MOBILITY MISSION REPORT

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MISSION TITLE

Geochemical & Reactive Transport Modelling for Geological Disposal

DESCRIPTION

Concerned organisations

Research entities

Concerned infrastructures or facilities

Other relevant infrastructure or facility to be specified

Concerned phases

Phase 2: Site characterisation

Themes and topics

Theme 4: Geoscience to understand rock properties, radionuclide transport and long-term geological evolution

- Long-term stability (uplift, erosion and tectonics)
- Perturbations (gas, temperature and chemistry)
- Aqueous pathways and radionuclide migration

Keywords

Modelling geochemical systems, thermodynamic modelling, reactive transport modelling, PHREEQC, geochemistry of the host rock

EXECUTIVE SUMMARY

The program consists of hour-long lectures and practical trainings where the participants had the opportunity to handle experimental data and practice on different software. The tutors are experts in the field of different modelling codes. The program lasted five days, each day had a different topic and theme. The course provided training sessions for some of the more widely-used codes (PHREEQC, GEMS and ORCHESTRA, and their coupling with transport models, as HPx) between which the participant could choose. During practical trainings I learned PHREEQC. I have been a research associate at the Centre for Energy Research since February 2022, where I started to work with total reflection X-ray fluorescence (TXRF) and micro-X-ray fluorescence (µ-XRF) spectrometry. I used them to study the sorption of cobalt on Boda claystone. My study is centred on the sorption and diffusion of cobalt ions on the potential host rock of a high-level radioactive waste repository. I also started investigating the sorption of nickel concerning cobalt. The opportunity for this training course was helpful in expanding my knowledge and expertise in geochemical and coupled reactive transport modelling, which will help in my following studies.

My final conclusion about the course is that it was incredibly important to further expand my knowledge on this subject. The presentations were given by experts, who helped me to get the most up-to-date information possible regarding geological disposal systems.

1. MISSION BACKGROUND

1.1. R&D background

The program consists of hour-long lectures and practical trainings where the participants had the opportunity to handle experimental data and practice on different software. The tutors were experts in the field of different modelling software. The program lasted five days, each day had a different topic and theme. During practical trainings I learned PHREEQC.

1.2. Mission objectives

I have been a research associate at the Centre for Energy Research since February 2022, where I started to work with total reflection X-ray fluorescence (TXRF) and micro-X-ray fluorescence (μ-XRF) spectrometry. I used them to study the sorption of cobalt on Boda claystone. My study is centred on the sorption and diffusion of cobalt ions on the potential host rock of a high-level radioactive waste repository. I also started investigating the sorption of nickel concerning cobalt. The opportunity for this training course was helpful in expanding my knowledge and expertise in geochemical and coupled reactive transport modelling, which will help in my following studies.

1.3. Mission request

I am very confident that this training opportunity can provide this, so I would be grateful if the Committee could provide financial support through the mobility program.

1.4. Mission composition

Host organisation

University of Bern

Host facility

Institute of Geological Sciences

Mission dates

06 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 solver PHREEQC

Description

The geochemical solver PHREEQC is a powerful geochemical code for aqueous speciation, mineral equilibria, multi-site cation exchange, complex surface complexation modelling, exchange with a gas-phase, solid solutions and kinetic reactions.

Usage

We learned the benefits of using PHREEQC for geochemical modelling. We understood the basics of the technique, how it can be used for modelling.

Benefits

It gives a large flexibility for modelling different geochemical systems and experimental set-ups including titration, speciation plots, etc. Moreover, PHREEQC has the possibility to perform one-dimensional advective-dispersive transport under steady-state flow conditions and multi-dimensional diffusive transport. The wrappers iPHREEQC and PHREEQCRM provides libraries to work with PHREEQC from Excel, python, R, fortran, C++, … In one or another form, PHREEQC has been coupled with different transport solvers which can be used for different areas and research questions for several engineering and environmental application.

Limitations

The lecture and practical training were adequate for understanding the theoretical background, but more time is needed to fully understand and interpret the modelling.

Applicability

The use of this code is preferable for my study, I will know the method and I will be able to apply the acquired knowledge.

My study is centred on the sorption and diffusion of cobalt ions on the potential host rock of a high-level radioactive waste repository. I also started investigating the sorption of nickel concerning cobalt. The opportunity for this training course was helpful in expanding my knowledge and expertise in geochemical and coupled reactive transport modelling.

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

Description

Usage

Benefits

Limitations

Applicability

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

Description

Usage

Benefits

Limitations

Applicability

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

Description

Usage

Benefits

Limitations

Applicability

3. MISSION FINDINGS AND CONCLUSIONS

3.1. Lessons learned and conclusions

During the training course, as a participant I was able to: understand the principles of geochemical thermodynamic and kinetic modelling and reactive transport modelling, use these principles for application in the field of radioactive waste disposal, transform specific research questions related to geochemical properties or evolution into a conceptual model, implement simple conceptual models into numerical codes for geochemical and reactive transport modelling.

My final conclusion about the course is that it was incredibly important to further expand my knowledge on this subject. The presentations were given by experts, who helped me to get the most up-to-date information possible regarding geological disposal systems.

3.2. Relevant findings and conclusions for home organisation

3.3. Relevant findings and conclusions for host organisation

3.4. Relevant findings and conclusions for other organisations

4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

4.1. Generic potentials

I was very satisfied with the course. Its organization and the quality of the presentations were excellent. In addition to the lectures, we had the opportunity to talk with our peers, and discuss professional topics.

4.2. Potentials for home organisation

4.3. Potentials for host organisation

APPENDICES

Mission journal

DAY-1

I have participated in two lectures namely Modelling geochemical systems and Thermodynamic modelling of cementitious systems and their evolution. There were a short overview of the three codes: PHREEQC, Orchestra, and GEMS.

I also started to use PHREEQC during the practical training sessions.

DAY-2

I have participated in two lectures namely Geochemistry of the host rock and natural barrier material (pore water chemistry, mineralogy, fracture-matrix) and Reactive Transport – Pore to Continuum scale. There were a short overview of the codes: iCP and CRUNCH. During the practical training I learned implementing the Primitive Cement system, and I started modelling of cement degradation (leaching, carbonation).

DAY-3

I have participated in two lectures namely Speciation of radionuclides – Including thermodynamic databases and Molecular aspect and thermodynamic modelling of sorption phenomena. There were a short overview of the code: MIN3P.

DAY-4

I have participated in a lecture namely Modelling of kinetically controlled processes in radioactive waste disposal, from radiolytic corrosion to microbial activity. There were a short overview of the code: CORE. During the practical training we started new examples, such as U sorption modelling on montmorillonite. We also started to use the graphical user interface HYDRUS-1D, which is used to implement the reactive transport model. HPGeochemistry is used to implement the geochemical models.

DAY-5

I have participated in two lectures namely Integration of processes at larger scale – sensitivity (uncertainty) analyses and Machine learning for accelerating reactive transport model simulations and analysis. There were a short overview of the code: porousMedia4Foam: an hybrid-scale solver to model coupled processes in porous media.

Mission bibliography

MISSION BENEFICIARY

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Centre for Energy Research, Hungary

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Eric C. Gaucher, University of Bern
- Sergey Churakov, PSI, Switzerland and University of Bern

Home organisation experts

Other organisations experts

- Barbara Lothenbach, EMPA, Switzerland
- Carl I. Steefel , LBNL, US
- Diederik Jacques, SCK CEN, Belgium
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- Laurent De Windt, Mines Paris, France
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- Ulrich Mayer, UBC, Canada
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REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
10.03.2023.	Fruzsina Szabó	János Osán	Diederik Jacques
	Fruzsina Szabó Digitálisan aláírta: Fruzsina Szabó Dátum: 2023.03.10 15:32:17 +01'00'	János Osán Digitálisan aláírta: János Osán Dátum: 2023.03.11 23:36:22 +01'00'	Diederik Jacques Digitally signed by Diederik Jacques Date: 2023.03.10 13:47:32 +01'00'