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NUCLEAR ENERGY AGENCY
RADIOACTIVE WASTE MANAGEMENT COMMITTEE

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Sorption Project

PROCEEDINGS OF THE SORPTION WORKSHOP: CONCLUSION OF NEA SORPTION PROJECT PHASE II AND STATUS ANALYSIS OF SORPTION MODELLING FOR PA

Held at the NEA premises
Issy-les-Moulineaux - France
on 10-11 October 2005

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FOREWORD

Surface uptake of radionuclides (sorption) is one of the most important processes that are instrumental in retarding radionuclide migration to the biosphere. For the purpose of performance assessment (PA) calculations, sorption is often described by equilibrium distribution coefficients (K_d). The K_d value is a conditional parameter that reflects the (geo)chemical conditions under which it was measured. Conversely, thermodynamic sorption models (TSMs) offer the possibility to quantitatively describe the major physical-chemical mechanisms determining the sorption of radioelements on different types of solid materials, and predict how the distribution coefficient may be determined by the various geochemical parameters.

The NEA sorption project (Phase II) was an international benchmarking exercise based upon a series of seven test cases that were prepared for this purpose. The objective of the individual test cases was for modelling teams to develop a TSM that quantitatively described sorption by the various materials as a function of chemical conditions. The project has recently been completed, and the present workshop was conceived to summarise the findings of the project, derive the most important lessons learned and determine the requirements for any future international collaborative effort.

INTRODUCTION

The NEA Sorption Project was established to address the propositions that:

- the uncertainty associated with K_d values used for PA arises to a large part from the necessity to transfer K_d values experimentally determined in the laboratory to the expected *in situ* conditions corresponding to different PA scenarios;
- thermodynamic sorption models (TSMs) are uniquely suited for accomplishing this transfer in a fully quantitative and traceable fashion, because of their potential ability to describe sorption under variable geochemical conditions and to integrate geochemical and sorption *equilibria* in a single coherent model.

Phase II of this international project involved the independent development of sorption models by participants for seven test cases based on the same sets of experimental data. In some cases the models derived were applied to the prediction of sorption in similar systems.

Phase II consisted of the following steps:

- selection and design of the test cases (by the technical direction team, TDT);
- implementation in spreadsheets and distribution (by the TDT);
- development and application of sorption models (participants);
- initial interpretation of test case results (by the TDT);
- a modellers' workshop in San Lorenzo de El Escorial (participants and TDT);
- detailed interpretation and synthesis of results;
- preparation and publication of the final report on Phase II [1] (by the TDT and NEA);
- this workshop concluding Phase II of the project.

1 J.A. Davis, M. Ochs, M. Olin, T.E. Payne and C.J. Tweed. NEA Sorption Project Phase II: Interpretation and Prediction of Radionuclide Sorption onto Substrates Relevant for Radioactive Waste Disposal Using Thermodynamic Sorption Models, Nuclear Energy Agency Report No 5992, OECD, 2005.

WORKSHOP AIMS AND STRUCTURE

The aims of the workshop were to:

- provide an overview and illustration of the main project results, with emphasis on merits and limitations of thermodynamic sorption models (TSMs) and recommendations on their use;
- share ideas and stimulate discussion on the best use and practical implementation of "top-down" and "bottom-up" TSM approaches for PA-relevant materials of different complexity;
- achieve a clear picture of the importance of uncertainty in K_d for various performance assessments, of the potential of TSMs for strengthening the respective safety cases, and of the corresponding present and plausible future needs for TSM-based quantification of radionuclide sorption.

The workshop was organised into the following main sessions:

- Session I: Key results of the NEA Sorption Project, Phase II.
- Session II: Thermodynamic sorption model (TSM) approaches for complex materials.
- Session III: Implementation of TSMs in PA programmes, present status, future plans, challenges & needs.

The agenda and participant list for this workshop are included in the Appendix to this note.

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SESSION I

KEY RESULT FROM PHASE II

In this session the main results were summarised. A detailed description and discussion of the results is given in the final report on Phase II[1].

Key results from test cases with simple minerals (T. Payne):

- the test cases demonstrated the capability of the modeller to predict K_d values as a function of chemical conditions (e.g. pH, pCO_2);
- model performance was not significantly determined by choice of EDL model, provided it was applied consistently;
- the importance of considering the chemical conditions and variables to significant to PA was stressed (e.g. major groundwater solutes such as carbonate);
- demonstration of the need to include ternary surface complexes under appropriate conditions;
- two-site models gave better fits to the experimental data than one-site models;
- TSM modellers do not yet have a consensus about how to determine the site density of strong sites;
- most modelling groups chose chemical plausible surface species, but the selected sets of surface species applied in a particular test case were sometimes quite dissimilar.

Key results from test cases with clays (M. Ochs):

- TSMs developed for Na-montmorillonite can be applied to different systems (e.g. other Na-montmorillonite, Ca-montmorillonite, bentonite);
- initial model set up can be decisive – rationale behind the choice of modelling approaches must be clear;
- few teams were willing to modify their initial model;
- models need to be adequately parameterised – where relevant processes are not included (due to insufficient parameter variation in underlying experiments or due to the chosen calibration procedure) the range of model validity is significantly diminished;
- now more wiling to admit lack of knowledge than in the past;
- where carbonate is present it is important to include carbonate in modelling;
- there is no formal analysis of the uncertainties in the thermodynamic data; sensitivity studies would be very useful.

Key results from complex materials (J. Davis):

- for component additivity (CA, bottom up) approach, better sample characterisations are needed for mineral composition determinations – it is difficult to assess surface coating compositions, surface areas of components in complex systems;
- for development of CA models key data for some radionuclides, mineral phases and groundwater compositions are lacking;
- in CA approach there may be an additivity problem due to unknown EDL factors and neglecting the competitive sorption from major ions;
- it was evident that there was a general lack of experience in applying the generalised composite (GC, top down) approach to modelling sorption to complex materials;
- few teams justified their choice of modelling approach;
- the generalised composite approach (GC, top down) appeared to work better than the CA approach but this was probably because the teams used data fitting approaches rather than mechanistic prediction from single minerals,
- fits to data were worst for extreme pHs,
- test cases involving sorption to humic acids were able to describe the data well.

Further key issues were identified in application of the TSM approach (T. Payne):

- experimental measured K_d values are not the same as large-scale K_d values measured in natural analogues,
- experiments were often not undertaken at realistic water/rock ratios nor under fully in-site conditions,
- ternary species, especially actinide – carbonate complexes need to be considered,
- component additive approach (bottom up) has been shown not to work even for binary mineral mixtures,
- little consensus on how to determine site density,
- teams appeared not to be confident in including organics, but where they were included the results appeared to be OK.

Some recommendations were presented (M. Ochs):

- where extrapolation is necessary to predict sorption outside the range of experimental conditions, it is important to understand the influence of key geochemical variables – this requires sufficient variation of such parameters in underlying datasets
- at present, the experimental dataset is a limiting factor for further development of TSMs.

In discussions and questions it was pointed out that:

CA and GC approach

- while the generalised composite model gave the best fit to data, only the component adding approach can be scaled up to PA sized model blocks;

- the CA approach might give as good a fit to the data as the GC approach, if a similar number of parameters were used as fitting parameters.

Uncertainty

- it was recognised that there was little systematic measure of model uncertainty in Phase II of the project;
- there is scope for the study of the TSM sensitivity to key parameters in future work.

Other issues

- it was suggested that there maybe scope for the development of guidelines on when ternary complexes are likely to be significant, for example based on analogy with aqueous complexes;
- use of EXAFS, spectroscopic data: this was rather limited within the relevant test cases, and could be improved.

SESSION II

THERMODYNAMIC SORPTION MODEL APPROACHES TO COMPLEX MATERIALS

Presentations were made on the application of TSM approaches to complex systems including sorption onto single minerals in clay tuff systems, bentonite and sediments and weathered rock. This was followed by further presentations on the CA and GC approaches and on practical issue. The coverage of the session is indicated by the titles of presentations:

- Developing thermodynamic radionuclide sorption models: experimental and modelling results (D. Turner).
- TSM approaches for complex materials bentonite (M. Ochs).
- Surface complexation models to compare additivity and inverse modelling approach (J. Davis).
- Application of thermodynamic modelling tools – experience from Phase II (T. Heath).
- Surface complexation databases (J. Lutzenkirchen).
- Practical usefulness and scientific credibility (T. Payne and V. Brendler).
- Comparison of batch-scale and column experiments (J. Davis).
- Migration data for bentonite (M. Ochs).

Some key points from the discussion were:

- In an exercise to compare the additivity and inverse modelling approaches (J. Davis) it was found that a good match could not be obtained with observed K_d values using an additive model. An inverse model was used instead to derive two simple reactions that matched the data very well.
- It was commented that problems with application of CA approaches are less to do with the chemistry and more to do with surface parameters such as surface area.
- In deriving robust sorption models it is just as important to have a clear understanding of the aqueous chemistry as the surface and sorption processes.
- It was emphasised that chemical plausibility should be a prerequisite in the selection of surface complexes in model development.

SESSION III

IMPLEMENTATION OF THERMODYNAMIC SORPTION MODELS IN PA PROGRAMMES: PRESENT STATUS FUTURE PLANS AND CHALLENGES

The presentations addressed the selection of K_d values for PA and included examples and viewpoints of regulators. The presentations covered application to bentonite, clayrocks, near-surface formations and crystalline rocks.

Selection of K_d for PA as a function of (evolving) conditions: Examples and viewpoints of PA and regulatory agencies (E. Giffaut):

- The fact that there are so many possible types of sorption model available is a major limitation on use.
- Lack of validation of TSM models, several models can be made to fit the data.
- Incomplete knowledge of relationship between batch and compacted data.
- Competition effects generally not considered.

Migration data for bentonite (P. Sellin):

- Presentation of the SKBs methodology for incorporation of sorption onto bentonite buffer in safety assessments.
- SKB has a new procedure that produces traceable records on expert input to data selection and uncertainty.

Implementation of TSMs in PA: present status, future plan, challenges and needs (A. Dierckx):

- It described the Belgian concept and noted that current concept derives K_d from migration experiments.
- A need for high quality batch sorption data was noted; the situation is complicated by the release of organic matter from the clays during batch experiments, which is not the case for *in situ* conditions.

Approach for the development of sorption databases for safety assessment for a repository in Opalinus clay (B. Schwyn):

- A TSM based on illite to represent sorption in Opalinus clay was used.
- Applied a number of correction factors to correct experimental data to specific conditions (pH, ionic strength, pCO_2 etc).
- There is evidence from in-situ experiments that Cs moves faster by diffusion than a K_d approach would indicate.

Applying thermodynamic radionuclide sorption models to performance assessments (D. Turner):

- CNWRAs sorption modelling for PAs was described, including the use of response surfaces to capture correlations between properties of g/w and K_d values and in between K_d values
- Use of stochastic approach: sample water chemistry first then look up K_ds from table.
- It provides a complementary approach to that of US DOE.

TSM for transport modelling at the Naturita UMTRA site (J. Davis):

- Semi-empirical TSMs can reduce modelling uncertainty with respect to sorption under varying chemical conditions.
- Spatial variability groundwater conditions may be more important than variability in surface properties in influencing the retardation of strongly sorbing species over large (km) distances.

Implementation of TSMs in PA (H. Wanner):

- The old NEA sorption database showed no relationship between sorption parameters.
- Many sorption profiles show the same general shape as a function of pH, with ion exchange important at low pH and surface complexation at higher pH.
- Elements with similar hydrolysis behaviour tend to show similar sorption behaviour and can be used to check sorption data.
- Treatment of uncertainties through comparison with conservative data, use of parameter variations including upper and lower limits and consideration of "what if" cases.

TSM in safety assessments (B. Sagar):

- There has been a general shift in the radwaste industry from relying on the geological barrier to engineered barriers because the geosphere is so complex and uncertain;
- US DOE have a Risk Informed Review process that means that only the most risk critical features are examined in detail.
- A Monte Carlo approach was applied in safety assessment using a sample from water chemistry and look-up appropriate K_d values.

Examples of regulatory viewpoints regarding treatment of sorption in the safety assessment for a Swedish spent fuel repository (B. Stromberg):

- The key uncertainty is groundwater flow.
- Risks are much more dependent on depth of rock matrix diffusion than K_d.

SESSION III

DISCUSSION

The discussion session reiterated and expanded on many of the points raised above, as well highlighting some areas for future work. Some of these were related to the establishment of guidelines for various aspects of TSM development and application.

Reversibility of sorption

The question was raised as to whether the reversibility of sorption had been demonstrated in the relevant experiments on which TSMs are based. Although irreversible sorption may be beneficial in most scenarios, reversibility is required for the proper application of TSMs. It was commented that in some cases this had been demonstrated (e.g. in work by PSI on sorption onto clay minerals).

External perceptions of TSM development and application

Has sorption modelling progressed? Most responses to this question indicated that it was felt that progress had been made and that there is increasing confidence in the use of TSMs to support of PA. It was commented that that there is a need to develop clear messages based on facts, e.g. good experimental data sets combined with a mechanistic understanding from the application of suitable TSMs? From the point of view of external perceptions, chemical plausibility in TSMs is especially important. One specific area, where external perceptions were felt to be an issue was related to the question of uniqueness. In particular, the use of various types of electrostatic SCMs that often give a similar quality of fit to experimental data was felt to give the impression that the development of sorption models was a 'hit-and-miss' process and lacked consistency.

Experimental and thermodynamic data

There is an ongoing need for good quality experimental data sets with sufficient mineralogical and surface characterisation data as well as sorption data covering sufficiently the variable chemical parameters. Experimental studies reported in the literature are frequently too limited or are lacking a sufficient characterisation of the sorbent phases to be useful for TSM development.

It was commented that a closer link between the sorption project and the NEA thermodynamic database would be beneficial. Any TSM parameterisation is dependent on the aqueous chemical data set applied and requires re-fitting if the thermodynamic data for significant aqueous species are revised.

It was also noted that there was a lot more information available now from spectroscopic studies on the nature of surface complexes than at the start of Phase II. TSM development should make use of these data where available, although in most cases little use was made of the data available for the Phase II test cases.

Lessons learned from the approaches to Phase II test cases

It was commented (with hindsight) that the TDT should have constrained the test cases more tightly to ensure that particular variables selected were adequately investigated. In many cases it was difficult to explain differences between the performance of various participants' models because of the number of variables involved in the models.

Training

The need for training in TSM development and application for new workers in this area was discussed. It was suggested that such activities could be incorporated into current EU projects such as NF-PRO or FUNMIG.

Suggested areas for further work

Many of the suggestions for further work involved the development of guidance on a wide variety of issues related to TSM development and application. The extent and detail of such guidance and methods by which they should be developed were not discussed in detail. Areas where guidelines or guidance was suggested or where agreement on a way forward might be helpful included:

- the use of TSMs in developing safety cases;
- the preferred method(s) for determining site densities;
- the use of spectroscopic data in TSM development;
- the criteria for selecting the number of fitting parameters;
- the reasons for selection the type of surface complexation model (DLM, TLM, etc.);
- the extent of experimental data required/preferred for model development;
- the recording and reporting of decisions made in model development;
- the inclusion of ternary complexes.

Other areas suggested for further work included:

- the assessment and treatment of uncertainties at all stages from experimental measurements, through model development and scale-up to the application of simplified treatments of sorption in PA;
- the further development of sorption databases and standard models for selected minerals; it was commented that this may not be the appropriate time for such developments but also that it would be useful to "clear out" the sorption database (e.g. FZR database) or to use some method to rank the usefulness of entries.

CONCLUSIONS AND RECOMMENDATIONS

The workshop showed that the thermodynamic sorption model (TSM) approach has made considerable advances in recent years. The model inter-comparison exercise demonstrated:

- the general validity of the TSM approach for describing sorption;
- the ability of TSMs to describe the dependence of K_d on geochemical parameters;
- the inherent chemical realism in TSMs;
- the general acceptance of the need for considering ternary surface complexes;
- the recognition that many sorption models for geological substrates are in reality a blend of conceptually different approaches for modelling complex materials;
- the potential for TSMs to form a bridge between geochemistry and performance assessment, combining mechanistic modelling with pragmatic applied geology.

However, despite the general satisfactory outcomes of the modelling exercise it is also recognised that TSM approaches, as implemented in the project, had several limitations, including:

- lack of standardisation in model development;
- inexperience of modelling teams, which in some cases resulted in sometimes inappropriate or deleterious individual modelling decisions;
- inadequate analysis of uncertainty and error propagation;
- lack of consensus on methods to parameterise key model components, such as site density.

Some participants also commented on the lack of uniqueness: although the models resulted a satisfactory fit to the data, this was possibly attributable to a sufficiently large number of fitting parameters, rather than the inherent merits of the model.

There is a requirement for greater consistency in sorption modelling as applied in PA exercises world-wide. It may be considered to produce a report on strategies for TSM development for a wide range of materials and chemical elements of interest to PA, written in a manner that facilitates their use in selecting K_d for use in safety cases. This could cover *inter alia*:

- Overall strategies and decision making.
- Appropriate methods for determining model parameters (e.g. surface sites, surface species and reaction stoichiometry).
- Identification of key model parameters by sensitivity analyses and relationship to K_d value uncertainty.
- Scientific basis for applying models and parameters to materials at *in situ* conditions.

There is also a continued need for a training and communication programme on TSM application to relevant systems. The project clearly identified a range of skill levels amongst participating teams, and at times uncertainty and inexperience in application of the modelling approaches. Thus, it is recommended that the NEA continue to provide a forum in which sorption modellers can be brought together to increase both the level of technical competency as well as improve international communication and discussion of TSM modelling activities.

APPENDIX A

WORKSHOP AGENDA

Day 1 - 10 October 2005

09:00 9:30	**Introduction** Welcome, purpose and topics of workshop Overview of Sorption Project Phase I & II	*M. Askarieh, S. Voinis*
09:30-10:30	**Session I: Key results from Phase II** • Complexity of PA-relevant substrates and relevance for sorption models • Key results and assessment of sorption models • Key issues in the consistent application of thermodynamic sorption models (TSMs) • Management of uncertainty in K_d • Recommendations for TSM approaches	Chair: *M. Askarieh* *J. Davis, M. Ochs T. Payne*
10:30-11:00	**Coffee break**	
11:00-12:30	**Session I,** (cont'd).	Chair: *M. Askarieh*
12:30-14:00	**Lunch**	
14:00-15:00	**Session II: Thermodynamic sorption model (TSM) approaches for complex materials** **Part I:** Introduction and examples • Introduction to the session • Examples: o Single minerals in clay/tuff systems o Bentonite o Sediments, weathered rock/fracture filling	Chair: *S. Altmann* *S. Altmann* *D. Turner* *M. Ochs* *J. Davis*
15:30-16:00	**Coffee break**	
16:00-18:00	**Session II,** (cont'd) **Part II:** Application of thermodynamic sorption models: strengths and limitations of "top-down" and "bottom-up" approaches, practical issues • Introduction: Different models for different tasks • Model parameters (fitted, other sources, chemical plausibility), data needs/bases, TDB • Practical usefulness and scientific defensibility • Application to intact systems, link with transport	Chair: *S. Altmann* *M. Ochs* *J. Davis, T. Heath, J.Lützenkirchen* *T. Payne, V. Brendler* *J. Davis, M. Ochs*
18:00	**Closing of sessions I and II**	

Day 2 - 11 October 2005

	Session III: Implementation of TSMs in PA programmes, present status, future plans and challenges, needs	Chair: *M. Randall*
09:00-10:30	**Summary of Day 1, outlook on Day 2**	*S. Altmann*
	Presentations and detailed discussions:	
	Selection of K_d for PA as a function of (evolving) conditions: Examples and viewpoints of PA and regulatory agencies	
	• Bentonite EBS • Clayrock (Boom/Opalinus Clay)	*E. Giffaut, P.Sellin* *A. Dierckx/L. Wang* *B. Schwyn*
10:30-11:00	**Coffee break**	
11:00-12:00	**Presentations and detailed discussions: cont.**	
	• Near-surface formations/US sites	*D. Turner*, *J. Davis*
12:00-13:30	**Lunch**	
13:30-15:00	**Presentations and detailed discussions: cont.**	
	• Crystalline rock/fractures • Viewpoint of regulators	*L. Knight* *H. Wanner*, *B. Sagar, B. Stromberg*
15:00-15:30	**Coffee break**	
15:30-17:00	**Session III: Discussion**	Chair: *P. Hernan*
	• Critical/less critical issues for using TSMs in PA • Foreseeable requirements for successful future TSM applications in PA • Discussion of priorities for a possible Phase III	*Panel:* M. *Askarieh, S. Altmann, J. Bruno, J. Davis, A. Dierckx, , P. Larue, M. Hakanen, M. Ochs, S. Voinis*
17:00-17:15	**Closing of the session III and workshop**	*M. Askarieh*

APPENDIX B

WORKSHOP ABSTRACTS

SESSION I: OVERVIEW OF SORPTION PROJECT PHASE I AND PHASE II

M. Askarieh
Nirex, UK

Motivation for and overall objectives of the Sorption Project is outlined with respect to Performance Assessment (PA) needs and a brief historical overview of Phase I & Phase II of the Sorption Project is provided with a particular emphasis on specific goals and conclusions of Phase II project.

In Performance Assessment (PA), a large number of parameters is used to represent the relevant processes along a given migration path. Ultimately, movement and fate of radionuclides is determined by their solubility in the respective aqueous solutions, and the partitioning of their dissolved forms between the solutions and the surfaces that they encounter along their migration path. Particularly critical in this regard is the determination and management of uncertainty in K_d as a function of geochemical conditions, which can have a major influence on the assessment of repository performance.

As K_d for most elements is sensitive to geochemical conditions (solution composition, the nature and amount of the solid material's wetted surface) it may vary significantly from one compartment to another if there are significant differences in solid or solution composition or, within a given compartment, if the composition evolves over time or is subject to uncertainty.

In many waste management programmes, confidence in PA may rely strongly upon confidence in K_d, and a reduction of uncertainty in K_d allows the use of excessively conservative safety factors to be avoided.

Phase II of the project illustrated not only the advances that had been made in the field of thermodynamic sorption models, but also the diversity in the details of thermodynamic descriptions of sorption processes. Accordingly, Phase II of the project was initiated towards demonstrating the consistency and applicability of different TSM approaches to support the selection of K_d values for safety assessments

The main aim of the workshop is to provide an overview and illustration of the main Phase II project results, with emphasis on merits and limitations of thermodynamic sorption models (TSMs) and recommendations on their use; sharing of expereince on the best use and practical implementation of "top-down" and "bottom-up" TSM approaches for PA-relevant materials of different complexity; and, achieving a clear picture of the importance of uncertainty in K_d for various performance assessments, of the potential of TSMs for strengthening the respective safety cases. It was also intended to identify present and plausible future needs for TSM-based quantification of radionuclide sorption.

SESSION I: KEY RESULTS FROM PHASE II

J. Davis[1], M. Ochs[2], and T. Payne[3]
[1]US Geological Survey, USA; [2]BMG Engineering Ltd, Switzerland and [3]ANSTO, Australia

In Session I, key concepts of thermodynamic sorption models (TSMs) are introduced to set the stage for the workshop. Subsequently, the most relevant results of Phase II of the NEA Sorption Project are discussed. Session I was aimed primarily at those participants that are less familiar with the NEA Sorption Project or sorption modelling in general.

Specifically, the following topics are covered:

- A general introduction to thermodynamic sorption models (TSMs) is given, emphasising how surface complexation and ion exchange models are coupled with an aqueous thermodynamic model to yield a TSM. It are described how different electrostatic correction models are available and how surface complexation models are valid regardless of which electrostatic model (if any) is chosen, as long as model consistency is maintained.
- Overview of the solid substrates that are most likely to play a relevant role for the safety of repositories in various PA-programmes through sorption of important radionuclides. Discussion of the characteristics of the different substrates with respect to the sorption of radionuclides and the respective modelling possibilities and challenges.
- Presentation and discussion of the key results of the sorption modelling benchmarking exercise carried out in Phase II of the NEA Sorption Project. This includes issues such as overall model performance and comparison of the suitability of various models for different modelling tasks.
- Discussion of critical issues for the consistent application of TSMs. This topic includes the use of TSM parameters from the literature, transfer of parameters from one model to another, and the relation between a TSM and the underlying aqueous thermodynamic data.

Recommendation for TSM approaches. Here, the main recommendations of Phase II of the NEA Sorption Project are presented. Further, important sources of uncertainty in K_d values selected for PA-purposes are pointed out, and the possibilities of using TSMs for minimising such uncertainties are discussed.

SESSION II: DEVELOPING THERMODYNAMIC RADIONUCLIDE SORPTION MODELS: EXPERIMENTAL AND MODELING RESULTS

D.R. Turner, R.T. Pabalan, and F.P. Bertetti
CNWRA, USA

Historically, performance assessment calculations have represented radionuclide sorption through using sorption coefficient (K_d) values that are assumed to be properties of the geologic medium. The K_d approach is favored for its simplicity, but it does not explicitly consider changes in system chemistry or variations in the mineral/water interface that may affect radionuclide sorption. Thermodynamically-based approaches such as surface complexation models provide a way to constrain the chemical effects on sorption, but they can not be directly implemented in current performance assessment models. We are investigating ways to abstract the results from these more detailed process models for performance assessment calculations.

We have worked with radionuclide sorption data for a variety of end-member minerals such as alumina, quartz, clinoptilolite, and montmorillonite to identify key geochemical parameters that control radionuclide sorption. In particular, pH, P_{CO2}, and mineral surface area are observed to exert the most influence on actinide sorption. We have developed and evaluated simplified, robust modeling approaches to capture these major geochemical effects on sorption for use in performance assessment calculations. Additional laboratory and modeling efforts are being developed to focus on radionuclide sorption behavior for composite materials.

SESSION II: APPLYING THERMODYNAMIC RADIONUCLIDE SORPTION MODELS TO PERFORMANCE ASSESSMENT

D.R. Turner, F.P. Bertetti, J. McMurry, and R.T. Pabalan
CNWRA, USA

Performance assessment studies are used to evaluate the overall ability of a given disposal concept to provide the long-term isolation of nuclear waste. The analysis may include both qualitative evaluations and quantitative simulations, but performance assessment studies are generally designed to link numerical computer models that represent the different features of the repository design. In performance assessment analyses, uncertainty and variability in sorption coefficients (K_d) are represented by parameter distributions that are sampled during individual numerical simulations or realizations. The model outputs (e.g. estimated dose to a receptor), and intermediate results (e.g. radionuclide release to the saturated zone) that result from multiple realizations (typically hundreds) are considered to reflect the likely range in outcomes due to parameter uncertainty and variability.

We have examined different approaches to include aspects of mechanistic sorption models into performance assessment calculations. Simplified surface complexation models are calibrated against laboratory experiments and used to calculate actinide transport parameters. In one approach, parameter distributions are calculated based on site-specific water chemistry. Model results are used to provide limits on K_d probability distribution functions as direct input into the performance assessment calculation. Another approach uses the detailed models to calculate actinide sorption behavior for a wide range in geochemical conditions. Response surfaces for actinide sorption are developed as a function of pH and P_{CO2} and normalized to surface area. Site specific water chemistry is then used to establish parameter distributions for these key groundwater parameters.

SESSION II: APPLICATION OF THERMODYNAMIC MODELLING TOOLS: EXPERIENCE FROM PHASE II

M. Askarieh[1] and T. Heath[2]
[1]Nirex and [2]Serco Assurance, UK

The modelling work performed under the Phase II of the Sorption Project used a wide range of approaches and modelling tools. The Thermodynamic Sorption Models (TSMs) tested in this projects were able to reproduce the trends and in most cases the magnitudes of the experimental data over a wide range of chemical conditions and complexity of mineral substrates. Absolute errors of model predictions compared to experimental data were in the range 0.5 to 1 log K_d units (or less) some significant variation was found dependent on the modelling approach, tool used and (possibly) effort applied.

Despite this success in the modelling studies, one useful outcome of the Phase II modelling exercises and discussions at the earlier San Lorenzo de El Escorial workshop was the identification of some limitations of the tools applied and suggestions for improvements. The various suggestions that were made for improvements and other issues raised concerning the modelling tools included:

- selection of fitting criteria
- types of fitting process
- weighting of fits by experimental errors
- application of appropriate activity treatments

These issues and the implications of limitations in the modelling tools applied are discussed with respect to model development. In addition, the question of finding the best model fit when fitting multiple data sets is addressed. The application of a Monte Carlo method for fitting experimental data is presented.

SESSION II: THERMODYNAMIC SORPTION MODEL (TSM) APPROACHES FOR COMPLEX MATERIALS

M. Ochs
BMG Engineering Ltd, Switzerland

As documented in the final report on Phase II of the NEA Sorption Project, available TSM approaches cover a wide range in terms of model complexity. The chemically most defensible approaches are invariably of a more mechanistic nature and aim at a detailed description of the structure of sorbed species and the solid/solution interface by the model. The surface chemical information required to parameterise such models is available for some simple minerals, but is difficult, and sometimes impossible, to obtain in case of complex substrates. The other end of the spectrum is formed by top-down models parameterised directly with macroscopic sorption data for a complex substrate. These models typically use generic surface sites and neglect electrostatic correction terms, emphasising a good fit of the model to the sorption data and direct applicability to a complex substrate. Regarding the best use of different TSM approaches for PA, a central issue is, therefore, to find the best compromise between chemical correctness and mathematical simplicity as required by the particular modelling task at hand.

SESSION II: SURFACE COMPLEXATION DATABASES: TOWARDS QUANTITATIVE EVALUATION OF EXPERIMENTAL DATA QUALITY – ACID-BASE TITRATIONS

J. Lützenkirchen and T. Fanghänel
FZK-INE, Germany

When developing surface complexation databases, it is necessary to have suitable quality criteria for the process of selecting molecular scale and the macroscopic experimental data that will be considered for the determination of the surface complexation parameters. Macroscopic data may encompass titration data, electrokinetic data, or classical batch (ad)sorption data. Nominally identical mineral surfaces may in many cases not be as easily comparable as would be the case for solutes. The method of preparation, subsequent treatment (washing, drying etc.) and ageing may have an influence on the resulting interfacial properties. In particular, surface contaminations may influence metal ion or ligand adsorption data.

We suggest an approach to verify whether a surface may have been contaminated. The approach consists in spline-fitting surface charge density versus pH curves (at various values of ionic strength) and calculating the first derivative of these curves. Two aspects may now be used to asses the state of the surface:

- the extremum of the derivative should coincide with the published or postulated point of zero of the sample and be independent of ionic strength;
- the shape of the derivative should not include various local extrema.

If the two criteria are met, it is probable that the surface was not significantly contaminated and would thus pass this part of data assessment.

The approach is illustrated based on model calculations. The success with model-generated data is a prerequisite before the application to experimental data.

SESSION II: PRACTICAL USEFULNESS AND SCIENTIFIC DEFENSIBILITY

V. Brendler[1] and T. Payne[2]
[1]Institute of Radiochemistry, Germany and [2]ANSTO, Australia

Sorption involves complex phenomena that can be simulated in a variety of ways using thermodynamic sorption models (TSMs). Assessing the "value" of a particular model is a complex task, and depends, to a large extent, on the proposed applications for the model and the scientific background of the individual. For example, a more rigorous mechanistic model may be more acceptable to a surface chemist but of less value to a PA modeller requiring defensible K_d values. Thus the issues of scientific defensibility and practical usefulness may in some cases lead to conflicting assessments of model value.

In this session, the issues of model usefulness, correctness and credibility are discussed. Usefulness is considered to centre on the data requirements, predictive capability and limitations of the model. Correctness refers to whether the model is scientifically reasonable and satisfactorily incorporates existing scientific knowledge regarding adsorption mechanisms and interfacial phenomena (for example, structural spectroscopic information, thermodynamic constraints, double layer electrostatics). Credibility is perhaps the most important issue in PA - can we trust the predictions of the model? It will be shown that the three characteristics of usefulness, correctness and credibility are not necessarily exhibited together. As demonstrated by the examples of uranium sorption onto goethite and onto KGa kaolinite, mechanistically correct sorption models are not necessarily useful or likely to lead to credible predictions.

After briefly outlining the specifics of the most often applied TSM types, the session will consider their respective data requirements. Many of the data requirements of a TSM can be facilitated by the existence of databases such as the NEA TDB project (inorganic aqueous complexes and solids) or the SCM database RES³T. In addition the appropriate codes must be on hand. Ultimately, the practical usefulness of a TSM can be considered to be partially a trade-off between complexity (high data requirements) and simplicity. Even so, it is not necessarily the case that a model with a large number of parameters is more accurate. The relationship between data requirements of a model and its credibility is quite complex. Finally, the gaps in the existing knowledge and priorities for further research are discussed.

SESSION III: BENTONITE EBS

E. Giffaut
Andra, France

Radionuclide migration in colloidal form through intact clayey barriers is considered to be negligible. This being the case, the contribution of solid-solution partitioning reactions to the migration behaviour becomes the most pertinent criterion for assessing radionuclides relevance for PA. While a K_d database is generally quite sufficient for assessing the upper limits for radionuclide transport rates through the far field of clayey host formations, this approach is not generally applicable to bentonite buffers due to the strong chemical couplings occurring in the near field. This is why TSMs have been developed to predict the effect of environmental variables on the retention properties of the clayey buffer materials. Data requirements concerning solution chemistry is supported by the Andra TDB, *ThermoChimie*, which takes the NEA/TDB data sets as a master reference.

TSMs include both surface complexation and ion exchange reactions, the corresponding equilibrium constants being deduced from sorption isotherms as a function of typical variables such as pH, pCO_2, ionic strength, etc. Such a methodological approach is possible for dispersed bentonite/water systems. These models have subsequently been used to assess K_d sensitivity with regard to changes in system chemical composition, focusing primarily on water composition and montmorillonite content. The effects of temperature elevation have also been studied using the same thermodynamic formalism. K_d selection for PA has then been performed with respect to these model results, taking into account environmental evolution as a source of uncertainty.

More accurate sorption modelling could be developed from TSMs for PA applications, but several limitations must be highlighted:

- An effect of bentonite density on radionuclide sorption has been observed, but still to be interpreted in a manner consistent with TSMs development.
- Macroscopic thermodynamic assumptions have to be verified for application to reactions taking place in micropore solutions, where electrical double layer overlap is prevalent.
- Reversibility of radionuclide sorption remains a questionable issue due to controversial observations.
- While competitive effects are easily assessed using TSMs, cooperative ones are still poorly understood because of a lack of extensive and systematic studies.

Nevertheless, use of TSMs remains the only comprehensive way to improve the coherence and credibility of sorption representation in PA exercises. The recent consistency in the approach of the scientific community is promising, introducing relevant spectroscopic characterisations as a model constraint, and using models with a good chemical sense.

SESSION III: MIGRATION DATA FOR BENTONITE

P. Sellin and F. Vahlund
SKB, Sweden

Background

SKB is currently pursuing site investigations for a deep repository in the municipalities of Östhammar and Oskarshamn. The aim is to build a deep repository at one of these candidate sites, provided that the bedrock and other relevant conditions are found suitable. Two safety reports will be produced within the next five years; one as a supporting document to the application to build an encapsulation plant, SR-Can, and another one for the application to build the repository, SR-Site.

Assessing input data – need for traceable expert decisions

All input data used in quantitative aspects of the safety assessment have uncertainties. The quality of the results of any calculation in the assessment will, among other factors, depend on the quality of the input data and on the rigor with which input data uncertainties have been handled. A methodological approach for the determination of input data with uncertainties and the subsequent handling of data uncertainty is therefore required.

For the SR-Can assessment a methodology has been developed to handle input data and the associated uncertainties. Each set of data is processed according to a standardized outline covering (with data for radionuclide migration in buffer as an example):

- **modelling in SR-Can**, radionuclide migration through the compacted bentonite buffer is predominantly a diffusional transport that may be modelled using Fick's law. In the buffer, radionuclides are (to different degrees) also assumed to sorb to the buffer material.
- **sensitivity to assessment results,** the release of nuclides from the near-field depends on half-life and canister containment time. However, for some nuclides, (such as I-129 and other long lived anions) the near field release is proportional to D_e. The impact of K_d is inversely proportional for some nuclides.
- **source of information**, a dedicated buffer migration data report (Ochs and Talerico, 2004) has been prepared. Details about sources of information and how they were used are found there.
- **conditions for which data are supplied,** the buffer is considered to be MX-80 at the reference dry density of 1590 kg/m^3 and a porosity of 0.41. Some variations with respect to dominant cation and amount of soluble impurities were considered. A reference porewater and two variations were also considered.
- **conceptual uncertainties**, conceptual uncertainties exist regarding the interpretation of, and self-consistency among, batch K_d values and diffusivities of sorbing radionuclides on the one hand, and of diffusivities and diffusion available porosities of anions on the other. There

are some open questions regarding the fundamental, underlying chemistry of radionuclides in aqueous solutions. There are significant scientific shortcomings regarding the derivation of the pore water composition in compacted bentonite and its evolution over time under repository conditions.

- **data uncertainty,** spatial and temporal variation**,** spatial variation and its related uncertainty is not considered relevant for the bentonite buffer since the bentonite can be considered homogeneous. Temporal variation becomes important for the evolution of the buffer/pore water. Experimental errors and other sources of data uncertainty are discussed at length.
- **correlations,** pH and buffer density will affect the transport properties. Based on their chemical characteristics, the radionuclides considered can be organised into groups of elements and oxidation states whose migration behaviour will generally show a similar response to variations in pore water composition caused by variations in groundwater composition, bentonite evolution, etc

The data selection procedure applied by (Ochs and Talerico, 2004) rely strongly on sorption data obtained in batch experiments. No element-specific D_e values were derived for reactive elements. Instead, the selected D_e value for HTO was relied upon. D_e values for anions and Cs were selected to take into account the electrostatic potential in bentonite pores.

References

Ochs M, Talerico C, **2004.** SR-Can. Data and uncertainty assessment. Migration parameters for the bentonite buffer in the KBS-3 concept, SKB TR-04-18, Svensk Kärnbränslehantering AB

SESSION III: IMPLEMENTATION OF TSMs IN PA: PRESENT STATUS, FUTURE PLANS, CHALLENGES & NEEDS – THE BOOM CLAY CASE IN BELGIUM

A. Dierckx[1] and L. Wang[2]
[1]ONDRAF/NIRAS and [2]SCK•CEN, Belgium

In Belgium, the Boom Clay is studied as the reference formation for methodological research in the context of high level waste and spent fuel disposal. Within the disposal system under study, Boom Clay fulfills the safety function "delaying and spreading the releases", aiming to slow down the migration of radionuclides towards the biosphere as much as possible to allow maximum radioactive decay within the disposal system. This is realized by the fact that transport in the Boom Clay is mainly diffusive, and by the strong retention properties of the Boom Clay.

Actually, the Belgian program relies exclusively on migration experiments on intact clay cores to obtain sorption parameters for PA. The interpretation of the migration experiments has so far been restricted in fitting the solute transport parameters without taking chemistry into account. Difficulties are thus encountered when studying radionuclides with complex chemistry and geochemistry. Also, because of the inflexibility of the migration experiment, it is difficult to study the sorption behaviour under varying chemical conditions.

Recently, ONDRAF/NIRAS and SCK•CEN started a sorption program based on a TSM approach. Utilising the advantage that a TSM accounts for system geochemistry, the motivation is to be able to scope the range of variation in K_d under expected geochemically perturbed conditions. A direct use of TSM-derived parameters to PA is not feasible at this stage because of the problems of upscaling, i.e. applicability of batch K_ds to a compact clay system. Further, it is believed that through a TSM approach we will increase the confidence in the performance of the clay barrier resulting in a strong assessment basis for PA. A strong assessment basis is an absolute requirement for a sound Safety and Feasibility Case.

The main obstacle for implementing TSM approaches in our PA program at this point is the lack of high quality data. The acquisition of these data is not certain because of the complex nature of the Boom Clay, especially because of a rather high amount (between 1 and 5%) of organic matter. This data acquisition is given first priority, together with a large characterization program that includes a study on repository induced perturbations.

Another main obstacle is the transfer of K_d-values (TSM-derived or not) from batch systems to confined systems. This item will receive attention in the frame of the current FUNMIG-program (an integrated project in the 6th EC Framework).

SESSION III: APPROACH FOR THE DEVELOPMENT OF SORPTION DATABASES USED FOR SAFETY ASSESSMENT FOR A REPOSITORY IN OPALINUS CLAY

B. Schwyn[1], M.H. Bradbury[2] and B. Baeyens[2]
[1]Nagra and [2]PSI, Switzerland

In a diffusion dominated system such as Opalinus Clay the spreading of radionuclides is mainly determined by the element specific apparent diffusion coefficient D_a. D_a can either be directly measured or it can be derived using distribution coefficients (K_d values) from batch sorption experiments.

In the recent performance assessment "Project Opalinus Clay" Nagra/PSI used the latter approach for Opalinus Clay (and also for bentonite) for the following reasons:

- A representative set of batch sorption measurements was available to derive a comprehensive K_d data set. Methods for the adjustment to in-situ conditions, including thermodynamic sorption models (TSMs), could be applied.
- In contrast, only a few results from diffusion measurements in compacted Opalinus Clay were available. Moreover, to measure the diffusion of strongly sorbing elements is difficult.

TSMs used to derive K_d values are of the component additivity (CA) type; they are based on sorption measurements on the single mineral illite. It could be shown that these models are applicable to Opalinus Clay, i.e. illite can be used as a representative mineral for radionuclide sorption in the rock.

For the majority of radionuclides no TSMs were available at the time of sorption database compilation for the Project Opalinus Clay. Therefore, a transparent and traceable method was developed to adjust K_d values to in-situ conditions. Conversion factors were used to adapt for deviations in mineralogy, pH and speciation.

It is foreseen to further develop TSMs to derive K_d values. Not only are these models convenient to adapt sorption values to in-situ conditions but, at least the component additivity type can be used to connect sorption values to structural information derived from spectroscopy and molecular modelling. The resulting scientific background strengthens confidence in the performance of the barrier system.

The retention efficiency of a rock not only depends on the sorption property of the radionuclides but also on their half life and the transport properties. Assuming steady state conditions and base case diffusion properties, the efficiency of Opalinus Clay was therefore assessed as a function of radionuclide half life and K_d value.

Whether TSMs are applicable to compacted systems (accessible surfaces, high amount of bound porewater/overlapping double layers) is currently the most important uncertainty; for diffusion dominated systems future work should therefore focus on this issue.

SESSION III: THE ROLE OF SORPTION MODELLING IN PARAMETERISING PROBABILISTIC PERFORMANCE ASSESSMENTS OF CRYSTALLINE ROCKS

L. Knight and M. Askarieh
Nirex, UK

Nirex has developed a phased geological repository concept for the safe long-term management of intermediate-level and certain low-level (ILW/LLW) radioactive wastes. The regulator in the UK has set a risk target, among other criteria, for assessing the safety of such a repository. Since risk is itself a combination of the probability of an event and the consequences should the event occur it is necessary to consider key parameters such as K_d in a probabilistic way.

In the context of sorption modelling a probabilistic approach may be used to represent uncertainties in expected K_d values. Uncertainties arise from many sources including:

1. experimental artefacts,
2. inability to measure K_ds under all possible relevant conditions,
3. incomplete understanding of future conditions.

Thermodynamic models are routinely used to aid the extrapolation of K_d values to conditions outside of the range of experimental results and so are of value in understanding the uncertainties of type (2) above. However, such model results are themselves uncertain due to uncertainties in thermodynamic data etc. More importantly the results of thermodynamic modelling can only be interpreted probabilistically if the probabilities of occurrence of the conditions being modelled are known or can be estimated. Nirex has used data elicitation techniques to determine probability distributions of K_d values that take account of experimental data, thermodynamic modelling coupled with expert judgement of the probability of occurrence of future conditions.

To summarise, thermodynamic modelling provides a tool to extrapolate K_ds across a range of possible future conditions and are vital to demonstrate to third parties that we understand the fundamental processes involved. They provide important tools to scope uncertainty but in themselves do not provide probabilistic data.

SESSION III: "VIEWPOINT OF REGULATORS"

H. Wanner
HSK, Switzerland

The licensing process in Switzerland includes a complete safety analysis at each licensing step of a radioactive waste repository. The safety analysis must show that the repository complies with the regulatory requirements.

In the current Swiss project of a HLW repository in Opalinus clay, sorption of radionuclides in the bentonite near field and in the geosphere contributes substantially to the retention of radionuclides. The final dose rate is very low and determined exclusively by very poorly or non-sorbing radionuclides (^{129}I, ^{36}Cl, ^{79}Se, $^{14}C_{org}$). In the transport calculations, sorption is usually accounted for by a single K_d value for each radioelement.

Uncertainty is a major concern in the safety analysis. Uncertainties in sorption parameters may be due to variable or evolving conditions, but also to scaling from laboratory to *in situ* conditions. Uncertainties can be reduced by improving the system understanding, i.e. by investigating the sorption mechanisms. Modern spectroscopic methods and theoretical modelling of surface phenomena may be useful supporting techniques. The sorption of certain poorly studied elements may be approached by justified analogies. Consistency checks with representative diffusion experiments are essential for confidence building.

SESSION III: THERMODYNAMIC SORPTION MODELS IN SAFETY ASSESSMENTS: REGULATORY EVALUATIONS

B. Sagar
CNWRA, USA

In the United States, regulations applicable to a potential deep geologic repository for high-level nuclear waste at Yucca Mountain, Nevada, apply a concept of "reasonable expectation" in evaluating a licensee's safety case. As defined in 10 CFR 63.304, reasonable expectation recognizes the difficulties inherent in projecting repository performance to several tens or thousands of years. Therefore, while *absolute proof* is not required, it is required that a safety assessment (i) accounts for uncertainties; (ii) includes important parameters, even if these are hard to quantify to high degree of confidence; and (iii) focuses on a full range of defensible and reasonable, rather than extreme, physical situations and parameters. The application of this concept to practical situations that will be encountered during review of any license application is documented in the Yucca Mountain Review Plan (YMRP), which provides guidance to regulatory evaluators and includes review methods and criteria for acceptance.

As an example, a YMRP acceptance criterion for sorption guides the reviewer to determine whether (i) estimated flow and transport parameters are appropriate and valid, based on techniques that may include laboratory experiments, field measurements, natural analog research, and process-level modeling studies conducted under conditions relevant to the saturated zone at Yucca Mountain; and (ii) models are demonstrated to adequately predict field transport test results. While this can be interpreted as the regulator's expectations, it leaves complete flexibility to the licensee to choose approaches and methods for its safety demonstration. Thermodynamic sorption models can be an important process-level modeling approach to define the site-scale parameters.

To enhance its understanding and as an aid in its evaluation of any safety case, the U.S. Nuclear Regulatory Commission (NRC) and the Center for Nuclear Waste Regulatory Analyses (CNWRA) have conducted experimental and modeling sorption studies of their own, a summary of which are presented in this workshop by David Turner. The primary goal of the NRC and CNWRA effort is to (i) relate the commonly used sorption coefficients in performance assessment more realistically by associating them with chemical conditions of the site and (ii) explicitly include uncertainties.

APPENDIX C

LIST OF PARTICIPANTS

AUSTRALIA

PAYNE, T.E.
ANSTO
Private mail bag 1
Menai NSW 2234
Tel: +61 2 9717 3118
Fax: +61 2 9717 9286
Eml: tep@ansto.gov.au

BELGIUM

DIERCKX, Ann
ONDRAF/NIRAS
Avenue des Arts 14
1210 Bruxelles
Tel: +32 (0)2 212 10 45
Fax: +32 (0)2 218 51 65
Eml: a.dierckx@nirond.be

MAES, Norbert
SCK•CEN
Boeretang, 200
2400 Mol
Tel: +32 (0)14 33 32 35
Fax: +32 (0)14 33 35 53
Eml: nmaes@sckcen.be

WANG, Lian
SCK•CEN
Boeretang 200
2400 Mol
Tel: +32 (0)14 33 32 36
Fax: +32 (0)14 33 35 53
Eml: lwang@sckcen.be

CZECH REPUBLIC

KONOPASKOVA, Sona
Radioactive Waste Repository Authority
Dlazdena 6
110 00 Praha 1
Tel: +420 2 21 42 1518
Fax: +420 2 21 42 1544
Eml: konopaskova@rawra.cz

VOPALKA, Dusan
Czech Technical University in Prague
Faculty of Nuclear Sciences
and Physical Engineering
Dept. of Nuclear Chemistry
Brehova 7
115 19 Praha 1
Tel: +420 2 24 35 8206
Fax: +420 2 22 32 0861
Eml: dusan.vopalka@fjfi.cvut.cz

FINLAND

HAKANEN, Martti
Dept. of Radiochemistry
University of Helsinki
Unioninkatu 35
FIN-00170 Helsinki
Tel: +358 (9) 191 50135
Fax: +358 (9) 191 50121
Eml: martti.hakanen@helsinki.fi

VUORINEN, Ulla
VTT Processes
PO BOX 1608
FIN-02044 VTT Espoo
Tel: +358 (9) 456 6389
Fax: +358 (9) 456 6390
Eml: ulla.vuorinen@vtt.fi

FRANCE

ALTMANN, Scott
ANDRA DS/TR
Parc de la Croix Blanche
1-7, rue Jean Monnet
92298 Chatenay-Malabry Cedex
Tel: +33 (0)1 46 11 84 81
Fax: +33 (0)1 46 11 84 40
Eml: scott.altmann@andra.fr

BEAUCAIRE, Catherine
CEA - Saclay
DEN/DPC/SECR
L3MR - Bât. 450
91191 Gif-sur-Yvette Cedex
Tel: +33 (0)1 69 08 56 09
Fax: +33 (0)1 69 08 32 42
Eml: catherine.beaucaire@cea.fr

GAUCHER, Eric
BRGM Research Division
EPI/DES Dechets et Stockage
3 Avenue Claude Guillemin
BP 6009
45060 Orleans Cedex 2
Tel: +33 (0)2 38 64 35 73
Fax: +33 (0)2 38 64 30 62
Eml: e.gaucher@brgm.fr

GIFFAUT, Eric
ANDRA
Parc de la Croix Blanche
1/7 rue Jean Monnet
92290 Chatenay-Malabry Cedex
Tel: +33 (0)1 46 11 82 02
Fax: +33 (0)1 46 11 84 08
Eml: eric.giffaut@andra.fr

LOMENECH, Claire
Université de Nice-Sophia Antipolis
LRSAE
28 avenue Valrose
06108 Nice Cedex 2
Tel: +33 (0)4 92 07 63 77
Fax: +33 (0)4 92 07 63 64
Eml: Claire.Lomenech@unice.fr

MOULIN, Valerie
CEA
Nuclear Energy Division
DDIN/MR
Bat 121, P307
91191 Gif-sur-Yvette Cedex
Tel: +33 (0)1 69 08 32 52
Fax: +33 (0)1 69 08 58 91
Eml: valerie.moulin@cea.fr

MUSIKAS, Claude
5 av. Moissan
91440 Bures-sur-Yvette
Tel: +33 (0)1 69 86 19 80
Fax: +33 (0)1 69 86 19 80
Eml: claude.musikas@wanadoo.fr

GERMANY

BRENDLER, Vinzenz
Research Center Rossendorf e.V.
Institute of Radiochemistry
P.O. Box 510119
01314 Dresden
Tel: +49 3 51 2 60 24 30
Fax: +49 3 51 2 60 35 53
Eml: v.brendler@fz-rossendorf.de

FISCHER-APPELT, Klaus
Gesellschaft fur Anlagen-
und Reaktorsicherheit (GRS) mbH
Schwertnergasse 1
50667 Köln
Tel: +49 221 2068 768
Fax: +49 221 2068 939
Eml: klaus.fischer-appelt@grs.de

HERBERT, Horst-Juergen
Gesellschaft fuer Anlagen-
und Reaktorsicherheit (GRS) mbH
Bereich Endlagersicherheitsforschung
Theodor Heuss Strasse 4
38122 Braunschweig
Tel: +49 531 8012 250
Fax: +49 531 8012 200
Eml: Horst-Juergen.Herbert@grs.de

LARUE, Peter Jürgen
Gesellschaft für Anlagen-
und Reaktorsicheheit (GRS) mbH
Schwertnergasse 1
D-50667 Köln
Tel: +49 (0)221 2068 791
Fax: +49 (0)221 2068 939
Eml: peter-juergen.larue@grs.de

LUTZENKIRCHEN, Johannes
INE-FZK
PO Box 3640
76021 Karlsruhe
Tel: +49 7247 82 40 23
Fax:
Eml: johannes@ine.fzk.de

NOSECK, Ulrich
Gesellschaft für Anlagen
und Reaktorsicheheit (GRS) mbH
Theodor-Heuss-Str. 4
38122 Braunschweig
Tel: +49 (0)531 8012 247
Fax: +49 (0)531 8012 200
Eml: Ulrich.Noseck@grs.de

WOLLRATH, Juergen
Bundesamt für Strahlenschutz (BfS)
Federal Office for Radiation Protection
Postfach 10 01 49
38201 Salzgitter
Tel: +49 (0)1888 333 1964
Fax: +49 (0)1888 333 1605
Eml: JWollrath@BfS.de

JAPAN

ISHIGURO, Katsuhiko
Nuclear Waste Management Organization (NUMO)
Mita NN bldg. 1-23 Shiba
4-Chome Minato-ku
Tokyo 108-0014
Tel: +81 3 4513 1503
Fax: +81 3 4513 1599
Eml: kishiguro@numo.or.jp

SEIDA, Yoshimi
Institute of Research and Innovation
1201 Takada
277-0861 Kashiwa
Tel: +81 4 7144 8845
Fax: +81 4 7144 7602
Eml: seida@iri.or.jp

SUZUKI, Kazunori
Institute of Research and Innovation
1201 Takada,
277-0861 Kashiwa
Tel: +81 4 7144 8845
Fax: +81 4 7144 7602
Eml: k-suzuki@iri.or.jp

UMEKI, Hiroyuki
Geological Isolation Research
& Development Directorate
Japan Atomic Energy Agency
Shinsei-Bank Bldg, 2-1-8 Uchisaiwaicho
Chiyoda-ku, Tokyo 100-8577
Tel: +81 3 3592 2390
Fax: +81 3 5157 1921
Eml: umeki.hiroyuki@jaea.go.jp

SPAIN

ALONSO, Jesus
ENRESA
Calle Emilio Vargas, 7
28043 Madrid
Tel: +34 91 566 8108
Fax: +34 91 566 8165
Eml: jald@enresa.es

BRUNO, Jordi
ENVIROS Spain SL
Paseo de Rubi, 29-31
08197 Valldoreix
Tel: +34 93 583 0500
Fax: +34 93 589 0091
Eml: jbruno@enviros.biz

HERNAN, Pedro
ENRESA
Emilio Vargas 7
28043 Madrid
Tel: +34 91 566 8192
Fax: +34 91 566 8165
Eml: pher@enresa.es

SAMPER, Javier
University of La Coruna
Escuela de Caminos
Campus de Elviña s/n
15192 La Coruna
Tel: +34 98 116 7000
Fax: +34 98 116 7170
Eml: jsamper@iccp.udc.es

SWEDEN

MALMSTROM, Maria
Royal Institute of Technology (KTH)
Industrial Ecology
Teknikngen 34
100 44 Stockholm
Tel: +46 8 790 8745
Fax: +46 8 790 5034
Eml: malmstro@ket.kth.se

SELLIN, Patrik
Swedish Nuclear Fuel & Waste Management Co. (SKB)
Box 5864
102 40 Stockholm
Tel: +46 8 459 8522
Fax: +46 8 662 4974
Eml: patrik.sellin@skb.se

STROMBERG, Bo
Office of Nuclear Waste
Swedish Nuclear Power Inspectorate (SKI)
10658 Stockholm
Tel: +46 8 698 8485
Fax: +46 8 661 9086
Eml: bo.stromberg@ski.se

SWITZERLAND

OCHS, Michael
BMG Engineering Ltd.
Ifangstrasse 11
8952 Schlieren-Zürich
Tel: +41 1 732 92 83
Fax: +41 1 730 66 22
Eml: michael.ochs@bmgeng.ch

SCHWYN, Bernhard
NAGRA
Hardstrasse 73
5430 Wettingen
Tel: +41 56 437 1231
Fax: +41 56 437 1317
Eml: bernhard.schwyn@nagra.ch

WANNER, Hans
Waste Management Section
Swiss Federal Nuclear Safety
Inspectorate (HSK)
5232 Villigen-HSK
Tel: +41 56 310 3868
Fax: +41 56 310 3907
Eml: hans.wanner@hsk.ch

UNITED KINGDOM

ASKARIEH, Mehdi (Chairperson)
United Kingdom Nirex Ltd
Curie Avenue
Harwell, Didcot
Oxfordshire OX11 0RH
Tel: +44 1235 825 403
Fax: +44 1235 820 560
Eml: mehdi.askarieh@nirex.co.uk

HEATH, Tim
Serco Assurance
Building 150
Harwell International Business Centre
Didcot
Oxfordshire
Tel: +44 1635 280 411
Fax: +44 1635 280 305
Eml: tim.heath@sercoassurance.com

KNIGHT, John Leslie
United Kingdom Nirex Ltd.
Curie Avenue,
Harwell, Didicot
Oxfordshire OX11 0RH
Tel: +44 1235 825 447
Fax: +44 1235 820 560
Eml: les.knight@nirex.co.uk

RANDALL, Matthew
Nexia Solutions
Hinton House
RISLEY, Warrington, WA3 6AS
Tel: +44 1925 832 922
Fax: +44 1925 833 267
Eml: matthew.randall@nexiasolutions.com

UNITED STATES OF AMERICA

DAVIS, James A.
U.S. Geological Survey
M.S. 465
345 Middlefield Rd.
Menlo Park, CA 94025
Tel: +1 650 329 4484
Fax: +1 650 329 4327
Eml: jadavis@usgs.gov

OTT, William
US Nuclear Regulatory Commission (NRC)
MS T9C34
11545 Rockville Pike
Rockville, MD 20852
Tel: +1 301 415 6210
Fax: +1 301 415 5385
Eml: WRO1@NRC.GOV

SAGAR, Budhi
CNWRA - Southwest Research
Institute, CNWRA
Post Office Drawer 28510
6220 Culebra Road
San Antonio, TX 78238
Tel: +1 210 522 5252
Fax: +1 210 522 5155
Eml: bsagar@swri.org

TURNER, David R.
Center for Nuclear Waste
Regulatory Analyses
Southwest Research Institute
6220 Culebra Road
San Antonio, TX 78238-5166
Tel: +1 210 522 2139
Fax: +1 210 522 6081
Eml: dturner@swri.org

VAN LUIK, Abraham E.
U.S. Department of Energy
Office of Repository Development
1551 Hillshire Drive
Las Vegas, NV 89134
Tel: +1 702 794 1424
Fax: +1 702 794 1435
Eml: abe_vanluik@notes.ymp.gov

International Organisations

VOINIS, Sylvie
OECD/NEA
Radiation Protection and Radioactive
Waste management Division
12, Boulevard des Îles
F-92130 Issy-les-Moulineaux
Tel: +33 (0)145241049
Fax: +33 (0)1 45241145
Eml: sylvie.voinis@oecd.org

MOMPEAN, Federico
OECD/NEA
Data Bank
12 Boulevard des Îles
F-92130 Issy-les-Moulineaux
Tel: +33 (0)1 45 24 10 83
Fax: +33 (0)1 45 24 11 28
Eml: federico.mompean@oecd.org

ILLEMASSENE, Myriam
OECD/NEA
Data Bank
12 Boulevard des Îles
F-92130 Issy-les-Moulineaux
Tel: +33 (0)1 45 24 10 38
Fax: +33 (0)1 45 24 10 28
Eml: myriam.illemassene@oecd.org

PERRONE, Jane
OECD/NEA
Data Bank
12 Boulevard des Îles
F-92130 Issy-les-Moulineaux
Tel: +33 (0)1 45 24 11 18
Fax: +33 (0)1 45 24 10 28
Eml : jane.perrone@oecd.org