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NUCLEAR ENERGY AGENCY RADIOACTIVE WASTE MANAGEMENT COMMITTEE

Sorption Project

Management Board of the OECD-NEA Sorption Project Phase III **Summary Record**

NEA Headquarters (Room 7B) Issy-les-Moulineaux, France

5-6 November 2009

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Management Board of the

OECD-NEA Sorption Project

Phase III

Venue: NEA HEADQUARTERS (Room 7B), ISSY-LES-MOULINEAUX

5-6 November 2009

INTRODUCTION

1. Opening of the Meeting and Adoption of the Agenda

Scott Altmann, Sorption III Chair

Scott Altmann opened the meeting and welcomed the members. There followed a short *tour de table*.

S. Altmann noted that the project was advancing largely on schedule. Key upcoming dates were the joint TDB/sorption workshop, now scheduled for 17-19 May 2010. As this fell outside the original project schedule a project extension was therefore necessary. He envisaged that the Management Board should nonetheless have the opportunity to review and discuss the draft final report before the Workshop, in order that the presentations and discussions there reflected the considered position of the Board. Following the Workshop, the report should be completed by the Technical Direction Team (TDT), taking account as necessary of outcomes from the discussions there, and prepared for publication.

Decisions:

The proposed agenda was adopted without changes.

Noting that the advancement of the project was broadly on schedule, but that the report cannot be fully completed until after the workshop planned for May 2010, it was decided to extend the duration of the project to 31 December 2010 to allow ample time to complete the publication process. It was noted that this change would have no budget implications given that the duration of the TDT contracts was already until this date. [ACTION: SECRETARIAT]

2. Approval of the Summary Record of the 2nd MB Meeting (4 December 2008)

Decisions:

The Summary Record was adopted without changes.

RECENT DEVELOPMENTS WITHIN THE NEA

3.a **RWMC and Nuclear Energy Outlook**

Hans Riotte

H. Riotte provided an update on recent developments concerning the NEA's Radioactive Waste Management Committee (RWMC), in particular:

- The 42nd annual meeting (RWMC-42) had included discussion items on human resource requirements, maintaining a long-term memory of geological repositories, the meaning of 'repository closure' and the RWMC's ongoing project on 'reversibility and retrievability'
- The Regulators' Forum (RF) was currently giving attention to the application of the optimisation principle to geological disposal
- The Integration Group for the Safety Case (IGSC) had recently began a project on Methodologies for Safety Assessment (MESA)
- The Forum for Stakeholder Confidence (FSC) was considering the linkage between R&D programmes and stake holder confidence
- An International Conference on reversibility and retrievability was planned for December 2010, at Rheims, France.

He noted also that NEA was in the process of developing a new strategic plan, to cover the period 2011 – 2016, and that outreach efforts to Russia. China, India and Poland were ongoing.

Decisions:

The Board noted the report on the latest developments in relevant NEA activities.

3.c Thermochemical database (TDB) project

Mireille Defranceschi

M. Defranceschi said phase 4 of the TDB project, which had begun in February 2008, would consider auxiliary data, in particular concerning inorganic species and compounds of molybdenum and iron. Two further volumes in the main TDB report series (for tin and iron) were expected to be published in 2010. She said the review process aimed to ensure the overall consistency of the published data, i.e. data that are not consistent are not published in the reports. It was noted in discussion that the comprehensiveness of the review process is matched to the extent to which the properties of the species in question are considered to be well defined.

Decisions:

The Board noted the report on the latest developments in the TDB project.

GENERAL REVIEW OF PROGRESS

4.a Progress Report by the Head of the TDT

Michael Ochs

M. Ochs provided the following overview of progress with each of the chapters:

- Ch. 1 some editing for consistency with later chapters
- Ch. 2 draft completed and reviewed (first time a comprehensive approach to sensitivity analysis is presented)
- Ch. 3 incomplete (needs to be condensed from its current size of 80/90 pages)
- Ch. 4 largely completed; references to be added
- Ch. 5 planned for Feb 2010
- Ch. 6 planned for Feb 2010

He noted a tension between the desires of the external experts to provide their latest thinking, as scientific experts, on the issues in question, and the need to produce a report suitable for a wider, non-expert, audience. The general view of the meeting was that the primary audience for the report was the sorption modelling community and other users of K_D distribution coefficients in developing safety cases, rather than scientific experts in this field. The report should focus on process issues rather than on detailed scientific arguments, with the latter being addressed through referencing. [See also the later discussion under Item 8.]

Decisions:

The Board approved the following amendments to the project plan:

- Draft of chapter 3: December 2009, taking account of decisions at the TDT meeting scheduled for 23-25 November
- First full draft of final report, chapters. 1-6 ("80% Draft"): mid-March 2010
- Revised full draft of final report ("95% draft"): mid-May 2010 (on the timeframe of the joint workshop)

The Board will meet in April to conduct a detailed review of the 80% draft (see below). It is currently intended that the review of the 95% draft version can be undertaken by e-mail.

4.b **Joint TDB/Sorption Workshop**

Cherry Tweed

C. Tweed provided an overview of the programme sessions, which included half-day sessions

on: thermochemical databases; using thermodynamic models; the sorption project; from thermodynamics to the safety case, with a 1½ hour session on 'Where next for the TDB and sorption projects?'. She anticipated that a second flyer would be prepared during the coming weeks.

Decisions:

The Board noted that a second announcement for the Workshop with details of the programme and speakers will be issued later in November. On this timescale the TDT was requested to review the current outline programme for the ½-day session on sorption and to provide a considered view [ACTION: TDT].

THE AGREEMENT/ADMINISTRATION

5.a Report by the Secretariat on Project Administration

Patrick O'Sullivan

P. O'Sullivan recalled that the total budget for the project was €427 280. In accordance with the project plan, €288 360 of this would be used to cover the costs of the technical direction team, with the remainder, €138 920, being allocated for the costs of the external experts. Most of the budget had already been committed, with approximately €8 500 still being unallocated.

Decisions:

It was agreed that the unallocated funds (approximately €8 500) should be used to draw up an additional contract with BMG Engineering for anticipated additional editorial work on the final report, e.g. to take account a Management Board review (of the 95% draft version) now envisaged to take place after the joint TDB/sorption workshop [ACTION: SECRETARIAT].

5.b. **Financial Report**

Patrick O'Sullivan

P. O'Sullivan said that the total contributions by the end of October 2009 stood at €379 217; an amount of €34 279 remained to be collected from the participants.

Decisions:

The Board approved the financial report of the project. Noting that an amount of €34 280 remained to be collected the Secretariat was asked to remind individual participants of any outstanding payments [ACTION: SECRETARIAT].

DETAILED REVIEW OF DRAFT REPORT

6. Presentation/discussion of Chapter 2

Vinzenz Brendler

V. Brendler presented the results of an analysis of the effects of key TSM or geochemical

parameter uncertainties, based on a number of test cases. He concluded:

- the most sensitive model parameter was log K for surface complex formation;
- pK of surfaces was much less relevant → electrical double layer (EDL) consistency may be sacrificed;
- variability of the geochemical environment ranked of equal importance to log K
- exploiting parameter uncertainty matrices (where available) is very helpful in reducing K_D errors.
- constraining K_D values within one order of magnitude is still challenging

As regards the effect of the propagation of uncertainties in TSM parameters to calculated K_D values:

- more comparison of different systems and modelling approaches is required; and
- it is still premature to estimate application limits for K_D values

The following points were noted in the subsequent discussion:

- the non uniqueness of sorption models remains an issue that leads to confusion regarding the scientific reasonableness of TSM
- as regards the primary importance of log K, the importance of this conclusion on the model set up needs to be clarified
- currently the only way to optimise log K for surface complexation is to use the richest available data set
- it should be emphasised that overall uncertainty is related to two different parameter sets those relating to the intrinsic properties of the surface species and those relating to the geochemical environment (pH etc.). It was noted that the issue of geochemical heterogeneity is well recognised; it is currently less clear how different surface species should be reflected in the model.

There followed a discussion about how the existing text might be restructured to meet the aim of including only the main messages and guidance to users, rather than underlying proofs, in the main text. The general view expressed was that the main aim should be to describe the assessments of TSM sensitivity and uncertainty. The details regarding code and the underlying proofs should either be moved to appendices or should be proposed for publication in specialist journals and covered by citations.

Decisions:

The Board noted that further refinement of the Chapter 2 text (including some reduction of the overall number of pages) was planned. As part of this, the authors were asked to consider the comments provided at this meeting. The next Board review of the text would occur as part of the review of the 80% draft report in March (see above).

7. Presentation/discussion of Chapter 4

Michael Ochs

M. Ochs provided an overview of the current status of Chapter 4, which was currently in draft and comprised three main sections:

- 4.1- Background and Identification of the Problem
- 4.2 State of the Art in deriving K_D for Intact Materials
- 4.3 Extent of applicability of Generalised TSMs to Intact Materials

As regards the state of the art for deriving K_D for intact materials he noted that modelling approaches had been developed for compacted clay systems, involving the application of batch-derived models to the compacted state. There remained difficulties in characterising such systems in terms of sorption-relevant parameters due to the limited accessibility of pore characteristics and the difficulties in defining pore water chemistry. As regards crystalline rock, he said that K_D derivation approaches had been developed but modelling was currently quite limited.

The following points were noted in the subsequent discussion:

- the sorption model needs to be supported by a geochemical model. The issue of pore water chemistry in compacted systems must be addressed before dealing with sorption model, though it is noteworthy that much work on this has already been done. It was important that guidance on this issue should be given.
- It may be helpful to introduce the idea of a "representative volume" for different systems.

Turning to the extent of applicability of generalised TSMs to intact materials (Section 4.3), M. Ochs said that the use of TSMs for predicting radionuclide sorption in intact crystalline rock was not considered feasible at present, due to experimental difficulties in obtaining relevant sorption data and difficulties in describing boundary conditions relevant for radionuclide uptake. For compacted clay systems most evidence suggests that TSMs based on single minerals/additivity are directly applicable, though boundary conditions such as pore water composition need to be carefully constrained.

The following points were noted in the subsequent discussion:

- models cannot have more degrees of freedom than justified by the data available, i.e. cannot be too complex. This issue needs to be addressed also in Ch. 3
- in systems without perfect external constraint for the geochemistry it is necessary to prepare the ground for the sorption modelling, i.e. an experimental programme is generally obligatory as the necessary data will not otherwise be available
- in the case of compacted clay, models are developed for dispersed systems and then applied to the compacted system this issue needs to be addressed in the report
- TSM is always a valid conceptual framework for analysing a compacted clay system the problem is dealing with coupled processes. It is not possible to 'impose'

geochemistry onto the model for a real system; this coupling exists intrinsically in the system and needs to be addressed in the sorption model as there can never be a decoupling between geochemical and sorption models.

• As regards crushed granitic rock, there are two problems to be overcome - accessibility (which can usually be solved) and the change of properties due to crushing.

It was suggested that uncertainty be dealt with as follows in the report: model uncertainty (chapter 2); parameter uncertainty (chapter 3); and system specific (substrate) uncertainty (chapter 4).

Decisions:

The Board noted that further refinement of the Chapter 4 text was planned, which may include a rebalancing of items between chapter 4 and 5. As part of this the authors were asked to consider the comments provided at this meeting. The next Board review of the text would occur as part of the review of the 80% draft report in March (see above).

8. General discussion/Conclusions

Scott Altmann

There followed a general discussion about the intended audience for the report, leading to a general view that the report should not be aimed at experts in the field of sorption but rather those who need to deal with sorption in safety cases (as implementers or regulators) and the interested scientific community. The report should not be highly technical but should provide key references to underlying technical arguments.

It was noted that TSMs are not yet used universally, e.g. some waste management organisations still use empirically-based K_D values, rather than being based on TSM approaches, though there is a growing acceptance that the latter approach is better in situations where K_D varies with time.

It was noted that the report deals primarily with bentonite and clay geologies, and is therefore of less relevance to those dealing with fractured rock geologies and with complex materials such as cement. The latter provides a greater level of complexity, e.g. due to evolution of materials over time, though in this situation sorption may anyway not be the principal phenomenon, but processes based on solid solution chemistry. To deal with this aspect, it was suggested that the report should include some text indicating where the guidance may be helpful, though recognising that cement and other complex substrates (solid humics, volcanic tuffs) are not addressed by this project.

Decisions:

The Board noted that the target audiences for the project report were:

- New countries building their programmes (i.e. need to know the basics; how to get up to speed; formulation of a research programme)
- Any WMO writing a safety case, (e.g. provides help in organising ideas,, checklist of issues to be considered)

- Regulators overview of issues; e.g. provides guidance when it is better to use one approach rather than another
- Interested scientific community

It was agreed that a 2-page summary of key aims of each chapter, to assist in ensuring the overall coherence of the report, should be produced for discussion at the TDT meeting on 23-25 November which S. Altmann will attend. To achieve this timeframe, he will prepare a first draft by Monday 16 November; a response from Board members is required by 19 November, allowing a final version to be prepared on 20 November [ACTION: SCOTT ALTMANN, ALL BOARD MEMBERS]

It was agreed that the contributions of the external experts should be clearly acknowledged in the report [ACTION: TECHNICAL DIRECTION TEAM].

9. **Date of the Next Meeting**

Decisions:

The next meeting will be held on 15-16 April 2010 at the NEA Offices at Issy-les-Moulineaux. The meeting will be devoted to a detailed review of the draft final report from the project.

10. **Review of Decisions**

Scott Altmann, Patrick O'Sullivan

SORPTION III Management Board Members Meeting -- Issy Room B List of attendees

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