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Development of JAEA Sorption Database (JAEA-SDB): Update of Sorption/QA Data in FY2024

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The sorption of radionuclides (RNs) on buffer materials (bentonites), rocks, and cementitious materials is a key process in the safe geological disposal of radioactive waste because it can retard the migration of RNs in these materials. Therefore, the RN sorption process should be fully understood and a database of reliable data and mechanistic/predictive models should be developed to allow the use of reliable parameters under various geochemical conditions relevant to performance assessment (PA). Thus, the Japan Atomic Energy Agency (JAEA) has developed a database of sorption parameters on bentonites, rocks, and cementitious materials. This sorption database (SDB) was first developed to be a basis for the H12 PA for high-level radioactive waste disposal and was made available online. JAEA continuously improves and updates the SDB based on potential future needs of data, especially focusing on assuring the desired quality level and testing the usefulness of the databases in setting PA-related sorption parameters.

This report focuses on updating the sorption database (JAEA-SDB) as a basis for an integrated approach to setting a PA-related distribution coefficient (K_d) and developing mechanistic sorption models. Moreover, this report includes an overview of the database structure and contents. The K_d data and their quality assurance (QA) results were updated based on the literature collected with wide ranges.

K_d data (7,670 entries) from 73 references were included in this update, bringing the total number of K_d values in the JAEA-SDB to more than 86,000. In addition, QA evaluation and classification were performed to the K_d data already recorded in the JAEA-SDB for which QA evaluation had not been performed. By incorporating the most recent K_d data and assigning QA levels to all K_d data, the reliability of the JAEA-SDB as fundamental information for setting K_d parameters in future PA was improved.

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

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JAEA 収着データベース（JAEA-SDB）の開発：
2024 年度における収着データ/信頼度情報の拡充

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（2025 年 1 月 30 日受理）

放射性廃棄物地層処分の性能評価において、緩衝材（ベントナイト）、岩石、およびセメント系材料中での放射性核種の収着現象は、その移行遅延を支配する重要な現象の一つである。収着現象の理解と、信頼性の高い収着データを集約したデータベースおよび現象論的モデル/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にあたって重要となる。日本原子力研究開発機構では、ベントナイト、岩石とその構成鉱物、およ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行ってきた。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、およ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の適用等に着目し、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説明したうえで、幅広く文献収集を行った K_d データと信頼度情報の拡充について報告する。

今回の更新において、73 の文献から 7,670 点の 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 86,000 点以上となった。加えて、JAEA-SDB にすでに収録されている K_d データで信頼度評価が行われていなかったものに対して信頼度評価を行った。最新の K_d データを取り込むとともにすべての K_d データに信頼度が付与されたことで、今後の性能評価における収着パラメータ設定に向けた基盤情報としての JAEA-SDB の信頼性を向上することができた。

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1. Introduction

Sorption of radionuclides (RNs) in buffer materials (bentonite), host rock (rock matrix) and cementitious materials is one of the key processes ensuring the safe geological disposal of radioactive wastes. The magnitude of RN sorption onto these materials is normally expressed as a distribution coefficient (K_d). K_d values 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 RN 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 mechanistic/predictive models so that reliable parameters can be set under various geochemical conditions relevant to a performance assessment (PA). Because of the conditional nature of sorption data, K_d values used in PA calculations need to be tied to a specific set of conditions. Moreover, geochemical variability and uncertainty, and their effects on K_d values have to be considered in reference and alternative scenarios in PA[1, 2)]. Because it is not feasible to measure K_d values for all PA conditions, using existing sorption data obtained under generic experimental conditions and adapting these data to PA-specific conditions are a key task. A sorption database (SDB) containing large amounts of sorption data from estimated, simplified or generic systems is used to set K_d values in PA conditions considering any differences in substrate and geochemical conditions.

The Japan Nuclear Cycle Development Institute (JNC), one of the predecessors of the Japan Atomic Energy Agency (JAEA), developed the SDB (JNC-SDB), which was first developed as an important basis for the second progress report on high-level waste (H12 report)[3-6)]. The JNC-SDB was updated for the second progress report on trans-uranic (TRU) waste (TRU-2 report)[7-9)]. The JAEA has continued to improve and update the JAEA-SDB, the successor to JNC-SDB, in view of potential future needs for data, focusing on:

1) addition of sorption data[10-17)]
2) assuring the desired quality level for SDB[12, 14-21)]
3) testing and applying the SDB to setting sorption parameters[18-27)].

The JAEA-SDB was developed as a web-based SDB system (https://migrationdb.jaea.go.jp/) to allow effective application for parameter setting. The JAEA-SDB can search and extract K_d data by element and solid phase, and can plot graphs of K_d values trends against environmental conditions such as pH. The K_d data in the JAEA-SDB are assigned quality assurance (QA) levels based on guidelines to ensure traceability and quality[28)].

A K_d setting approach is needed that can be applied to various rock types and geochemical conditions, and that can be adapted from site-generic to site-specific assessment stages using the information obtained from forthcoming site investigations. Since available information varies at different stages of site investigation, the K_d setting approach should be based on the quality and quantity of available information. Such a comprehensive approach was developed based on international state-of-the-art knowledge[1, 22, 23, 26, 29, 30)] that integrate three different methods (**Fig. 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.

It is assumed that at the stage where no site has been identified or at the initial stage of site selection, an approach of extracting data relevant to the conditions to be evaluated from existing measured data will be adopted27). However, since K_d values vary depending on geochemical conditions, it is unlikely that measured K_d values will be available for all assumed conditions. Therefore, an approach to scale differences between experimental and assumed conditions and an approach to estimate K_d variations based on mechanistic understanding (thermodynamic sorption model; TSM) are also important27). All approaches require a reliable SDB, and the JAEA-SDB, which contains K_d data with QA levels, can play a role. 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 under complex geochemical conditions in compacted bentonites31-33). We have also tested these parameter setting approaches to estimate K_d values and their uncertainties for rock matrices like the Horonobe mudstones and generic granites22-27).

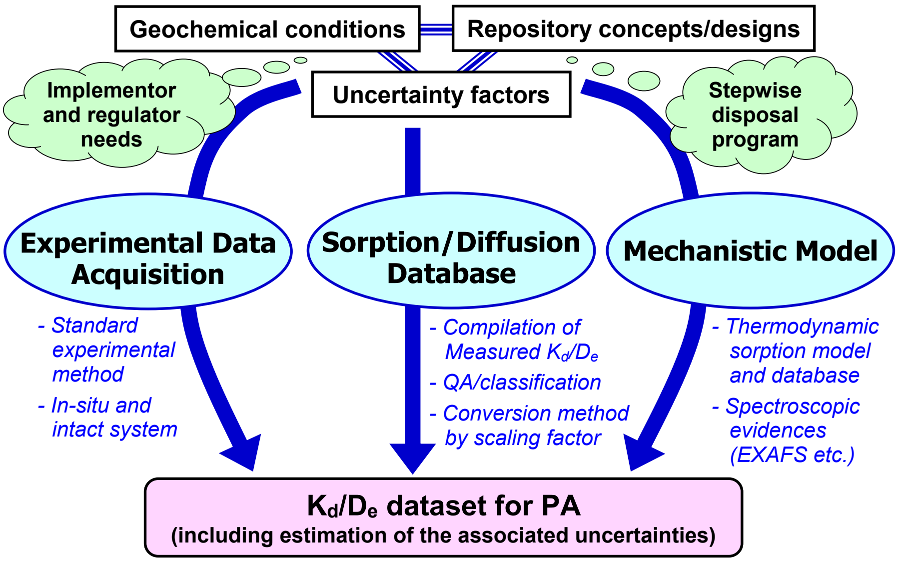

Fig. 1-1 Integrated approach for sorption/diffusion parameter setting for PA.

In this report, we focused on updating the JAEA-SDB as a basis for an integrated approach to PA-related K_d setting and the development of mechanistic sorption models. This report also includes an overview of the database structure and its contents. K_d data and their QA results are updated to focus on the following systems based on our recent activities on K_d setting and mechanistic sorption model development:

1) K_d data for clay minerals to develop and validate the mechanistic sorption models
2) K_d data for rocks to cover wider ranges of conditions for the K_d parameter setting
3) K_d data for cementitious materials to enhance dataset for the K_d parameter setting.

2. Contents, functions and systems of the JAEA-SDB

2.1 Overview and status of the JAEA-SDB

The JAEA-SDB is a compilation of experimental K_d values for key RN sorption onto bentonite, various rocks, cementitious materials and soils related to radioactive waste disposal. The K_d values were determined by batch sorption experiments and their entries include experimental conditions. These data are managed by a database software to allow quick searching and plotting of data as a function of selected parameters. The contents, functions and systems are briefly summarized in **Table 2.1-1**. As pointed out in the NEA SDB project[1, 2)], an SDB cannot be used in PA-related K_d setting without an understanding of the experimental details because K_d values were obtained under various conditions, and thus have different reliability levels. Therefore, the JAEA-SDB has been developed so that reliable data relevant to 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 (**Section 2.2**)
2) QA/classification scheme to check the reliability (**Section 2.3**).

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

Contents/functions	Brief description for status
Number of K_d data/references	- K_d data; over 86,000 (7,670 entries were added in this update*) - References; over 900 (73 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, and Zr - 2nd group; Ag, Ba, Ca, Ce, Cl, Co, Eu, Fe, I, Mn, Mo, Na, Nd, Ru, Sr, and Zn - Minor group; 41 elements
Solid phase	- Bentonite (smectite) - Rocks; basaltic rocks, granitic rocks, mudstone, sandstone, and tuff - Clay minerals (illite, kaolinite, etc.) - Other minerals (Fe-oxides/hydroxide, calcite, etc.) - Cementitious materials (cement/concrete) - Soils - Solid phases having special influence (grout, organic substance, etc.)
Search parameters	Element and solid phase group Detailed search parameters; solid phase, water type, pH, E_h, ionic strength, temperature, liquid/solid ratio, contact time, initial concentration, separation method, and atmosphere/redox condition
Graphing/data evaluation	- K_d plot as a function of pH, E_h, ionic strength, temperature, liquid/solid ratio, contact time, and 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; The evaluation of all K_d data was completed with this update*
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 the JAEA-SDB

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

Table 2.2-1 Main data table of the 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 value
	pH end		-	Final pH value
	E_h init		mV	Initial E_h value
	E_h end		mV	Final E_h value
Experimental condition	Atm/redox condition		-	Atmosphere, reducing reagent, 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 the 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 the JAEA-SDB

As described in **Section 2.1**, it is important to assess the reliability of a wide variety of K_d data in the SDB for PA-related K_d setting. The reliability of K_d values in the JAEA-SDB is assessed based on the following three main criteria:

Criterion I) Completeness of documentation and type of K_d information:
- the documentation of each entry is detailed enough to allow further examination in Criterion II.
- the reliability of K_d data input; available in table format in comparison to graph format.

Criterion 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.

Criterion III) Consistency of data:
- the examination of the level of internal consistency in the JAEA-SDB by comparing other K_d values in similar systems.

The QA/classification guidelines describing details of each criterion and overall classification scheme is shown in Appendix[18)] and briefly summarized in **Table 2.3-1**.

In accordance with the guideline, an entry is evaluated by Criterion I and key checkpoints II-b, II-c, II-d and II-h in Criterion II first. The 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 found in the JAEA-SDB[12)]. The JAEA-SDB uses QA levels (Class 1–6) classified in accordance with the sum of points obtained from Criterion II, with the results of unreliable evaluation in Criteria I and II as the main reliability information. All results and evidence of Criteria I and II are also recorded in tabular form and can be found in PDF format in the JAEA-SDB to keep traceability. The results relevant to Criterion 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 found in PDF format in the JAEA-SDB.

Table 2.3-1 Reliability information table of the JAEA-SDB.

QA-criteria / checkpoints		Brief description	SDB parameters related	Rating	
Criterion 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	
Criterion 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
Criterion III) Consistency of data:					
III	Evaluation of K_d reliability from the perspective of consistency among data*.		K_d	The evaluation is given in the form of comments. If there is clear mismatching with K_d of another similar experimental condition and the reason is not explained, the case is classified as unreliable.	

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

3. Updating the sorption data and their QA/classification

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

As mentioned above, SDB plays important roles in PA-related K_d setting and mechanistic sorption model development. Therefore, the most recent literatures were surveyed, focusing on data relevant to our recent PA-related setting[23-27)] and mechanistic sorption models[32-34)]. The literature survey was performed with Web of Science or Google Scholar, using solid phase names and words such as “sorption” and “retention” as keywords. Literatures published after 2021 were mainly included, but any literatures published before 2020 that were not included in the JAEA-SDB were also included. Detailed information on the 73 selected literatures is listed in **Table 3.1-1**.

Table 3.1-1 Overview of the 73 literatures selected for updating the JAEA-SDB (1/7).

Reference	Title	Element	Solid phase	Solution type
Almendros-Ginestà et al. (2023)[35)]	Analysis of radionuclide retention by the cement hydrate phase portlandite: A novel modelling approach	Ba, Cd, Cs, Eu, Pu, Se	portlandite	0.02 M $Ca(OH)_2$
Barker et al. (2024)[36)]	Effect of grain size variation of strontium sorption to heterogeneous aquifer sediments	Sr	sediment	2.5 mM–1 M NaCl
Bezzina et al. (2022)[37)]	Combining batch experiments and spectroscopy for realistic surface complexation modelling of the sorption of americium, curium, and europium onto muscovite	Am, Cm, Eu	synthetic muscovite	0.1 M NaCl
Bruneel et al. (2021)[38)]	Characterisation of the highly selective caesium sorption on glauconite rich sands of contrasting geological formations	Cs	sand	background solution
Chen et al. (2022)[39)]	Sorption mechanism of Fe(II) on illite: Sorption and modelling	Fe	Na-illite	0.1 M NaCl
Chikkamath et al. (2021)[40)]	Sorption and surface complexation modeling of ^{137}Cs on Fe(II)-montmorillonite clay mineral relevant to nuclear waste disposal	Cs	Fe(II)-montmorillonite, Na-montmorillonite	1 mM–1 M NaCl
Comarmond et al. (2021)[41)]	Radionuclide sorption studies of Co, Cs and Sr on LFLS soils	Co, Cs, Sr	clay, sandstone, shale, shaley clay, shalelyclay/siltstone, siltstone, silty clay, soil	0.01 M NaCl, 0.1 M NaCl
Czömpöly et al. (2023)[42)]	Adsorption and diffusion of selenite on Boda Claystone Formation	Se	sandstone	SPW
Dettmann et al. (2023)[43)]	Influence of gluconate on the retention of Eu(III), Am(III), Th(IV), Pu(IV), and U(VI) by C-S-H (C/S = 0.8)	Am, Eu, Pu, Th, U	CSH(0.8)	0.01 M NaCl, 0.01 M NaCl+GLU, deionized water, deionized water+GLU
Durce et al. (2022)[44)]	Sn(IV) sorption onto illite and Boom clay: Effect of carbonate and dissolved organic matter	Sn	clay, illite	0.015 M $NaHCO_3$, 0.017 M NaCl+DOM, SPRING water
Elhefnawy and Elabd (2022)[45)]	Adsorption of UO_2^{2+} by AlBaNi-layered double hydroxide nano-particles: Kinetic, isothermal, and thermodynamic studies	U	AlBaNi-LDH	U(VI) solution
Engates and Shipley (2021)[46)]	Batch studies of heavy metal sorption using nano-metal oxides	Cd, Cu, Ni, Pb, Zn	Al_2O_3, Fe_2O_3	0.01 M $NaNO_3$
Fabritius et al. (2022)[47)]	Radium sorption on biotite; Surface complexation modeling study	Ra	K-biotite	ALLMR, OLBA, OLGA, OLSR
Fiorito et al. (2022)[48)]	Calcium carbonate as sorbent for lead removal from wastewaters	Pb	$CaCO_3$	$Pb(NO_3)_2$ solution

Table 3.1-1 Overview of the 73 literatures selected for updating the JAEA-SDB (2/7).

Reference	Title	Element	Solid phase	Solution type
García et al. (2019)[49]	Sorption of Eu(III) on quartz at high salt concentration	Eu	quartz	0.1 M–5 M NaCl
Guo et al. (2024)[50]	Speciation studies at the illite-solution interface: Part 1 - Sorption of phosphate ion	P	Na-illite	5 mM NaCl
Guo et al. (2024)[51]	Speciation studies at the illite - solution interface: Part 2 - Co-sorption of uranyl and phosphate ions	P, U	Na-illite	5 mM NaCl, 5 mM NaCl+U, 5 mM NaCl+P
He et al. (2017)[52]	Migration of ^{75}Se(IV) in crushed Beishan granite: Effects of the iron content	Se	granite	0.3 M–1 M NaClO$_4$, groundwater
Hemmi et al. (2021)[53]	Experimental study on modeling of Pu sorption onto quartz	Pu	quartz, muscovite	mixed solution
Hwang et al. (2023)[54]	Diverse sorption capacities and contribution of multiple sorptive sites on illitic clays to assess the immobilization of dissolved cesium in subsurface environments	Cs	illitic clay	1 mM NaCl, 0.1 M NaCl, distilled water
Isaacs et al. (2020)[55]	Retention of technetium-99 by grout and backfill cements: Implications for the safe disposal of radioactive waste	Tc	AFm-CO$_3$, AFm-SO$_4$, hydrogarnet, calcite, cebama, CEM-I, CSH, ettringite, portlandite	ACW, CH, ES
Ishidera et al. (2023)[56]	Sorption of Sn and Nb on montmorillonite at neutral to alkaline pH	Nb, Sn	Na-montmorillonite	0.5 M NaCl
Jiang et al. (2022)[57]	Sorption of cesium on surrounding granite of Chinese low- and medium-level nuclear waste repository in the groundwater environment	Cs	granite	deionized water, groundwater
Jin et al. (2024)[58]	Batch, modeling and XPS study	U	chlorite	0.01 M NaCl, 0.1 M NaCl
Kamatchi et al. (2022)[59]	Thermodynamic, kinetic, batch adsorption and isotherm models for he adsorption of nickel from an artificial solution using Chloroxylon Swietenia Activated Carbon	Ni	CSAC	Ni solution
Kang et al. (2020)[60]	Adsorption characteristics of cesium onto calcium-silicate-hydrate in concrete powder and block	Cs	concrete	50 mM KCl, 50 mM KCl+100 mM NaCl
Karimzadeh et al. (2020)[61]	Effect of DTPA on europium sorption onto quartz - Batch sorption experiments and surface complexation modeling	Eu	quartz sand	0.01 M-NaClO$_4$, 0.01 M-NaClO$_4$+DTPA
Klinkenberg et al. (2021)[62]	Adsorption of barium and radium on montmorillonite: A comparative experimental and modelling study	Ba, Ra	Na-montmorillonite	0.02 M–0.3 M NaCl, 0.02 M NaCl+Ba, 0.02 M NaCl+Ra

Table 3.1-1 Overview of the 73 literatures selected for updating the JAEA-SDB (3/7).

Reference	Title	Element	Solid phase	Solution type
Kyllonen et al. (2014)63)	Modeling of cesium sorption on biotite using cation exchange selectivity coefficients	Cs	Na-biotite, K-biotite, Ca-biotite	0.1 M $CaCl_2$, 0.1 M KCl, 0.1 M NaCl
Lange et al. (2020)64)	Uptake and retention of molybdenum in cementitious systems	Mo	AFm-CO_3, AFm-SO_4, calcite, CEM-I, CSH, ettringite, hydrogarnet, portlandite	ACW, CH, ES
Lihareva et al. (2020)65)	Ion exchange of Cs^+ and Sr^{2+} by natural clinoptilolite from bi-cation solutions and XRD control of their structural positioning	Cs, Sr	clinoptilolite	distilled water
Liu et al. (2022)66)	Characterization of adsorption behaviors of U(VI) on bentonite colloids: Batch experiments, kinetic evaluation and thermodynamic analysis	U	bentonite colloid	0.007 mM–0.01 M NaCl, 0.1 mM $CaCl_2$, 0.1 mM $MgCl_2$, 0.1 mM NaCl, 0.1 mM $SrCl_2$, distilled water
Ma et al. (2020)67)	Factors influencing the reduction of U(VI) by magnetite	U	magnetite, magnetite+iron	uranyl acetate+Na_2CO_3, uranyl nitrate+Na_2CO_3
Marques Fernandes et al. (2023)68)	Adsorption of Ba and ^{226}Ra on illite: A comparative experimental and modelling study	Ba, Ra	Na-illite	0.02 M–0.3 M NaCl, 0.02 M NaCl+Ba, 0.02 M NaCl+Ra
Mei et al. (2022)69)	Uranium(VI) sorption on illite under varying carbonate concentrations: Batch experiments, modeling, and cryogenic time-resolved laser fluorescence spectroscopy study	U	Na-illite	0.1 M NaCl, 0.1 M NaCl+DIC
Mei et al. (2024)70)	U(VI) sorption on illite in the presence of carbonate studied by cryogenic time-resolved laser fluorescence spectroscopy and parallel factor analysis	U	Na-illite	0.1 M NaCl+DIC
Missana et al. (2022a)71)	Nickel retention by calcium silicate hydrate phases: Evaluation of the role of the Ca/Si ratio on adsorption and precipitation processes	Ni	CSH, portlandite, SiO_2	ultrapure water
Missana et al. (2022b)72)	Effect of presence of isosaccharinate on nickel adsorption by calcium silicate hydrate (CSH) gels: Experimental analysis and surface complexation modelling	Ni	CSH	distilled water, distilled water+ISA
Missana et al. (2023)73)	Analysis of cadmium retention mechanisms by a smectite clay in the presence of carbonates	Cd	Na-smectite	0.01 M $NaClO_4$, 0.1 M $NaClO_4$, 0.1 M $NaClO_4$+^{109}Cd

Table 3.1-1 Overview of the 73 literatures selected for updating the JAEA-SDB (4/7).

Reference	Title	Element	Solid phase	Solution type
Montavon et al. (2022)[74]	Uranium retention in a Callovo-Oxfordian clay rock formation: From laboratory-based models to *in natura* conditions	U	COx-clay, COx-claystone, illite	0.1 M NaCl, 0.1 M $NaNO_3$, SPW
Murota et al. (2023)[75]	Hydration states of europium(III) adsorbed on silicas with nano-sized pores	Eu	aerosil, silica	0.001 M–0.05 M $NaNO_3$
Nagasaki et al. (2019)[76]	Contribution of ternary reaction to Pd sorption on MX-80 in Na-Ca-Cl solution at high ionic strength	Pd	bentonite	0.1 M–4 M Na-Ca-ClO_4, 4 M Na-Ca-Cl-ClO_4
Noli et al. (2021)[77]	The effect of humic acid and competing cations Na^+ and Ca^{2+} on the sorption of uranium and europium, onto bentonite from Kimolos island (Greece)	Eu, U	bentonite	$Eu(NO_3)_3$, $Eu(NO_3)_3$+$Ca(NO_3)_2$, $Eu(NO_3)_3$+HA, $Eu(NO_3)_3$+$NaNO_3$, $Eu(NO_3)_3$+$UO_2(NO_3)_2$, $UO_2(NO_3)_2$, $UO_2(NO_3)_2$+$Ca(NO_3)_2$, $UO_2(NO_3)_2$+HA, $UO_2(NO_3)_2$+$NaNO_3$
Orucoglu et al. (2022)[78]	Competitive adsorption processes at clay mineral surfaces: A coupled experimental and modeling approach	Co, Pb	Kunipia-F, Kunipia-P	0.1 M NaCl, 0.3 M NaCl, 0.3 M NaCl+Mg, 0.3 M NaCl+Zn, 0.3 M NaCl+Mg+Zn
Papry et al. (2023)[79]	Investigating bisulfide sorption onto bentonite through laboratory batch experiments	S	bentonite	deoxygenated water
Parrotin et al. (2023)[80]	Competitive ion-exchange reactions of Pb(II) (Pb^{2+}/$PbCl^+$) and Ra(II) (Ra^{2+}) on smectites: Experiments, modeling, and implication for ^{226}Ra(II)/^{210}Pb(II) disequilibrium in the environment	Pb	beidellite	0.027 M NaCl, 0.11 M NaCl
Patel et al. (2021)[81]	Retention behaviour of Ba(II) on argillaceous rocks of Cuddapah system	Ba	clay	0.001 M–1 M NaCl

Table 3.1-1 Overview of the 73 literatures selected for updating the JAEA-SDB (5/7).

Reference	Title	Element	Solid phase	Solution type
Philipp et al. (2022)82)	Effect of Ca(II) on U(VI) and Np(VI) retention on Ca-bentonite and clay minerals at hyperalkaline conditions - New insights from batch sorption experiments and luminescence spectroscopy	Ca, Np, U	Ca-bentonite, muscovite, natural kaolinite, synthetic kaolinite	0.2 mM $CaCl_2$, 0.1 M NaCl, 0.1 M NaCl+0.02 M NaClO, 0.1 M NaCl+0.02 M NaClO, 0.1 M NaCl+0.02 M $SrCl_2$
Racette et al. (2023)83)	Influence of Ca-Na-Cl physicochemical solution properties on the adsorption of Se(−II) onto granite and MX-80 bentonite	Se	bentonite, granite	0.05 M–1 M Ca-Na-Cl
Ribet et al. (2023)84)	Temperature effect of U(VI) retention on the Callovo-Oxfordian clay rock	U	clay, claystone, illite	0.1 M NaCl, 0.1 M $NaNO_3$+$NaHCO_3$, SPW
Rodríguez et al. (2020)85)	New insights into ^{99}Tc(VII) removal by pyrite: A spectroscopic approach	Tc	pyrite	0.1 M NaCl, distilled water
Romanchuk et al. (2022)86)	U(VI), Np(V), Eu(III) sorption on goethite: A wide-ranging multiradionuclide dataset and uncertainty-aware parametrization of surface complexation models	Eu, Np, U	goethite	0.1 M $NaClO_4$
Satpathy et al. (2022)87)	Reduction of U(VI) on chemically reduced montmorillonite and surface complexation modeling of adsorbed U(IV)	U	Na-montmorillonite, reduced Na-montmorillonite	0.01 M–0.1 M NaCl, distilled water
Savoye et al. (2021)88)	Mobility of selenium oxyanions in clay-rich media: A combined batch and diffusion experiments and synchrotron-based spectroscopic investigation	Se	claystone	SPW
Schacherl et al. (2023)89)	Np(V) retention at the illite du Puy surface	Np	Na-illite du Puy-A, Na-illite du Puy-B, iron-free synthetic montmorillonite, Na-Wyoming smectite	0.1 M NaCl
Semenkova et al. (2023)90)	Eu(III) sorption on kaolinite: Experiments and modeling	Cs, Eu	kaolinite-76%, kaolinite-99%	0.01 M–1 M $NaClO_4$, 0.01 M $NaClO_4$+Al
Söderlund et al. (2019)91)	The sorption of alkaline earth metals on biotite	Ba, Ca, Ra, Sr	Na-biotite	0.01 M–1 M $NaClO_4$, groundwater
Stockmann et al. (2022)92)	New insights into U(VI) sorption onto montmorillonite from batch sorption and spectroscopic studies at increased ionic strength	U	Na-montmorillonite	0.1 M–3 M NaCl+$NaHCO_3$, 0.3 M–3 M $CaCl_2$, 0.3 M–3 M NaCl

Table 3.1-1 Overview of the 73 literatures selected for updating the JAEA-SDB (6/7).

Reference	Title	Element	Solid phase	Solution type
Tsai et al. (2009)93)	Cesium adsorption and distribution onto crushed granite under different physicochemical conditions	Cs	granite	0.1 µM–1 mM $CsNO_3$, 7 mM–0.2 M NaCl, 7 mM–0.2 M KCl, 7 mM–0.27 M $MgCl_2$, 7 mM–0.27 M $CaCl_2$, SGW, SSW, distilled water
Voronina et al. (2022)94)	The study of ^{137}Cs and ^{90}Sr sorption by natural and modified aluminosilicates in presence of humic acids	Cs, Sr	clinoptilolite, glauconite, NPF-CL, NPF-GL	tap water+HA
Walker et al. (2022)95)	Sorption of Se(−II) on illite, MX-80 bentonite, shale, and limestone in Na-Ca-Cl solutions	Se	limestone, Na-bentonite, Na-illite, shale	0.1 M–6 M Na-Ca-Cl
Wu et al. (2021)96)	Insight into the adsorption of europium(III) on muscovite and phlogopite: Effects of pH, electrolytes, humic substances and mica structures	Eu	muscovite, phlogopite	0.01 M $CaCl_2$, 0.01 M CsCl, 0.01 M CsCl+FA, 0.01 M KCl, 0.01 M NaCl, 0.01 M NaCl+FA, 0.1 M NaCl
Xu et al. (2021)97)	Selenium isotope fractionation during adsorption onto montmorillonite and kaolinite	Se	kaolinite, montmorillonite	0.01 M–0.1 M NaCl
Yang et al. (2020)98)	An approach for the efficient immobilization of ^{79}Se using Fe-OOH modified GMZ bentonite	Se	FeOOH-bentonite, Na-bentonite	0.5 mM–1 M NaCl
Yang et al. (2021)99)	Investigation on the efficient separation and recovery of Se(IV) and Se(VI) from wastewater using Fe-OOH-bent	Se	FeOOH-bentonite	0.001 M NaCl, 0.001 M NaCl+HA
Yang et al. (2023)100)	The adsorption behavior of niobium(V) on kaolin clay and kaolinite	Nb	kaolin clay, kaolinite	$Nb(HC_2O_4)_5$
Zabulonov et al. (2021)101)	Effect of the surface hydration of clay minerals on the adsorption of cesium and strontium from dilute solutions	Cs	kaolinite, montmorillonite, nontronite, palygorskite	Cs solution+Na
Zhang et al. (2019)102)	Adsorption uptake Th(IV) by red soil and black soil	Th	black soil, red soil	0.0075 M–0.75 M $NaNO_3$
Zhang et al. (2020)103)	Sorption of cesium on Tamusu clay in synthetic groundwater with high ionic strength	Cs	clay	0.6 mM–0.6 M $NaNO_3$, distilled water, distilled water+HA, SGW, SGW+HA

Table 3.1-1 Overview of the 73 literatures selected for updating the JAEA-SDB (7/7).

Reference	Title	Element	Solid phase	Solution type
Zhang et al. (2022)[104]	Oxidation and adsorption of Sb(III) in the presence of iron (hydr)oxides and dissolved Mn(II)	Sb	hematite, synthetic ferrihydrite	0.05 M NaCl, 0.05 M NaCl+Mn(II), 0.05 M NaCl+Mn(II)+PP, 0.05 M NaCl+Mn(II)+TBA, 0.05 M NaCl+Mn(II)+catalase
Zhang et al. (2022)[105]	Adsorption behavior of Cs(I) on natural soils: Batch experiments and model-based quantification of different adsorption sites	Cs	soil	0.01 M NaCl, 0.01 M NaCl+HA
Zheng et al. (2024)[106]	Sorption of U(VI) on MX-80 bentonite and granite in Ca-Na-Cl saline solutions	U	bentonite, granite	0.05 M–3 M Ca-Na-Cl
Zhou et al. (2022)[107]	Sorption/desorption of Eu(III) on halloysite and kaolinite	Eu	halloysite, kaolinite	0.01 M $NaNO_3$

3.2 QA evaluation based on Criteria I and II

This section discusses the results of the QA/classification of the K_d data included in this update. The detailed evaluation procedures are described in a previous report[12]. For transparency and simplicity, all results of Criteria I and II are presented in a tabular form using the following table format throughout this report. The results relevant to Criterion III were discussed in **Section 3.3** and illustrated in the form of plots of K_d vs. a relevant master parameter (typically pH or the initial concentration), where applicable. As mentioned in **Section 2.3**, an entry is first evaluated based on Criterion I and Checkpoints II-b, II-c, II-d, and II-h. Each entry is then subjected to points calculation and QA levels classification (Class 1–6) only when the entry is judged to be reliable based on the checkpoints. If an entry contains deficiencies, it is labeled unreliable and excluded from further evaluation. In this report, typical three QA results are shown as examples:

1) a case in which K_d data were evaluated as unreliable in Criterion I
2) a case in which K_d data were evaluated as unreliable at the critical checkpoints of Criterion II
3) a case in which K_d data evaluation was completed at all checkpoints in Criterion II.

Data table Cs/177: REF: Voronina et al. (2022)
JAEA-SDB version 5 - DATA: Cs/Other minerals; clinoptilolite, glauconite, NPF-CL, NPF-GL, #110527～110554
GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint		**Evaluation**	**Rating**
I-a.1	SDB	Information on pH values is missing.	unreliable

Data table Pb/37: REF: Fiorito et al. (2022)
JAEA-SDB version 5 - DATA: Pb/Other minerals; $CaCO_3$, #110770～110773
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 are given.	Yes
I-b	SDB	A linear graph shown in %-sorbed values is given.	class 4
II-a	SDB	The solid phase used in the experiments is $CaCO_3$. No information on accessory minerals and CEC are given.	C/D
II-b	SDB	The final pH values are given.	A
II-c	SDB REF	No information on redox conditions is given. Pb(II) is not a redox-sensitive element.	A/B
II-d	SDB REF	The experiments were performed in $Pb(NO_3)_2$ solution. The solution composition after the experiments is not given.	C/D
II-e	SDB	The experiments were performed at room temperature (293.2 K).	A/B
II-f	SDB	The specific surface area is not given.	C/D
II-g	REF	From the K_d values and L/S ratios, % sorbed values can be calculated as follows; ・#110770, #110771 : $0<\%\leq 2$ or $98\leq\%<100$ ・#110772 : $2<\%\leq 5$ or $95\leq\%<98$ ・#110772 : $5<\%<95$	C/D B A
II-h	SDB REF	The initial Pb concentrations were 1.0×10^{-4}–8.0×10^{-2} M. Assuming the solubility-limiting phases to be plumbonacrite or cerussite (JAEA-TDB; 201203.tdb), the initial Pb concentrations are calculated to be higher than the solubilities under all conditions.	unreliable

Data table Cs/170: REF: Comarmond et al. (2021)
JAEA-SDB version 5 - DATA: Cs/Clay minerals; clay, shaley clay, silty clay, #109642～109699
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 are given.	Yes
I-b	SDB	A table of K_d values (mL/g) is given.	class 1
II-a	SDB	The solid phases used in the experiments were clay, shaley clay, and silty clay. No information on the mineralogical properties is given.	B
II-b	SDB REF	The final pH values are given. The pH values were adjusted with NaOH or HCl solutions.	A
II-c	SDB REF	The experiments were performed under atmospheric conditions. Cs(I) is not a redox-sensitive element.	A/B
II-d	SDB REF	The experiments were performed in 0.01 M or 0.1 M NaCl solutions. The final solution composition is not given but can be estimated.	C/D
II-e	SDB	The experiments were performed at 25˚C.	A/B
II-f	SDB	The specific surface area is given, but the solid phase weight is not.	C/D
II-g	REF	From the K_d values and L/S ratios, %-sorbed values can be calculated as follows; ・#109644 : 0<%≤2 or 98≤%<100 ・#109643, #109645, #109647, #109660, #109669, #109696, #199697, #190699 : 2<%≤5 or 95≤%<98 ・Other datapoints : 5<%<95	C/D B A
II-h	SDB REF	The initial Cs concentration was 1.13×10^{-9} M. Cs(I) is not a solubility-limited element.	A
II-i	SDB	Phase separation was performed by centrifugation (8,000×*g*, 20 minutes).	B
II-j	SDB REF	The duration of the experiments was 2 days. The duration was confirmed to be sufficient to attain thermodynamic equilibrium.	A/B
II-k	REF	No information on agitation method is given.	C/D
II-l	REF	No experiments were performed with varying initial Cs concentrations.	C/D
II-m	REF	The experiments were performed using Nalgene centrifuge tubes. Wall sorption was regarded as negligible.	B
II-n	REF	Error bars are given, but information on uncertainty estimates is not.	C
II-o	SDB	The experiments were performed by varying one parameter (pH).	C

* SDB: Information from the SDB system, REF: Information from original literature

3.3 QA evaluation based on Criterion III

Some literatures obtain K_d values by varying experimental conditions such as pH, ionic strength, and initial concentration to investigate the sorption mechanism. In Criterion III, the newly added K_d values will be compared with K_d values for similar experimental conditions recorded in the JAEA-SDB to evaluate their consistency. The K_d values of some important elements on bentonite (smectite), rocks and clay minerals, and cementitious materials have been compared to confirm their consistency in our previous reports[12-17]. In this report, the literatures that systematically obtained K_d values by varying pH or initial concentration were targeted to check the consistency with the data already recorded in the JAEA-SDB. This section focuses on the literature examining sorption on bentonite (smectite) and clay minerals, for which much data has been obtained by varying pH or initial concentration. Specifically, Cs sorption on bentonite (smectite)[40], U(VI) sorption on bentonite (smectite)[92, 106], Np(V) sorption on bentonite (smectite)[89], and U(VI) sorption on clay minerals[51, 69, 70, 74] were reviewed. First, the data sets, in which K_d values were obtained by systematically varying the pH or initial element concentrations, were selected from the JAEA-SDB. These data were then reviewed to observe the trends of K_d values and describe the sorption mechanisms. Next, the new data retrieved from the literature that are added in this update were compared with the previous ones, and the possibility of interpreting the trends of the K_d values based on the sorption mechanisms was discussed.

3.3.1 Evaluation of the data for Cs sorption on bentonite (smectite)

Figure 3.3.1-1 shows some of the K_d values of Cs sorbed on bentonite (smectite) that are recorded in the JAEA-SDB. The data sets selected here are for purified Na-montmorillonite and were obtained by systematically varying the initial Cs concentrations in NaCl or $NaClO_4$ solutions (**Table 3.3.1-1**). The data are color-coded according to the ionic strength of the solutions. The K_d values exhibit an ionic strength dependence, in which they decrease with the increase in the ionic strength, which can be attributed to the sorption of Cs on the planar sites of the montmorillonite via cation exchange. The K_d values determined by Tachi and Yotsuji (2014)[31] exhibited little dependence on the initial Cs concentration. In contrast, the K_d values of Missana et al. (2014)[108] exhibited a decrease in the K_d values at low initial Cs concentrations, suggesting the presence of sorption sites with small capacity and high affinity for Cs, which are known as frayed edge sites and are found in illite, in addition to the planar sites. Missana et al. (2014)[108] suggested that the initial Cs concentration dependence is due to the presence of an illite–smectite mixed layer in the smectite they used.

Herein, the trends of the K_d values reported by Chikkamath et al. (2021)[40] were reviewed. They investigated the K_d values of Na- and Fe(II)-montmorillonite in an NaCl solution (0.1 M). These K_d values exhibited little initial Cs concentration dependence. The values of Na-montmorillonite were slightly higher than those of Fe(II)-montmorillonite. This can be attributed to the difference in the selectivity coefficients for Na^+–Cs^+ and Fe^{2+}–Cs^+. Thus, the K_d values obtained by Chikkamath et al. (2021)[40] can be interpreted as the sorption on montmorillonite via cation exchange similar to the other K_d values shown in **Figure 3.3.1-1**.

Table 3.3.1-1 Cs sorption data shown in Fig. 3.3.1-1.

Reference	Solid phase	Solution type
Missana et al. (2014)[108]	Na-montmorillonite (purified from bentonite (FEBEX))	0.001–1 M NaClO$_4$
Tachi and Yotsuji (2014)[31]	Na-montmorillonite (Kunipia P)	0.01, 0.05 M NaCl
Chikkamath et al. (2021)[40]*	Na-montmorillonite (Kunipia F), Fe(II)-montmorillonite (Kunipia F)	0.1 M NaCl

* Newly added data

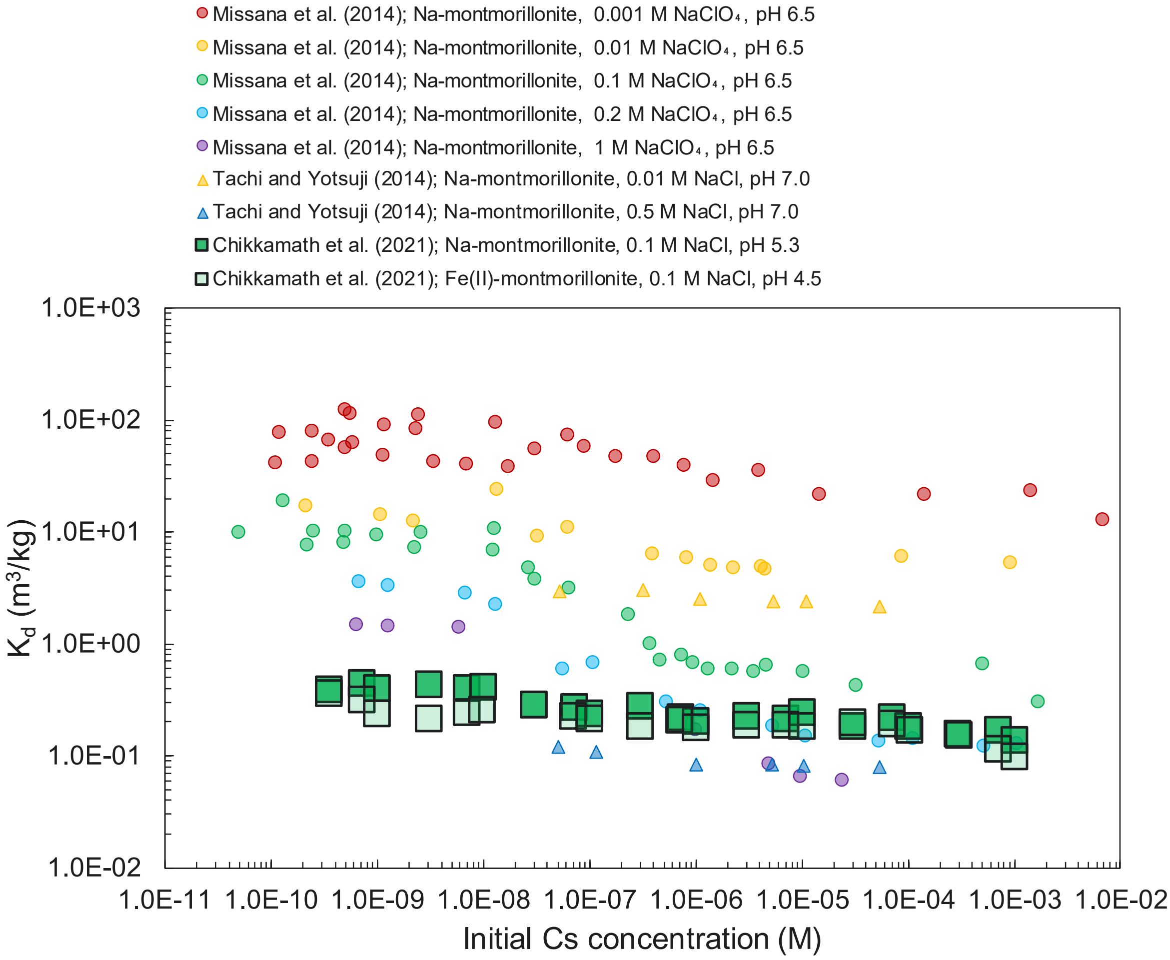

Fig. 3.3.1-1 K$_d$ of Cs sorbed on bentonite (smectite).

3.3.2 Evaluation of the data for U(VI) sorption on bentonite (smectite)

Figure 3.3.2-1 shows some of the K_d values of U(VI) sorbed on bentonite (smectite) that are recorded in the JAEA-SDB. The data sets selected here are for purified Na-montmorillonite and were obtained in NaCl, $NaClO_4$, or $NaNO_3$ solutions at different pH values (**Table 3.3.2-1**). The data are color-coded according to the ionic strength of the solutions. The data obtained under inert gas atmosphere and under atmospheric equilibrium conditions are represented by closed and open symbols, respectively. Under inert gas atmosphere, the K_d values increase with the pH values, reaching its maximum at $pH \approx 6$, after which it starts to slightly decrease. This pH dependence of the K_d values is attributed to the sorption of U(VI) on the montmorillonite edge sites owing to the surface complexation. The decrease in the K_d values at pH values higher than 6 is likely due to an increase in the proportion of negatively charged U(VI) species. In contrast, at $pH < 5$, the K_d values show an ionic strength dependence because U(VI) is mainly present as UO_2^{2+} in this pH range and sorbs on planar sites via cation exchange. Under atmospheric equilibrium conditions, the K_d values decrease at $pH > 7$ because bicarbonate ions form complexes with U(VI) and inhibit the sorption of U(VI) on the solid phase. The K_d values vary widely even under similar experimental conditions. For example, the K_d values obtained at an ionic strength of 0.1 M and $pH = 6$ under inert gas atmosphere exhibited a variation of more than two orders of magnitude. Even at the same ionic strength and pH, the K_d values can be affected by the initial U(VI) concentration and the solid-to-liquid ratio. Moreover, the carbonate ions, which are present in trace amounts as impurities in the solutions even under inert gas atmosphere, can affect the K_d values117).

Herein, we reviewed the trends of the K_d values reported by Stockmann et al. (2022)92) and Zheng et al. (2024)106). Stockmann et al. (2022)92) investigated the effect of the ionic strength of the solutions and carbonate concentration in them on K_d values. The K_d values show an ionic strength dependence in the low pH region, which is attributed to the sorption of U(VI) via cation exchange. In the presence of carbonate, the K_d values reported by Stockmann et al. (2022)92) considerably decrease at $pH = 10$ because, as mentioned above, the carbonate ions inhibit the sorption of U(VI) on the solid phase. Zheng et al. (2024)106) obtained K_d values at various ionic strengths under inert gas atmosphere. The K_d values reach its maximum at pH 6 and slightly decrease at $pH > 6$. This trend of pH dependence was the same with the other data shown in **Figure 3.3.2-1**, though the pH dependence was not entirely clear. In summary, the trend of K_d values in these two studies generally corresponded to the other data and can be interpreted based on the typical sorption mechanisms of U(VI) on montmorillonite.

Table 3.3.2-1 U(VI) sorption data shown in Fig. 3.3.2-1.

Reference	Solid phase	Solution type
Zachara and McKinley (1993)[109]	Na-montmorillonite (SWy-1)	0.01, 0.1 M $NaClO_4$
McKinley et al. (1995)[110]	Na-montmorillonite (SWy-1)	0.001–0.1 M $NaClO_4$
Pabalan and Turner (1997)[111]	Na-montmorillonite (SAz-1)	0.1 M $NaNO_3$
Boult et al. (1998)[112]	Na-montmorillonite (purified from bentonite (Kunigel V1))	0.01 M NaCl
Korichi and Bensmaili (2009)[113]	Na-montmorillonite (purified from bentonite (Maghnia, Algeria))	0.001–0.1 M $NaNO_3$
Missana et al. (2009)[114]	Na-montmorillonite (purified from bentonite (FEBEX))	0.003–0.1 M $NaClO_4$
Yang et al. (2010)[115]	Na-montmorillonite (purified from bentonite (Jinchuan, China))	0.1 M NaCl
Marques Fernandes et al. (2012)[116]	Na-montmorillonite (SWy-1)	0.1 M $NaClO_4$
Tournassat et al. (2018)[117]	Na-montmorillonite (SWy-2)	0.1 M NaCl
Stockmann et al. (2022)[92]*	Na-montmorillonite (SWy-2)	0.3, 3 M NaCl, 0.3, 3 M NaCl + $NaHCO_3$
Zheng et al. (2024)[106]*	bentonite (MX-80)	0.05–3 M Ca-Na-Cl

* Newly added data

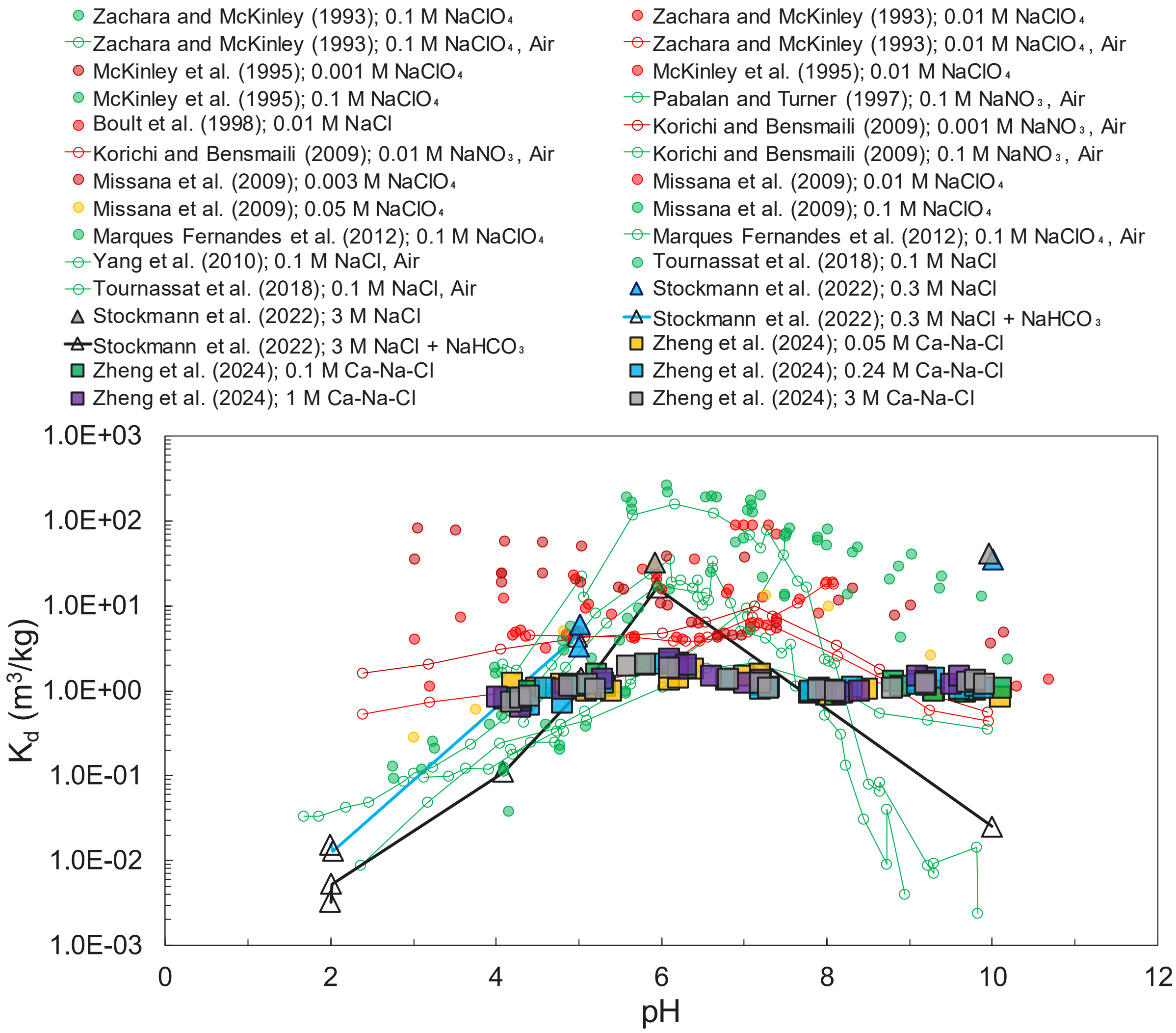

Fig. 3.3.2-1 K_d of U(VI) sorbed on bentonite (smectite).

3.3.3 Evaluation of data for Np(V) sorption on bentonite (smectite)

Figure 3.3.3-1 shows some of the K_d values of Np(V) sorbed on montmorillonite that are recorded in the JAEA-SDB. The data sets selected here are for purified Na-montmorillonite and were obtained in NaCl, $NaClO_4$, or $NaNO_3$ solutions at different pH values (**Table 3.3.3-1**). The legends are represented in the same manner as in **Section 3.3.2**. At pH < 5, the K_d values exhibit an ionic strength dependence. Under inert gas atmosphere, the K_d values increase with the pH values at pH > 5. This ionic strength and pH dependence occurs owing to the sorption of Np(V) on montmorillonite via cation exchange and surface complexation, which is similar to the case of U(VI). However, at pH < 5, the K_d values of U(VI) show pH dependence, whereas those of Np(V) exhibit little pH dependence. This is probably because Np(V) is less likely to form surface complexes compared to U(VI) and sorption via cation exchange is the dominant mechanism, whereas U(VI) forms surface complexes even at this pH range. Under atmospheric equilibrium conditions, the K_d values decrease at pH > 8 because, similar to U(VI), Np(V) forms carbonate complexes.

Herein, we reviewed the trends of the K_d values reported by Schacherl et al. (2023)89). Schacherl et al. (2023)89) obtained K_d values in a NaCl solution (0.1 M) under inert gas atmosphere. The K_d values increased with the pH values and were comparable to the data obtained in other studies under similar conditions.

Table 3.3.3-1 Np(V) sorption data shown in Fig. 3.3.3-1.

Reference	Solid phase	Solution type
Turner et al. (1998)118)	Na-montmorillonite (SAz-1)	0.1 M $NaNO_3$
Bradbury and Baeyens (2006)119)	Na-montmorillonite (SWy-1)	0.01, 0.1 M $NaClO_4$
Wendt (2009)120)	Na-montmorillonite (STx-1)	0.1 M NaCl
Elo et al. (2017)121)	Na-montmorillonite (purified from bentonite (MX-80))	0.01, 0.1 M NaCl
Scholze et al. (2019)122)	Na-montmorillonite (STx-1)	0.1, 1 M NaCl
Schacherl et al. (2023)89)*	Na-montmorillonite (purified from bentonite (Wyoming, USA))	0.1 M NaCl

* Newly added data

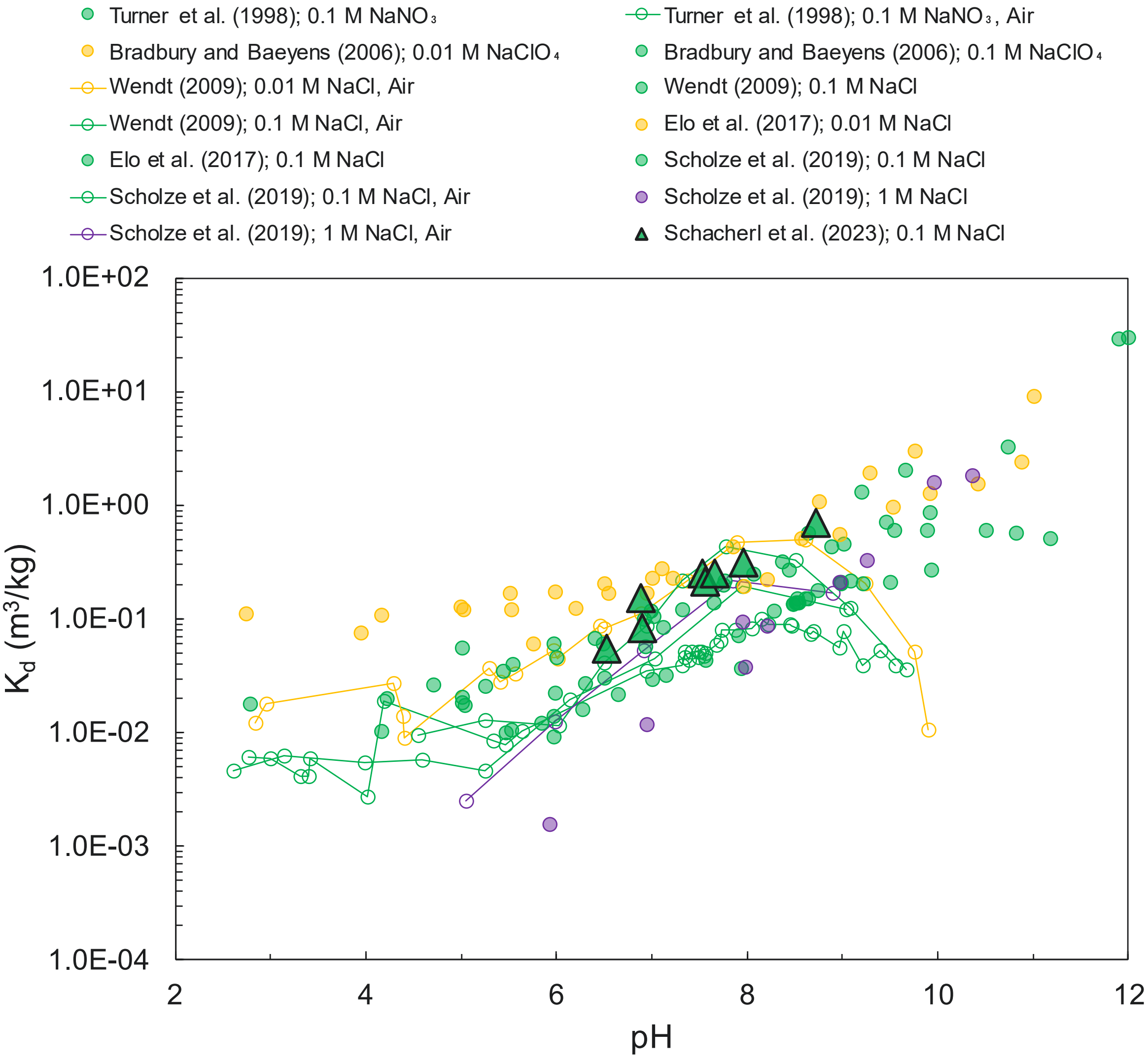

Fig. 3.3.3-1 K_d of Np(V) sorbed on bentonite (smectite).

3.3.4 Evaluation of the data for U(VI) sorption on clay minerals

Figure 3.3.4-1 shows some of the K_d values of U(VI) sorbed on clay minerals that are recorded in the JAEA-SDB. The data sets selected here are for purified Na-illite and were obtained in NaCl, $NaClO_4$, or $NaNO_3$ solutions at different pH values. The data are color-coded according to the ionic strength of the solution. The data obtained under inert gas atmosphere and under atmospheric equilibrium conditions (or in the presence of carbonate) are represented by closed and open symbols, respectively. The K_d values increase with the pH values, reaching a maximum at pH ≈ 6 and slightly decrease at pH > 6. This pH dependence is similar to that of the K_d values on bentonite (smectite) (**Fig. 3.3.2-1**). In contrast, little difference in the K_d values is observed at ionic strengths of 0.01 and 0.1 M in the low pH region probably because (1) U(VI) tends to form surface complexes and (2) sorption via cation exchange is not pronounced at an ionic strength of 0.01 M.

Herein, we reviewed the trends of K_d values reported by Montavon et al. (2022)[74)], Mei et al. (2022)[69)], Guo et al. (2024)[51)], and Mei et al. (2024)[70)]. Montavon et al. (2022)[74)] obtained K_d values under inert gas atmosphere and atmospheric equilibrium conditions. The data obtained under inert gas atmosphere showed values and trends similar to those obtained by Bradbury and Baeyens (2005)[122)]. In contrast, the K_d values obtained under atmospheric equilibrium conditions exhibit a sharp decrease at pH ≥ 7. Guo et al. (2024)[51)] determined K_d values under atmospheric equilibrium conditions. Their K_d values also exhibit similar trend with those reported by Montavon et al. (2022)[74)] under atmospheric equilibrium conditions. Mei et al. (2022)[69)] and Mei et al. (2024)[70)] obtained K_d values at different dissolved inorganic carbon (DIC) concentrations. The K_d values decreased with increasing the DIC concentrations. As mentioned in **Section 3.3.2**, these decrease in the K_d values observed under atmospheric equilibrium condition or in the presence of carbonate are due to the weak sorption of U(VI) carbonate complexes on the solid phase. The data obtained in the presence of carbonate by Mei et al. (2022)[69)] and Mei et al. (2024)[70)] indicated an increase in the K_d values at pH > 9, likely due to the change in the dominant dissolved species of U(VI) from carbonate complexes to hydroxide complexes at pH > 9[69, 70)]. The K_d values shown in **Figure 3.3.4-1** are in good agreement with each other. Thus, the trend of K_d values in these four references can be explained based on the sorption mechanisms of U(VI) on the solid phase in the presence or absence of carbonate.

Table 3.3.4-1 U(VI) sorption data shown in Fig. 3.3.4-1.

Reference	Solid phase	Solution type
Bradbury and Baeyens (2005)[123)]	Na-illite (illite du Puy)	0.01, 0.1 M $NaClO_4$
Marques Fernandes et al. (2012)[116)]	Na-montmorillonite (SWy-1)	0.1 M $NaClO_4$ + $NaHCO_3$
Mei et al. (2022)[69)]*	Na-illite (illite du Puy)	0.1 M $NaClO_4$ + $NaHCO_3$
Montavon et al. (2022)[74)]*	Na-illite (illite du Puy)	0.1 M $NaClO_4$ + $NaHCO_3$
Guo et al. (2024)[51)]*	Na-illite (illite du Puy)	0.1 M NaCl
Mei et al. (2024)[70)]*	Na-illite (illite du Puy)	0.1 M $NaClO_4$ + $NaHCO_3$

* Newly added data

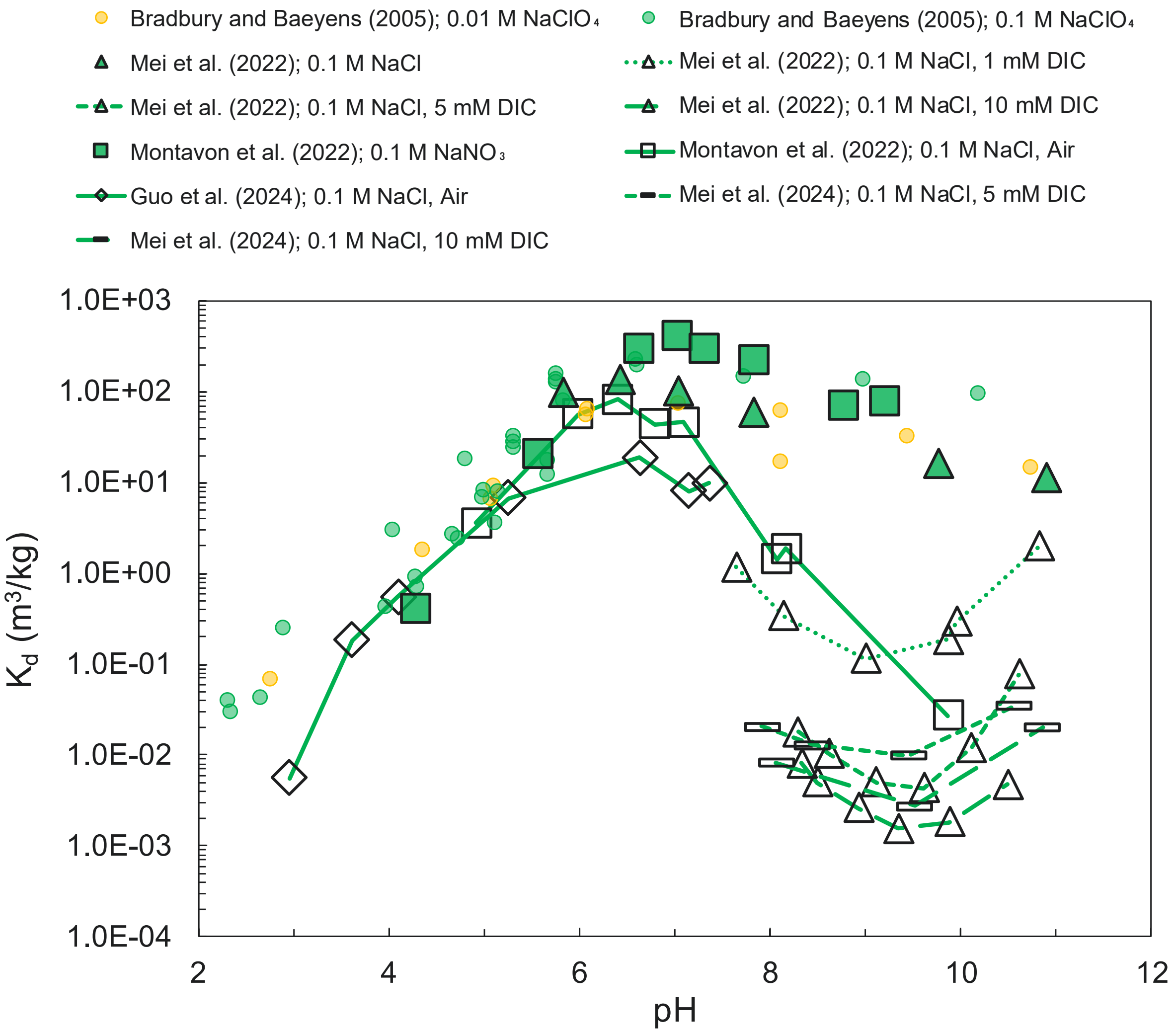

Fig. 3.3.4-1 K_d of U(VI) sorbed on clay minerals.

3.4 Data revision

QA evaluation and classification were performed to the K_d data already recorded in the JAEA-SDB for which QA evaluation had not been performed.

The data corrected in this update are shown in **Table 3.4-1**. The details of the changes are given in the additional/information column of the data.

Table 3.4-1 Data corrected in this update.

Data number	Data source	Correction details
#38261, #38262, #38264, #38265, #38267~#38269, #38271, #38290~#38292, #38774~#38776, #38784~#38786, #38794~#38796, #38804~#38806, #38814~#38816, #38824~#38826, #38834~#38836, #38844~#38846, #38854~#38856, #38864~#38866, #38874~#38876, #38884~#38886, #38901~#38908, #39060~#39071, #39724, #39755, #39772, #39923, #39934, #39939, #39964~#40199	Bradbury and Baeyens (2011)124)	Deleted data due to duplication
#40757~#40900	Inoue and Morisawa (1976)125)	Deleted data due to duplication
#54065~#54091	Kozai et al. (1994)126)	Deleted data due to duplication
#55949	Matsumoto et al. (1994)127)	Deleted data due to duplication
#63171~#63199	Kitamura et al. (2002)128)	Deleted data due to duplication
#107742~#107855, #107953~#108021	Missana et al. (2021)129)	Corrected solid phase group classification

Typos and garbled characters in the author and reference information columns of the data already included in the JAEA-SDB were corrected.

4. Conclusions

To contribute to the PA-related K_d setting and mechanistic sorption model development, a survey of the latest literature on sorption was conducted. K_d data (7,670 entries) were obtained from 73 references and were subjected to QA classification. The total number of K_d data entries in the JAEA-SDB reached more than 86,000 after this update. In addition, QA evaluation and classification were performed to the K_d data already recorded in the JAEA-SDB for which QA evaluation had not been performed. This assigned QA levels to all K_d data in the JAEA-SDB.

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Abbreviations

Solid phases

AFm	alumina ferric oxide monosulfate
CL	clinoptilolite
CSH	calcium-silicate-hydrate
CSAC	chloroxylon swietenia activated carbon
CEM	cement paste
GL	glauconite
LDH	layered double hydroxide
NPF	nickel-potassium ferrocyanide

Solution types

ACW	artificial cement water
CH	saturated portlandite solution
DW	distilled water
ES	equilibrium solution
SGW	synthetic groundwater
SPW	synthetic porewater

Ligands

DIC	dissolved inorganic carbon
DOM	dissolved organic matter
DTPA	diethylenetriaminepentaacetic acid
FA	fulvic acid
GLU	gluconate
HA	humic acid
ISA	isosaccharinic acid
PP	pyrophosphate
TBA	tert-butyl alcohol

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 an 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-C/D × 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