

# Reference database with diffusion properties

OPERA-PU-NRG6132

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-Produktie maatschappij Zuid-Nederland (EPZ) and coordinated by COVRA. Further details on OPERA and its outcomes can be accessed at [www.covra.nl](http://www.covra.nl).

This report concerns a study conducted in the framework of OPERA. The conclusions and viewpoints presented in the report are those of the author(s). COVRA may draw modified conclusions, based on additional literature sources and expert opinions. A .pdf version of this document can be downloaded from [www.covra.nl](http://www.covra.nl).

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Date of publication: 7 February 2017

Keywords: radionuclide diffusion, Boom Clay, modelling, anion diffusion, clay charge, molecular dynamics

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## Summary

This report contains the reference database with diffusion properties and represents deliverable M6.1.3.2 which forms part of the results of the research proposed for Task 6.1.3. A description of the underpinning calculations and assumptions is given in the accompanying report OPERA-PU-NRG6131 [Meeussen, 2016].

## Samenvatting

Dit rapport bevat de referentie database met diffusie parameters en vertegenwoordigt OPERA deliverable M6.1.3.2 en vormt onderdeel van de resultaten van Task 6.1.3. De berekeningen die ten grondslag liggen aan deze waarden worden beschreven in het bijbehorende rapport OPERA-PU-NRG6131 [Meeussen, 2016].

# 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 (M6.1.3.2) presents results of the OPERA research project RANMIG (Radionuclide migration), as part of OPERA Task 6.1.3, Modelling approach for diffusion 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], [Hart et al., 2012], [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 disposals 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.

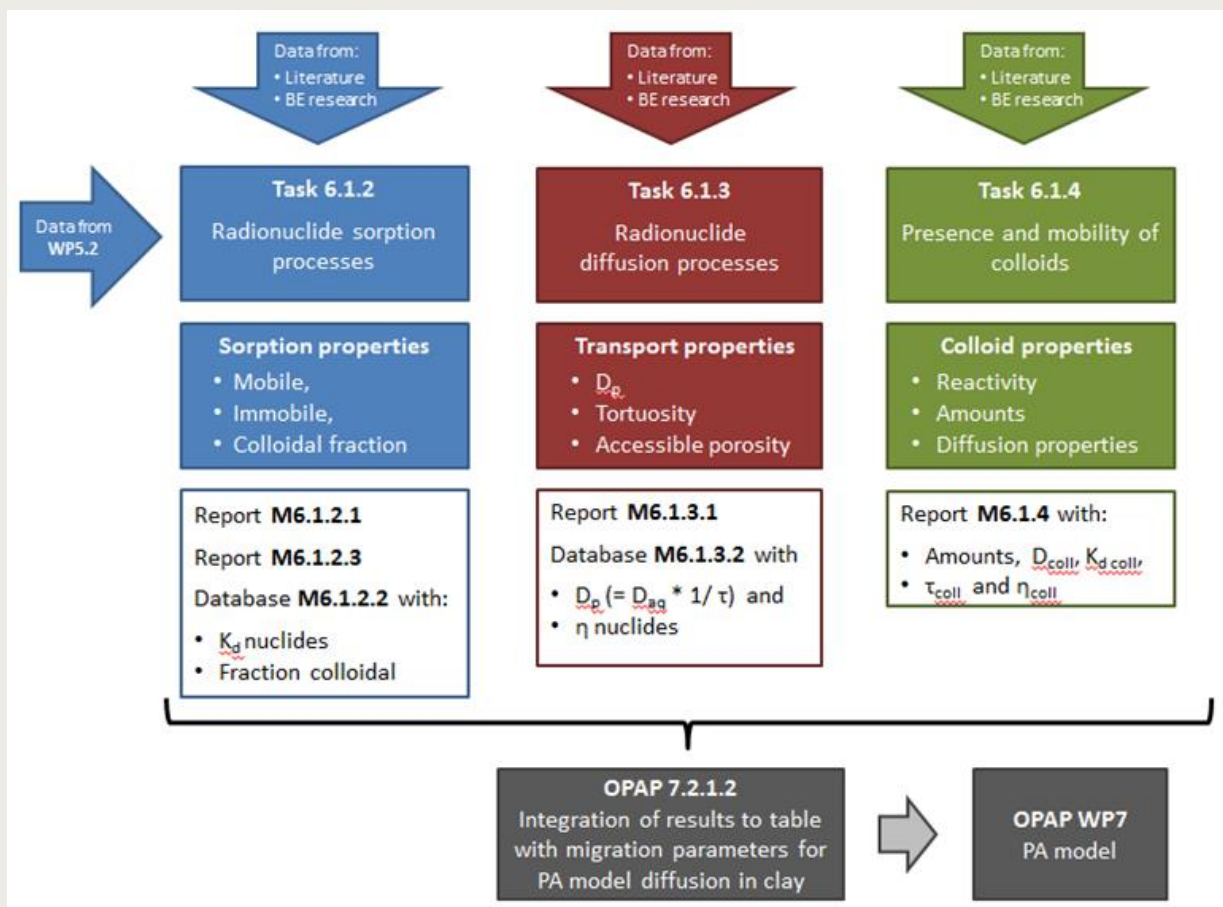


Table 1-1 Schematic overview of relationship between OPERA WP6.1 tasks and WP7

### *1.2. Objectives*

This report contains the reference database with diffusion properties and represents deliverable M6.1.3.2 which forms part of the results of the research proposed for task 6.1.3

### *1.3. Realization*

The values for the reference database with diffusion properties are the result of the work described in the accompanying report M6.1.3.1 [Meeussen, 2016].

### *1.4. Explanation contents*

Chapter 2 contains the reference database with diffusion properties

## 2. Reference database with diffusion properties

The database presented in the table below summarizes the migration parameters values deduced for the Boom Clay for conditions as expected for the OPERA reference disposal concept. These values are based on the parameter ranges estimated by SCK•CEN for the Boom Clay in the Mol region. This data were adapted for conditions as expected for the future Dutch disposal facility and address uncertainties caused by the lack of geochemical characteristics of the Boom Clay in the Netherlands. The estimation of the parameters ranges was carried out in line with the recommendations given by SCK•CEN and TNO. The diffusion properties listed in Table 2-1 are valid for salinities and in situ effective stress ranging from the Belgian conditions (low salinity and in situ effective stress 2.4 MPa) and the highest expected salt level and in situ effective stress for a Dutch situation (sea water +/-0.6 M, in situ effective stress 6.9 MPa).

The used methods, data and assumptions are documented in [Meeussen, 2016]. Together with the  $K_d$  values resulting from task 6.1.2 these will provide an estimation of overall apparent diffusion coefficient for the PA calculations within WP7.

Table 2-1 Reference database with diffusion properties

Element	Diffusion accessible porosity $\eta$ [-]		Pore diffusion coefficient $D_{pore}$ [ $m^2s^{-1}$ ]	
	min	max	min	max
H	0.14	0.40	2.00E-10	2.60E-10
Be	0.07	0.17	5.70E-12	5.70E-11
C	0.05	0.40	1.50E-11	1.00E-10
Si	0.14	0.40	2.00E-10	2.60E-10
Cl	0.05	0.40	1.00E-10	1.60E-10
Ar	0.14	0.40	2.00E-10	2.60E-10
K	0.14	0.40	1.40E-10	8.10E-09
Ca	0.14	0.40	1.90E-10	3.30E-10
Ti	0.07	0.17	5.70E-12	5.70E-11
Ni	0.07	0.17	5.70E-12	5.70E-11
Se (I)	0.05	0.40	8.40E-11	1.30E-10
Se (II)	0.05	0.40	5.00E-11	8.00E-11
Kr	0.14	0.40	2.00E-10	2.60E-10
Sr	0.14	0.40	1.90E-10	3.30E-10
Mo	0.05	0.40	5.00E-11	8.00E-11
Nb	0.05	0.40	6.70E-11	1.10E-10
Zr	0.07	0.17	5.70E-12	5.70E-11
Tc	0.07	0.17	5.70E-12	5.70E-11
Pd	0.07	0.17	5.70E-12	5.70E-11
Ag	0.07	0.17	5.70E-12	5.70E-11
Cd	0.07	0.17	5.70E-12	5.70E-11
Sn	0.07	0.17	5.70E-12	5.70E-11
I	0.05	0.40	1.00E-10	1.60E-10

Element	Diffusion accessible porosity $\eta$ [-]		Pore diffusion coefficient $D_{pore}$ [ $m^2s^{-1}$ ]	
	min	max	min	max
Ba	0.14	0.40	1.90E-10	3.30E-10
Cs	0.14	0.40	1.40E-10	8.50E-09
Pm	0.07	0.17	5.7E-12	5.7E-11
Sm	0.07	0.17	5.70E-12	5.70E-11
Eu	0.07	0.17	5.70E-12	5.70E-11
Ho	0.07	0.17	5.70E-12	5.70E-11
Re*	0.05	0.40	5.7E-12	8.5E-09
Pb	0.07	0.17	5.70E-12	5.70E-11
Bi*	0.05	0.40	5.7E-12	8.5E-09
Po*	0.05	0.40	5.7E-12	8.5E-09
Ra	0.14	0.40	1.80E-10	3.10E-10
Ac	0.07	0.17	5.70E-12	5.70E-11
Th	0.07	0.17	5.70E-12	5.70E-11
Pa	0.07	0.17	5.70E-12	5.70E-11
Np	0.07	0.17	5.70E-12	5.70E-11
U	0.07	0.17	5.70E-12	5.70E-11
Pu	0.07	0.17	5.70E-12	5.70E-11
Am	0.07	0.17	5.70E-12	5.70E-11
Cm	0.07	0.17	5.70E-12	5.70E-11
Cf	0.07	0.17	5.70E-12	5.70E-11

\* There are no thermodynamic and chemical data on Bi, Po and Re in the standard databases so it is difficult to estimate the form they occur. For these radionuclides we will assume the most conservative migration parameters (see Section 5.4 in [Meeussen et al., 2016] for more detail).



### 3. References

[Verhoef et al., 2011] Verhoef, E, E Neeft, JB Grupa, A Poley, *OPERA. Outline of a disposal concept in clay*, OPERA report OPERA-PG-COV008, COVRA N.V., July 2011, 1-17.

[Verhoef & Schröder 2011] Verhoef, E and TJ Schröder, *OPERA Research plan*, OPERA-PG-COV004, COVRA N.V., 2011, 1-48.

[NEA, 1999] Nuclear Energy Agency (NEA), *Confidence in the Long-term Safety of Deep Geological Repositories. Its Development and Communication*, OECD, Paris, 1999, 1-80.

[NEA, 2004] Nuclear Energy Agency (NEA), *Stepwise Approach to Decision Making for Long-term Radioactive Waste Management. Experience, Issues and Guiding Principles*, NEA report No. 4429 - ISBN 92-64-02077-2OECD, Paris, 2004, 1-72.

[Hart et al., 2012] Hart, J, P Davis, D-A Becker, U Noseck, L Hendriksen, AFB Wildenborg, M Winegram, *OSCAR. Evaluation of current state-of-the art on Safety Case methodologies*, OPERA Deliverable M2.1.1.a. OPERA Report OPERA-CF-NRG211A/NRG-report NRG-23194/12.117766/P, December 2012, 1-209.

[Grupa & Davis, 2013] Grupa, JB, P Davis, *Report on the OPERA Safety Case structure*, OPERA report OPERA-PU-NRG008, October 2013, 1-24.

[Meeussen et al., 2016] J.C.L. Meeussen, E. Rosca-Bocancea, T.J. Schröder, M. Koenen, F. Valega Mackenzie, N. Maes, C. Bruggeman, *Model representation of radionuclide diffusion in Boom Clay*, OPERA report OPERA-PU-NRG6131, submitted.

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