investigations for Nuclide Sorption Mechanism in Natural Barrier (II) -Relationship of Sorption Ability between Rock and Its Constituent Minerals-, 2001 Fall Meeting of the Atomic Energy Society of Japan, No.O27, p.905 (2001).	Cs	granite, quartz, microcline, albite, biotite	pure water, synthetic groundwater, synthetic seawater
Kaukonen et al.(1997)	Kaukonen, V. , Hakanen, M. and Lindberg, A. : Diffusion and sorption of HTO, Np, Na and Cl in rocks and minerals of Kivetty and Olkiluoto., Univ. Helsinki, FIN, POSIVA 97-07 (1997).	Np	biotite, calcite, chlorite, granite, hornblende, kaolinite, K-feldspar, muscovite, plagioclase, pyrite, quartz	groundwater, seawater
Kitamura et al.(1999c)	Kitamura, A. , Fujiwara, K. , Yamamoto, T. , Nishikawa, S. and Moriyama, H. : Mechanism of Adsorption of Cations onto Rocks, JAERI-Conf 99-004, pp.617-626 (1999).	Ba, Sr	granite	0.01M-0.1M NaClO4
Kitamura et al.(2008)	Kitamura, A. , Tomura, T. , Sato, H. and Nakayama, M. : Sorption Behavior of Cesium onto Bentonite and Sedimentary Rocks in Saline Groundwaters, JAEA Technical Report, JAEA-Research 2008-004 (2008), 39p.	Cs	Kunigel V1, mudstone, sandstone	0.02M-0.7M KCl, 0.02M-0.7M NaCl, synthetic porewater
Koskinen et al.(1985)	Koskinen, A., Alaluusa, M., Pinnioja, S., Jaakola, T. and Lindberg, A. : Sorption of Iodine, Neptunium, Technetium, Thorium and Uranium on Rocks and Minerals, YJT Report, YJT-85-36 (1985).	I, Np, Tc, U, Th	mica gneiss, tonalite	groundwater
Kulmala and Hakanen(1992)	Kulmala, S. and Hakanen, M. : Review of the sorption of radionuclides on the bedrock of Haestholmen and on construction and backfill materials of a final repository for reactor wastes, YJT-92-21 (1992).	C, Ca, Cl, Co, Cs, I, Nb, Ni, Np, Sr, Tc, Zr	basalt, concrete, granite, mica gneiss, organic, tonalite	cement solution, groundwater, saline water

Table 3.2 Overview of references additionally evaluated the QA (8/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Kulmala and Hakanen(1993)	Kulmala, S. and Hakanen, M. : The Solubility of Zr, Nb and Ni in Groundwater and Concrete Water, and Sorption on Crushed Rock and Cement, YJT Report, YJT-93-21 (1993).	Nb, Ni, Zr	cement, granite, tonalite	concrete water, groundwater
Kulmala et al.(1998a)	Kulmala, S. , Hakanen, M. and Lindberg, A. : Sorption of iodine on rocks from Posiva investigation sites, POSIVA 98-05 (1998)	I	granite, granodiorite, mica gneiss, tonalite	groundwater, saline water
Kulmala et al.(1998b)	Kulmala, S. , Hakanen, M. and Lindberg, A. : Sorption of Plutonium on Rocks in Groundwaters from Posiva Investigation Sites, POCIVA 98-12 (1998).	Pu	granite, granodiorite, mica gneiss, tonalite	natural groundwater
Kumata and Vandergraaf(1993)	Kumata, M. and Vandergraaf, T. T. : Technetium Behaviour under Deep Geological Conditions, Radioactive Waste Management and the Nuclear Fuel Cycle, vol.17, pp.107-117 (1993).	Tc	granite	groundwater
Lee et al.(2008)	Lee, C.-P. , Tsai, S.-C. , Jan, Y.-L. , Wei, Y.-Y. , Teng, S.-P. and Hsu, C.-N. : Sorption and diffusion of HTO and cesium in crushed granite compacted to different lengths, Journal of Radioanalytical and Nuclear Chemistry, vol.275, pp.371-378 (2008).	Cs	granite	synthetic groundwater
Liu et al.(2006)	Liu, D. J. , Fan, X. H. , Yao, J. and Wang, B. : Diffusion of 99Tc in granite under aerobic and anoxic conditions, Journal of Radioanalytical and Nuclear Chemistry, vol.268, pp.481-484 (2006).	Tc	granite	simulated groundwater
Lujaniene et al.(2007)	Lujaniene, G. , Motiejunas, S. and Sapolaite, J. : Sorption of Cs, Pu and Am on clay minerals, Journal of Radioanalytical and Nuclear Chemistry, vol.274, pp.345-353 (2007).	Cs, Pu	clay	cement water, saline water
Maclean et al.(1978)	Maclean, S. C. , Coles, D. G. and Weed, H. C. : The Measurement of Sorption Ratios for Selected Radionuclides on Various Geologic Media (1978).	Cs, Pu, Sr, Tc	basalt, biotite, dolomite, granite, limestone, shale, tuff	natural groundwater, synthetic groundwater
Morooka et al.(2005)	Morooka, K. , Nakazawa, T. , Saito, Y. , Suyama, T. , Shibata, M. and Sasamoto, H. : Measurements of distribution coefficient for Sm on tuff and granodiorite in synthesized sea water and distilled water, JNC Technical Report, JNC TN8400 2005-015 (2005), 63p.	Sm	granodiorite, tuff	distilled water, synthetic seawater
Mucciardi et al.(1979)	Mucciardi, A. N. , Johnson, T. C. and Saunier, J. : Statistical Investigation of the Mechanics Controlling Radionuclide Sorption, Annual Report, Battelle-Pacific Northwest Laboratories, ADI Ref. 548, pp.1-75 (1979).	Am, Cs, I, Np, Pu, Sr, Tc	albite, anorthite, augite, basalt, biotite, enstatite, granite, hornblende, illite, kaolinite, limestone, microcline, montmorillonite, quartz, shale, vermiculite	30-$CaCl_2$, 30-NaCl, 30-$NaHCO_3$, 5130-NaCl

Table 3.2 Overview of references additionally evaluated the QA (9/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Murali and Mathur(2002)	Murali, M. S. and Mathur, J. N. : Sorption characteristics of Am(III), Sr(II) and Cs(I) on bentonite and granite, Journal of Radioanalytical and Nuclear Chemistry, vol.254, No.1, pp.129-136 (2002).	Am, Cs, Sr	bentonite, granite	brine water
Nakayama et al.(1986)	Nakayama, S. , Moriyama, H. , Arimoto, H. and Higashi, K. : Distribution Coefficients of Americium, Neptunium and Protoactinium for Selected Rocks, The Memories of the Faculty of Engineering, Kyoto University, vol.48, pp.275-286 (1986).	Am. Np, Pa	granite, quartz, tuff	distilled water, equilibrated water
Nakayama et al.(1994)	Nakayama, S. , Vandergraaf, T. T. and Kumada, M. : Experimental Study on Nuclides Migration under the Deep Geological Condition. -Column Tests on Neptunium and Plutonium with Granite and Groundwater at Lac du Bonnet, Manitoba, Canada, Journal of Nuclear Fuel Cycle and Environment, vol.1, pp.67-76 (1994).	Np, Pu	granite	natural groundwater
Oda et al.(1999)	Oda, C. , Ikeda, T. and Shibata, M. : Experimental Studies for Sorption Behavior of Tin on Bentonite and Rocks, and Diffusion Behavior of Tin in Compacted Bentonite, JNC Technical Report, JNC TN8400 99-073 (1999).	Sn	Kunigel V1, granodiorite, tuff	0.01M-0.1M NaCl
Ohe and Nakaoka(1982)	Ohe, T. and Nakaoka, A. : Radionuclide transfer in underground media, (3). Ion exchange reactions in geological materials, CRIEPI Report, Central Research Institute of Electric Power Industry, No.282026 (1982).	Co, Cs, Mn, Sr	granite	solution
Okuyama et al.(2007)	Okuyama, K. , Sasahira, A. and Noshita, K. : Cesium Sorption Rate on Non-Crushed Rock Measured by a New Apparatus Based on a Micro-Channel-Reactor Concept, Materials Research Society Symposium Proceedings, vol.985, pp.449-454 (2007).	Cs	biotite/granite	distilled water
Okuyama et al.(2008)	Okuyama, K. , Sasahira, A. , Noshita, K. and Ohe, T : A method for determining both diffusion and sorption coefficients of rock medium within a few days by adopting a micro-reactor technique, Applied Geochemistry, vol.23, pp.2130-2136 (2008).	Cs	biotite/granite	distilled water

Table 3.2 Overview of references additionally evaluated the QA (10/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Palmer and Meyer(1981)	Palmer, D. A. and Meyer, R. E. : Adsorption of Technetium on Selected Inorganic Ion-exchange Materials and on a Range of Naturally Occurring Minerals under Oxic Conditions, Journal of Inorganic and Nuclear Chemistry, vol.43, No.11, pp.2979-2984 (1981).	Tc	albite, apatite, attapulgite, augite, basalt, beryl, biotite, chacocite, chalcopyrite, chlorite, corundum, dolomite, epidote, galena, gibbsite, granite, gypsum, hematite, hornblende, illite, ilmenite, kaolinite, limonite, magnetite, microcline, molybdenite, monazite, montmorillonite, muscovite, olivine, pyrite, pyroxene, quartz, serpentine, sphene, triphylite, zircon	NaCl solution
Sato et al.(1997)	Sato, H. , Shibutani, T. , Tachi, Y. , Ota, K. , Amano, K. and Yui, M. : Diffusion Behavior of Nuclides Considering Pathways in Fractured Crystalline Rocks, PNC Technical Report, PNC TN8410 97-127 (1997), 57p.	Cs, Pu, Se, Sr, U	granodiorite	groundwater
Sazarashi et al.(1996)	Sazarashi, M. , Ikede, Y. , Kumagai, M. , Lin, K.-H. and Kawakami, Y. : A Study on Behavior of Solution Radioactive Species and Biodegradation of Bituminized Radioactive Waste, PNC Technical Report, Institute of Research and Innovation, PNC TJ1564 96-001 (1996).	C, I	albite, anhydrite, anorthite, basalt, biotite, boulangerite, bournonite, calcite, cement, chalk, charcoal, clay, concrete, dolomite, glauconite, gneiss, granite, illite, kaolinite, limestone, marl, microcline, montmorillonite, quartz, sand, sandstone, shale, silt, soil, tetrahedrite, tuff, vermiculite	equilibrated water, synthetic groundwater, 0.01M-5M NaCl
Shimooka et al.(1985)	Shimooka, K. , Nakamura, H. , Yanagida, T. and Muraoka, S. : Measurement of diffusion and sorption of radionuclides in rocks, Journal of Nuclear Science and Technology, No.22, pp.833-840 (1985).	Am, Cs, Np, Sr	andesite, basalt, granite, granodiorite, rhyolite	distilled water
Siitari-Kauppi et al.(1999)	Siitari-Kauppi, M. , Hoelttae, P. , Pinnioja, S. and Lindberg, A. : Cesium sorption on tonalite and mica gneiss, Materials Research Society Symposium Proceedings, vol.556, pp.1099-1106 (1999).	Cs	mica gneiss, tonalite	groundwater

Table 3.2 Overview of references additionally evaluated the QA (11/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Suksi et al.(1989)	Suksi, S. , Siitari-Kauppi, M. , Hoelttae P. , Jaakola, T. and Lindberg, A. : Sorption and diffusion of radionuclides (C, Tc, U, Pu, Np) in rock samples under oxic and anoxic conditions, YJT Report, YJT-89-13 (1989).	Np, Pu, U	granite	Allard water
Tachi et al.(1999d)	Tachi, Y. , Shibutani, T. , Sato, H. and Shibata, M. : Sorption and Diffusion Behavior of Palladium in Bentonite, Granodiorite and Tuff, JNC Technical Report, JNC TN8400 99-088 (1999), 58p.	Pd	bentonite, granodiorite, tuff	0.01M-0.1M NaCl
Takebe and Deying(1995)	Takebe, S. and Deying, X. : Studies on Sorption Behavior of Technetium in Soils, JAERI-Research 95-024 (1995), 14p.	Tc	loam, sand, sandstone, soil, tuff	RI water
Taki and Hata(1991)	Taki, H. and Hata, K. : Measurement Study on Distribution Coefficient and Effective Diffusion Coefficient for Some Rocks and Bentonite, JNC Technical Report, PNC TJ1214 91-010 (1991).	Nb, Ra, Sn, Zr	basalt, granodiorite, Kunigel V1, mudstone, tuff	distilled water, seawater
Tanaka et al.(1999)	Tanaka, T. , Sakamoto, Y. and Muraoka, S. : Modeling of Neptunium(V), Plutonium(IV) and Americium(III) Sorption on Soils in the Presence of Humic Acid, Japan Atomic Energy Research Institute, JAERI-Conf 99-004, pp.662-673 (1999).	Np, Am, Pu	sand, soil	0.01M NaNO3
Ticknor(1994)	Ticknor, K. V. : Sorption of Nickel on Geological Materials, Radiochimica Acta, vol.66/67, pp.341-348 (1994).	Ni	biotite, granite, hematite, kaolinite, K-feldspar, quartz	groundwater
Ticknor and McMurry(1996)	Ticknor, K. V. and McMurry, J. : A Study of Selenium and Tin Sorption on Granite and Goethite, Radiochimica Acta, vol.73, pp.149-156 (1996).	Se, Sn	granite, goethite	groundwater
Torstenfelt et al.(1981)	Torstenfelt, B. , Andersson, K. and Allard, B. : Sorption of Sr and Cs on Rocks and Minerals Part I : Sorption in Groundwater, Prev 4.29 (1981).	Cs, Sr	apatite, biotite, calcite, diabase, fluorite, gneiss, granite, hematite, hornblende, magnetite, muscovite, orthoclase, quartz, serpentine	groundwater
Torstenfelt et al.(1988)	Torstenfelt, B. , Rundberg, R. S. and Mitchell, A. J. : Actinide Sorption on Granites and Minerals as a Function of pH and Colloids/ Pseudocolloids, Radiochimica Acta, vol.44/45, pp.111-117 (1988).	Np, Pu, U	albite, anorthite, bentonite, granite, hornblende, illite, microcline	groundwater
Wernli et al.(1985)	Wernli, B. , Bajo, C. and Bischoff, K. : Bestimmung des Sorptions Koeffizienten von Uran(VI) an Grimsel-und Bottsteingranit, EIR-Bericht, Nr.543 (1985).	U	granite	distilled water, synthetic groundwater

Table 3.2 Overview of references additionally evaluated the QA (12/12)

Reference	Details of reference	Element	Solid Phase	Solution Type
Widestrand et al.(2001)	Widestrand, H. , Byegard, J. , Skarnemark, G. and Skalberg, M. : In situ migration experiments at Aspo Hard Rock Laboratory, Sweden : Results of radioactive tracer migration studies in a single fracture, Journal of Radioanalytical and Nuclear Chemistry, vol.250, pp.501-517 (2001).	Ba, Ca, Cs, Na, Rb, Sr	biotite, cation exchange resin, diorite, granite, mylonite	groundwater
Xia et al.(2006a)	Xia, X. , Iijima, K. , Kamei, G. and Shibata, M. : Comparative study of cesium sorption on crushed and intact sedimentary rock, Radiochimica Acta, vol.94, pp.683-687 (2006).	Cs	mudstone, shale	deionized water, natural groundwater, synthetic groundwater
Xia et al.(2006b)	Xia, X. , Kamei, G. , Iijima, K. , Shibata, M. , Ohnuki, T. and Kozai, N. : Selenium sorption in a sedimentary rock/saline groundwater system and spectroscopic evidence, Materials Research Society Symposium Proceedings, vol.932, pp.933-941 (2006).	Se	mudstone, shale	synthetic groundwater, natural groundwater
Yamaguchi and Nakayama(2002)	Yamaguchi, T. and Nakayama, S. : Present status of the study on radionuclide diffusion in barrier materials, JAERI-Conf 2002-004, pp.325-332 (2002).	Ba, Cs, I, Pu	granite	deionized water

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

QA-evaluated 95 references listed in Table 3.2 are not included in this reference list.

3.3 QA evaluation on Criteria III

Only the entries for data sets classified as reliable are being considered for Criteria III. All unreliable entries, or entries where classification according to Criteria I and II could not be completed, are excluded.

3.3.1 Evaluation of data for trivalent of actinide and lanthanide

The following entries are evaluated in this section; the respective data are shown in Figure 3.3-1.

Reference	Element	Data table	Solid phase
Allard et al.(1979b)	Am	—	Granite
Allard et al.(1979b)	Ce	Ce/2	Granite
Allard et al.(1979b)	Eu	Eu/2	Granite
Berry et al.(2007)	Ac	Ac/2	Granodiorite
Berry et al.(2007)	Cm	Cm/1	Granodiorite
Erdal et al.(1979a)	Am	—	Granite
Erdal et al.(1979a)	Ce	Ce/5	Granite
Erdal et al.(1979a)	Eu	Eu/3	Granite
Eriksen and Locklund(1987)	Eu	Eu/4	Granite
Eriksen and Locklund(1989)	Eu	Eu/5	Granite
Ikeda and Amaya(1998)	Am	—	Granodiorite
Kitamura et al.(1999a)30)	Am	—	Granite

Figure 3.3-1 summarizes the data for the sorption of trivalent of actinide and lanthanide in fresh water system (ionic strength < 1.0×10^{-2} M). Some K_d dataset with wider variations can be explained by different particle size of solid phases (Erdal et al.,1979a ; Eriksen and Locklund,1987 ; Eriksen and Locklund,1989). The K_d values tend to increase basically as the particle size decreases. Considering the differences of experimental conditions and composition of used granitic rocks, all K_d values of elements on granitic rocks are evaluated as being consistent with each other.

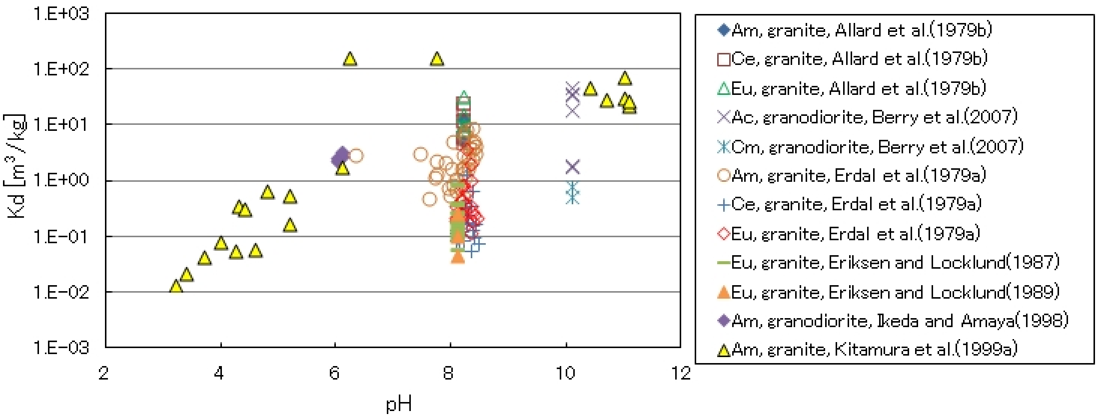

Figure 3.3-1 Overview of sorption data for trivalent of actinide and lanthanide on granitic rocks

3.3.2 Evaluation of data for radium and strontium

The following entries are evaluated in this section; the respective data are shown in Figure 3.3-2.

Reference	Element	Data table	Solid phase
Allard et al.(1979b)	Ra	Ra/2	granite
Allard et al.(1979b)	Sr	Sr/2	granite
Andersson et al.(1983b)	Sr	Sr/6	gneiss
Andersson et al.(1983b)	Sr	Sr/6	granite
Barney and Brown(1979)	Sr	Sr/10	granite
Daniels(1981)	Sr	Sr/13	granite
Erdal et al.(1979a)	Sr	Sr/14	granite
Eriksen and Locklund(1987)	Sr	Sr/15	granite
Eriksen and Locklund(1989)	Sr	Sr/16	granite
Igarashi et al.(1998)	Sr	Sr/17	granite
Maclean et al.(1978)	Sr	Sr/25	granite
Torstenfelt et al.(1981)	Sr	Sr/37	gneiss
Torstenfelt et al.(1981)	Sr	Sr/37	granite

Figure 3.3-2 shows the available data for radium and strontium sorption on granitic rocks in fresh water system (ionic strength < 1.0×10^{-2} M). Although K_d values lie in wide ranges, a fairly clear trend of increasing K_d with increasing pH was found. Some K_d dataset with wider variations can be explained by different particle size of solid phases (Erdal et al.,1979a ; Eriksen and Locklund,1987 ; Eriksen and Locklund,1989 ; Maclean et al.,1978 ; Torstenfelt et al.,1981). The K_d values tend to increase basically as the particle size decreases. It is difficult to evaluate because of lack of detailed information on the mineralogy of the granitic rocks, but they are approximately consistent with each other.

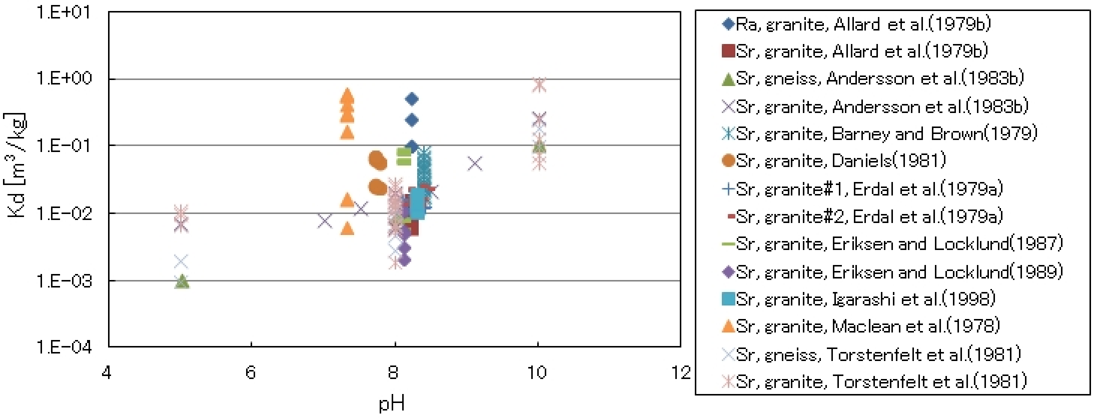

Figure 3.3-2 Overview of sorption data for radium and strontium on granitic rocks

3.3.3 Evaluation of data for selenium

The following entries are evaluated in this section; the respective data are shown in Figure 3.2-3.

Reference	Element	Data table	Solid phase
Sato et al.(1997)	Se(IV)	—	granodiorite
Ticknor and McMurry(1996)	Se(IV)	—	granite
Iida et al.(2011)	Se(-II)	Se/2	granodiorite

Figure 3.3-3 shows the available data for selenium sorption on granitic rocks in fresh water system (ionic strength < 1.0×10^{-2} M). Although K_d values lie in wide ranges, a fairly clear trend of increasing K_d with decreasing pH was found. The solid phases used for Sato et al. (1997) are altered granodiorite, fracture fillings granodiorite and intact granodiorite. The lowest K_d value for Ticknor and McMurry (1996) is considered to be not reached at equilibration, because of 1 day reaction time. All K_d values of elements on granitic rocks are evaluated as being consistent with each other in spite of different valences of Se.

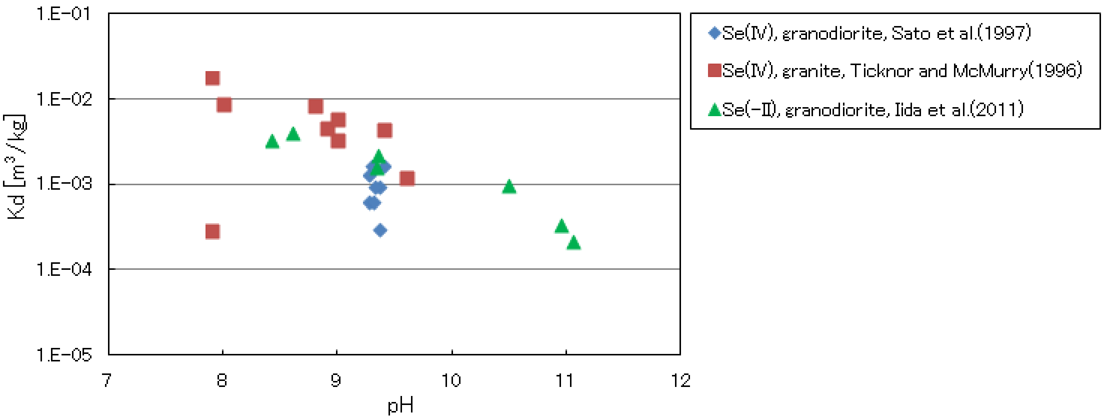

Figure 3.3-3 Overview of sorption data for selenium on granitic rocks

3.3.4 Evaluation of data for technetium

The following entries are evaluated in this section; the respective data are shown in Figure 3.3-4.

Reference	Element	Data table	Solid phase
Allard et al.(1979b)	Tc(VII)	Tc/3	granite
Amaya et al.(1995)	Tc(VII)	Tc/5	granite
Amaya et al.(1995)	Tc(IV)	Tc/5	granite
Baston et al.(1995a)	Tc(VII)	Tc/10	granodiorite
Baston et al.(1995a)	Tc(IV)	Tc/10	granodiorite
Berry et al.(2007)	Tc(VII)	Tc/12	granodiorite
Berry et al.(2007)	Tc(IV)	Tc/12	granodiorite
Erdal et al.(1979a)	Tc(VII)	Tc/16	granite
JGC Corporation(1991)	Tc(VII)	Tc/28	granodiorite

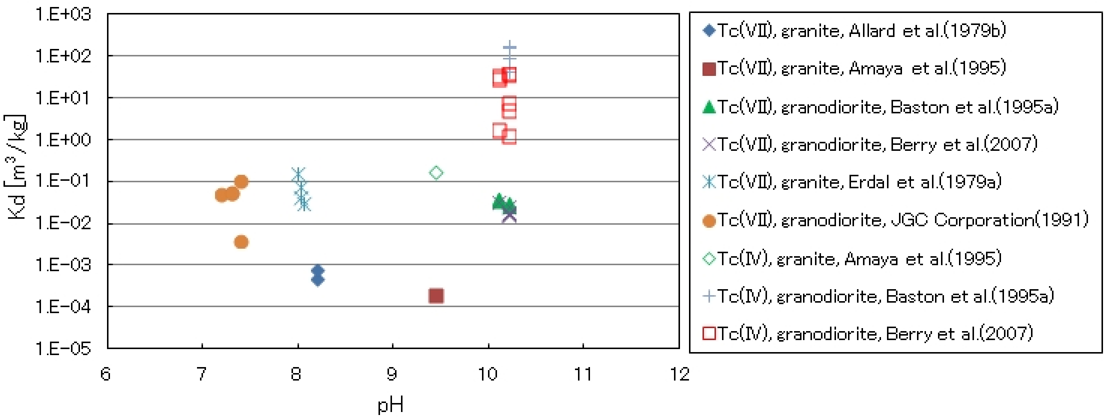

Figure 3.3-4 Overview of sorption data for technetium on granitic rocks

Figure 3.3-4 shows the available data for technetium sorption on granitic rocks in fresh water system (ionic strength < 1.0×10^{-2} M). Although K_d values lie in wide ranges, It is seemed that sorption of Tc(IV) is generally higher than that of Tc(VII). The K_d values of Tc(IV) for Berry et al. (2007) are seemed to be different by the separation methods (centrifugation or filtration). It is difficult to evaluate because of lack of detailed information on the mineralogy of the granitic rocks, but they are approximately consistent with each other.

3.3.5 Evaluation of data for tetravalent of actinide

The following entries are evaluated in this section; the respective data are shown in Figure 3.3-5.

Reference	Element	Data table	Solid phase
Allard et al.(1978)	Np(IV)	—	granite
Allard et al.(1978)	Pu(IV)	Pu/1	granite
Allard et al.(1979b)	Th(IV)	—	granite
Barney and Brown(1979)	Pu(IV)	Pu/6	granite
Daniels(1981)	Pu(IV)	Pu/12	granite
Erdal et al.(1979a)	Pu(IV)	Pu/13	granite
Maclean et al.(1978)	Pu(IV)	Pu/21	granite
Sato et al.(1997)	Pu(IV)	Pu/26	granodiorite
Suksi et al.(1989)	Pu(IV)	Pu/27	granite
Torstenfelt et al.(1988)	Pu(IV)	Pu/29	granite

Figure 3.3-5 shows the available data for technetium sorption on granitic rocks in fresh water system (ionic strength < 1.0×10^{-2} M). Although K_d values lie in wide ranges, a clear trend of pH was not found. Some K_d dataset with wider variations can be explained by different particle size of solid phases (Erdal et al.,1979a). The solid phases used for Sato et al. (1997) are altered granodiorite, fracture fillings granodiorite and intact granodiorite. It is difficult to evaluate because of lack of detailed information on the mineralogy of the granitic rocks, but they are approximately consistent with each other.

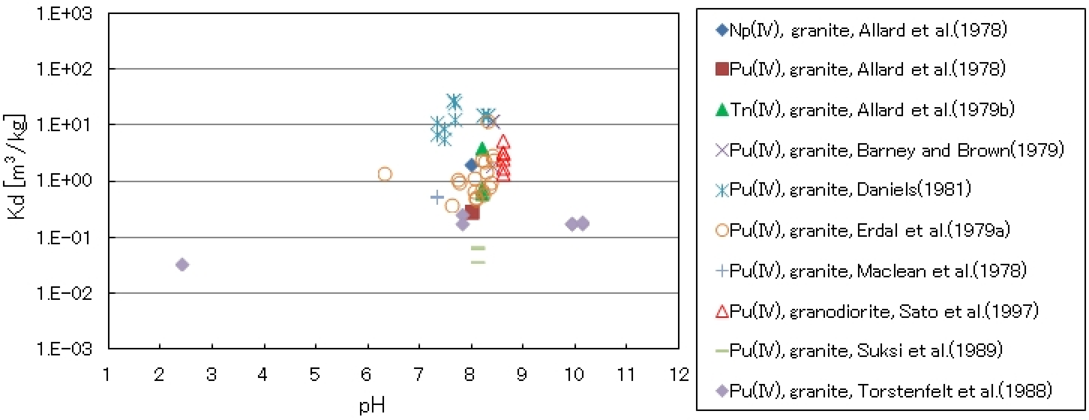

Figure 3.3-5 Overview of sorption data for tetravalent of actinide on granitic rocks

4. Conclusions

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

- To support the setting of the K_d values and their uncertainty range, two functions for data evaluation were added ; i) Function of statistical data evaluation to support PA-related K_d and uncertainty setting, and ii) Function of grouping for K_d data related to the potential perturbations.
- 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, 11,206 K_d data from 83 references were added, total number of K_d values in the JAEA-SDB reached about 58,000. The QA/classified K_d data reached about 60% 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.

Acknowledgments

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Appendix

QA/classification guideline for JAEA-SDB

(Ochs et al. 2007)

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1. Introduction, description of main Criteria

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

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

a) It needs to be verified that the documentation of each entry is detailed enough to allow further examination according to the main Criteria II-III. At this point, only the completeness of the documentation is examined; the appropriateness of the reported data and approaches is evaluated under Criteria II below.

b) This point takes also into account that the reliability of data input to the JAEA-SDB will be substantially high if K_d values are directly available in table format in comparison to literature that reports e.g. %-adsorbed values in a graph. The latter way of reporting requires the operator to i) manually read values off a graph and ii) to calculate K_d from the %-adsorbed and Solid/water ratio (s/w) values given, which significantly increases the likelihood of an operator error during data input.

Criteria II － Quality of reported data

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

Criteria III － Consistency of data:

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

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

2. Description of checkpoints within each main Criteria

2.1 General

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

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

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

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

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

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

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

- units

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

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

→ The following levels are distinguished:

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

2.3 Criteria II: Technical and scientific quality of reported data

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

II-a Solid phase (substrate)

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

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

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

1. It needs to be known whether a substrate consists of a single pure mineral phase, or whether it contains impurities or additional minerals. In general, some measure of site density per mass (e.g. CEC) needs to be known to properly design experiments, in particular with respect to achieving reasonable surface loading.

2. In case of simple substrates (pure minerals), no further information is necessary.
3. In case of complex substrates (i.e., where significant impurities are present, or where a substrate is composed of several minerals), and in particular in case of natural samples, detailed information on composition has to be provided in addition.
4. In cases where sample treatment (such as crushing or sieving) had been performed, the respective information on particle size also needs to be provided (see II-f). Where any chemical treatments (e.g. acid washing to remove calcite; but also change of redox conditions in case of redox-sensitive substrates, see II-c) had been applied, the applied method and resulting mineralogy should be given as well.
5. In case of many commercially available substrates (e.g., MX-80 or Kunigel-V1 bentonite; standard clay minerals from the Clay Minerals Society, such as SWy-1; Min-U-Sil SiO_2, 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 sobbing RN, not with redox control of an overall redox-sensitive system. If the experimental system comprises a range of redox-sensitive dissolved (e.g. organics) and solid (e.g. Fe- and Mn-phases) components, imposing redox conditions different from the original level may influence many redox-equilibria simultaneously. In such a case it can be very difficult to ascertain equilibrium or to know which solid phases are present. Such effects on solution and solid phase chemistry are addressed by checkpoints II-a and II-d. It also needs to be pointed out in this context that "imposed redox condition" does not necessarily refer only to imposing reducing conditions by adding a reducing agent, it also includes imposing oxidizing conditions by e.g. transferring a reduced natural sediment to the laboratory and exposing it to O_2 (as a matter of fact, the latter may be the more common problem).

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

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

→ Two levels of reliability:

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

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

- Experiments where reducing conditions are imposed on redox-sensitive RN (in otherwise stable systems) and where similar results are obtained using several reducing agents.

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

- Reducing conditions imposed on redox-sensitive RN (in otherwise stable systems) using one reducing agent that can be estimated (e.g. from experience or from the literature) to be effective and to be sufficiently inert with respect to influencing RN behavior.
- In cases where complexing reducing agents have been used, level C/D still can be achieved if the influence of the reducing agent on RN speciation has been estimated.
- All cases where redox conditions may be less well defined than for level A/B, but where it can be assumed that no significant artifacts regarding RN behavior are introduced and where the oxidation state of RN has been measured independently (in some cases, this may include low-O_2 conditions with a subsequent confirmation of RN oxidation state). Evaluating the reliability of such measurements is likely to require an expert decision by the operator.

→ If a lower quality than required for level C/D is evident, the respective entry is excluded from further evaluation as unreliable. For example, cases where it has been attempted to achieve reducing conditions only by minimizing the level of O_2 (e.g., by performing experiments in a N_2 atmosphere) generally should be labeled "unreliable" (except where the oxidation state of a RN somehow has been confirmed, see description of level C/D). Also, if a strongly complexing reducing agent (such as many organic acids) is used at unspecified concentration levels, the respective entry is excluded from further evaluation as unreliable.

II-d Final solution composition

Note that solution composition includes dissolved carbonate concentration, which may be controlled through, or expressed as pCO_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) [surface area sorbent] » [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 are (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 $\leq 2\times10^{-9}$ 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-l RN loading

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

→ Three levels of reliability:

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

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

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

II-m Reaction vessels

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

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

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

→ Three levels of reliability:

A) An appropriate vessel has been used (taking into account sorption as well as tightness with respect to CO_2 or O_2, where required), and corrections for sorption on vessel wall have been performed or no sorption on vessel wall has been observed by blank tests. If effects of vessel walls are corrected for, it has to be done by extracting any RN sorbed to vessel walls after experimentation (e.g. by acid washing) and establishing a complete mass balance. If the sorption on vessel wall has been determined as significantly lower (at least two orders of magnitude in terms of K_d) than the actual K_d value and thus corrections for sorption on vessel wall have not been performed, such a case would also correspond to level A.

B) An appropriate vessel has been used, and corrections for sorption on vessel walls have not been performed.

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

II-n Uncertainty estimates

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

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

→ Four levels of reliability:

A) Uncertainties in K_d are derived based on entire, replicated sorption experiments (i.e., at least duplicate experiments).

B) Uncertainties in K_d are derived based on single sorption experiments that are sampled and analyzed repeatedly. This may be supplemented by error propagation.

C) Uncertainties in K_d are based on error propagation of estimated analytical and/or procedural uncertainties.

D) No error estimate is given, no repeated sampling is done.

II-o Parameter variation

Studies with a systematic variation of key parameters are much more valuable and reliable than single K_d measurements. In this context, key parameters are those that influence sorption (for example, chemical parameters such as RN concentration, pH, pCO_2, but also temperature, 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 pCO_2 (edge), or e.g. [Na] in case of ion exchange, are varied systematically.

B) Either RN concentration (isotherm) and/or chemical parameters, such as pH or pCO_2 (edge), or e.g. [Na] in case of ion exchange (i.e., at least two parameters in total), are varied. These variations are less systematic than in A, but still allow to observe trends.

C) As B, but only one parameter in total is varied.

D) No parameter variation is done.

2.4 Criteria III: Consistency of data

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

→ Therefore, the evaluation of criteria III will only be reported in the form of a comment. Any such comments will be included both in a classification report as well as in the corresponding rating summary sheets.

→ If the K_d values under investigation are clearly inconsistent with the majority of related reliable studies, and if the reason for this observation cannot be explained, they may also be labeled unreliable based on criteria III. As this requires an expert decision by the operator, the underlying reasoning needs to be clearly documented.

3. Overall classification

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

- The three criteria I-III are evaluated separately, the respective results are reported separately as well.
- Criteria I: The checkpoints under I-a are used in a yes/no screening fashion, entries not fulfilling I-a are labeled as unreliable and are not evaluated further.
- Criteria I-b is then used to assign classes 1-6 for documentation.
- Criteria II: a) The datasets that pass Criteria I are again classified according to a 6-level system, where classes 1-6 represent the highest and lowest levels of reliability. To ensure a minimum quality level, certain checkpoints are regarded as critical (marked with * in Table 3.1). If the quality of the data does not correspond to the respective minimum requirements, the entries are not to be used and are classified as unreliable.
  b) To facilitate transparent averaging of all checkpoints, the following numerical system is suggested: A=3, B=2, C=1, D=0 (A/B=3 and C/D=0 in some cases).
  c) Initially, checkpoints II-b, II-c, II-d, and II-h are evaluated (indicated in bold letters below). If an entry is rated unreliable for any of these checkpoints, it is excluded

from further evaluation.

d) Weighting of individual checkpoints at this level is done according to the factors given in Table 3.1 below.

e) The total sum of points obtained for Criteria II is then used to indicate the level of reliability. With the present system, the maximum number of points would be 183, leading to an overall classification as follows (Table 3.2).

Table 3.1 Weighting of individual checkpoints under Criteria II.

checkpoint	description	weighting factor
II-a	solid phase (substrate)	A-C/D × 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).

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

国際単位系（SI）

表１．SI 基本単位

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

表２．基本単位を用いて表されるSI組立単位の例

組立量	SI 組立単位	
	名称	記号
面積	平方メートル	m^2
体積	立方メートル	m^3
速さ，速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	m/s^2
波数	毎メートル	m^{-1}
密度，質量密度	キログラム毎立方メートル	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	1
比透磁率(b)	（数字の）　1	1

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

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

表３．固有の名称と記号で表されるSI組立単位

組立量	SI 組立単位			
	名称	記号	他のSI単位による表し方	SI基本単位による表し方
平面角	ラジアン(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	ジーメンス	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)	℃		K
光束	ルーメン	lm	cd sr(c)	cd
照度	ルクス	lx	lm/m^2	$m^{-2}\ cd$
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	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
粘度	パスカル秒	Pa s	$m^{-1}\ kg\ s^{-1}$
力のモーメント	ニュートンメートル	N m	$m^2\ kg\ s^{-2}$
表面張力	ニュートン毎メートル	N/m	$kg\ s^{-2}$
角速度	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	$m^{-3}\ s\ A$
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	名称	記号	乗数	名称	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=60 s
時	h	1 h =60 min=3600 s
日	d	1 d=24 h=86 400 s
度	°	1°=(π/180) rad
分	’	1’=(1/60)°=(π/10 800) rad
秒	”	1”=(1/60)’=(π/648 000) rad
ヘクタール	ha	$1\ ha=1\ hm^2=10^4m^2$
リットル	L，l	$1\ L=1\ l=1\ dm^3=10^3cm^3=10^{-3}m^3$
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	$1\ eV=1.602\ 176\ 53(14)\times10^{-19}J$
ダルトン	Da	$1\ Da=1.660\ 538\ 86(28)\times10^{-27}kg$
統一原子質量単位	u	1 u=1 Da
天文単位	ua	$1\ ua=1.495\ 978\ 706\ 91(6)\times10^{11}m$

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	$1\ bar=0.1MPa=100\ kPa=10^5Pa$
水銀柱ミリメートル	mmHg	1 mmHg≈133.322Pa
オングストローム	Å	$1\ Å=0.1nm=100pm=10^{-10}m$
海里	M	1 M=1852m
バーン	b	$1\ b=100fm^2=(10^{-12}cm)^2=10^{-28}m^2$
ノット	kn	1 kn=(1852/3600)m/s
ネーパ	Np	SI単位との数値的な関係は、対数量の定義に依存。
ベル	B	
デシベル	dB	

表９．固有の名称をもつCGS組立単位

名称	記号	SI 単位で表される数値
エルグ	erg	$1\ erg=10^{-7}\ J$
ダイン	dyn	$1\ dyn=10^{-5}N$
ポアズ	P	$1\ P=1\ dyn\ s\ cm^{-2}=0.1Pa\ s$
ストークス	St	$1\ St=1cm^2\ s^{-1}=10^{-4}m^2\ s^{-1}$
スチルブ	sb	$1\ sb=1cd\ cm^{-2}=10^4cd\ m^{-2}$
フォト	ph	$1\ ph=1cd\ sr\ cm^{-2}=10^4lx$
ガル	Gal	$1\ Gal=1cm\ s^{-2}=10^{-2}ms^{-2}$
マクスウエル	Mx	$1\ Mx=1G\ cm^2=10^{-8}Wb$
ガウス	G	$1\ G=1Mx\ cm^{-2}=10^{-4}T$
エルステッド(a)	Oe	$1\ Oe \triangleq (10^3/4\pi)A\ m^{-1}$

(a) ３元系のCGS単位系とSIでは直接比較できないため、等号「 ≙ 」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	$1\ Ci=3.7\times10^{10}Bq$
レントゲン	R	$1\ R=2.58\times10^{-4}C/kg$
ラド	rad	$1\ rad=1cGy=10^{-2}Gy$
レム	rem	$1\ rem=1\ cSv=10^{-2}Sv$
ガンマ	γ	$1\ \gamma=1\ nT=10^{-9}T$
フェルミ		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$=0.2\ g=2\times10^{-4}kg$
トル	Torr	1 Torr = (101 325/760) Pa
標準大気圧	atm	1 atm = 101 325 Pa
カロリー	cal	1 cal=4.1858J（「15℃」カロリー），4.1868J（「IT」カロリー），4.184J（「熱化学」カロリー）
ミクロン	µ	$1\ \mu=1\mu m=10^{-6}m$

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