MOBILITY MISSION REPORT

This work has been partially supported by the EURAD project that has received funding from H2020-EURATOM 1.2 under grant agreement ID 847593.

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).

REPORT TEMPLATE GUIDELINES — REMOVE THIS ENTIRE SECTION BEFORE SUBMITTING

- *This template consists of "sections" (fixed headings) and "fields" (text boxes for custom information)*
- *All sections and fields are mandatory unless specified otherwise*
- *Appendix "A. Mission journal" should be prepared during the course of the mission*
- *All template guidelines shall be replaced with custom text or removed as specified*
- *The report shall be approved by the official mission mentors or supervisors before submission (use the signature block at the very end of the report template)*
- *The report shall be submitted in both editable (.doc) and portable (.pdf) file formats*
- *Both files shall use the code of the mission as the filename's suffix, i.e. "Mission_Report_SXXXXX" : the word "Template" shall be replaced with the initial code assigned automatically to the application (letter "S" followed by 5 digits)*
- *The report shall be submitted via email to euradwp13@sckcen.be*

MISSION TITLE

Geochemical and Reactive Transport Modelling for Geological Disposal

DESCRIPTION

Concerned organisations

- Geology institue, University of Bern

Concerned infrastructures or facilities

- High-performance computing
- Underground research laboratory

Concerned phases

- Phase 3: Facility construction
- Phase 4: Facility operation and closure
- Phase 5: Post-closure

Themes and topics

- Theme 3: Engineered barrier system (EBS) properties, function and long-term performance
    - Cementitious-based backfills, plugs and seals
- Theme 4: Geoscience to understand rock properties, radionuclide transport and long-term geological evolution
    - Aqueous pathways and radionuclide migration

Keywords

Reactive transport codes; geochemical modelling; phreeqC; cement.

EXECUTIVE SUMMARY

In the first year of my thesis work, I implemented a model to simulate the chemical degradation of cement paste at macro scale, taking into account carbonation and calcium leaching. This model was incorporated into the Cast3M finite element code since the final objective of my work is to do a mechanical calculation on a chemically deteriorated tunnel. This model is based on many hypothesis and simplification to reduce the size of the chemical model. As part of this training, I gained experience in simulating cement degradation from a different perspective, using geochemical model at a smaller scale. This code take into account all relevant species and solves various nonlinear equations to achieve equilibrium. This models depends on the input database, we used the CEMDATA18 during the trainning. Implementation examples on cement hydration and hardned cement paste carbonation have been carried out also an example on unidirectional reactive transport with uranium sorption. In addition, differents lectures have been given and have broadened information on various parts of geochemical modelling and reactive trasport. After having taken this course, I have the ability to confidently discuss and justify my hypotheses and models during project presentations and my thesis defense.

1. MISSION BACKGROUND

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1.1. R&D background

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1.2. Mission objectives

The training aims at enlarging knowledge and expertise in geochemical and coupled reactive transport modelling in the framework of disposal of radioactive waste with the focus on geological disposal.

The theoretical basis is on

(i) principles of geochemical and reactive transport modelling
(ii) their applications for processes and evolution of materials in a geological disposal (cementitious materials, clay)
(iii) speciation and migration of radionuclides
(iv) advanced topics related to uncertainty and machine learning.

1.3. Mission request

The regestrion for this trainning was done through the website of euradschool.

1.4. Mission composition

Host organisation

EURAD WP13

Host facility

Institue of geology, University of Bern.

Mission dates

6 February 2023 – 10 February 2023

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

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

During this mission we used the interface Hpx wich is a interface connecting the geochemical calculation code (Phreec C) with reactive transport simulations (Hydrus) .

Description

In geochemical modelling the partial equilibrium is used to setting up the thermodynamics equilibrium.

PhreeqC is a geochemical model based on the Law mass action LMA. Using the Newton Raphson method, the mass balance residuals is minimized at the boundary conditions of LMA expressions for all product species formation reaction with their logK values.

The calculation in this type of models is based on the database given, wish contains the species, their properties and all reactions can occurs.

The coupling with the reactive transport model is based on an non iterative sequantieal approach. The reactive transport model in HYDRUS is based on a partial differential equations that describe the movement of water, and solutes through the porous media.

Usage

Geochemical models have a wide range of applicability in the fields of geology, environmental science, and engineering.

Benefits

Geochemical models are a powerful tool for understanding and predicting the behavior of chemical elements and compounds in geological and environmental systems

Limitations

Geochemical models require accurate input data, this can lead to errors and uncertainties in the model results. In addition to the scaling issue, when performing structure-scale mechanical calculations, it is sometimes possible to encounter issues with non-convergence.

Applicability

During this training we used the geochemical models to simulate the cement hydration, and cement degradation due to carbonation.

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

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Description

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Usage

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Benefits

Klikněte nebo klepněte sem a zadejte text.

Limitations

Klikněte nebo klepněte sem a zadejte text.

Applicability

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

Replace this entire field with the name of the practice, technique, method, tool or system that is the object of this mission.

Description

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Usage

Klikněte nebo klepněte sem a zadejte text.

Benefits

Klikněte nebo klepněte sem a zadejte text.

Limitations

Klikněte nebo klepněte sem a zadejte text.

Applicability

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

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Description

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Usage

Klikněte nebo klepněte sem a zadejte text.

Benefits

Klikněte nebo klepněte sem a zadejte text.

Limitations

Klikněte nebo klepněte sem a zadejte text.

Applicability

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3. MISSION FINDINGS AND CONCLUSIONS

3.1. Lessons learned and conclusions

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3.2. Relevant findings and conclusions for home organisation

Klikněte nebo klepněte sem a zadejte text.

3.3. Relevant findings and conclusions for host organisation

Klikněte nebo klepněte sem a zadejte text.

3.4. Relevant findings and conclusions for other organisations

Klikněte nebo klepněte sem a zadejte text.

4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

This entire section shall be maximum one page (remove this entire sentence).

4.1. Generic potentials

4.2. Potentials for home organisation

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4.3. Potentials for host organisation

Klikněte nebo klepněte sem a zadejte text.

APPENDICES

Mission journal

This course consists of lectures sessions and practical sessions on geochemical software :

- Day 1 :
  Lecture 1 is about the thermodynamics equilibrium
  Introduction for the modelling geochemical systems
  Presentation of three geochemical software Gems, Orchestra, phreeqC
  Lecture 2 describes the cement and its hydration
  I choose phreeq C for the practical sessions
  Hands on phreeqC
- Day 2 :
  Lecture 3 on the Clay water and the minerals
  Lecture 4 on the geochemical and reactive transport modelling for geological disposal
  Presentation of the code ICP and and the code Crunsh
  Hands on PhreeqC (exercice on the cement hydration)
- Day 3 :
  Lecture 5 on the speciation of radionuclides includingthermodynamics datbases
  Lecture 6 on the reactive transport pore to continuum scale
  Presentation of the code Mine3p
  Hands ob phreeqC (continue the exercice of cement hydration and carbonation)
- Day 4 :
  Lecture 7 about the modelling of the reaction kinetick and reactive transport using Hytec
  Lecture 8 about the modelling of reactive transport for saturated and unsaturated water flow and heat transfer using the code CORE
  Hands on phreeqC (exercice Uranium sorption)
- Day 5 :
  Lecture 8 on the integration of processes at larger scale sensitivity (uncertainty) analysis.
  Lecture 9 on the machine learning for accelerating reactive transport model simulation and analysis
  Presentation of the code openFoam
  Hands on phreeqC coupled with Hydrus (exercice on the reactive transport)

Mission bibliography

MISSION BENEFICIARY

Layla Ibrahim
PhD student
Centre de génie civil UPS-INSA
Labortary of Materials and Durability of Constructions, Toulouse, France

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Dr. Diederik Jacques

Home organisation experts

- Pr. Alain Sellier
- Pr. Laurie Lacarriere
- Dr. Thiery Vidal

Other organisations experts

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REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
Date of last signee	Layla Ibrahim	Alain Sellier	Diederik Jacques
	Visa LI	Visa sellier Signé numériquement par sellier Raison : Je suis l'auteur du document Date : 2023.03.09 17:48:38+01'00' Foxit PDF Reader Version: 12.1.0	Visa Diederik Jacques Digitally signed by Diederik Jacques Date: 2023.03.08 06:09:27 +01'00'