MOBILITY MISSION REPORT

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The information included in this mission report consists of personal data of applicants, and in the frame of GDPR we ask you place emphasis on its integrity: the personal data in this mission report cannot be used for purposes other than the evaluation and the management of EURAD Mobility Programme. For the avoidance of doubt, this information – out of its nature – is confidential information as mentioned in Article 10.1 of the EURAD Consortium Agreement Version [17/09/2019] with effective date of 1 June 2019 (although it might not be explicitly marked as such).

MISSION TITLE

Participation in the training course "Geochemical and Reactive Transport Modelling for Geological Disposal"

DESCRIPTION

Concerned organisations

- Research entities (VTT Technical Research Centre of Finland Ltd)

Concerned infrastructures or facilities

- High-performance computing

Concerned phases

- Phase 2: Site characterisation
- Phase 5: Post-closure

Themes and topics

- Theme 3: Engineered barrier system (EBS) properties, function and long-term performance
    - Clay-based backfills, plugs and seals
    - Cementitious-based backfills, plugs and seals
    - Salt backfills
    - EBS system understanding

Keywords

Reactive transport; geochemical modelling; ORCHESTRA

EXECUTIVE SUMMARY

The safe disposal of spent nuclear fuel requires detailed knowledge of the processes and geochemical evolution of the engineered barrier system and the chosen final repository site. When it comes to high level radioactive waste, the time scales related to these processes range from tens of thousands to hundreds of thousands of years, which can only be obtained through numerical models.

With previous experience in nano scale simulations of bentonite clay and cement, the objective of the mobility was to widen the applicant's expertise into chemical transport modelling in crystalline rock and engineered barrier systems related to the KBS-3 disposal concept planned in Finland and Sweden.

This 5-day training course introduced participants into the basics of geochemical and reactive transport modelling, from theory to application, in the form of classroom lectures and hands-on exercises to learn some practical skills. Multitude of real research examples were given in the context of geological disposal of radioactive waste and a number of different available software with their capabilities were introduced.

This training course provided a strong background on which to build: with enough knowledge to continue model building independently and more easily adapt to other related simulation codes. Additionally, the course gave a broad idea on the type of research that is done in other research groups world wide.

1. MISSION BACKGROUND

1.1.R&D background

In Finland and Sweden, the safe disposal of spent nuclear fuel is planned according to the KBS-3 concept: geological disposal of nuclear waste with a multibarrier system to prevent/retard the release of radionuclides into the biosphere. Spent fuel is incased in copper canisters with cast iron insert, and the canisters are placed into boreholes approximately 400 m deep in the bedrock. The boreholes are lined with bentonite clay, which is also used as tunnel backfill. In this concept, the retardation of radionuclides is mainly based on diffusional transport and sorption on solid mineral surfaces. To ensure the long-term safety of the disposal system, numerical modelling is utilized to evaluate solute transport and chemical interactions in different parts of the system.

1.2.Mission objectives

The attendance of a researcher in a five-day (6.-10.2.2023) training course “Geochemical and Reactive Transport Modelling for Geological Disposal” organized by EURAD WP13 at the University of Bern in Switzerland. Having previously worked on nano scale simulations of bentonite and cement, the applicant plans to widen their expertise into larger scale simulations and chemical transport modelling in the bedrock and engineered barrier systems. Participation in the training course provides an opportunity for speedy and effective learning as the course covers a wide variety of topics in this area with introduction to different simulation codes and includes hands-on exercises to learn practical skills.

1.3.Mission request

To cover the funding needed for the participation of research scientist A. Seppälä in the training course Geochemical and Reactive Transport Modelling for Geological Disposal on 6.2.-10.2.2023

1.4.Mission composition

Host organisation

SCK CEN

Host facility

University of Bern, Baltzerstrasse 3, Bern, 3012 Switzerland

Mission dates

5 February 2023 – 10 February 2023

2.MAJOR PRACTICES, TECHNIQUES, METHODS, TOOLS OR SYSTEMS OPERATED OR STUDIED

2.1.Practice, technique, method, tool or system operated or studied during the mission

Geochemical modelling

Description

Classroom lectures into the theory behind geochemical and reactive transport modelling and its usage in current research in the context of radioactive waste disposal.

Usage

During the training we followed lectures from multiple experts in the field who presented the theory (thermodynamics, reactions, kinetics etc.) and its application with examples from recent research. Additionally, there were introductions to nine different modelling codes and their capabilities.

Benefits

Numerical methods enable the prediction of the geochemical evolution of a radioactive waste site in large enough time scales (up to hundreds of thousands of years), which cannot be attained experimentally.

Limitations

Modelling relies on experimentally obtained parameters so the applicability of the parameters depends on conducted experiments.

Applicability

Participation in the course provided me with the understanding of the basics of geochemical and reactive transport modelling and how to implement the related research questions into a numerical code. This provided me with the competence to adapt to other codes (those used in home organization) and continue learning and building models related to engineered barrier systems.

2.2.Practice, technique, method, tool or system operated or studied during the mission

ORCHESTRA geochemical modelling code

Description

Introductory lecture to the capabilities of the tool and hands-on exercises covering different types of modelling cases in the context of radioactive waste disposal.

Usage

During the training course we used ORCHESTRA in hands-on training sessions to simulate Ca-CO2 system, cement hydration and uranium sorption and kinetics in claye systems.

Benefits

ORCHESTRA allows for more flexibility than many other geochemical modelling tools as it is possible to modify the code when needed.

Limitations

The documentation of the tool is quite sparse which makes learning its usage challenging.

Applicability

Although, continuing to apply this particular tool is not very likely in my case, the lessons provided deeper understanding of the modelling processes which will be useful and facilitate the transfer to other geochemical modelling codes.

3.MISSION FINDINGS AND CONCLUSIONS

3.1.Lessons learned and conclusions

This training course offered an intensive introduction into the world of geochemical modelling. Lectures taught us the basic principles of geochemical modelling from thermodynamics to kinetics to reactive transport modelling. Multiple examples were given to demonstrate how these principles are applied to investigate material evolution and the relevant processes in geological disposal concepts for radioactive waste disposal. The more advanced lectures gave information on sensitivity and uncertainty analysis, when upscaling the models, and machine learning applications. The presentation of different modelling codes and their capabilities was very useful as there are numerous software available and written in different coding languages.

During hands-on exercise sessions using ORCHESTRA software, going through simple practical examples that closely followed the course topics, we learned how problems are input into a numerical code and resulting data analysed. In addition, the instructor gave us many functional tips and tricks about the code that are not easy to come by on our own.

The knowledge gained from this course will be applied in the creation of reactive transport models related to the concept of geological disposal of radioactive waste in Finland.

APPENDICES

Mission journal

6.2.2023
9.00-9.30 Welcome and introductions
9.30 -10.30 Lecture: Modelling geochemical systems – Equilibrium, Thermodynamics, Reaction Progress (D. Kulik)
10.30-11.00 Introduction to course – hands-on examples
11.30-12.00 Code: GEM-selektor (D. Kulik)
12.00-12.30 Code: ORCHESTRA (H. Meeussen)
12.30-13.00 Code: PHREEQC (D. Jacques)
14.00-15.00 Lecture: Thermodynamic modelling of cementitious systems (B. Lothenback)
15.00-17.30 Hands-on session: ORCHESTRA

7.2.2023
9.00-10.00 Lecture: Geochemical & Reactive Transport Modelling for Geological Disposal (E. Gaucher)
10.00-12.30 Hands-on session: ORCHESTRA
13.30-14.00 Code: iCP (E. Coene)
14.00-16.30 Hands-on session: ORCHESTRA
16.30-17.30 Lecture: Reactive Transport: Pore to Continuum (C. Steefel)
17.30-18.00 Code: CrunchTope/CrunchClay (C. Steefel)

8.2.2023
9.00-10.00 Lecture: Radionuclide speciation incl. thermodynamic databases (V. Montoya)
10.00-12.30 Hands-on session: ORCHESTRA
13.30-14.30 Lecture: Sorption processes (S. Churakov)
14.30-17.00 Hands-on session: ORCHESTRA
17.00-17.30 Code: Min3P (U. Mayer)

9.2.2023
9.00-10.00 Lecture: Kinetic processes in radwaste disposal (L. de windt)
10.00-10.30 Code: Hytec (L. de Windt)
10.30-13.00 Hands-on session: ORCHESTRA
14.00-14.30 Code: Core2 (J. Samper)
14.30-17.00 Hands-on session: ORCHESTRA

10.2.2023
9.00-9.30 Code: PHREEQC-OpenFoam (C. Soulaine)
9.30-11.30 Hands-on session: ORCHESTRA
11.30-12.30 Lecture: Uncertainty and sensitivity analysis (J. Samper)
14.00-15.00 Lecture: Machine learning for accelerating reactive transport modelling (N. Prasianakis & D. Jacques)

MISSION BENEFICIARY

ANONYMOUS
Research Scientist
Nuclear Waste Management
VTT Technical Research Centre of Finland Ltd., Finland

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Diederik Jacques, Head of Unit, Engineered and Geosystem Analysis.
- Eric Laloy, Research Scientist, Engineered and Geosystem Analysis
- Vanessa Montoya, Research Project Leader, Engineered and Geosystem Analysis

Other organisations experts

- Barbara Lothenbach, Leader of Cement Chemistry and Thermodynamics group, Concrete and Asphalt Laboratory, EMPA, Switzerland
- Dmitrii Kulik, Senior Scientist, PSI, Switzerland
- Hans Meeussen, NRG Petten, Netherlands
- Laurent de Windt, Lecturer/Researcher, Centre of Geosciences, Mines Paris - PSL, France
- Emilie Coene, Senior Consultant, Materials Engineering, Amphos 21 Consulting S.L., Spain
- Sergey Churakov, Head of Laboratory of Waste Management, Department of Nuclear Energy and Safety, PSI, Switzerland.
- Ulrich Mayer, Professor of hydrogeology, Department of Earth, Ocean and Atmospheric Sciences, University of British Columbia, Canada
- Eric C. Gaucher, Associate Researcher, Institute of Geological Sciences, University of Bern, Switzerland
- Carl Steefel, Head of the Geochemistry department, Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, USA
- Javier Samper, Professor, University of Coruna, Spain
- Cyprien Soulaine, Associate Scientist, Institute of Earth Sciences of Orléans, CNRS, France

REPORT APPROVAL

Date of last sign.	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
	ANONYMOUS	Veli-Matti Pulkkanen	Diederik Jacques