MOBILITY MISSION REPORT

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MISSION TITLE

Participation in iCP (interface between Comsol Multiphysics and Phreeqc) training course

DESCRIPTION

Concerned organisations

Research entities (Lithuanian Energy Institute)

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

Keywords

Coupled processes, THMC, groundwater flow, geochemical ineractions, modelling, Phreeqc, Comsol Multiphysics, iCP, radioactive waste disposal

EXECUTIVE SUMMARY

As in other nuclear countries, the operation of the Ignalina nuclear power plant (INPP) in Lithuania has led to the accumulation of around 22 thousand of spent nuclear fuel (SNF) assemblies. A country's responsibility for the safe management of its SNF is acknowledged worldwide. 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 will be stored in dry interim storage facilities (new and existing) for at least 50 y prior to possible deep geological disposal. Some investigations of the possibilities to dispose of the SNF in Lithuania have been initiated.

Researchers of Nuclear Engineering Laboratory have been actively involved in the analysis of 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 thermo-hydro-mechanical-chemical processes.

Powerful numerical tools COMSOL Multiphysics and Phreeqc are already available at LEI; however, currently they can be operated in separate modes. To simulate reactive solute transport with groundwater requires a communication between flow ant transport simulator such Comsol Multiphysics and the solver of chemical interactions (dissolution, precipitation, ion exchange, surface complexation, etc.) such as Phreeqc. iCP (interface Comsol–PhreeqC) developed at Amphos 21 is powerful and flexible tool for this communication and have used to simulate a wide variety of geochemical systems. Participation in 3 days iCP training course allowed to get basics about iCP framework, preparation of input files, run the simulations, analysis of the results.

Taking this training increased my competence in modelling complex coupled THMC processes in backfill materials (cementitious, clay based). 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 geological repository conditions and in the provision of scientific support to the decision making bodies within the Lithuanian repository development programme. Also, the gained knowledge and skills will allow LEI scientists to contribute to the analysis of HM, THC processes in the geological repository within the framework of EURAD WP MAGIC, Donut 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. The topics of my research evolved over time from the research of radionuclide release from a disposal facility and migration in porous and fractured media, uncertainty and sensitivity analysis to the modelling of coupled thermo-hydro, hydro-mechanical, thermo-hydro-mechanical processes and, most recently, to the coupling of THM and chemical processes in the repository environment.

1.2. Mission objectives

The participation of dr. Asta Narkūnienė in iCP Training Course, 8–10th November 2022.

iCP (interface Comsol–PhreeqC) is powerful and flexible reactive transport modelling software developed at Amphos 21, which can be used to simulate a wide variety of geochemical systems, such as the geological disposal of radioactive waste, carbon capture and storage, or mining. The numerical tools COMSOL Multiphysics and Phreeqc are already available at LEI; however, currently they can be operated in separate modes.

1.3. Mission request

To cover the fee for the participation of dr. Asta Narkūnienė in iCP Training Course, 8–10th November 2022.

1.4. Mission composition

Host organisation

Amphos21 (Spain).

Host facility

Online training course.

Mission dates

2022 November 8-10.

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 iCP (interface Comsol–PhreeqC)

Description

Lectures and hands-on exercises with iCP followed by the introduction to advanced topics of iCP and on-going developments

Usage

During the training course we have introductory lectures on reactive transport modelling, flow and solute transport in porous media, Phreeqc, Comsol Multiphysics and iCP. We have a hands-on exercises to simulate cation echange, calcite dissolution and nitrate leaching processes which are relevant in the context of radioactive waste disposal.

Benefits

The training course allowed to get knowledge on working with iCP, which increased my competence and capabilities in modelling complex coupled THMC processes in backfill materials (cementitious, clay based) considering various couplings (one-way, two-way). The fee of training course included a permanent R&D licence for iCP.

Limitations

The reactive transport simulation time is highly dependent on problem scale in space and time. Reliable solute transport modelling results need to consider criterions for mesh and timestep size and may require very fine discretization.

Applicability

Participation in this training course expanded the LEI researchers' competence to evaluate the properties of the engineered barrier system and its long-term performance in geological repository conditions. iCP license will allow to continue development of numerical models for simulations of complex coupled THMC processes in the repositories.

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

Replace this entire field with a description of your operation or study of this practice, technique, method, tool or system during the mission.

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 mission provided an great opportunity to get effective training on iCP (set up of input files, running the simulations, analysis of the results, etc.) from iCP developers and experienced users. The key aspects of modelling of solute transport with numerical methods, operator splitting, mesh and time size criterions for diffusive and advective transport were introduced and discussed. Amphos 21 experts also presented iCP applications for modelling complex problems where reactive transport simulations are needed. During discussions and hands-on exercises with experienced instructors we get information on important features, tips, criteria to follow while setting the problem and analysing modelling results. Practical hands-on exercises were extremely useful to get familiar with iCP environment and setting-up input files for particular problem. This training course enhanced my knowledge and skills about the development of reactive transport models relevant within the context of radioactive waste management and deep geological disposal of radioactive waste.

3.2. Relevant findings and conclusions for home organisation

Participation in this training course expanded the LEI researchers' competence in the evaluation of the properties of the engineered barrier system and its long-term performance in geological repository conditions and in the provision of scientific support to the decision making bodies within the Lithuanian repository development programme. The gained knowledge and skills will allow LEI scientists to contribute to the analysis of HM, THC processes in the geological repository within the framework of EURAD WP MAGIC, Donut 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

4.1. Generic potentials

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4.2. Potentials for home organisation

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4.3. Potentials for host organisation

The training course was very well planned and organized. The lectures, instructions and exercises were prepared in details. While giving the training course online it would be advisable to have a dedicated time slot (0.5 or 1 day) for users to test iCP by their own following instructions and new information given by lecturers.

APPENDICES

Mission journal

8th November

9:00-10:00 Welcome & iCP Installation
10:00-11:30 Introduction to PhreeqC
11:30-13:00 Introduction to COMSOL - flow and solute tramsport in Porous Media
14:00-16:00 Hands on: Cation exchanger Part I (set up of Comsol, Phreeqc files)

9th November
9:00-10:00 Introduction to Reactive Transport Modelling & iCP
10:00-11:30 Hands on: Cation exchanger Part II (set up of iCP files)
11:30-13:00 Hands on: Calcite dissolution (set up of Comsol, Phreeqc files)
14:00-16:00 Hands on: Calcite dissolution (set up of iCP file)

10th November
9:00-11:30 Advanced topics of iCP and on-going developments: multiphase flow, fractures, mechanics, Oil&Gas, biosphere
11:30-13:00 Advanced hands-on iCP example Part I (set up of Comsol, Phreeqc files)
14:00-16:00 Advanced hands-on iCP example Part II (set up of iCP file)

Mission bibliography

MISSION BENEFICIARY

Asta NARKUNIENE
Senior researcher
Nuclear Engineering Laboratory
Lithuanian Energy institute

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Jorge Molinero is the Scientific and Technical Director of Amphos 21. He has 20 years of experience working with reactive transport simulations.

- Elena Abarca is Group Manager in hydrogeology and reactive transport modelling at Amphos 21. Her work focusses in numerical modelling of groundwater flow and transport of (conservative and reactive) contaminants in porous media.

- Andrés Idiart is a Civil Engineer with a PhD in Solid Mechanics and works as a Group Manager in engineering materials at Amphos 21. Andrés fields of expertise include geomechanics and the coupling between multiphysics and geochemistry.

- Emilie Coene is a consultant and iCP developer at Amphos 21. She is an expert in numerical model development and application.

- Marcelo Laviña is a consultant of the Modelling Solutions team at Amphos 21 Barcelona since 2016. He develops geomechanical and reactive transport models, specialising in the coupling of hydro-chemo-mechanical (HCM) processes in porous media.

- Diego Sampietro is a consultant in the Modelling Solutions team at Amphos 21 since 2014. His main field of expertise includes the modelling of hydro-chemical processes in porous and fractured media.

- Albert Nardi is Group Manager in Hydroinformatics, Software and Data Science at Amphos 21. He is an expert in numerical modelling and software development. He is one of the main developers of iCP and GibbsStudio.

Home organisation experts

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Other organisations experts

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REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
Date of last signee	Asta Narkūnienė	Povilas Poškas	Albert Nardi
2022/12/01			