MOBILITY MISSION REPORT

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MISSION TITLE

Reactive transport and geochemical modelling in engineered and geological barrier systems.

DESCRIPTION

Concerned organisations

Research entities (Lithuanian Energy Institute, SCK-CEN)

Concerned infrastructures or facilities

High-performance computing

Concerned phases

Phase 1: Site evaluation and site selection

Phase 5: Post-closure

Themes and topics

Theme 3: Engineered barrier system (EBS) properties, function and long-term performance

    - Containers for long-lived intermediate and low level wastes
    - Clay-based backfills, plugs and seals
    - Cementitious-based backfills, plugs and seals
- Theme 4: Geoscience to understand rock properties, radionuclide transport and long-term geological evolution
    - Perturbations (gas, temperature and chemistry)
    - Aqueous pathways and radionuclide migration

Keywords

Reactive transport, coupled processes, groundwater flow, geochemical interactions, modelling, PHREEQC, Hydrus, radioactive waste disposal, cementitious barrier degradation, carbonation.

EXECUTIVE SUMMARY

As in other nuclear countries, the operation of the Ignalina nuclear power plant (INPP) in Lithuania has led to the accumulation of large amount of radioactive waste (RAW) and spent nuclear fuel (SNF) assemblies. Within the European Union (EU), directive 2011/70/EURATOM contains the provision for every member state (country) to be responsible for the implementation of the safe and sustainable solution for SNF and radioactive waste management and disposal. Currently, it is envisaged that Lithuanian SNF and long-lived intermediate level waste will be disposed of in a deep geological repository. Some investigations of the possibilities to dispose of this waste in Lithuania have been initiated.

Researchers of Nuclear Engineering Laboratory have been actively involved in the analysis of the problems related to the management of radioactive waste from INPP since 1994. For this purpose, the Laboratory performs assessments of the release of radionuclides from waste repositories, safety assessments of waste treatment technological equipment, storage and disposal facilities, and environmental impact studies. Typically, the safety and performance analysis are supported with the numerical modelling of coupled processes.

While numerical tools Hydrus and HPx are available at LEI, additional work is necessary to improve the competence of LEI researchers to use these numerical tools to the fullest extent. Internship at Belgian Nuclear Research Centre SCK-CEN provided valuable experience in using these numerical tools for reactive transport modelling, necessary to perform nuclear disposal site analysis. The main topics covered during the internship included: performance of engineered barriers, chemical evolution in the near field of the repository, radionuclide sorption, organic and inorganic carbon behaviour in cementitious/geological environment, modelling of kinetically controlled reactions, sensitivity analysis. During the visit the theoretical background was combined with the numerous practical exercises and models, which were implemented in the HPx tool.

This internship increased my competence in modelling coupled HC processes in various geochemical configurations (cementitious barriers, clay materials). It will also expand the LEI researchers' competence in the evaluation of the properties of the engineered barrier system and its long-term performance in various geochemical conditions and in the provision of scientific support to the decision making bodies within the Lithuanian repository development programme.

In addition, the gained experience and skills will allow LEI scientists to contribute to the analysis of the chemical evolution in a disposal cell of the deep geological repository in the framework of EURAD WP ACED more effectively.

1. MISSION BACKGROUND

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1.1. R&D background

The Lithuanian Energy Institute (LEI) and our Nuclear Engineering Laboratory in particular participate in radioactive waste and spent nuclear fuel management activities and, especially, in activities related to the disposal of radioactive waste in Lithuania. Typically, the safety and performance analysis of the disposal facilities are supported with the numerical modelling of coupled processes. This is a complex task and capabilities to perform it heavily relate on the staff's competences and skills. Therefore, to gain experience and increase the skills are of great importance in implementation of the radioactive waste disposal facilities.
In addition, the gained experience and skills will allow LEI scientists to contribute to the analysis of the chemical evolution in a disposal cell of the deep geological repository in the framework of EURAD WP ACED more effectively.

1.2. Mission objectives

The participation of Povilas Balčius in an internship programme in SCK-CEN 23rd April – 18th May 2023.

The main goal of the internship is to gain knowledge about the interactions of the engineered barriers with the environment and to increase experience in reactive transport and geochemical modelling with the focus on the cementitious barriers and carbon behaviour in the disposal system.

1.3. Mission request

To cover the cost of Povilas Balčius internship at SCK-CEN 24th April –17th May 2023, total 2893.80 EUR, which includes travelling to and from SCK-CEN (travel on April 23rd and May 18th), accommodation and daily expenses (for a period from 23th April to 18th May 2023).

1.4. Mission composition

Host organisation

Belgian Nuclear Research Centre SCK-CEN (Belgium)

Host facility

SCK-CEN, SCH building (chemistry centre)

Mission dates

2023 April 23rd – May 18th.

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

Numerical software Hydrus and HPx (PHREEQC interface).

Description

Lectures on sorption and exercises on chemical reaction and reactive transport modelling using Hydrus 1D and HPx software.

Usage

Lectures on radionuclide sorption and hands on exercises on chemical modelling topics: cement hydration, carbonation, chemical reactant speciation, sorption, kinetics and degradation. Implementing such reactions into reactive transport modelling systems using Hydrus software.

Benefits

The internship gave valuable knowledge and skills on working with Hydrus and HPx software, which increased my competence and capabilities in modelling reactive transport modelling in systems under various geochemical conditions (cementitious materials, clay soils).

Limitations

Reactive transport simulations are computationally expensive and as such are highly time dependent on problem scale in space and time. To achieve reliable reactive transport modelling results it is necessary to consider criterions for mesh and time step size and may need fine discretization.

Applicability

Participation in the internship expanded LEI researchers' competence to evaluate the properties of engineered barrier systems and their long-term performance under various conditions. The gained experience can be used for modelling of chemical evolution in a deep geological repository as well as in a near-surface repository and can serve in the provision of scientific support to the decision making bodies within the Lithuanian repository development programme.

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

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Limitations

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Applicability

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2.3. 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

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Limitations

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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

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Benefits

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Limitations

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Applicability

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3. MISSION FINDINGS AND CONCLUSIONS

3.1. Lessons learned and conclusions

The mobility action provided an opportunity to get effective training on the use of Hydrus and HPx for reactive transport modelling (setting up input, running the simulations, determining issues with the code, analysing results, etc.) from the developers and experienced users of these software packages. The key aspects discussed: modelling of various scenarios of the chemical evolution of cementitious materials, modelling of sorption of radionuclides, kinetic reactant modelling, organic degradation modelling, carbonation modelling and modelling of permeability/porosity change due to the aforementioned processes. During the internship part of the exercises were performed together with the experienced instructors and part of the work was studied independently and later analysed and discussed with the supervisors. Such method was very useful for identifying the weak points in modelling and smooth progress. This training course enhanced my knowledge and skills about reactive transport modelling, relevant within the context of radioactive waste management under various geochemical conditions (near surface repositories, deep geological disposal facilities).

3.2. Relevant findings and conclusions for home organisation

Participation in this internship significantly expanded my personal competence and, as knowledge sharing between researchers in LEI is a common practice and is encouraged, LEI researchers' competence in the evaluation of properties of engineered barrier systems and their long-term performance assessment under various geochemical conditions. The gained knowledge and skills will allow LEI scientists to contribute to the analysis of reactive transport modelling problems within the framework of EURAD WP2 ACED more effectively.

3.3. Relevant findings and conclusions for host organisation

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3.4. Relevant findings and conclusions for other organisations

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4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

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4.1. Generic potentials

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4.2. Potentials for home organisation

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4.3. Potentials for host organisation

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APPENDICES

Mission journal

23rd April

Travel from Vilnius to Belgium, Brussels and then to Mol

24th April

Arrival at SCK-CEN, security quiz, welcome, discussion about internship goals. Initial lectures about radionuclide sorption course material study.

25th April

Course material study and discussion with the mentor. First hands on tasks on cement hydration modelling.

26th April

Discussion of results and issues of cement hydration modelling, further work of implementation of various HPx features for cement hydration modelling.

27th April

Discussion of issues of use of HPx features for cement hydration modelling, study of cement hydration and carbonation modelling.

28th April

Implementation of cement hydration/carbonation modelling, study and discussion of implementation of cement carbonation/leaching modelling

29th April-1st May

Weekend

2nd May

Discussion of cement carbonation/leaching modelling issues, study and implementation of Uranium speciation modelling under different pH conditions (sensitivity analysis).

3rd May

Study and implementation on Uranium sorption modelling on montmorillonite.

Study and implementation of Kinetics implementation for montmorillonite dissolution.

4th May

Discussion of 3rd May topics and issues that arose, discussion of implementation of kinetic reactions for further tasks, study and implementation of kinetic reactions for Dual Arrhenius and Michaelis-Mentin model for mineral dissolution.

5th May

Discussion of implementation first order degradation reaction networks in modelling. Implementation of first order degradation reactions and discussion of results.

6th – 7th May

Weekend

8 th May

Discussion of acquired results, discussion of implementation of HPx (PHREEQC) code in reactive transport models including kinetic reactions in Hydrus reactive transport models. Implemntation of first order degradation networks in reactive transport models.

9th May

Discussion of issues and results of modelling results. Further discussion in carbon behaviour in cementitious/geochemical conditions and potential implementation in reactive transport models.

10th May

Discussion of kinetic reaction modelling in reactive transport models. Implementation of trapped organic PCE degradation modelling. Discussion of permeability change modelling.

11th May

Implementation on organic reactant degradation and reactive transport modelling, discussion of issues and results.

12th May

Discussion of implementation of permeability/porosity change due to degradation of organic reactant modelling. Discussion of results and issues.

13th-14th May

Weekend

15th May

Discussion of implementation of combined carbonation/organic carbon degradation/porosity/permeability change in reactive transport models. Exercise to to implement these models under different flow parameters (sensitivity study).

16th May

Discussion of results and issues, potential modelling improvement. Implementation of corrections and discussion of results, potential future work.

17th May

Discussion of tasks completed during the internship, acquired results and problems solving during modelling attempts. Departure from SCK-CEN for Brussels.

18th May

Travel from Brussels, Belgium to Vilnius, Lithuania.

Mission bibliography

https://doi.org/10.1016/j.apgeochem.2020.104539 Geochemical modelling of the effect of waste degradation processes on the long-term performance of waste forms. E. Wieland, G. Kosakowski, B. Lothenbach, D. A. Kulik.

MISSION BENEFICIARY

Povilas BALČIUS
P.h.d. student and junior research associate.
Nuclear Engineering Laboratory
Lithuanian Energy Institute

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Diederik Jacques, Head of Unit Engineered and Geosystem Analysis at SCK-CEN and group leader since 2011. Has long-term experience, that covers various areas of geochemical modelling such as flow and transport phenomena, reactive transport modelling, parameter estimation, geostatistical characterization, with the most recent research being focused on long-term evolution of cement-based materials, contaminant and colloid transport in porous media and performance assessment of near-surface and deep radioactive waste disposal systems. Diederik Jacques is the WP leader of the EURAD WP2 ACED
- Vanessa Montoya, Research project leader at SCK-CEN since April 2022, has more than 15 years of professional and research experience, covering areas of applied geoscience, radiochemistry, modelling of coupled processes and safety analysis, thermodynamics, engineering, geochemistry and material sciences with the application in radioactive waste management.
- Sanheng Liu, researcher at SCK-CEN, more than 10 years of experience in geochemical and reactive transport modelling in the framework of geological disposal of radioactive waste.
- Janez Perko, senior researcher at SCK-CEN, main occupation – safety analysis of Belgian low level waste disposal facility.

Home organisation experts

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Other organisations experts

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REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
2023	Povilas Balčius	Povilas Poškas	Diederik Jacques
	Visa	Visa	Visa Diederik Jacques Digitally signed by Diederik Jacques Date: 2023.06.05 15:20:13 +02'00'