# ASSESSMENT OF SORPTION AND DIFFUSION IN THE ROCK MATRIX IN THE NUMO SAFETY CASE

T. Hamamoto<sup>a</sup>, S. Shibutani<sup>a</sup>, K. Ishida<sup>a</sup>, K. Fujisaki<sup>a</sup>, M. Yamada<sup>a</sup>, Y. Tachi<sup>b</sup>

<sup>a</sup> Nuclear Waste Management Organization of Japan (NUMO) <sup>b</sup> Japan Atomic Energy Agency (JAEA)

<sup>a</sup> Mita NN Bldg. 1-23, Shiba 4-Chome, Minato-ku, Tokyo 108-0014 Japan
<sup>b</sup> 4-33, Muramatsu, Tokai-mura, Naka-gun, Ibaraki, 319-1194 Japan

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# Abstract

NUMO has developed a generic safety case to demonstrate the feasibility and safety of geological disposal of high-level radioactive waste (HLW) and low and intermediate level waste generated from reprocessing and MOX fabrication (named TRU waste) in Japan. In this pre-siting safety case, the performance assessment was carried out for the repositories tailored to site descriptive models developed for three representative rock groups (plutonic, Neogene sedimentary and Pre-Neogene sedimentary rocks). Radionuclide migration parameters in rocks, *i.e.* distribution coefficients and effective diffusion coefficients, were derived to allow performance assessment for a range of scenarios. The values of these parameters were given statistically from data for certain rock types. The data were extracted from the latest sorption and diffusion database, with interpretation based on the speciation by thermodynamic modeling using relevant groundwater chemistry. In the performance assessment, the parameters assessed as the most realistic were used for a dose calculation of a "likely" scenario. The variations of the parameters to account for the uncertainties were analyzed in "less-likely" scenarios.

### 1. Introduction

## 1.1 NUMO safety case

NUMO has developed a safety case (NUMO-SC) to confirm a generic demonstration of feasibility of geological disposal of HLW and TRU waste in Japan and extend this to consider the geological settings that may result from the volunteering approach to siting. A consequence of volunteer siting is that the design of the repository has to be tailored to the geological setting encountered.

For the long-term performance assessment after the closure of the repository, parameters to characterise the migration of nuclides in the geological environment relevant to each host rocks have to be defined. We first develop the relevant models of groundwater chemistry for each host rocks, then assess key parameters such as solubility, speciation, distribution coefficient (Kd) and effective diffusion coefficient (De) in the engineered material and rocks. This paper describes the setting of Kd and De of three representative host rocks for target radionuclides for performance assessment.

# 1.2. The engineered repository

For disposal of HLW, two different designs of the engineered barrier system layout have been developed (Fig. 1), although these both feature a massive steel overpack, a bentonite-based buffer and backfill (Ref. 1). HLW will be co-disposed with TRU waste, which will be placed in concrete vaults infilled with a cementitious material. Following the classification concept (Ref. 2), 4 groups of TRU waste packages was defined. For some TRU waste groups, a bentonite-based buffer layer is also included (Fig. 2). TRU waste group 3 contains large amount of nitrate which influences the radionuclide migration.



Fig. 1. Cross section of HLW drift. (modified from Ref. 1)



#### 1.3. Site descriptive models

In this pre-siting safety case, site descriptive models are developed for representative rock groups (plutonic, Neogene sedimentary and Pre-Neogene sedimentary rocks) in Japan (Ref. 3). The nationwide geoscientific information suggested that plutonic rocks and Pre-Neogene sedimentary rocks are characterised by the network of faults/fractures where flow predominatly occurs while Neogene sedimentary rocks are characterised by the permeable sedimentary layers and water conducting fracture systems (Ref. 3). As the result of the repository design based on the site descriptive models, the repository of the plutonic rocks and the both sedimentary rocks are assumed to be located in granite and mudstone, respectively (Ref. 3). Higher porosity mudstone in Neogene sedimentary rocks than that in Pre-Neogene sedimentary rocks in response to the site descriptive models.

Groundwater chemistry reflects its origins, as rainwater, seawater, deep-seated fluids, etc., together with processes along its flow path, including mixing and rock-water interactions. It is thus difficult to set the groundwater chemistry based on specification of the host rock alone. In NUMO-SC, two salinity types of groundwater chemistry for each host rock are specified based on average values from the limited number of high quality measurements of relevant deep groundwaters (Refs. 4 to 8) to understand a wide variation in groundwater chemistry (salinity) in Japan. However, there is no high quality groundwater deep measurements of for the Pre-Neogene sedimentary rocks so the Neogene sedimentary groundwater chemistry data are substituted for the setting of the Pre-Neogene sedimentary groundwater. Sampling groundwater from deep underground is inherently problematic, introducing errors due to artefacts such as degassing, and hence considerations of the equilibrium of mineral such as quartz, feldspar, mica, carbonate minerals and the redox equilibrium with thermodynamic calculation are coupled. Table 1 show the resulting groundwater chemistries.

#### 3. Scenario analysis

In performance assessment, scenarios are developed based on the state-of-the-art understanding

TABLE 1. Chemical composition of model groundwater. High salinity (HS) and Low salinity (LS) groundwater are set for each rocks.

	Plutonic rocks		Neogene sedimentary		Pre-Neogene	
			rocks		sedimentary rocks	
	HS	LS	HS	LS	HS	LS
pH	7.6	8.2	6.5	8.4	6.3	8.2
Eh (mV)	-260	-300	-170	-280	-170	-290
		Element	concentration	[mol/dm <sup>3</sup> ]		
Na	$1.7 \times 10^{-2}$	$3.1 \times 10^{-3}$	$2.2 \times 10^{-1}$	$2.8 \times 10^{-3}$	$2.2 \times 10^{-1}$	$2.8 \times 10^{-3}$
Ca	$1.6 \times 10^{-2}$	$4.0 \times 10^{-4}$	$3.5 \times 10^{-3}$	$2.3 \times 10^{-4}$	$3.5 \times 10^{-3}$	$2.3 \times 10^{-4}$
K	$1.0 \times 10^{-4}$	$1.6 \times 10^{-5}$	$3.2 \times 10^{-3}$	$3.0 \times 10^{-5}$	$3.2 \times 10^{-3}$	$3.0 \times 10^{-5}$
Mg	$6.2 \times 10^{-5}$	$8.2 \times 10^{-6}$	$5.0 \times 10^{-3}$	$1.5 \times 10^{-5}$	$5.0 \times 10^{-3}$	$1.5 \times 10^{-5}$
Fe	$4.9 \times 10^{-7}$	$9.0 \times 10^{-7}$	$3.3 \times 10^{-5}$	$8.5 \times 10^{-7}$	$3.3 \times 10^{-5}$	$8.5 \times 10^{-7}$
Al	$2.8 \times 10^{-7}$	$7.9 \times 10^{-7}$	$1.3 \times 10^{-9}$	$2.2 \times 10^{-8}$	$2.4 \times 10^{-9}$	$4.3 \times 10^{-8}$
Si	$3.0 \times 10^{-4}$	$3.2 \times 10^{-4}$	$6.6 \times 10^{-4}$	$7.5 \times 10^{-4}$	9.2×10 <sup>-4</sup>	$1.0 \times 10^{-3}$
S	$2.0 \times 10^{-5}$	$7.3 \times 10^{-6}$	$4.1 \times 10^{-6}$	$1.2 \times 10^{-4}$	$4.1 \times 10^{-6}$	$1.2 \times 10^{-4}$
С	$2.2 \times 10^{-4}$	$9.5 \times 10^{-4}$	$4.0 \times 10^{-2}$	$1.7 \times 10^{-3}$	$4.7 \times 10^{-2}$	$1.7 \times 10^{-3}$
Cl	$4.9 \times 10^{-2}$	$2.3 \times 10^{-3}$	$2.1 \times 10^{-1}$	$1.1 \times 10^{-3}$	$2.1 \times 10^{-1}$	$1.1 \times 10^{-3}$
F	$1.3 \times 10^{-4}$	$5.7 \times 10^{-4}$	$6.5 \times 10^{-6}$	$1.9 \times 10^{-4}$	$6.5 \times 10^{-6}$	$1.9 \times 10^{-4}$
В	$2.7 \times 10^{-4}$	$4.6 \times 10^{-6}$	$1.0 \times 10^{-2}$	$4.6 \times 10^{-6}$	$1.0 \times 10^{-2}$	$4.6 \times 10^{-6}$
Р	5.3×10 <sup>-6</sup>	6.5 × 10 <sup>-7</sup>	$5.9 \times 10^{-6}$	$5.6 \times 10^{-6}$	$5.9 \times 10^{-6}$	$5.6 \times 10^{-6}$
N	$2.8 \times 10^{-5}$	$2.0 \times 10^{-5}$	1.0×10 <sup>-2</sup>	2.5×10 <sup>-6</sup>	1.0×10 <sup>-2</sup>	2.5 × 10 <sup>-6</sup>
Br	$3.9 \times 10^{-5}$	$4.3 \times 10^{-6}$	$8.0 \times 10^{-4}$	$4.4 \times 10^{-6}$	$8.0 \times 10^{-4}$	$4.4 \times 10^{-6}$
I	$5.5 \times 10^{-6}$	$7.9 \times 10^{-6}$	$1.8 \times 10^{-4}$	3.9 × 10 <sup>-6</sup>	$1.8 \times 10^{-4}$	3.9 × 10 <sup>-6</sup>

of the evolution of repository system. At the first step of scenario development regarding to the radionuclide migration in the host rock, we extract FEPs (feature, event, process) which may influence it. The FEP analysis showed the retention of radionuclides to host rocks might be inhibited by nitrate from the TRU waste and high pH plume from cement porewater. Note that we do not assess the microbes effects in this generic safety case because of its high regionality.

Reactive transport analyses have been conducted to understand the processes, such as transport of perturbing species and alteration of rock. The results show the high pH plume from cementitious materials have low effect on the sorption and diffusion because of pore clogging at the boundary of cement and rock. We assume no influence of high pH plume in the likely scenario and less-likely scenarios.

Radionuclide migration near the TRU waste group 3 containing nitrate is assessed considering the nitrate effect in the likely case. The nitrate may not influence the groudwater in the pathway of radionuclides from the other wastes because the nitrate waste is located at the downstream of the other waste. In less-likely scenario, the nitrate effect on the migrationi of the radionuclides from the waste is evaluated in case that nitrate transports to the pathway of radionuclides considering the uncertainties on the assessment of nitrate transport.

#### 4. Parameter setting

## 4.1 Effective diffusion coefficient

De for rocks has been reported to depend on electric charge of species and porosity of host rock. Since De is well known to have temperature dependency, correction is made according to the expected temperature at each repository depth. The temperature of 30°C for the Neogene sedimentary rocks and 45°C for the plutonic rocks and the Pre-Neogene sedimentary rocks is set.

*De* values for specified conditions are derived from empirical equations based on measured data from the JAEA-DDB (Diffusion Database) (Ref. 9). The trends of *De* of the plutonic rock and the porosity showed no clear dependency with electric charged states of elements (Fig. 3, Ref. 10). Thus, *De* values of the plutonic rocks at 25°C are obtained from the following relation: equation (1).

$$De = 8.55 \times 10^{-13} \cdot \varepsilon^{1.3} \tag{1}$$

where  $\varepsilon$  is the porosity.

On the other hand, the dataset in the sedimentary rocks show the relations of electric charge of diffusing species and De (Fig. 4). This is consistent with the setting of De for clay rocks assessed in SGT-E2 report (Ref. 11). De values of the both sedimentary rocks at 25°C are obtained from the following relations: equation (2)-(4).

Cations;	$De = 1.1 \times 10^{-13} \cdot \epsilon^{2.2}$ (2)
Neutral species;	$De = 3.5 \times 10^{-13} \cdot \epsilon^{1.6}$ (3)
Anions;	$De = 2.0 \times 10^{-14} \cdot \epsilon^{2.0}$ (4)

where  $\varepsilon$  is the porosity.

Table 2 show the *De* values corrected for the repository temperature. The Neogene sedimentary rocks are more porous than Pre-Neogene sedimentary rocks so the *De* values of Neogene sedimentary rocks are higher. *De* values of some elements, such as Co, Ni, Zr, Pd, Sn and Pu (in addition Am, Ac and Cm for Neogene sedimentary groundwater), for high salinity sedimentary groundwater and low salinity one are different reflecting their speciation in the groundwater.



Fig. 3 The relation of De (m<sup>2</sup>/s) of the granitic rock at 25°C and porosity (%). The reference value (orange) and the lower limit (green) are set with the porosity of 0.8%. (Modified from Ref. 10)



Fig. 4 The relation of De (m<sup>2</sup>/s) of the mudstone at 25°C and porosity (%).The reference values (orange) and the lower limits (green) are set with the porosity of 3.5% and 24.5% for the Pre-Neogene sedimentary rock and the Neogene sedimentary rock, respectively.

TABLE 2. De (m<sup>2</sup>/s) dataset corrected for the repository temperature for high salinity groundwater (HS) and low salinity groundwater (LS) of three representative host rocks.

	plutonic rocks		Neogene sedimentary rocks		Pre-Neogene sedimentary rocks	
GW type	HS	LS	HS	LS	HS	LS
C(inorg)	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$1 \times 10^{-11}$	$1 \times 10^{-11}$	3×10 <sup>-13</sup>	$3 \times 10^{-13}$
C(org)	$1 \times 10^{-12}$	$1 \times 10^{-12}$	6×10 <sup>-11</sup>	6×10 <sup>-11</sup>	4×10 <sup>-12</sup>	$4 \times 10^{-12}$
Cl	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-11</sup>	$1 \times 10^{-11}$	3×10 <sup>-13</sup>	$3 \times 10^{-13}$
Co	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$1 \times 10^{-10}$	6×10 <sup>-11</sup>	$2 \times 10^{-12}$	$4 \times 10^{-12}$
Ni	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-10</sup>	6×10 <sup>-11</sup>	$2 \times 10^{-12}$	$4 \times 10^{-12}$
Se	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$1 \times 10^{-11}$	$1 \times 10^{-11}$	3×10 <sup>-13</sup>	$3 \times 10^{-13}$
Sr	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-10</sup>	$1 \times 10^{-10}$	$2 \times 10^{-12}$	$2 \times 10^{-12}$
Zr	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-11</sup>	6×10 <sup>-11</sup>	3×10 <sup>-13</sup>	$4 \times 10^{-12}$
Nb	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-11</sup>	$1 \times 10^{-11}$	3×10 <sup>-13</sup>	$3 \times 10^{-13}$
Mo	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-11</sup>	1×10 <sup>-11</sup>	3×10 <sup>-13</sup>	3×10 <sup>-13</sup>
Tc	$1 \times 10^{-12}$	$1 \times 10^{-12}$	6×10 <sup>-11</sup>	6×10 <sup>-11</sup>	4×10 <sup>-12</sup>	$4 \times 10^{-12}$
Pd	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-10</sup>	6×10 <sup>-11</sup>	$2 \times 10^{-12}$	$4 \times 10^{-12}$
Sn	$1 \times 10^{-12}$	$1 \times 10^{-12}$	6×10 <sup>-11</sup>	1×10 <sup>-11</sup>	$4 \times 10^{-12}$	3×10 <sup>-13</sup>
Ι	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-11</sup>	$1 \times 10^{-11}$	3×10 <sup>-13</sup>	$3 \times 10^{-13}$
Cs	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-10</sup>	1×10 <sup>-10</sup>	$2 \times 10^{-12}$	$2 \times 10^{-12}$
Pb	$1 \times 10^{-12}$	$1 \times 10^{-12}$	6×10 <sup>-11</sup>	6×10 <sup>-11</sup>	$4 \times 10^{-12}$	$4 \times 10^{-12}$
Ra	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$1 \times 10^{-10}$	$1 \times 10^{-10}$	$2 \times 10^{-12}$	$2 \times 10^{-12}$
Ac	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-10</sup>	1×10 <sup>-11</sup>	$2 \times 10^{-12}$	$2 \times 10^{-12}$
Th	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-11</sup>	$1 \times 10^{-11}$	3×10 <sup>-13</sup>	$3 \times 10^{-13}$
Pa	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-11</sup>	1×10 <sup>-11</sup>	3×10 <sup>-13</sup>	3×10 <sup>-13</sup>
U	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$1 \times 10^{-11}$	$1 \times 10^{-11}$	3×10 <sup>-13</sup>	3×10 <sup>-13</sup>
Np	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-11</sup>	1×10 <sup>-11</sup>	3×10 <sup>-13</sup>	3×10 <sup>-13</sup>
Pu	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$1 \times 10^{-10}$	1×10 <sup>-11</sup>	$2 \times 10^{-12}$	3×10 <sup>-13</sup>
Am	$1 \times 10^{-12}$	$1 \times 10^{-12}$	1×10 <sup>-10</sup>	1×10 <sup>-11</sup>	2×10 <sup>-12</sup>	$2 \times 10^{-12}$
Cm	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$1 \times 10^{-10}$	1×10 <sup>-11</sup>	$2 \times 10^{-12}$	$2 \times 10^{-12}$

## 4.2 Distribution coefficient

The Kd setting approach was developed by the integration of three methods; direct use of measured Kd data extracted from the sorption database, semi-quantitative estimation procedures by scaling differences between experiment and performance assessment conditions, and thermodynamic sorption models (Ref. 12). An trial of the integrated Kd setting method for the Kd of granitic rock for Cs and Am indicated that Kd can be quantitatively evaluated by all approaches when adequate data and models are available (Ref. 12). In this paper, the dataset for the all host rocks based on the direct use of measured data was adopted because of the limitation of data under the situation of this generic stage.

*Kd* values for host rocks are logarithmic mean values of data in JAEA-SDB (Sorption Database) obtained under similar conditions to the groundwater chemistry. In particular, pH, ionic strength, redox condition and carbonate concentration are considered in the data extracting process. Table 3 show the *Kd* datasets.

TABLE 3. Kd (m<sup>3</sup>/kg) dataset for high salinity groundwater (HS) and low salinity groundwater (LS) of three representative host rocks.

	Plutoni	c rocks	Neogene sedimentary		Pre-Neogene	
	(Re	f. 9)	rocks		sedimentary rocks	
GW type	HS	LS	HS	LS	HS	LS
C(inorg)	0	0	0	0	0	0
C(org)	0	0	0	0	0	0
Cl	0	0	0	0	0	0
Co	0.1	0.1	0.5	3	0.5	3
Ni	0.1	0.1	0.5	3	0.5	3
Se	0.001	0.001	0.05	0.04	0.05	0.04
Sr	0.008	0.008	0.07	0.2	0.07	0.2
Zr	0.8	0.8	0	2	0	2
Nb	0.4	0.4	6	6	6	6
Mo	0	0	0	0	0	0
Tc	8	8	0	0.01	0	0.01
Pd	0.6	0.6	3	1	3	1
Sn	10	10	100	100	100	100
Ι	0	0	0	0	0	0
Cs	0.04	0.04	0.1	1	0.1	1
Pb	1	1	0	2	0	2
Ra	0.1	0.1	0.03	0.3	0.03	0.3
Ac	1	1	20	200	20	200
Th	0.3	0.3	5	30	5	30
Pa	2	2	2	2	2	2
U	0.3	0.3	$2 \times 10^{-6}$	6	$2 \times 10^{-6}$	6
Np	0.3	0.3	5	30	5	30
Pu	0.3	0.3	5	30	5	30
Am	1	1	20	200	20	200
Cm	1	1	20	200	20	200

In this situation, a large uncertainty on geological environment remained. For plutonic rocks, the datasets have the same value for two types of groundwater chemistry. Sorption of the alkali and alkaline earth elements generally have an dependency on ionic strength, but the both plutonic groundwater have so similar ionic strength that the defference of the Kd is negligible. For the high salinit y sedimentary groundwater, lower sorption of the alkali and alkaline earth elements (Sr, Cs and Ra) are estimated because these elements assumed to be adsorbed by ion exchange. Moreover, high carbonate concentration (ca. 40 mM) indicates the low sorption of many elements (Co, Ni, Zr, Tc, Pb, Ac, Th, U, Np, Pu, Am and Cm) due to carbonate complexation. No sorption of Zr, Tc and Pb are conservatively set because of the limitation of adequate data to evaluate the effect of such high carbonate concentration although these elements are usually assumed to be somewhat adsorbed to host rocks. Note that relatively low sorption of U under high salinity Neogene groundwater, due to the stabilization of U(VI) by forming carbonate complexation, may be somewhat over-conservative because the value is estimated from the data under oxidizing condition.

The results show low sorption in plutonic and high sorption in sedimentary rock except for the species associated with carbonate. This trend can be interpreted by the fact that mudstone usually contains large amount of clay minerals which have good retardation properties.

## 4.3 Parameter variability and uncertainty

Kd and De values are set from the dataset extracted from the database. The range of the values dataset is extracted from relatively wide conditions due to a high uncertainty of geological environment. The Kdvalue of the element which has large number of data, such as Sr, exhibits a log-normal distribution approximately (Fig. 3). Thus, the 95% confidence interval is estimated as the variation of Kd and Devalues. The lower limit of the 95% confidence interval is used in the less-likely scenario (see Table 4 and 5).

Uncertainties on the scenarios have also been considered in less-likely scenarios. As described in section 3, nitrate is assumed to influence the water chemistry of near-field pathways for radionuclides from all of the TRU waste in the less-likely scenario of nitrate transport. Because there is less amount of data obtained under high nitrate concentration, the effect of nitrate is evaluated with the reduction factors for Kd (Ref. 13). These factors are acquired by analysis of the effect of ionic strength from the JAEA-SDB and the effect of complex formation using the sorption dependency of sodium nitrate concentration for tuff. The nitrate reduction factors are shown as Table 6. The factors of Co, Ni, Pd and Pb are estimated considering the association with ammonia/ammonium. The factors which assessed for highest concentration of ammonia the are conservatively used because it is hard to estimate the concentration of ammonia produced by the nitrate reduction bacteria.



Fig. 3 Histogram of the logarithmic value of mudstone Kd (m<sup>3</sup>/kg) of Sr. The red line show the log-normal distribution with the mean value and standard deviation of the dataset.

TABLE 4. Lower De (m<sup>2</sup>/s) dataset corrected for the repository temperature for high salinity groundwater (HS) and low salinity groundwater (LS) of three representative host rocks including 95% confidence interval.

	plutonic rocks		Neogene sedimentary		Pre-Neogene	
	1		rocks		sedimentary rocks	
GW type	HS	LS	HS	LS	HS	LS
C(inorg)	$5 \times 10^{-14}$	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$5 \times 10^{-14}$	$5 \times 10^{-14}$
C(org)	5×10 <sup>-14</sup>	5×10 <sup>-14</sup>	3×10 <sup>-12</sup>	3×10 <sup>-12</sup>	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Cl	$5 \times 10^{-14}$	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$1 \times 10^{-12}$	5×10-14	5×10-14
Co	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	3×10 <sup>-12</sup>	3×10 <sup>-12</sup>	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Ni	5×10-14	$5 \times 10^{-14}$	3×10-12	3×10-12	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Se	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$5 \times 10^{-14}$	5×10-14
Sr	5×10-14	$5 \times 10^{-14}$	3×10-12	3×10-12	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Zr	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$3 \times 10^{-12}$	$5 \times 10^{-14}$	9×10 <sup>-14</sup>
Nb	5×10-14	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$1 \times 10^{-12}$	5×10-14	5×10-14
Mo	5×10 <sup>-14</sup>	5×10-14	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$5 \times 10^{-14}$	5×10 <sup>-14</sup>
Tc	5×10 <sup>-14</sup>	5×10-14	3×10 <sup>-12</sup>	3×10 <sup>-12</sup>	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Pd	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	3×10 <sup>-12</sup>	3×10 <sup>-12</sup>	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Sn	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	3×10 <sup>-12</sup>	$1 \times 10^{-12}$	9×10 <sup>-14</sup>	5×10-14
Ι	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$5 \times 10^{-14}$	$5 \times 10^{-14}$
Cs	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	3×10 <sup>-12</sup>	3×10 <sup>-12</sup>	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Pb	$5 \times 10^{-14}$	$5 \times 10^{-14}$	3×10-12	3×10-12	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Ra	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	3×10 <sup>-12</sup>	$3 \times 10^{-12}$	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Ac	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	3×10 <sup>-12</sup>	$1 \times 10^{-12}$	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Th	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$5 \times 10^{-14}$	$5 \times 10^{-14}$
Pa	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$5 \times 10^{-14}$	5×10-14
U	5×10-14	$5 \times 10^{-14}$	$1 \times 10^{-12}$	$1 \times 10^{-12}$	$5 \times 10^{-14}$	$5 \times 10^{-14}$
Np	5×10-14	5×10-14	1×10 <sup>-12</sup>	$1 \times 10^{-12}$	$5 \times 10^{-14}$	5×10-14
Pu	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	3×10 <sup>-12</sup>	$1 \times 10^{-12}$	9×10 <sup>-14</sup>	$5 \times 10^{-14}$
Am	5×10-14	5×10-14	3×10 <sup>-12</sup>	$1 \times 10^{-12}$	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>
Cm	5×10 <sup>-14</sup>	$5 \times 10^{-14}$	3×10 <sup>-12</sup>	$1 \times 10^{-12}$	9×10 <sup>-14</sup>	9×10 <sup>-14</sup>

TABLE 5. Lower Kd (m<sup>3</sup>/kg) dataset for high salinity groundwater (HS) and low salinity groundwater (LS) of three representative host rocks including 95% confidence interval.

	Plutonic rocks		Plutonic rocks Neogene		Pre-Neogene	
	(Ref. 10)		sedimentary rocks		sedimentary rocks	
GW type	HS	LS	HS	LS	HS	LS
C(inorg)	0	0	0	0	0	0
C(org)	0	0	0	0	0	0
Cl	0	0	0	0	0	0
Co	0.006	0.006	0.4	0.8	0.4	0.8
Ni	0.006	0.006	0.4	0.8	0.4	0.8
Se	0.0003	0.0003	0.05	0.02	0.05	0.02
Sr	0.0005	0.0005	0.02	0.01	0.02	0.01
Zr	0.1	0.1	0	2	0	2
Nb	0.05	0.05	6	6	6	6
Mo	0	0	0	0	0	0
Tc	0.3	0.3	0	0.01	0	0.01
Pd	0.04	0.04	0.7	0.07	0.7	0.07
Sn	0.5	0.5	60	60	60	60
Ι	0	0	0	0	0	0
Cs	0.001	0.001	0.005	0.04	0.005	0.04
Pb	0.2	0.2	0	1	0	1
Ra	0.01	0.01	0.01	0.1	0.01	0.1
Ac	0.07	0.07	10	100	10	100
Th	0.008	0.008	5	20	5	20
Pa	0.009	0.009	2	2	2	2
U	0.008	0.008	$8 \times 10^{-8}$	4	$8 \times 10^{-8}$	4
Np	0.008	0.008	5	20	5	20
Pu	0.008	0.008	5	20	5	20
Am	0.07	0.07	10	100	10	100
Cm	0.07	0.07	10	100	10	100

TABLE 6. Nitrate reduction factor of *Kd* for all representative groundwater for 1 - 6 M and 0.1 - 1 M nitrate (Ref. 13).

	Reduction factor (Ref. 13)				
	1-6M nitrate	0.1-1M nitrate			
Co	10000	10000			
Ni	10000	10000			
Sr	1000	100			
Pd	100	100			
Cs	1000	100			
Pb	1000	1000			
Ra	1000	100			

#### 5. Conclusion

As part of the performance assessment in NUMO-SC, the Kd and De of rocks and their variables and uncertainties are estimated reflecting the characteristics of site descriptive models and performance assessment scenarios. The results show low sorption and fast diffusion of plutonic rocks, high sorption and slow diffusion in Neogene sedimentary rocks and high sorption and fast diffusion in Pre-Neogene sedimentary rocks, relatively. However, the uncertainties on perturbing species, such as carbonate and nitrate, indicate that this trend can change. In particular, the limitation of sorption data under high carbonate concentration makes large uncertainties. NUMO is planning to promote experimental stueies at high carbonate concentration in reducing conditions.

In this paper, the uncertainties are assessed based on output from speciation calculation and simple statistical analysis of sorption and diffusion data. NUMO will implement a structured program to improve understanding and to develop more rigorous models using long-term experiments under realistic conditions coupled to appropriate natural analogues.

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