# Introduction to OECD/NEA Sorption Project Phase III

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## 1. Introduction

Deep or near-surface underground repositories are being considered for the safe long-term storage and/or final disposal of radioactive wastes in many countries. A key safety feature is to prevent or sufficient retard radionuclide migration to the biosphere. Radionuclide sorption is one of the most important processes which provide this safety feature. Sorption is generally characterized by equilibrium distribution coefficients  $(K_d \text{ values})$  for performance assessment (PA) of a repository. The NEA Sorption Project was established to reduce uncertainty in K<sub>d</sub> and to increase confidence in PA. The overall objective of the NEA Sorption Project is to clarify and demonstrate how the use of thermodynamic sorption models (TSMs) can serve to improve confidence in the K<sub>d</sub> values used to represent radionuclide sorption in most PA models [1].

## 2. History of NEA Sorption Project

The first phase of the NEA Sorption Project ran from 1997 to 1998 and illustrated not only the advances that had been made in the field of thermodynamic sorption models, but also the diversity in the details of the thermodynamic descriptions of sorption processes. Accordingly, Phase II of the NEA Sorption Project from 2000 to 2005 was initiated as a major international contribution towards demonstrating the consistency and applicability of different TSM approaches to support the selection of K<sub>d</sub> values for safety assessments (SA). The results of the NEA Sorption Project II conclusively show that 1) the conceptual and methodological tools needed for characterizing, interpreting and justifying the K<sub>d</sub> values provided for PA needs are largely available; 2) with respect to complex materials, what is mainly needed are good quality and more complete sets of pertinent sorption data [1].

#### 2. Sorption Modeling for Performance Assessment

Radionuclide sorption along the migration path is significantly influenced by the various geochemical conditions. Because of the highly conditional nature of  $K_d$ , different estimates of  $K_d$  values for each relevant radionuclide are required for each environmental compartment along the migration path. It is obvious that it is not feasible to determine  $K_d$  for every system and condition experimentally, and many of the relevant systems are difficult to reproduce in the laboratory. The relationship between data obtained in approximated

and/or simplified experimental systems and the derivation of  $K_d$  for conditions being modeled in PA, as well as the associate principal uncertainties, are schematically illustrated in Fig. 1 [1]. As shown in Fig. 1,  $K_d$  data transfer includes many procedures to take into account differences in mineralogy and solution composition. Uncertainties in data transfer are almost unavoidable; their magnitude is critically dependent on how well the relations between  $K_d$  and the key geochemical parameters are constrained.



Fig. 1. A schematic and simplified illustration of the derivation of  $K_d$  values for PA based on sorption data from approximated experimental systems and of the associated uncertainties.

In modeling sorption processes, thermodynamic sorption models (TSMs) offer a distinct advantage over the sorption coefficient K<sub>d</sub> since TSMs represent surface chemical reactions with a set of thermodynamic constants which are independent of changes in the solution conditions. The application of TSM to single mineral sorption systems has mostly been considered to be successful. However, for the composite natural sorption systems like rocks and soils it has been considered to be partially successful. TSMs have been routinely used to aid the extrapolation of K<sub>d</sub> values to the conditions outside of the range of experimental results. Thus TSMs are very useful in understanding the uncertainties inherent in using K<sub>d</sub> values. TSM is not restricted to predictive applications. TSM can also provide a thermodynamic framework to integrate quantitatively the influence of all relevant geochemical parameters on K<sub>d</sub>.

#### 3. NEA Sorption Project Phase III

The objective of the Sorption Project, Phase III, will be to develop and publish a Guideline Document to address the key needs identified at the end of Phase II regarding TSM development and use within the framework of performance assessment and building safety cases. The Guideline Document includes following chapters [2]:

- Chapter 1. Introduction, overview and background
- Chapter 2. Overall strategies and decision making during TSM development
- Chapter 3. Identification of key model parameters by sensitivity analysis; assessment of uncertainties
- Chapter 4. Methods for determining fundamental model parameters, model physical and chemical reasonableness
- Chapter 5. Scientific basis for applying models and parameters to field situations (up-scaling)
- Chapter 6. Conclusions and recommendations.

Control of the Sorption Project (Phase III) will be vested in the Management Board (MB) consisting of one member designated by each Participant. The MB may invite one or more members of the Technical Direction Team (TDT). A TDT will provide the technical direction of the Sorption Project. The TDT will consist of three international experts with experience on sorption modeling and also an understanding of the requirements of the safety assessments for radioactive waste disposal systems. Certain inputs to the Guideline Document will be provided by External Experts (EE). These experts will be nominated by the Management Board during the first six months of the project, on the basis of advice provided by the TDT.

Table 1. Summary of the Sorption Project Phase III

	13 organizations (12 countries):					
Participating organization	ANSTO (Australia)					
	ONDRAF/NIRAS(Belgium)					
	RAWRA (Czech Republic)					
	Posiva Oy (Finland)					
	ANDRA (France)					
	GRS (Germany)					
	JAEA (Japan)					
	ENRESA (Spain)					
	HSK/NAGRA/PSI (Switzerland)					
	Nexia Solution Ltd. (UK).					
	NDA (UK)					
	NRC (USA)					
	KAERI (Korea Republic)					
Project						
neriod	2007. 11 ~ 2010. 04 (30 months)					
Expenses	Total 427 300 Euros					
	(32,860) Euros per organization)					
	(52,009 Euros per organization)					

A total project timescale of about 30 months is envisaged, with an intermediate milestone after the first 12 months. The principal project activities are associated with the production of the Guideline Document. Fig. 2 summarizes the planned schedule of production of the 6 chapters by the Technical Direction Team and External Experts. The final phase of the project will involve holding a OECD-NEA Workshop to present and discuss the draft Guideline Document contents to all interested parties and publication by the OECD-NEA of the final Guideline Document.

Overall Action Planning	07.06 ~ 07.10	07.11 ~ 07.12	08.01 ~ 08.06	08.07~ 08.12	09.01 ~ 09.06	09.07 ~ 09.12	10.01 ~ 10.04
Preliminary work							
Organization of TDT & EE (TDT meeting #1)							
Draft of Chapters 1 and 2							
Draft of Chapter 3 (TDT Meeting #2)							
Draft of Chapter 4							
Draft of Chapters 5 and 6							
Final editing and revision (TDT Meeting #3) (NEA Workshop)							

Fig. 2. A planned schedule of the Sorption Project Phase III.

# REFERENCES

[1] J. A. Davis et al., NEA Sorption Project Phase II, OECD-NEA, 2005.

[2] Arrangement of the OECD/NEA Sorption Project (Phase III), 2007.