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Development of JAEA Sorption Database (JAEA-SDB) : Update of Sorption/QA Data in FY2019

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

This report focuses on updating of the sorption database (JAEA-SDB) as a basis of integrated approach for the PA-related distribution coefficient (K_d) setting and development of mechanistic sorption models. This report also includes an overview of the database structure and contents. K_d data and their quality assurance (QA) results were updated by focusing on the following systems as potential needs extracted from our recent activities on the K_d setting and development of mechanistic models: i) K_d data for clay systems to develop and validate the mechanistic sorption models, ii) K_d data for sedimentary rocks to cover wider ranges of conditions for the K_d parameter setting, and iii) K_d data for cementitious materials to enhance dataset for the K_d parameter setting

As a result, 7,696 K_d data from 66 references related to the above-mentioned systems were added and the total number of K_d values in JAEA-SDB reached 70,673. The QA/classified K_d data reached about 73% for all K_d data in JAEA-SDB. The updated JAEA-SDB is expected to make it possible to give a basis for the next-step PA-related K_d setting.

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

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JAEA 収着データベース（JAEA-SDB）の開発：
2019 年度における収着データ/信頼度情報の拡充

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

今回，性能評価における収着分配係数（K_d）設定のための統合的手法の構築の基礎として，収着データベース（JAEA-SDB）のデータ拡充を行った。本報告では，はじめに JAEA-SDB のデータベースの構造と内容の概要を確認したうえで，K_d 設定や収着モデル開発の最近の取り組みにおいて課題として抽出された系に着目して実施した，K_d データと信頼度情報の拡充について報告する。具体的な対象は，i) 収着モデルの開発・確証のための粘土系 K_d データ，ii) 幅広い条件に対応したパラメータ設定のための堆積岩系 K_d データ，そして iii) パラメータ設定のデータセット拡充のためのセメント系 K_d データである。

今回の更新において，上記の 3 つの系に関連した 66 の文献から 7,696 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 70,673 件となり，全データのうちの約 73%のデータに対して信頼度情報が付与されたこととなる。今回更新された JAEA-SDB によって，今後の性能評価における収着パラメータ設定に向けて，有効な基盤情報を提供するものと期待される。

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1. Introduction

Sorption behavior of radionuclides (RNs) in buffer materials (bentonite), host rock (rock matrix) and cementitious materials is one of the key processes in a safe geological disposal of radioactive waste. The magnitude of RNs sorption onto these materials is normally expressed as a distribution coefficient (K_d). K_d values extremely depend on geochemical conditions such as pH, E_h, ionic strength and solution composition[1-2]. Therefore, it is necessary to understand the detailed processes of RNs sorption onto these materials under wide ranges of geochemical conditions. Additionally, it is important to develop a database containing extensive compilation of K_d data and a mechanistic/predictive models so that reliable parameters can be set under a variety of geochemical conditions relevant to a performance assessment (PA). Because of the conditional nature of sorption data, K_d values used in the PA calculations need to be corresponded to the specific conditions which characterize the respective PA-setting. Moreover, geochemical variability and uncertainty and their effects on K_d values have to be considered for the reference and alternative scenarios in the PA[1]. Because it is not feasible to measure K_d values for all PA conditions, using existing sorption data obtained under generic experimental conditions and converting these data to the range of PA-specific conditions is a key task. A sorption database (SDB) containing large amount of sorption data for estimated, simplified or generic systems is used to set K_d values for the PA conditions taking into account any differences in substrate and geochemical conditions.

We have developed the SDB, which were firstly developed as an important basis for the second progress report on high-level waste (H12 report)[3-6]. We have also developed the SDB for the second progress report on trans-uranic (TRU) waste (TRU-2 report) [7-9]. We have continued to improve and update the SDB in the view of potential future needs of data focusing on:

1) updating sorption data[10-15]

2) assuring the desired quality level for SDB[12, 14-19]

3) testing and applying of the SDB to a parameter-setting[16-26]

The web-based SDB system (JAEA-SDB) has been developed to utilize a quality assuring procedure and to allow effective application for a parameter setting[27] (https://migrationdb.jaea.go.jp/).

A K_d setting approach is needed to apply for various rock types and geochemical conditions and to evolve from site-generic stages to site-specific stages by considering the information obtained from forthcoming site investigation stages. Such comprehensive K_d setting approach which is applicable for various conditions and situations was developed on the basis of the international state-of-the-art knowledge integrating the three different methods as follows (Figure 1-1):

1) experimental data acquisition for specific/reference conditions

2) extraction and conversion of K_d data from existing sorption and diffusion data

3) prediction by mechanistic sorption and diffusion models

These procedures can be done through an expert judgment and a semi-quantitative way by considering differences of parameters such as surface sites of the solid phase, speciations of the RNs and the presence of competitive RNs[1, 20, 21, 24, 28, 29]. As shown in NEA[1], a thermodynamic sorption model (TSM) makes it possible to estimate K_d variations directly on the basis of the mechanistic understanding. We have developed an integrated sorption/diffusion (ISD) database combined with thermodynamic sorption and diffusion models and tested the ISD database to explain sorption and diffusion behavior of various RNs with a complex geochemical conditions in compacted bentonites[30-32]. We have also tested these K_d setting approaches for the derivation of K_d values and their uncertainties for rock matrix such as Horonobe mudstones and generic granites[20-26].

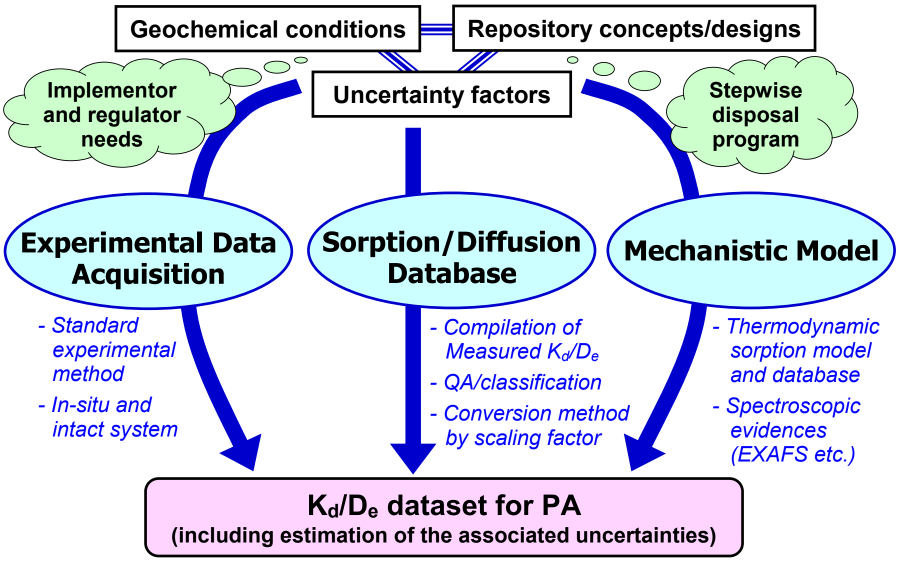

Figure 1-1 Integrated approach for sorption/diffusion parameter setting for PA

In this report, we focused on updating of JAEA-SDB as a basis for integrated approach for the PA-related K_d setting and development of mechanistic sorption models. This report also includes an overview of the database structure and contents. K_d data and their quality assurance (QA) results are updated by focusing on the following systems as potential needs extracted from our recent activities on the K_d setting and mechanistic model development:

i) K_d data for clay systems to develop and validate the mechanistic sorption models

ii) K_d data for sedimentary rocks to cover wider ranges of conditions for the K_d parameter setting

iii) K_d data for cementitious materials to enhance dataset for the K_d parameter setting

2. Contents, functions and systems of JAEA-SDB

2.1 Overview and status of JAEA-SDB

JAEA-SDB is a compilation of experimental K_d values of key RNs sorption onto bentonite, various rocks, cementitious materials and soils related to the radioactive waste disposal. The K_d values were determined by batch sorption experiments and they include experimental conditions. These data are operated by a database software to allow quick search and plotting data as a function of selected key parameters. The contents, functions and systems are briefly summarized in Table 2.1-1. As pointed out in NEA SDB project[1)], a SDB cannot be used in the PA-related K_d setting without understanding and checking of the experimental details because it includes great varieties of K_d values obtained under various conditions and has different reliability levels. Therefore, JAEA-SDB has been developed so that reliable data relevant to the PA conditions can be extracted from the SDB in an effective way by focusing on the following points:

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

Table 2.1-1 Summary of the contents, functions and systems of JAEA-SDB

Contents/functions	Brief description for status
Number of K_d values/references	K_d ; 70,673 (7,696 was added in this update or revise*) Reference ; 780 (66 references were added in this update*)
Elements	79 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; 41 elements
Solid phase	Bentonite (clay minerals); Rocks – 5 groups; Basaltic rock, granitic rock, mudstone, sandstone, tuff; Other minerals (Fe, Al-oxides/hydroxide, calcite, etc.); Cementitious materials (cement/concrete); Soils; Having special influence (grout, organic substance, etc.)
Search parameters	Element, solid phase group Detailed – Solid phase, water type, pH, Eh, ionic strength, temperature, liquid/solid ratio, contact time, initial concentration, separation method, atmosphere/redox condition
Graphing/data evaluation	K_d plot as a function of ; pH, Eh, ionic strength, temperature, liquid/solid ratio, contact time, initial concentration; Grouping function to evaluate multi-parameter dependence; Statistical data evaluation; Grouping of K_d data related to perturbations
QA/classification	QA information evaluated by QA guideline, and related evidences 51,234 K_d (about 73% of total K_d)* for key RNs have been evaluated
Database systems	- Web application based database (since 2009) - Microsoft Access® database (since 2003/stand-alone/limited functions)

*; Contents and functions updated or revised in this report.

2.2 Main data table and contents of JAEA-SDB

Main data table of JAEA-SDB contains K_d values and a large number of additional key information. Each K_d value is associated with the information of solid and liquid phase, experimental condition and the reference (Table 2.2-1). The hierarchical structure comprising primary and detailed information is used to allow effective database operations.

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

Category	Parameters and notes recorded		Unit	Remarks
No.	Save No.		-	Number for managing data record
Elements	Element		-	Chemical symbol (basic search condition)
	Redox		-	Valency
Solid phase	Solid phase group		-	Solid phase group (basic search condition)
	Solid phase		-	Name of solid phase as rocks, clay minerals, minerals, etc.
	Detailed Info.	Specific surface area	m^2/g	
		CEC	meq/100 g	Cation exchange capacity
		Chemical/mineral composition	-	
		Note	-	Particle size, source, name, conditions and methods for sample preparation, etc.
Liquid/solid ratio	Liquid/solid		mL/g	Liquid to solid ratio
	Detailed Info.	Liquid	mL	Amount of liquid phase
		Solid	g	Amount of solid phase
Liquid phase	Water type		-	Type and name of solution/groundwater
	Detailed Info.	Ca	ppm	Final or initial composition (concentration)
		Na	ppm	
		K	ppm	
		Mg	ppm	
		Cl	ppm	
		HCO_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 2.2-1 Main data table of JAEA-SDB (2/2)

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

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

As described in 2.1, it is important to assess the reliability of a wide variety of K_d data in the SDB for the PA-related K_d setting. The reliability of K_d values in JAEA-SDB is assessed on the basis of 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 the 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[16)] and briefly summarized in Table 2.3-1.

In accordance with the guideline, an entry is evaluated by Criteria I and key checkpoints II-b, II-c, II-d and II-h in Criteria II first. Classification and final numerical rating of the entry are only completed if the entry is evaluated as “reliable” on the basis of these checkpoints. If the entry is evaluated as “unreliable”, it is excluded from further evaluation. The entries are evaluated by the three criteria separately, and the all results can be referred in JAEA-SDB[12)]. JAEA-SDB uses QA levels (Class 1–6) classified in accordance with the sum of points obtained from Criteria II, the result of unreliable evaluation in Criteria I and II as main reliability information. All results and evidence of Criteria I and II are also recorded in tabular form and can be referred as a PDF format in JAEA-SDB to keep a traceability. The results relevant to Criteria III are discussed subsequently and illustrated in the form of plots of K_d vs. a relevant master parameter (typically pH). The results can be referred as a PDF format in JAEA-SDB.

Table 2.3-1 Reliability information table of JAEA-SDB

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

* Critical checkpoints with minimum requirements related with the judgment to be “unreliable”.

3. Updating of sorption data and its QA classification

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

As mentioned above, the SDB plays important roles in the PA-related K_d setting and development of mechanistic sorption models. Therefore, we added 66 references to JAEA-SDB in relation to our recent activities on the development of mechanistic models[31-33)] and the PA-related K_d setting[21-26)] in this update. We selected the references focusing on three solid phase systems; i.e., i) clay minerals, ii) sedimentary rocks and iii) cementitious materials. 66 references selected in this update and their details are shown in Table 3.1-1. In i) clay minerals, bentonite/smectite which is the main component of buffer materials was especially targeted. Sorption models such as TSM have been developed, therefore, collecting reliable sorption data of the clay mineral contribute to confirm the validity of the modeling. ii) Sedimentary rocks are important rock matrix. They were focused to cover wider ranges of conditions and mineral compositions. Compared with the reports on clay minerals and sedimentary rocks, those on iii) cementitious materials are scarce. Therefore, collecting reliable RNs sorption data of cementitious materials is important.

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (1/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
1)	ANDRA(2005)	ANDRA : Référentiel de comportement des radionucléides et des toxiques chimiques d'un stockage dans le Callovo-Oxfordien jusqu'à l'homme, Site de Meuse/Haute-Marne, Tome 1/2: Chapitres 1 à 4, Dossier 2005 Argile (2005).	Ni	CSH	-
2)	Ashikawa et al.(2001)	Ashikawa, N. , Tajima, T. , Saito, H. and Fujiwara, A. : Sorption behavior of radionuclides on calcium-leached mortar, Material Research Society Symposium Proceedings, vol.663, pp.97-104 (2001).	Ag, Am, C, Cs, I, Sr, Tc	mortar	equilibrated solution
3)	Banik et al.(2017)	Banik, N. L. , Marsac, R. , Lutzenkirchen, J. , Marquardt, C. M. , Dardenne, K. , Rothe, J. , Bender, K. and Geckeis, H. : Neptunium sorption and redox speciation at the illite surface under highly saline conditions, Geochimica et Cosmochimica Acta, vol.215, pp.421-431 (2017).	Np	illite	1.0M-NaCl, 3.2M-NaCl
4)	Bayliss et al.(1992)	Bayliss, S. , Haworth, A. , McCrohon, R. , Moreton, A. D. , Oliver, P. , Pilkington, N. J. , Smith, A. J. and Smith-Briggs, J. L. : Radioelement behaviour in a cementitious environment, Materials Research Society symposia proceedings, vol.257, pp.641-648 (1992).	Tc	OPC/limestone	non-saline water, saline water
5)	Berry et al.(2000)	Berry, J. A. , Bond, K. A. , Green, A. , Linklater, C. M. and Smith, A. J. : An experimental study of actinide sorption onto calcite, aluminium oxide and hematite, AEA Technology, AEA Report, AEAT/R/ENV/0205 (2000).	Pu, Th, U	aluminium oxide, calcite, hematite	0.1M-$NaNO_3$, 0.02M-$Ca(NO_3)_2$+0.1M $NaNO_3$, 0.1M-$NaNO_3$+CO_3
6)	Bonhoure et al.(2002)	Bonhoure, I. , Scheidegger, A. M. , Wieland, E. and Dahn, R. : Iodine species uptake by cement and CSH studied by I K-edge X-ray absorption spectroscopy, Radiochimica Acta, vol.90, pp.647-651 (2002).	I	HCP	ACW
7)	Boult et al.(1998)	Boult, K. A. , Cowper, M. M. , Heath, T. G. , Sato, H. , Shibutani, T. and Yui, M. : Towards an understanding of the sorption of U(VI) and Se(IV) on sodium bentonite, Journal of Contaminant Hydrology, vol.35, pp.141-150 (1998).	Se, U	goethite, Na-smectite	0.01M-NaCl, 0.01M-NaCl+CO_3^{2-}, 0.1M-NaCl, 1M-NaCl
8)	Bradbury and Baeyens(2011b)	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, PSI Bericht Nr. 11-05 (2011).	Cs, Eu, I, Ni, Se, Th, U	MX-80	SBPW

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (2/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
9)	Chen et al.(2016)	Chen, Z. , Chen, L. and Lu, S. : Effect of solution chemistry on the interaction of radionuclide 63Ni(II) onto montmorillonite, Journal of Radioanalytical and Nuclear Chemistry , vol.308, pp.505-516 (2016).	Ni	montmorillonite	0.001M-, 0.01M-, 0.1M $NaClO_4$, 0.01M-$Ca(ClO_4)_2$, 0.01M-$KClO_4$, 0.01M-NaCl, 0.01M-$NaNO_3$
10)	Cowan et al.(1990)	Cowan, C. E. , Zachara, J. M. and Resch, C. T. : Solution ion effects on the surface exchange of selenite on calcite, Geochimica et Cosmochimica Acta, vol.54, pp.2223-2234 (1990).	Mg, P, Se	$CaCO_3$	$CaCO_3$(aq), $CaCO_3$(aq)/$CaSO_4$(aq), $CaCO_3$(aq)+ Mg, $CaCO_3$(aq)+ PO_4, $CaCO_3$(aq)+ Se, $CaCO_3$(aq)+ SeO_3
11)	Cowper et al.(2005)	Cowper, M. M. , Green, A. , Myatt, B. J. , Swanton, S. W. and Williams, S. J. : A laboratory study of the lmpact of picolinate and anion exchange resin degradation products on nickel, americium and plutonium behaviour in a repository, Serco Assurance, SA/ENV-0693 (2005).	Am, Ni, Pu	CSH, NRVB	CSH equilibrated water, CSH equilibrated water+picolinate, leachate, NRVB equilibrated water, NRVB equilibrated water+picolinate
12)	Dahn et al.(2011)	Dahn, R. , Baeyens, B. and Bradbury, M. H. : Investigation of the different binding edge sites for Zn on montmorillonite using P-EXAFS - The strong/weak site concept in the 2PNES SC/CE sorption model, Geochimica et Cosmochimica Acta, vol.75, pp.5154-5168 (2011).	Zn	Na-montmorillonite	0.1M-$NaClO_4$
13)	Druteikiene et al.(2017)	Druteikiene, R. , Sapolaite, J. , Ezerinskis, Z. and Juodis, L. : Batch-type study of Ca, Co, and Tc binding with hydrated cement under hyperalkaline conditions, Journal of Radioanalytical and Nuclear Chemistry, vol.313, pp.299-307 (2017).	Co, Cs, Tc	HCP	cement water, cement water+$Na_2S_2O_4$, deionized water, deionized water+$Na_2S_2O_4$
14)	Elo et al.(2017)	Elo, O. , Muller, K. , Ikeda-Ohno, A. , Bok, F. , Scheinost, A. C. , Holtta, P. and Huittinen, N. : Batch sorption and spectroscopic speciation studies of neptunium uptake by montmorillonite and corundum, Geochimica et Cosmochimica Acta, vol.198, pp.168-181 (2017).	Np	corundum, Na-montmorillonite	0.01M-$NaClO_4$

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (3/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
15)	Fukushi et al.(2013)	Fukushi, K. , Hasegawa, Y. , Maeda, K. , Aoi, Y. , Tamura, A. , Arai, S. , Yamamoto, Y. , Aosai, D. and Mizuno, T. : Sorption of Eu(III) on granite: EPMA, LA-ICP-MS, batch and modeling studies, Environmental Science and Technology, vol.47, pp.12811-12818 (2013).	Eu	biotite, granite	0.01M-, 0.1M-NaCl
16)	Geibert and Usbeck(2004)	Geibert, W. and Usbeck, R. : Adsorption of thorium and protactinium onto different particle type: Experimental findings, Geochimica et Cosmochimica Acta, vol.68, No.7, pp.1489-1501 (2004).	Pa, Th	$CaCO_3$, MnO_2, opal, smectite	seawaer
17)	Goldberg(2014)	Goldberg, S. : Modeling selenate adsorption behavior on oxides, clay minerals, and soils using the triple layer model, Soil Science, vol.179, pp.568-576 (2014).	Se	Al-oxide, Fe-oxide, illite, kaolinite, soil	0.1M-NaCl
18)	Higgo and Rees (1986)	Higgo, J. J. W. and Rees, L. V. : Adsorption of actinides by marine sediments: Effect of the sediment/seawater ratio on the measured distribution ratio, Environmental Science and Technology, vol.20, pp.483-490 (1986).	Am, Np, Pu	sediment	seawater
19)	Hu et al.(2018)	Hu, W. , Lu, S. , Song, W. , Chen, T. , Hayat, T. , Alsaedi, N. S. , Chen, C. and Liu, H. : Competitive adsorption of U(VI) and Co(II) on montmorillonite: A batch and spectroscopic approach, Applied Clay Science, vol.157, pp.121-129 (2018).	Co, U	montmorillonite	0.0001M-, 0.001M-, 0.01M-NaCl
20)	Huber et al.(2017)	Huber, F. M. , Totskiy, Y. , Marsac, R. , Schild, D. , Pidchenko, I. , Vitova, T. , Kalmykov, S. , Geckeis, H. and Schafer, T. : Tc interaction with crystalline rock from Aspo (Sweden): Effect of in-situ rock redox capacity, Applied Geochemistry, vol.80, pp.90-101 (2017).	Tc	diorite	AGWS
21)	Hyun et al.(2001)	Hyun, S. P. , Cho, Y. H. , Hahn, P. S. and Kim, S. J. : Sorption mechanism of U(VI) on a reference montmorillonite: Binding to the internal and external surfaces, Journal of Radioanalytical and Nuclear Chemistry, vol.250, pp.55-62 (2001).	U	chlorite, kaolinite, montmorillonite	0.001M-, 0.01M-, 0.1M-$NaNO_3$
22)	Iida et al.(2016a)	Iida, Y. , Yamaguchi, T. , Tanaka, T. and Hemmi, K. : Sprption behavior of thorium onto granite and its constituent minerals, Journal of Nuclear Science and Technology, vol.53, pp.1573-1584 (2016).	Th	albite, biotite, granite, quartz	0.01M-, 0.05M-, 0.1M-$NaHCO_3$
23)	Iida et al.(2016b)	Iida, Y. , Barr, L. , Yamaguchi, T. and Hemmi, K. : Sorption behavior of thorium onto montmorillonite and illite, Journal of Nuclear Fuel Cycle and Environment, vol.23, No.1, pp.3-8 (2016).	Th	illite, montmorillonite	0.01M-, 0.05M-, 0.1M-$NaHCO_3$

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (4/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
24)	Johnson et al.(2000)	Johnson, E. A. , Rudin, M. J. , Steinberg, S. M. and Johnson, W. H. : The sorption of selenite on various cement formulations, Waste Management, vol.20, pp.509-516 (2000).	Se	cement/silica fume/clay mixture	deionized water
25)	Lakshtanov and Stipp(2007)	Lakshtanov, L. Z. and Stipp, S. L. S. : Experimental study of nikel(II) interaction with calcite: Adsorption and coprecipitation, Geochimica et Cosmochimica Acta, vol.71, pp.3686-3697 (2007).	Ni	calcite	equilibrated solution
26)	Leng et al.(2016)	Leng, Y. , Henderson, M. J. , Courtois, J. , Li, H. , Xiong, K. , Tuo, X. and Yan, M. : Sorption of plutonium on geological materials associated with a Chinese radioactive waste repository: influence of pH, Journal of Radioanalytical and Nuclear Chemistry, vol.308, pp.895-903 (2016).	Pu	bentonite, Ca-bentonite, Na-bentonite, slate, soil	distilled water, distilled water+0.01M-$FeCl_2$, distilled water+0.1M-$FeCl_2$
27)	Lothenbach et al.(1999)	Lothenbach, B. , Ochs, M. and Hager, D. : Confinement of radioactive waste in cementitious barriers for surface and deep geological disposal, Andra 2005 report 1999, C. RP.0BMG.99-001 (1999).	Se	cement	pre-equilibrated pore solutions
28)	Maiti et al.(1989)	Maiti, T. C. , Smith, M. R. and Laul, J. C. : Sorption of uranium, thorium, and radium on matrices under oxic environments, Radioactive Waste Management and the Nuclear Fuel Cycle, vol.11, No.3, pp.269-278 (1989).	Ra, Th, U	anhydrite, calcite, dolomite	synthetic brine
29)	Marques Fernandes and Baeyens(2019)	Marques Fernandes, M. and Baeyens, B. : Cation exchange and surface complexation of lead on montmorillonite and illite including competitive adsorption effects, Applied Geochemistry, vol.100, pp.190-202 (2019).	Pb	Na-illite, Na-montmorillonite	0.02M-, 0.1M-, 0.3M-NaCl
30)	Marques Fernandes et al.(2016)	Marques Fernandes, M. , Scheinost, A. C. and Baeyens, B. : Sorption of trivalent lanthanides and actinides onto montmorillonite: Macroscopic, thermodynamic and structural evidence for ternary hydroxo and carbonate surface complexes on multiple sorption sites, Water Research, vol.99, pp.74-82 (2016).	Eu	Na-montmorillonite	0.1M-$NaClO_4$
31)	Marsac et al.(2015)	Marsac, R. , Banik, N. , Lutzenkirchen, J. , Marquardt, C. M. , Dardenne, K. , Schild, D. , Rothe, J. , Diascorn, A. , Kupcik, T. , Schafer, T. and Geckeis, H. : Neptunium redox speciation at the illite surface, Geochimica et Cosmochimica Acta, vol.152, pp.39-51 (2015).	Np	Na-illite	0.1M-NaCl

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (5/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
32)	Montavon et al.(2009)	Montavon, G. , Guo, Z. , Lutzenkirchen, J. , Alhajji, E. , Kedziorek, M. A. M. , Bourg, A. C. M. and Grambow, B. : Interaction of selenite with MX-80 bentonite: Effect of minor phases, pH, selenite loading, solution composition and compaction, Colloids and Surfaces A: Physicochemical and Engineering Aspects, vol.332, pp.71-77 (2009).	Se	bentonite, montmorillonite	0.01M-, 0.05M-, 0.1M-NaCl, 0.05M-NaCl+Ca, 0.016M-Na_2SO_4, 0.05M-$NaNO_3$, SGW
33)	Montoya et al.(2018)	Montoya, V. , Baeyens, B. , Glaus, M. A. , Kupcik, T. , Marques Fernandes, M. , Van Laer, L. , Bruggeman, C. , Maes, N. and Schafer, T. : Sorption of Sr, Co and Zn on illite: Batch experiments and modelling including Co in-diffusion measurements on compacted samples, Geochimica et Cosmochimica Acta, vol.223, pp.1-20 (2018).	Co, Sr, Zn	Na-illite	0.001M-, 0.01M-, 0.03M-, 0.1M-, 0.3M-, 0.5M-, 1M-$NaClO_4$, 0.1M-, 0.5M-NaCl
34)	Muuri et al.(2017)	Muuri, E. , Siitari-Kauppi, M. , Natara-aho, M. , Ikonen, J. , Lindberg, A. , Qian, L. and Koskinen, L. : Cesium sorption and diffusion on crystalline rock: Olkiluoto case study, Journal of Radioanalytical and Nuclear Chemistry, vol.311, pp.439-446 (2017).	Cs	biotite, gneiss, granite, K-feldspar, plagioclase	synthetic groundwater
35)	Muurinen et al.(2014)	Muurinen, A. , Tournassat, C. , Hadi, J. and Greneche, J.-M. : Sorption and diffusion of Fe(II) in bentonite, Posiva, Working Report 2014-04 (2014).	Fe	bentonite, smectite	0.05M-, 0.3M-NaCl
36)	Nagasaki et al.(2017)	Nagasaki, S. , Riddoch, J. , Saito, T. , Goguen, J. , Walker, A. and Yang, T. T. : Sorption behaviour of Np(IV) on illite, shale and MX-80 in high ionic strength solutions, Journal of Radioanalytical and Nuclear Chemistry, vol.313, pp.1-11 (2017).	Np	bentonite, illite, shale	0.1M-NaCl+$CaCl_2$, 0.5M-NaCl+$CaCl_2$, 1M-NaCl+$CaCl_2$, 2M-NaCl+$CaCl_2$, 3M-NaCl+$CaCl_2$, 4M-NaCl+$CaCl_2$, 6M-NaCl+$CaCl_2$+$NaClO_4$, brine solution
37)	Ochs et al.(2001)	Ochs, M. , Lothenbach, B. and Talerico, C. : Support of Kd models and datasets for the retention of radionuclides in cementitious repositories, ANDRA Report, C.RP.0BMG.01-001 (2001).	I, Se	CSH, portlandite, calcite, hydrogarnet	synthetic pore water
38)	Ochs et al.(2006)	Ochs, M. , Pointeau, I. and Giffaut, E. : Caesium sorption by hydrated cement as a function of degradation state: Experiments and modelling, Waste Management, vol.26, pp.725-732 (2006).	Cs	CEM, CSH	AGW, distilled water, NH_4NO_3

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (6/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
39)	Orucoglu et al.(2018)	Orucoglu, E. , Tournassat, C. , Robinet, J.-C. , Made, B. and Lundy, M. : From experimental variability to the sorption related retention parameters necessary for performance assessment models for nuclear waste disposal system: The example of Pb adsorption on clay minerals, Applied Clay Science, vol.163, pp.20-32 (2018).	Pb	bentonite, claystone, illite	0.025M-, 0.1M-NaCl
40)	Patel et al.(2017)	Patel, M. A. , Kar, A. S. , Garg, D. , Kumar, S. , Tomar, B. S. and Bajpai, R. K. : Sorption studies of radionuclides on argillaceous clays of Cuddapah System, Journal of Radioalalytical and Nuclear Chemistry, vol.313, pp.555-563 (2017).	Cs, Eu	clay	0.1M NaCl
41)	Pointeau(2000)	Pointeau, I. : Etude mécanistique et modélisation de la retention de radionucléides par les phases de silicate de calcium des ciments hydrates, Thèse de l'Université de Reims-Champagne- Ardennes, France (2000).	Cs	CSH	synthetic pore water
42)	Pointeau et al.(2001)	Pointeau, I. , Marmier, N. , Fromage, F. , Fedoroff, M. and Giffaut, E. : Cesium and lead uptake by CSH phases of hydrated cement, Material Research Society Symposium Proceedings, vol.663, pp.105-113 (2001).	Cs, Pb	CSH	WCSH, WCSH+$NaNO_3$
43)	Pointeau et al.(2008)	Pointeau I. , Coreau N. and Reiller P. E. : Uptake of anionic radionuclides onto degraded cement pastes and competing effect of organic ligands, Radiochimica Acta, vol.96, pp.367-374 (2008).	C, Cl, Cs, I, Se, U	HCP	HCP-equilibrated water, HCP-equilibrated water+EDTA
44)	Pratopo et al.(1993)	Pratopo, M. I. , Yamaguchi, T. , Moriyama, H. and Higashi, K. : Sorption and colloidal behavior of Np(IV) in a bentonite-carbonate solution system, Journal of Nuclear Science and Technology, vol.30, No.6, pp.560-566 (1993).	Np	bentonite	0.1M-$NaClO_4$+0.1M-$NaHCO_3$
45)	Richter(2015)	Richter, C. : Sorption of environmentally relevant radionuclides (U(VI), Np(V)) and lanthanides (Nd(III)) on feldspar and mica, 133p (2015).	Nd, Np, U	muscovite, orthoclase	0.01M-, 1M $NaClO_4$, 0.01M-$NaClO_4$+0.0015M-Ca
46)	Richter(2015)	Richter, C. : Sorption of environmentally relevant radionuclides (U(VI), Np(V)) and lanthanides (Nd(III)) on feldspar and mica, 133p (2015).	Nd, Np, U	muscovite, orthoclase	0.01M-, 1M $NaClO_4$, 0.01M-$NaClO_4$+0.0015M-Ca
47)	Rouff et al.(2005a)	Rouff, A. A. , Reeder, R. J. and Fisher, N. S. : Electrolyte and pH effects on Pb(II)-calcite sorption processes: the role of the PbCO30(aq) complex, Journal of Colloid and Interface Science, vol.286, pp.61-67 (2005).	Pb	calcite	0.0015M-, 0.15M-, 0.2M-, 0.3M-, 0.5M-$NaNO_3$, 0.15M-, 0.3M-, 0.5M-NaCl

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (7/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
48)	Rouff et al.(2005b)	Rouff, A. A. , Elzinga, E. J. , Reeder, R. J. and Fisher, N. S. : The influence of pH on the kinetics, reversiblility and mechanisms of Pb(II) sorption at the calcite-water interface, Geochimica et Cosmochimica Acta, vol.69, No.22, pp.5173-5186 (2005).	Pb	calcite	equilibrated solution
49)	Rouff et al.(2006)	Rouff, A. A. , Elzinga, E. J. , Reeder, R. J. and Fisher, N. S. : The effect of aging and pH on Pb(II) sorption processes at the calcite-water interface, Environmental Science and Technology, vol.40, pp.1792-1798 (2006).	Pb	calcite	equilibrated water
50)	Sasaki et al.(2016)	Sasaki, T. , Ueda, K. , Saito, T. , Aoyagi, N. , Kobayashi, T. , Takagi, I. , Kimura, T. and Tachi, Y. : Sorption of Eu^{3+} on Na-montmorillonite studied by time-resolved laser fluorescence spectroscopy and surface complexation modeling, Journal of Nuclear Science and Technology, vol.53, No.4, pp.592-601 (2016).	Eu	Na-montmorillonite	0.01M-, 0.1M-, 1M-$NaNO_3$
51)	Savoye et al.(2015)	Savoye, S. , Beaucaire, C. , Grenut, B. and Fayette, A. : Impact of the solution ionic strength on strontium diffusion through the Callovo-Oxfordian clayrocks: An experimental and modeling study, Applied Geochemistry, vol.61, pp.41-52 (2015).	Sr	clay	PW
52)	Schnurr et al.(2015)	Schnurr, A. , Marsac, R. , Rabung, T. , Lutzenkirchen, J. and Geckeis, H. : Sorption of Cm(III) and Eu(III) onto clay minerals under saline conditions: Batch adsorption, laser-fluorescence spectroscopy and modeling, Geochimica et Cosmochimica Acta, vol.151, pp.192-202 (2015).	Cm, Eu	Na-illite, Na-montmorillonite	0.09M-, 0.1M-, 0.92M-, 1.02M-, 3.9M-NaCl
53)	Schulthess and Huang(1990)	Schulthess, C. P. and Huang, C. P. : Adsorption of heavy metals by silicon and aluminium oxide surfaces on Bentonite (Clay minerals), Soil Science Society of America Journal, vol.54, pp.679-688 (1990).	Cd	montmorillonite	0.01M-$NaClO_4$
54)	Siroux et al.(2017)	Siroux, B. , Beaucaire, C. , Tabarant, M. , Benedetti, M. F. and Reiller, P. E. : Adsorption of strontium and caesium onto an Na-MX80 bentonite: Experiments and building of a coherent thermodynamic modelling, Applied Geochemistry, vol.87, pp.167-175 (2017).	Cs, Sr	Na-montmorillonite	0.05M-, 0.1M-, 0.15M-NaCl
55)	Stathi et al.(2010)	Stathi, P. , Papadas, I. T. , Tselepidou, A. and Deligiannakis, Y. : Heavy-metal uptake by a high cation-exchange-capacity montmorillonite: The role of permanent charge sites, Global NEST Journal, vol.12, No.3, pp.248-255 (2010).	Cd, Cu, Pb, Zn	Na-montmorillonite	$Cd(NO_3)_2$, $Cu(NO_3)_2$, $Pb(NO_3)_2$, $Zn(NO_3)_2$

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (8/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
56)	Tachi et al.(2020)	Tachi, Y. , Suyama, T. and Mihara, M. : Data acquisition for radionuclide sorption on barrier materials for performance assessment of geological disposal of TRU wastes, JAEA Technical Report, JAEA-Data/Code 2019-021 (2020).	Am, C, Cl, Cs, I, Nb, Ni, Se, Sn, Sr, Th	OPC, DOPC, tuff	alkali solution, distilled water, synthetic seawater, nitric acid solution, ammonia solution
57)	Tamamura et al.(2014)	Tamamura, S. , Takada, T. , T. Tomita, J. , Nagao, S. , Fukushi, K. and Yamamoto, M. : Salinity dependence of ^{226}Ra adsorption on montmorillonite and kaolinite, Journal of Radioanalytical and Nuclear Chemistry, vol.299, pp.569-575 (2014).	Ra	kaolinite, montmorillonite	0.01M-, 0.1M-, 0.5M-, 1M-NaCl
58)	Titis et al.(2003)	Tits, J. , Stumpf, T. , Rabung, T. , Wieland, E. and Fanghanel, T. : Uptake of Cm(III) and Eu(III) by calcium silicate hydrates: A solution chemistry and time-resolved laser fluorescence spectroscopy study, Environmental Science and Technology, vol.37, No.16, pp.3568-3573 (2003).	Eu	CSH	ACW
59)	Tits et al.(2005)	Tits, J. , Wieland, E. and Bradbury, M. H. : The effect of isosaccharinic acid and gluconic acid on the retention of Eu(III), Am(III) and Th(IV) by calcite, Applied Geochemistry, vol.20, pp.2082-2096 (2005).	Am, Eu, Th	calcite	ACW, ACW+ISA, ACW+GLU, 0.3M-NaOH, 0.3M-NaOH+ISA, 0.3M-NaOH+GLU
60)	Tournassat et al.(2018)	Tournassat, C. , Tinnacher, R. M. , Grangeon, S. and Davis, J. A. : Modeling uranium(VI) adsorption onto montmorillonite under varying carbonate concentrations: A surface complexation model accounting for the spillover effect on surface potential, Geochimica et Cosmochimica Acta, vol.220, pp.291-308 (2018).	U	Na-montmorillonite	0.002M-, 0.01M-, 0.1M-NaCl
61)	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
62)	Um et al.(2009)	Um, W. , Serne, R. J. , Last, G. V. , Clayton, R. E. and Glossbrenner, E. T. : The effect of gravel size fraction on the distribution coefficients of selected radionuclides, Journal of Contaminant Hydrology, vol.107, pp.82-92 (2009).	Np, Tc, U	sediment, gravel	simulated groundwater

Table 3.1-1 Overview of 66 references selected for updating JAEA-SDB (9/9)

No.	Reference	Details of reference	Element	Solid phase	Solution type
63)	Verma et al.(2017)	Verma, P. K. , Romanchuk, A. Y. , Vlasova, I. E. , Krupskaya, V. V. , Zakusin, S. V. , Sobolev, A. V. , Egorov, A. V. , Mohapatra, P. K. and Kalmykov, S. N. : Np(V) uptake by bentonite clay: Effect of accessory Fe oxides/hydroxides on sorption and speciation, Applied Geochemistry, vol.78, pp.74-82 (2017).	Np	clay	0.01M-, 1M-$NaClO_4$
64)	Viallis-Terrisse(2000)	Viallis-Terrisse, H. : Interactions des silicates de calcium hydratés, principaux constituants du ciment, avec let chlorures d’alcalins. Analogies avec les argile, Thèse de l’Université de Bourgogne, Dijon, France (2000).	Cs	CSH	Synthetic pore water
65)	Wieland and Van Loon(2003)	Wieland , E. and Van Loon, L. R. : Cementitious near-field sorption data base for performance assessment to an ILW repository in Opalinus clay, PSI, PSI Bericht Nr. 03-06 (2003).	Eu, Ni, Sn, Sr, Th	cement	ACW, ACW+ISA
66)	Zachara et al.(1991)	Zachara, J. M. , Cowan, C. E. and Resch, C. T. : Sorption of divalent metals on calcite, Geochimica et Cosmochimica Acta, vol.55, pp.1549-1562 (1991).	Ba, Cd, Co, Mn, Ni, Sr, Zn	calcite	equilibrium solution

3.2 QA evaluation on Criteria-I and -II

This section shows the results of QA/classification for K_d data in this update and revises. In addition to the 60 references newly selected in this update (see 3.1), several existing data were revised. The list of revised data is shown in Table 3.2-1. The evaluation procedures are described in detail in the previous report12). For transparency and simplification, all results of Criteria I and II were presented in tabular form using the following table format throughout. The results relevant to Criteria III were discussed (in next section 3.3) subsequently and illustrated in the form of plots of K_d vs. a relevant master parameter (typically pH), where applicable. As mentioned in section 2.3, an entry is evaluated by Criteria I and checkpoints II-b, II-c, II-d and II-h first. Classification and final numerical rating of the entry is only carried out when the entry is evaluated as reliable on the basis of the checkpoints. If the entry has deficiencies, the entry is labeled as unreliable and excluded from further evaluation. In this report, the QA results for only Am data newly selected for this update are shown as an example.

Data table Am/1: Tits et al. (2005)
JAEA-SDB version 5 - DATA: Am/Other minerals ; calcite, #96644－96665
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint*		**Evaluation**	**Rating**
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	A figure with R_d value [L/kg] are provided.	class 5
II-a	REF	The solid phase used in the experiments was The Merck calcite. CEC value of the solid was not provided.	C/D
II-b	SDB	Initial pH values are provided.	C
II-c	SDB	It is indicated that the experiments were carried out under N_2 atmosphere condition. Am(III) is not a redox-sensitive element.	A/B
II-d	SDB REF	It is indicated that the experiments were carried out in 0.3 M NaOH solution. The solution composition after experiments is not provided.	C/D
II-e	SDB	It is indicated that the experiments were carried out at 23 ± 3 [°C].	A/B
II-f	SDB	It is indicated that the specific surface area is 0.31 m^2/g, but the solid weight is not provided.	C/D
II-g	REF	From the direct information on % sorbed values in the figure and on the basis of K_d values and L/S ratios, % sorbed values can be calculated as follows: ・#96644－96649, #96651, #96652, #96658 : 0<%≤2 or 98≤%<100 ・#96650, #96653, #96659 : 2<%≤5 or 95≤%<98 ・Other datapoints : 5<%<95	C/D B A
II-h	SDB	It is indicated that the initial Am concentrations were 1.0×10^{-11} M. Solubility calculations performed using the JAEA-TDB (140331c0.tdb) assuming solubility limit of $Am(OH)_3(cr)$ show that the initial concentration of all datapoints are higher than a one-fifth of the solubility.	B
II-i	SDB	It is indicated that phase separation was carried out by centrifugation (95,000*rpm* for 1 hour).	C/D
II-j	SDB	It is indicated that the reaction times were 3 days. On the basis of kinetic experiments for Eu or Th, it is assumed that the experiments have reached equilibrium.	A/B
II-k	REF	It is indicated that the samples were agitated by end-over-end shaker.	A/B
II-l	REF	The initial Am concentration was not varied.	C/D
II-m	REF	It is indicated that the experiments were carried out in polyallomere centrifuge tubes.	B
II-n	REF	The experiments were carried out at least in duplicates. Error was estimated with error bar in the figure.	A
II-o	SDB	The effect of organic ligand was investigated.	D

*; SDB…Information from SDB system, REF…Information from original literature

Data table Am/2: REF: Ashikawa et al. (2001)
JAEA-SDB version 5 - DATA: Am/Cementitious materials ; mortar, # 97680－97703
GUIDELINE: Revision 4b (May 19, 2005)

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

Data table Am/1: REF: Cowper et al. (2005)
JAEA-SDB version 5 - DATA: Am/Cementitious materials ; NRVB, #99361－99376
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		**Evaluation**	**Rating**
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	A table with R_d $[cm^3/g]$ values is provided.	class 1
II-a	SDB	The solid phase used in the experiments was NRVB (Nirex Reference Vault Backfill, a mix of Portland cement, limestone flour and lime). CEC value of the solid was not provided.	C/D
II-b	SDB	The final pH values are reported. The pH values were adjusted with NaOH.	A
II-c	SDB REF	It is indicated that the experiments were carried out in N_2 atmosphere. Am(III) is not a redox-sensitive element.	A/B
II-d	SDB REF	The sorption experiments were carried out in NRVB equilibrated water in the presence and absence of picolinate, anion exchange resin, degradation product and leachate. Composition of the solutions is not reported.	C/D
II-e	SDB	No information on the temperature is provided.	C/D
II-f	SDB	The specific surface area is not provided.	C/D
II-g	REF	% sorbed values were calculated from R_d values and L/S ratios. The % sorbed values of all datapoints are $98 \leq \% < 100$.	C/D
II-h	SDB REF	It is indicated that the initial Am concentrations were 7.42×10^{-12}–8.66×10^{-12} [M]. The initial Am concentration is decided on the basis of the solubility experiments.	A
II-i	SDB REF	It is indicated that phase separation was carried out by filtration (30,000 MWCO).	B
II-j	SDB REF	It is indicated that the reaction times were 26–35 days. It is assumed that the time is sufficiently long.	A/B
II-k	REF	No information on agitation method is provided.	C/D
II-l	REF	The initial Am concentration was almost same.	C/D
II-m	REF	No information on the material of vessels is provided. R_d values are estimated considering wall sorption of Am.	A
II-n	SDB REF	The experiments were carried out in quadruplicate. The uncertainties are quoted to be ± two standard deviations.	A
II-o	SDB	Parameters were not varied.	D

Table 3.2-1 Overview of references revised data

No.	Reference	Revised points
1)	Pointeau et al.(2004a)	Addition of data
2)	Pointeau et al.(2004b)	Addition of data
3)	Pointeau et al.(2008)	Addition of data
4)	Schulthess and Huang(1990)	Addition of data

3.3 QA evaluation on Criteria III

Only the entries for datasets classified as reliable are evaluated in accordance with Criteria III. All unreliable entries and the entries whose classification could not be completed in accordance with Criteria I and II are excluded.

As an example for bentonite system, Ni sorption was evaluated as one of key elements for our modelling studies. Additionally, Th and U(VI) sorption datasets onto cementitious materials were evaluated as key representative actinide elements.

1) Evaluation of data for Ni sorption onto bentonite/smectite

Table 3.3-1 shows evaluated entries in this section. The respective data are shown in Figure 3.3-1 and the data added in this update are represented with black rims.

Table 3.3-1 List of evaluated data for Ni sorption onto bentonite/smectite

Reference	Data table	Solid phase
Baeyens and Bradbury (1997)[35)]	—	Montmorillonite
Chen and Dong (2013)[36)]	—	Montmorillonite
Lothenbach et al. (1997)[37)]	—	Montmorillonite
Tertre et al. (2005a)[38)]	—	Montmorillonite
Bradbury and Baeyens (2011b)	Ni/1	MX-80
Chen et al. (2016)	Ni/2	Montmorillonite
Schulthess and Huang (1990)	Ni/28	Montmorillonite

The K_d values of Ni sorption onto bentonite/smectite (e.g., Na-Swy-1 montmorillonite) as a function of pH are shown in Figure 3.3-1. According to the data from JAEA-SDB, the K_d values tend to increase with increasing pH values ($4 < pH < 10$). In the data of Chen et al. (2016), ionic strength dependence can be observed below pH 7. This trend is similar to the data obtained by Bradbury and Baeyens (1997) and Chen and Dong (2013); however, the differences among ionic strength conditions are smaller than the data by Bradbury and Baeyens (1997). Above pH 8, no ionic strength dependence can be observed in the data of Chen et al. (2016). This trend is similar to the data by Bradbury and Baeyens (1997) and Chen and Dong (2013). The data obtained by Schulthess and Huang (1990) in 0.01 M $NaClO_4$ condition represent a similar trend to the data obtained in 0.025 M $NaClO_4$ condition (Tertre et al., 2005a). However, the data obtained by Schulthess and Huang (1990) shows weak pH dependence above pH 7 unlike Tertre et al. (2005a).

The sorption isotherms of Ni sorption onto bentonite/smectite are shown in Figure 3.3-2. On the basis of the sorption edges (Figure 3.3-2), the K_d values would be expected to increase with increasing pH values ($4 < pH < 10$). However, the data obtained by Bradbury and Baeyens (2011b) (pH 7.5) represent a similar trend and values to the data obtained by Bradbury and Baeyens (1997) (pH5.9). Additionally, the data by Bradbury and Baeyens (2011b) (pH 7.5) are smaller than the data by Bradbury and Baeyens (1997) (pH 7.0). One of the possible reasons is the differences of cation exchange capacity (CEC) values. The CEC value of MX-80 for Bradbury and Baeyens (2011b) is 78.7 meq/100 g, but that of Na-SWy-1 montmorillonite for Bradbury and Baeyens (1997) is 87 meq/100 g. The data Chen et al. (2016) (pH 6.0) are higher than other data. In this case, not only the CEC values (90.0 meq/100 g; Chen et al., 2016) but also ionic strength conditions affect the difference of K_d values. The solution used in Chen et al. (2016) is 0.01 M $NaClO_4$, and one used in Bradbury and Baeyens (1997) is 0.1 M $NaClO_4$. Dispersion of the K_d values of Chen et al. (2016) can be explained the differences of the temperature (20, 40 and 60°C). The data obtained by Schulthess and Huang (1990) are higher than the data by Bradbury and Baeyens (1997). One of the reasons of the difference is ionic strength conditions. The solution used in Schulthess and Huang (1990) is 0.01 M $NaClO_4$, and the one used in Bradbury and Baeyens (1997) is 0.1 M $NaClO_4$. Among the data obtained by Schulthess and Huang (1990), the K_d values increase with increasing pH values. This trend is consistent with Figure 3.3-1.

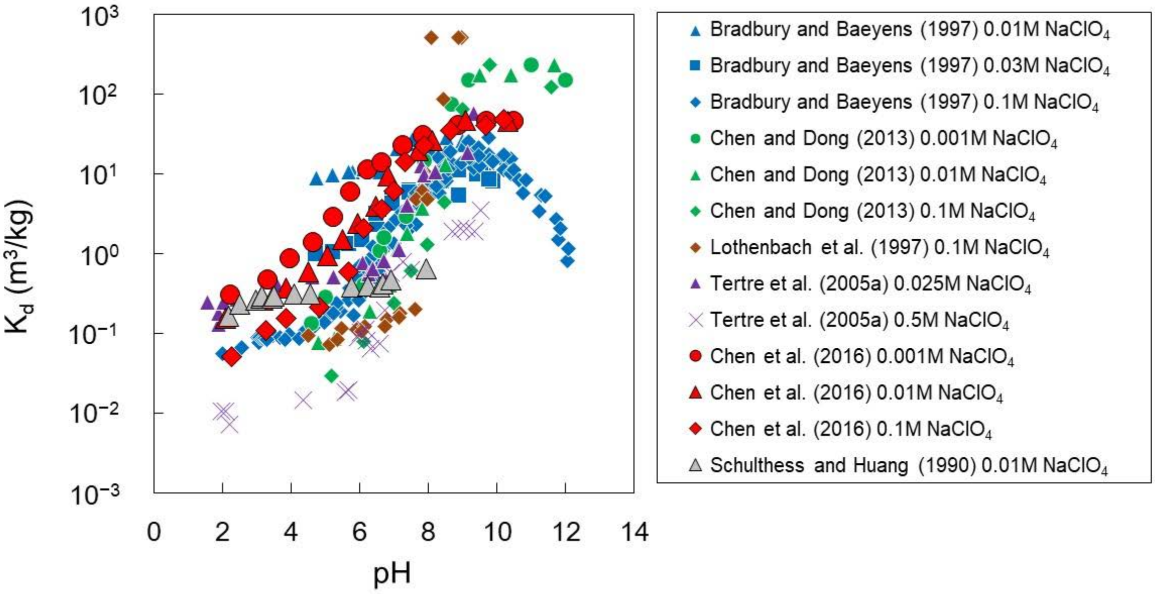

Figure 3.3-1 Overview of sorption data for Ni onto bentonite/smectite

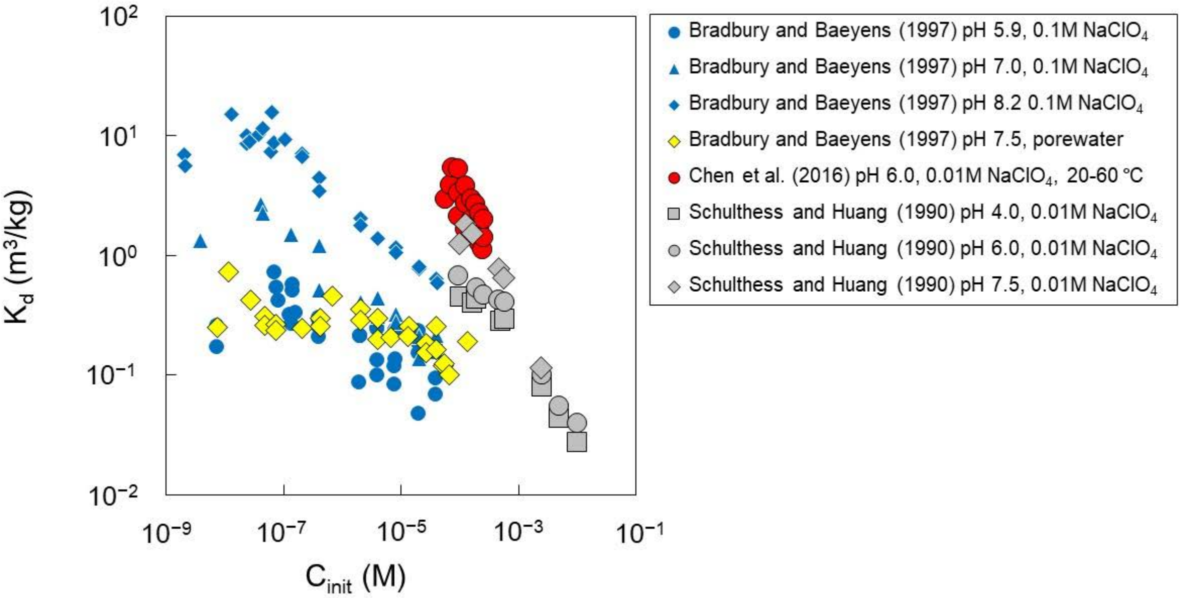

Figure 3.3-2 Overview of sorption isotherm for Ni onto bentonite/smectite

2) Evaluation of data for Th sorption onto cementitious materials

Table 3.3-2 shows evaluated entries in this section. The respective data are shown in Figure 3.3-3 and the data added in this update are represented with black rims.

Table 3.3-2 List of evaluated data for Th sorption on cementitious materials

Reference	Data table	Solid phase
Allard et al. (1984)39)	—	Cement, Slag cement
Cowper et al. (2006)40)	—	Cement hydrate, Altered cement hydrate
Höglund et al. (1985)41)	—	Cement
Sugiyama et al. (2000)42)	—	Cement
Sugiyama et al. (2003a)43)	—	Cement paste, Cement hydrate
Sugiyama et al .(2003b)44)	—	Cement hydrate, Portlandite, Calcite, CSH, Tobermonite, Ettringite, Monosulphate, Hydrotalcite
Wieland et al. (1998)45)	—	HCP
Wieland and Van Loon (2003)	Th/10	Cement

The K_d values of Th sorption onto cementitious materials (e.g., cement, cement hydrate, CSH, HCP) as a function of pH are shown in Figure 3.3-3. Unlike the case of Ni sorption onto bentonite/smectite, there is no literature data collected as a function of pH. Additionally, the solid and liquid phases vary among the literatures. No obvious pH dependence was observed. The solid and liquid used in Wieland and Van Loon (2003) is the sulfate-resisting Portland cement (water/cement = 1.3) and artificial cement porewater + 2.0 × 10^{-3} M ISA(isosaccharinic acid), respectively. It was found that these K_d values are lower than other data. It is thought that isosaccharinic acid decreased sorption of Th on cement. It is thought that solid-liquid ratio cause the dispersion for data.

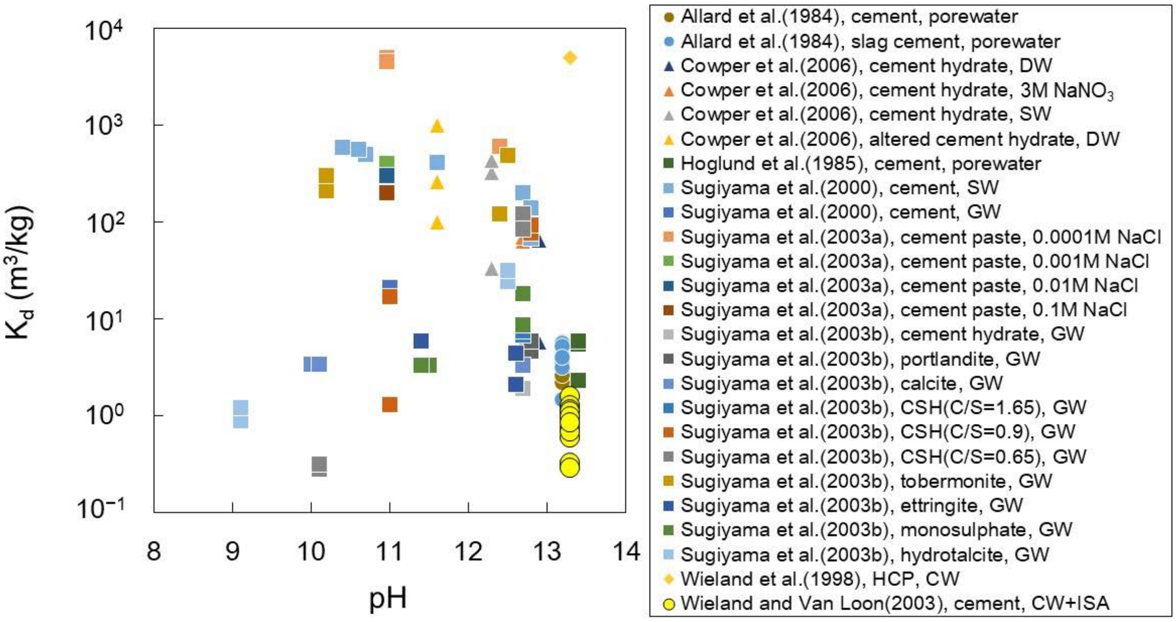

Figure 3.3-3 Overview of sorption data for Th onto cementitious materials

3) Evaluation of data for U(VI) sorption onto cementitious materials

Table 3.3-3 shows evaluated entries in this section. The respective data are shown in Figure 3.3-4 and the data added in this update are represented with black rims.

Table 3.3-3 List of evaluated data for U(VI) sorption on cementitious materials

Reference	Data table	Solid phase
Allard et al. (1984)[39]	—	Cement
Höglund et al. (1985)[41]	—	Cement
Morgan et al. (1988)[46]	—	Concrete
Sugiyama et al. (2003a)[43]	—	Cement
Sugiyama et al. (2003b)[44]	—	Cement
Sugiyama et al. (2008)[47]	—	OPC, FAC
Tits et al. (2008)[48]	—	CSH
Zhao et al. (2000)[49]	—	Concrete
Pointeau et al. (2008)	U/12	HCP
Pointeau et al. (2004a)	U/13	CEM

The K_d values of U(VI) onto cementitious materials as a function of pH are shown in Figure 3.3-4. Unlike the case of Ni sorption onto bentonite/smectite, there is no literature data collected as a function of pH. Additionally, the solid and liquid phase vary among the literatures. The solid used in Pointeau et al. (2008) is degraded the Ordinary Portland Cement, a degraded hardened cement pastes (HCP). The water/cement ratio of these cement paste is 0.38. The liquid is HCP-equilibrated water. These K_d values decreased with increase of pH. The solid used in Pointeau et al. (2004a) are CEM I (Ordinary Portland Cement), CEM V (blast furnace slag (BFS) and fly ash added to OPC) and CSH phase. The liquids are equilibrated with each solid. These K_d values do not vary at pH range between 9.5 and 11.5. At pH > 11.5, K_d value decreased with increase of pH. Also, the sorption isotherms indicates liner shape (slope = 1). It is observed that the sorption is not affected by difference of solid phase.

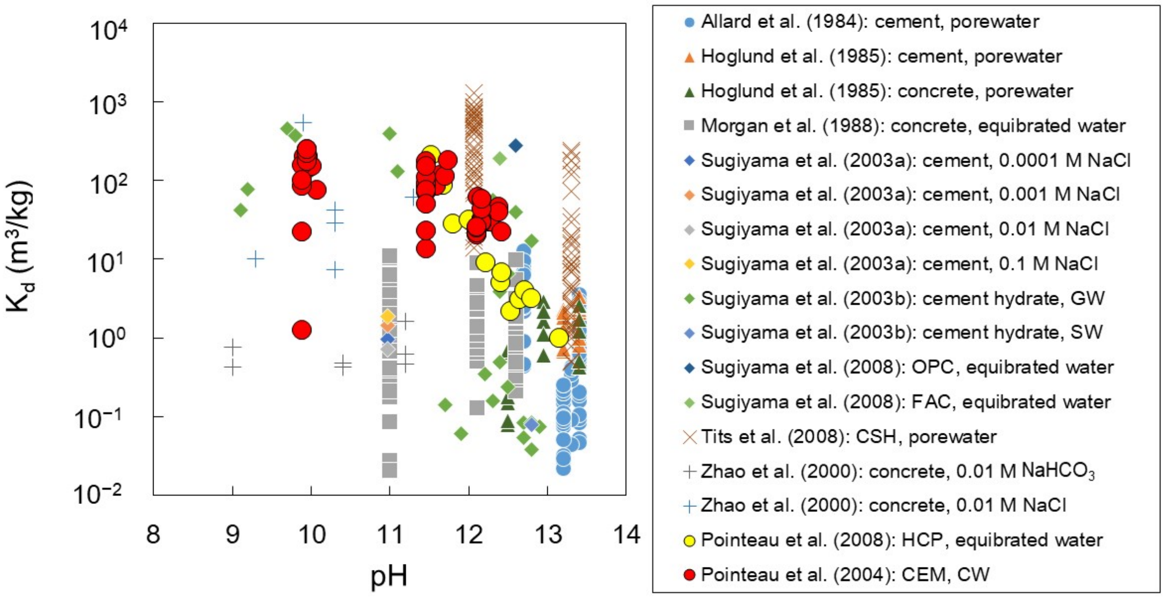

Figure 3.3-4 Overview of sorption data for U(VI) onto cementitious materials

4. Conclusions

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

- K_d data and their QA results are updated by focusing on our recent activities on the K_d setting and development of mechanistic models. As a result, 7,696 K_d data from 66 references were added and the total number of the K_d values in JAEA-SDB reached about 70,673. The QA/classified K_d data reached about 73% for all K_d data in JAEA-SDB.
- Further study is required to test the applicability of JAEA-SDB and improve their functions and contents by focusing on the site-specific K_d setting including uncertainty assessment and the combination with modeling approaches including ISD 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	$\mathrm{m^2}$
体積	立方メートル	$\mathrm{m^3}$
速さ，速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	$\mathrm{m/s^2}$
波数	毎メートル	$\mathrm{m^{-1}}$
密度，質量密度	キログラム毎立方メートル	$\mathrm{kg/m^3}$
面積密度	キログラム毎平方メートル	$\mathrm{kg/m^2}$
比体積	立方メートル毎キログラム	$\mathrm{m^3/kg}$
電流密度	アンペア毎平方メートル	$\mathrm{A/m^2}$
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	$\mathrm{mol/m^3}$
質量濃度	キログラム毎立方メートル	$\mathrm{kg/m^3}$
輝度	カンデラ毎平方メートル	$\mathrm{cd/m^2}$
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)	$\mathrm{m^2/m^2}$
周波数	ヘルツ(d)	Hz		$\mathrm{s^{-1}}$
力	ニュートン	N		$\mathrm{m\ kg\ s^{-2}}$
圧力，応力	パスカル	Pa	$\mathrm{N/m^2}$	$\mathrm{m^{-1}\ kg\ s^{-2}}$
エネルギー，仕事，熱量	ジュール	J	N m	$\mathrm{m^2\ kg\ s^{-2}}$
仕事率，工率，放射束	ワット	W	J/s	$\mathrm{m^2\ kg\ s^{-3}}$
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	$\mathrm{m^2\ kg\ s^{-3}\ A^{-1}}$
静電容量	ファラド	F	C/V	$\mathrm{m^{-2}\ kg^{-1}\ s^4\ A^2}$
電気抵抗	オーム	Ω	V/A	$\mathrm{m^2\ kg\ s^{-3}\ A^{-2}}$
コンダクタンス	ジーメンス	S	A/V	$\mathrm{m^{-2}\ kg^{-1}\ s^3\ A^2}$
磁束	ウエーバ	Wb	Vs	$\mathrm{m^2\ kg\ s^{-2}\ A^{-1}}$
磁束密度	テスラ	T	$\mathrm{Wb/m^2}$	$\mathrm{kg\ s^{-2}\ A^{-1}}$
インダクタンス	ヘンリー	H	Wb/A	$\mathrm{m^2\ kg\ s^{-2}\ A^{-2}}$
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	$\mathrm{lm/m^2}$	$\mathrm{m^{-2}\ cd}$
放射性核種の放射能(f)	ベクレル(d)	Bq		$\mathrm{s^{-1}}$
吸収線量, 比エネルギー分与, カーマ	グレイ	Gy	J/kg	$\mathrm{m^2\ s^{-2}}$
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	$\mathrm{m^2\ s^{-2}}$
酸素活性	カタール	kat		$\mathrm{s^{-1}\ mol}$

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

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	°	$1° = (\pi/180)$ rad
分	’	$1’ = (1/60)° = (\pi/10\,800)$ rad
秒	”	$1” = (1/60)’ = (\pi/648\,000)$ rad
ヘクタール	ha	$\mathrm{1\ ha=1\ hm^2=10^4 m^2}$
リットル	L，l	$\mathrm{1\ L=1\ l=1\ dm^3=10^3 cm^3=10^{-3} m^3}$
トン	t	$\mathrm{1\ t=10^3\ kg}$

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	$\mathrm{1\ eV=1.602\ 176\ 53(14)\times10^{-19}J}$
ダルトン	Da	$\mathrm{1\ Da=1.660\ 538\ 86(28)\times10^{-27}kg}$
統一原子質量単位	u	1 u=1 Da
天文単位	ua	$\mathrm{1\ ua=1.495\ 978\ 706\ 91(6)\times10^{11}m}$

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	$\mathrm{1\ bar=0.1MPa=100\ kPa=10^5Pa}$
水銀柱ミリメートル	mmHg	1 mmHg≈133.322Pa
オングストローム	Å	$\mathrm{1\ Å=0.1nm=100pm=10^{-10}m}$
海里	M	1 M=1852m
バーン	b	$\mathrm{1\ b=100fm^2=(10^{-12}cm)^2=10^{-28}m^2}$
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	$\mathrm{1\ erg=10^{-7}\ J}$
ダイン	dyn	$\mathrm{1\ dyn=10^{-5}N}$
ポアズ	P	$\mathrm{1\ P=1\ dyn\ s\ cm^{-2}=0.1Pa\ s}$
ストークス	St	$\mathrm{1\ St=1cm^2\ s^{-1}=10^{-4}m^2\ s^{-1}}$
スチルブ	sb	$\mathrm{1\ sb=1cd\ cm^{-2}=10^4cd\ m^{-2}}$
フォト	ph	$\mathrm{1\ ph=1cd\ sr\ cm^{-2}=10^4lx}$
ガル	Gal	$\mathrm{1\ Gal=1cm\ s^{-2}=10^{-2}ms^{-2}}$
マクスウエル	Mx	$\mathrm{1\ Mx=1G\ cm^2=10^{-8}Wb}$
ガウス	G	$\mathrm{1\ G=1Mx\ cm^{-2}=10^{-4}T}$
エルステッド(a)	Oe	$\mathrm{1\ Oe} \triangleq (10^3/4\pi)\mathrm{A\ m^{-1}}$

(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	$\mathrm{1\ Ci=3.7\times10^{10}Bq}$
レントゲン	R	$\mathrm{1\ R=2.58\times10^{-4}C/kg}$
ラド	rad	$\mathrm{1\ rad=1cGy=10^{-2}Gy}$
レム	rem	$\mathrm{1\ rem=1\ cSv=10^{-2}Sv}$
ガンマ	γ	$\mathrm{1}\ \gamma=\mathrm{1\ nT=10^{-9}T}$
フェルミ		1 フェルミ=1 fm=$\mathrm{10^{-15}m}$
メートル系カラット		1 メートル系カラット= 0.2 g = $\mathrm{2\times10^{-4}kg}$
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	$\mathrm{1\ µ=1µm=10^{-6}m}$

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