OPERA

Reference database with sorption properties

OPERA-PU-NRG6122

Radioactive substances and ionizing radiation are used in medicine, industry, agriculture, research, education and electricity production. This generates radioactive waste. In the Netherlands, this waste is collected, treated and stored by COVRA (Centrale Organisatie Voor Radioactief Afval). After interim storage for a period of at least 100 years radioactive waste is intended for disposal. There is a world-wide scientific and technical consensus that geological disposal represents the safest long-term option for radioactive waste.

Geological disposal is emplacement of radioactive waste in deep underground formations. The goal of geological disposal is long-term isolation of radioactive waste from our living environment in order to avoid exposure of future generations to ionising radiation from the waste. OPERA (OnderzoeksProgramma Eindberging Radioactief Afval) is the Dutch research programme on geological disposal of radioactive waste.

Within OPERA, researchers of different organisations in different areas of expertise will cooperate on the initial, conditional Safety Cases for the host rocks Boom Clay and Zechstein rock salt. As the radioactive waste disposal process in the Netherlands is at an early, conceptual phase and the previous research programme has ended more than a decade ago, in OPERA a first preliminary or initial safety case will be developed to structure the research necessary for the eventual development of a repository in the Netherlands. The safety case is conditional since only the long-term safety of a generic repository will be assessed. OPERA is financed by the Dutch Ministry of Economic Affairs and the public limited liability company Electriciteits-Produktiemaatschappij Zuid-Nederland (EPZ) and coordinated by COVRA. Further details on OPERA and its outcomes can be accessed at www.covra.nl.

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Summary

This report contains the reference database with sorption property values and represents deliverable M6.1.2.2 which forms part of the results of the research proposed for Task 6.1.2. A description of the underpinning calculations is given in the accompanying report OPERA-PU-NRG6123 [Schröder, 2017].

Samenvatting

Dit rapport bevat de referentie database met sorptie parameterwaardes en vormt OPERA deliverable M6.1.2.2, onderdeel van de resultaten van het onderzoek voor Taak 6.1.2. De berekeningen die ten grondslag liggen aan de in dit rapport beschreven waarden worden beschreven in het bijbehorende rapport OPERA-PU-NRG6123 [Schröder, 2017].

1. Introduction

1.1. Background

The five-year research programme for the geological disposal of radioactive waste – OPERA- started on 7 July 2011 with an open invitation for research proposals. In these proposals, research was proposed for the tasks described in the OPERA Research Plan [Verhoef & Schröder, 2011]. This report (M6.1.2.2) presents results of the OPERA research project RANMIG (Radionuclide migration), as part of OPERA Task 6.1.2, Modelling approach for sorption processes.

In the OPERA research programme, all safety relevant aspects of a given generic reference disposal concept for radioactive waste [Verhoef et al., 2011] are evaluated and assessed in order to evaluate the long-term safety of such a facility [Verhoef & Schröder, 2011]. The programme follows in general terms the methodology known as 'Safety Case' [NEA, 1999], [NEA, 2004], [Grupa & Davis, 2013]. Central part of the Safety Case are safety assessment calculations that will be performed in order to investigate potential risks of a disposal concept. In case of the OPERA Safety Case for a disposal concept in Boom Clay, the slow migration of radionuclides is expected to have a relevant role in the long-term safety of such a disposal concept.

The interaction between the OPERA Tasks 6.1.2, 6.1.3, 6.1.4 and WP7 is given in Figure 1-1.

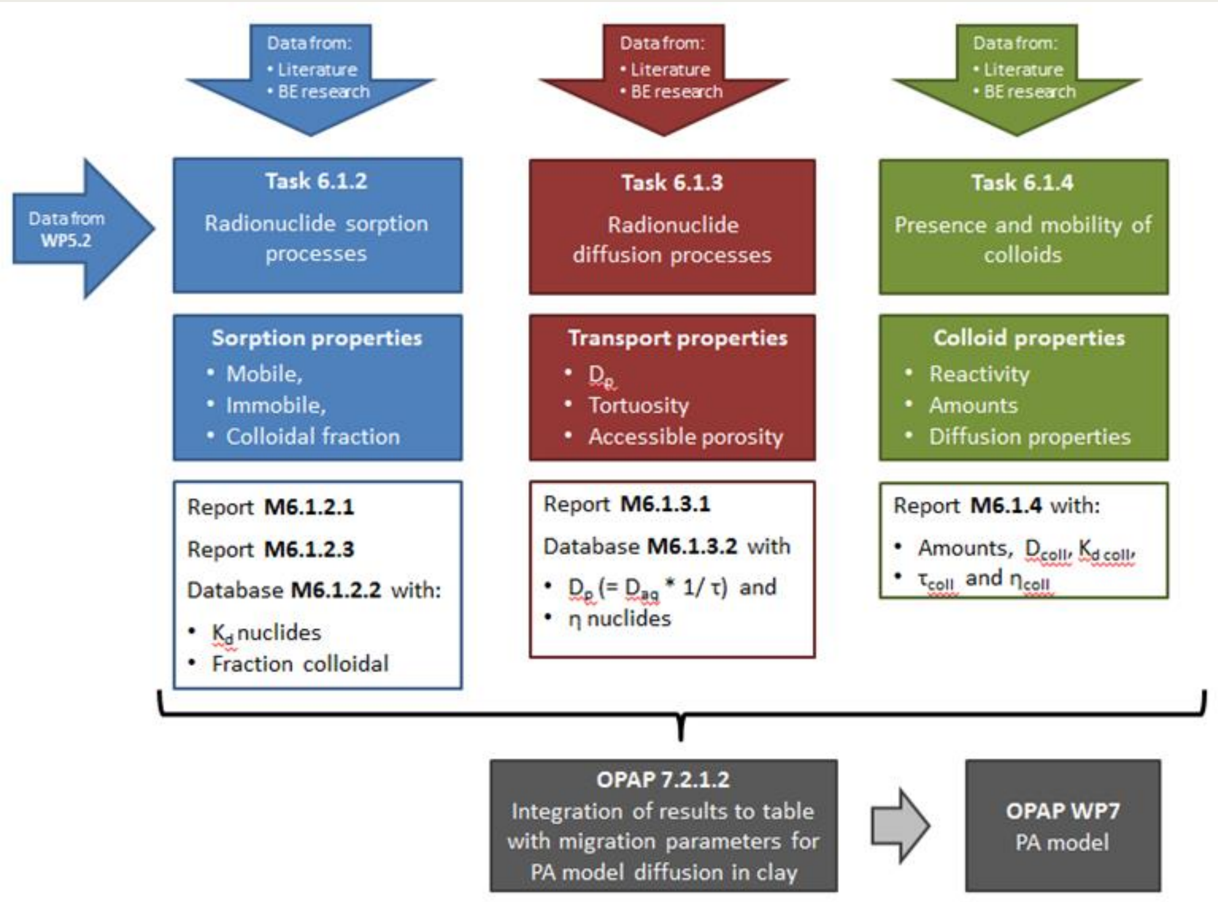

Figure 1-1 Schematic overview of relationship between OPERA WP6.1 tasks and WP7

1.2. Objectives

This report contains the reference database with sorption property values and represents deliverable M6.1.2.2 which forms part of the results of the research proposed for Task 6.*1.2*.

1.3. Realization

The values for the reference database with sorption property values are the result of the work described in the accompanying report M6.1.2.3 [Schroder, 2016].

1.4. Explanation contents

Chapter 2 contains tables with:

Table 2-1:	input parameters ranges for the OPERA reference sorption model to be used for the uncertainty analyses in OPERA WP7
Table 2-2 - 2-5:	the reference database with element specific sorption and distribution properties to be used for the deterministic calculations for the Central Assessment Case ([Grupa et al, 2015], Section 4.2) of the normal evolution Scenario , to be performed as part of OPERA WP 7

2. Reference database with sorption properties

In the reference database with sorption properties, three cases are distinguished:

- a ***base case*** with a DOC concentration of 100 mg/l,
- a ***low DOC*** **case** with a DOC concentration of 20 mg/l, and
- a ***high DOC case*** with a DOC concentration of 200 mg/l.

Table 2-1 shows the input values ranges for the OPERA reference sorption model (see Table 4-1 in [Schröder & Meeussen, 2017]), to be used for securing the correlations between K_d's for and mobility of the various radionuclides in the uncertainty analyses in OPERA WP7.

Table 2-1: Boom Clay input ranges for use in the OPERA reference sorption model

property	min - max	
Bulk wet density [kg/m^3]	1.900 – 2.150	
Porosity [%]	29 – 43	
CEC Boom Clay [meq/100g Boom Clay]	2.0 – 42	
SOC [wt. %]	0.35 – 2.0	
Proton exchange capacity SHA [meq/g]	1 – 2	
DOC [mg/L]	***base case:***	100 mg/l
	low DOC case:	20 mg/l
	high DOC case:	200 mg/l
Proton exchange capacity DHA [meq/g]	2 – 6	
HFO [g/kg]	0.4 – 3.3	
Inorganic carbon [wt. %]	0.0 – 2.5	
Total amount Ca [wt. %]	0.2 – 7.3	
Total amount Fe [wt. %]	2.2 – 5.4	
Total amount S [wt. %]	0.35 – 2.6	
Soluble concentration Cl [mg/L]	4 – 20'000	
Soluble concentration Na [mg/L]	4 – 11'000	
pH [-]	7.7 – 9.2	
pe + pH [-]	3.8 – 5.8	

Table 2-2 to Table 2-4 show the resulting lower, upper and central K_d-*values* and retardation factors for all three cases. The tables distinguish between dissolved, aqueous radionuclides and radionuclides bound to dissolved organic matter (DOC).

Table 2-2: Ranges of calculated K_d- and R-values in Boom Clay of the Netherlands for the '*base case*' (100 mg/l DOC). Lower, central, and upper values correspond to 5-, 50- and 95-percentiles of the calculated values, respectively.

Element	$K_{d\text{-}diss}$			$K_{d\text{-}DOC}$			R_{dis}			R_{DOC}		
	lower	central	upper	lower	central	upper	lower	central	upper	lower	central	upper
Se	0	0	0	51	129	247	1	1	1	236	621	1263
U	7	>10'000	>10'000	16	46	95	33	>50'000	>50'000	77	221	489
Tc	>10'000	>10'000	>10'000	16	46	95	>50'000	>50'000	>50'000	77	221	489
Th	>10'000	>10'000	>10'000	16	46	95	>50'000	>50'000	>50'000	77	221	489
Np	>10'000	>10'000	>10'000	16	46	95	>50'000	>50'000	>50'000	77	221	489
K	0	7	387	113	485	1068	3	34	1997	525	2300	5694
Ca	9	1114	>10'000	133	603	1831	46	5409	>50'000	611	2881	9584
Pu	>10'000	>10'000	>10'000	16	46	95	>50'000	>50'000	>50'000	77	221	489
Am	>10'000	>10'000	>10'000	24	71	366	>50'000	>50'000	>50'000	116	349	1676
Sn	>10'000	>10'000	>10'000	16	46	95	>50'000	>50'000	>50'000	77	221	489
Eu	>10'000	>10'000	>10'000	20	56	146	>50'000	>50'000	>50'000	95	267	706
Ni	>10'000	>10'000	>10'000	17	47	96	>50'000	>50'000	>50'000	81	227	494
Cs	103	1329	7596	3413	>10'000	>10'000	476	6454	38'699	16611	>50'000	>50'000
Cm	>10'000	>10'000	>10'000	16	46	95	>50'000	>50'000	>50'000	78	222	489
Sr	33	2762	>10'000	35	95	273	160	13'329	>50'000	161	461	1375
Ra	18	1554	>10'000	34	95	275	87	7320	>50'000	161	458	1364
Pb	>10'000	>10'000	>10'000	25	69	237	>50'000	>50'000	>50'000	120	338	1145

Table 2-3: Ranges of calculated K_d- and R-values in Boom Clay of the Netherlands for the '*low DOC case*' (20 mg/l DOC). Lower, central, and upper values correspond to 5-, 50- and 95-percentiles of the calculated values, respectively.

Element	$K_{d\text{-}diss}$			$K_{d\text{-}DOC}$			R_{dis}			R_{DOC}		
	lower	central	upper	lower	central	upper	lower	central	upper	lower	central	upper
Se	0	0	0	257	646	1235	1	1	1	1178	3100	6311
U	7	>10'000	>10'000	81	231	473	33	>50'000	>50'000	382	1103	2442
Tc	>10'000	>10'000	>10'000	81	231	473	>50'000	>50'000	>50'000	382	1103	2442
Th	>10'000	>10'000	>10'000	81	231	473	>50'000	>50'000	>50'000	382	1103	2442
Np	>10'000	>10'000	>10'000	81	231	473	>50'000	>50'000	>50'000	382	1103	2442
K	0	7	387	567	2423	5339	3	34	1996	2619	11496	28464
Ca	9	1114	>10'000	663	3016	9153	46	5400	>50'000	3051	14'398	47'917
Pu	>10'000	>10'000	>10'000	81	231	473	>50'000	>50'000	>50'000	382	1103	2442
Am	>10'000	>10'000	>10'000	119	357	1829	>50'000	>50'000	>50'000	578	1741	8379
Sn	>10'000	>10'000	>10'000	81	231	473	>50'000	>50'000	>50'000	382	1103	2442
Eu	>10'000	>10'000	>10'000	100	278	732	>50'000	>50'000	>50'000	473	1332	3527
Ni	>10'000	>10'000	>10'000	86	236	481	>50'000	>50'000	>50'000	402	1130	2468
Cs	103	1328	7594	>10'000	>10'000	>10'000	476	6453	38'699	>50'000	>50'000	>50'000
Cm	>10'000	>10'000	>10'000	82	231	473	>50'000	>50'000	>50'000	384	1105	2442
Sr	33	2761	>10'000	173	474	1365	160	13'289	>50'000	802	2303	6873
Ra	18	1550	>10'000	173	475	1373	87	7315	>50'000	799	2287	6816
Pb	>10'000	>10'000	>10'000	125	347	1184	>50'000	>50'000	>50'000	595	1685	5722

Table 2-4: Ranges of calculated K_d- and R-values in Boom Clay of the Netherlands for the '*high DOC case'* (200 mg/l DOC). Lower, central, and upper values correspond to 5-, 50- and 95-percentiles of the calculated values, respectively.

Element	$K_{d\text{-}diss}$ lower	$K_{d\text{-}diss}$ central	$K_{d\text{-}diss}$ upper	$K_{d\text{-}DOC}$ lower	$K_{d\text{-}DOC}$ central	$K_{d\text{-}DOC}$ upper	R_{dis} lower	R_{dis} central	R_{dis} upper	R_{DOC} lower	R_{DOC} central	R_{DOC} upper
Se	0	0	0	26	65	123	1	1	1	119	311	632
U	7	>10'000	>10'000	8	23	47	33	>50'000	>50'000	39	111	245
Tc	>10'000	>10'000	>10'000	8	23	47	>50'000	>50'000	>50'000	39	111	245
Th	>10'000	>10'000	>10'000	8	23	47	>50'000	>50'000	>50'000	39	111	245
Np	>10'000	>10'000	>10'000	8	23	47	>50'000	>50'000	>50'000	39	111	245
K	0	7	387	57	242	534	3	34	1999	263	1151	2847
Ca	9	1114	>10'000	66	302	915	46	5427	>50'000	306	1441	4793
Pu	>10'000	>10'000	>10'000	8	23	47	>50'000	>50'000	>50'000	39	111	245
Am	>10'000	>10'000	>10'000	12	36	183	>50'000	>50'000	>50'000	58	175	838
Sn	>10'000	>10'000	>10'000	8	23	47	>50'000	>50'000	>50'000	39	111	245
Eu	>10'000	>10'000	>10'000	10	28	73	>50'000	>50'000	>50'000	48	134	353
Ni	>10'000	>10'000	>10'000	9	24	48	>50'000	>50'000	>50'000	41	114	248
Cs	103	1329	7597	1706	>10'000	>10'000	476	6457	38'699	8302	>50'000	>50'000
Cm	>10'000	>10'000	>10'000	8	23	47	>50'000	>50'000	>50'000	39	111	245
Sr	34	2764	>10'000	17	47	136	160	13'382	>50'000	81	231	688
Ra	18	1557	>10'000	17	47	137	87	7330	>50'000	81	230	682
Pb	>10'000	>10'000	>10'000	12	35	118	>50'000	>50'000	>50'000	60	169	573

Table 2-5 summarizes the values to be used for the radionuclides for which no speciation calculations are performed.

Table 2-5: Recommended lower, central, and upper K_d-values of dissolved and DOC-bound fractions of the radionuclides considered in OPERA. '-':no model representation necessary, because the contribution can be neglected in comparison to the other K_d

Element	K_{d_diss} [l/kg] Lower value	K_{d_diss} [l/kg] Central value	K_{d_diss} [l/kg] Upper value	K_{d_DOC} [l/kg] Lower value	K_{d_DOC} [l/kg] Central value	K_{d_DOC} [l/kg] Upper value
H, C, Si, Cl, Ar, Ti, Kr, Mo, Nb, Ba, Pm, Ho, Re, Bi, Po, I		0			-	
Be	as *Ca*					
Zr, Pd, Ag, Sm, Ac	as *Sn*					
Pa, Cf	as *U*					

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