MOBILITY MISSION REPORT

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MISSION TITLE

Integrating Thermo-Hydro-Mechanical (THM) Processes in Geomaterials: A Multiscale and Multiphysics Approach for Deep Geological Facilities.

DESCRIPTION

Concerned organisations

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- Research entities: TU Delft, Uleige, CIEMAT (TSO), ANDRA.
- Waste management organisations: Nuclear Waste Service (NWS), ENRESA, British Geological Survey (BGS), NAGRA.

Concerned infrastructures or facilities

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- Underground research laboratory: EURIDICE_HADES.
- CIEMAT laboratories.
- NAGRA.
- ENRESA.

Concerned phases

This report does not concern facility construction, but rather focuses on summarizing the knowledge acquired during my study of thermos-hydro-mechanical behaviour in clay rock while attending the workshop at the University of Liege.

Themes and topics

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- Theme 3: Engineered barrier system (EBS) properties, function and long-term performance
    - Spent Fuel and high-level waste disposal canisters
    - Containers for long-lived intermediate and low level wastes
    - Clay-based backfills, plugs and seals
    - EBS system understanding
- 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
- Theme 7: Performance assessment, safety case development, and safety analyses
    - Integration of safety-related information
    - Performance assessment and system models
    - Treatment of uncertainties

Keywords

Couplying processes (THM); Modelling; Validation; Clay; Geomaterials.

EXECUTIVE SUMMARY

Low-strength sedimentary rocks (LSSRs), mainly clay rocks, are highly desirable formations for geological deep facilities (GDF) with clay content, particularly when considering gas migration due to their low permeability and mineral distribution. Hydrogen is considered the most dominant gas in GDF generated by corrosion. Accurate prediction and understanding of the gas migration process within the GDF and surrounding formations are essential for ensuring long-term safe storage of nuclear waste disposal. Multiscale modelling aims to address the challenges at the engineering meso-scale while considering engineering micro-scale physical and chemical processes and phenomena. Considering the micro-scale structure, complex methods has been established to handle relevant phenomena effectively. Understanding the thermo-hydro-mechanical (THM) behaviour of clay is crucial for long-term safety management.

The study that I am conducting is focused on the evaluation of simulation results from meso (cm) scale models over a period of approximately 200 years, specifically focusing on two-phase flow simulation using TOUGH2. Following the study, and perceiving the importance of early-time diffusion of hydrogen in the aqueous phase compared to two-phase advection of gas, the diffusion transport of gas in clay formations at the micro-scale

was investigated using single-phase modelling in COMSOL. The micro-scale model will generate an ``overall diffusion coefficient'' for the mesoscale simulation.

Sensitivity analysis for three models with varying overall diffusion coefficient values for the continuum scale has shown an indirect relationship between the value of diffusion coefficient and pressure build-up. The lowest overall diffusion coefficient model had a pressure build-up value of 70 bar, while the highest magnitude of diffusion coefficient value had a pressure value of 20 bar. The observed build-up pressure is attributed to the advection mechanism that becomes gradually dominant surpassing diffusion in the system. In the micro-scale modelling, the mineralogy of clay and the heterogeneous distribution of clay have been taken into account to determine the overall diffusion coefficient. The effective ''input'' diffusion coefficient values for the minerals range from $6.5 \times 10^{-12}\ \mathrm{m}^2 \cdot \mathrm{s}^{-1}$ to $4.6 \times 10^{-9}\ \mathrm{m}^2 \cdot \mathrm{s}^{-1}$, which consequently lead to overall diffusion coefficient values ranging between $6.49 \times 10^{-12}\ \mathrm{m}^2 \cdot \mathrm{s}^{-1}$ and $7.95 \times 10^{-10}\ \mathrm{m}^2 \cdot \mathrm{s}^{-1}$.

1. MISSION BACKGROUND

In this section, mission background will be explained.

1.1. R&D background

During my first year of PhD at the University of Manchester, I dedicated significant time and effort to investigate the deep geological facility and the characterization of hydrogen in low-strength sedimentary rocks, specifically focusing on Mercia Mudstone Group (MMG). My research aimed to establish a connection between micro and meso-scale (cm) modelling by examining the effective diffusion coefficient of distributed minerals derived from various SEM images. By utilizing TOUGH2 and COMSOL software, I successfully obtained results that underscored the importance of comprehending the migration of hydrogen gas in a low strength sedimentary rocks. Hence, attending the workshop in the University of Leige was essential.

1.2. Mission objectives

• Analysing the mechanical and the hydraulic properties of clayey (e.g. retention capacity, swelling , porosity, permeability) by interperating the experimental results.

• Examining the impact of the temprature on the hydro-mechanical (HM) properties of the clay materials and the drill cores.

• Designing and recording the experimental results to identify the impact of temperature elevation on the mineralogical and geochemical composition, as well as the hydraulic and mechanical attributes of the rock mass and the engineering barrier.

1.3. Mission request

I was invited by my supervisors from the Nuclear Waste Service to attend the workshop in Liege since the content is very relevant to my PhD project. Multiscale modelling is crucial to prevent /or anticipate the initial build up in the facility for the long term safety.

1.4. Mission composition

Host organisation

EURAD.

Host facility

ULiege (Sart-Tilman campus), Liege, Belgium.

Mission dates

28 August – 1 September 2023, Liege (BE).

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

Coupling of THM processes effects on the clay within the saturated medium focusing on the TH processes. “Basic of thermo-hydro-mechanical processes in geomaterials”

Description

Considering the THM processes have been covered. Explanation of the four stages of the life time of the GDF such as excavation, maintenance, repository and long-term storage were aligned with the THMG processes and their interactions. Gas generation of hydrogen “dominant gas ” due to the corrosion was highlighted. Considering the low permeability of the clay rock and the barriers (e.g. bentonite) and how it affects on the gas migration in a saturated medium.

Usage

Numerical models become a powerful tool. It delivers high accuracy results since the above considerations are taken.

Benefits

Considering the properties of the solid, liquid ,and gas were vital for managing the GDF. Heat generation due to the radionuclides interactions should be considered. This will support not only to predict the initial build-up pressure of gas but also to control the migration of the radionuclides gases.

Limitations

Experimental study will always be a limitation for model validation.

Applicability

Knowledge gained improved my understanding of the TH processes. It is also aligned with my modelling approach with considering that the diffusion is dominant over the advection in the saturated medium within an extended period of time.

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

Lectures “ In situ THM and gas experiments”and Advanced multiphysics modelling of geomaterial : multiscale approches and heterogenities.

Description

It highlights the importance of understanding gas migration experiments to validate the numerical approach. Also, upscaling techniques of heterogeneity are crucial to capture the behaviour of the mechanical effects on the bentonite samples.

Usage

Clay material (e.g. bentonite) is crucial for the GDF. Studying the mechanical stress and its affect on a low permeability medium will be vital to add it as an objective in my PhD project.

Benefits

Available experiments could validate my numerical model of gas transport through the clay rock. Then I will be able to use the deep learning tool to cut off the computational cost.

Limitations

Hydrogen gas diffusivity experiments on micro and meso scale for determining the diffusion coefficients since diffusion mechanism is dominant for an extensive period.

Applicability

I contacted Dr Anne as she may have the experiments to validate my obtained results.

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

“Development, validation and maintenance of numerical codes” lecture and HADES visit.

Description

Overview on “OpenGeoSys” software and hands on field experimental facility “HADES”.

Usage

OpenGeoSys software and the available data are crutial for long term safety of the GDF.

Benefits

Results of heat field experiments from HADES could validate our numerical modelling.

Limitations

Modelling the plasticity by utilizing “OpenGeoSys” software is a current challenge.

Applicability

I may use the results of the heat transfer in HADES to merge them with my objectives.

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

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3.1. Lessons learned and conclusions

The workshop has enhanced my comprehension of the Thermo-Hydro-Mechanical (THM) behaviour of clay materials. My PhD at the University of Manchester primarily concerns different clay types behaviours aligned with the types that have been introduced in the workshop such as Boom clay and Opalinus clay. Furthermore, I gained insight into different approaches internationally, including, Belgium, Italy, Switzerland, France, Spain and the United Kingdom for future nuclear waste storage, and that each employs distinct multi-barrier concepts.

Additionally, the course equipped me with knowledge about modelling THM processes, which enhanced my understanding of the overview of the physical processes within the geological deep facility. Modelling THM processes in geomaterials is involving mathematical and numerical models that describe how clay materials respond to variations in water content, temperature and mechanical effects. Visiting EURIDICE_HADES was an immensely valuable experience for my PhD journey and my overall career. Being on-site provided me with a tangible connection to the importance of modelling gas migration, a main aspect of my PhD research. This hands-on experience not only aligned perfectly with my academic objectives but also offered a wealth of insights and inspiration that will undoubtedly enhance the quality and depth of my work. Moreover, introducing an open-source software “OpenGeoSys” was beneficial for future developments.

Finally, understanding the THM behaviour of clay materials is a multidisciplinary and complex field. It involves the interaction of thermal, hydraulic, and mechanical processes, as well as chemical reactions and the alteration of microstructure. Clay materials exhibit high sensitivity to temperature fluctuations, resulting in changes such as increased hydraulic conductivity and the diffusion coefficient of hydrogen gas, reduced water retention capacity, and modified mechanical properties that may increase the permeability of the host rock and affect negatively the main concept of radionuclides storage. It is crucial to enhance our understanding and management of the GDF, ensuring long-term safety and optimizing resource utilisation.

3.2. Relevant findings and conclusions for home organisation

Not applicable.

3.3. Relevant findings and conclusions for host organisation

Not applicable.

3.4. Relevant findings and conclusions for other organisations

Not applicable.

4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

Not applicable (N/A).

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

The mission comprised of a week workshop at the University of Liege, part of the PhD school of EURAD GAS and HITEC, focusing on THM processes in geomaterials. The daily schedule was as follows:

Monday, August 28th:

Two lectures were conducted. The first lecture demonstrated the fundamentals of TH processes in geomaterials, emphasizing a comparison between saturated and unsaturated conditions and their impact on clay material behaviour such as bentonite. It explored hysteresis effects between dry and wet phases. It emphasized that the diffusion mechanism is dominant for an extensive period over the advection mechanism. The second lecture focused on experimental testing and the effect of the mechanic loads on the medium, covering parameters (e.g. representative elementary volume (REV) for upscaling, total stress, and stiffness of the rock.

Tuesday, August 29th:

Lectures focused on modelling THM processes in geomaterials, providing insights into the mathematical equations used in soil studies. Furthermore, OpenGeoSys, a freely available software, was introduced, along with some essential benchmarks for generating THMC models.

Wednesday, August 30th:

In the morning, PhD students presented their research and posters, offering opportunities for networking and discussions. In the afternoon, four lectures have been presented, focusing on different types of clay materials with varying approaches for long-term management of the GDF in Spain, Belgium, France, and United Kingdom.

Thursday, August 31st:

These lectures delved into advanced multiphysics modelling of geomaterials, building upon the concepts introduced in previous sessions. Upscaling of heterogeneity were presented to consider the mechanical effect. In the afternoon, we explored in situ THM and gas experiments, including those conducted at CIEMAT concerning FEBEX bentonite.

Friday, September 1st:

The day involved a visit to the HADES underground research laboratory and the Tabloo exhibitions, which covered topics related to nuclear power and nuclear waste management. We managed to explore the facility and the experiments that takes place. Gas diffusivity result of an experiment that took place were demonstrated which align with the nature of the clay rock.

MISSION BENEFICIARY

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PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Replace this entire field with the names of the experts and their affiliation (position, department) from the host organisation who participated directly in overseeing or implementing the mission
- Add as many lines as appropriate

Home organisation experts

- Replace this entire field with the names of the experts and their affiliation (position, department) from your home host organisation who participated directly in overseeing or implementing the mission
- Add as many lines as appropriate

Other organisations experts

- Replace this entire field with the names and affiliations of the experts and their affiliation (position, department, organisation) from any other organisation who contributed directly to oversee or implement the mission
- Add as many lines as appropriate

REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
Date of last signee	Abdelrazik Elfar	Masoud Babaei, Lin Ma	Not applicable
	Visa	26/09/2023 Signed by Masoud Babaei	Visa