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European Joint Programme
on Radioactive Waste Management

MOBILITY MISSION REPORT

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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

Research internship at SCK CEN (identical to the title in the mobility mission request)

DESCRIPTION

Concerned organisations

Research entities:

- Aalto University (Finland)
- SCK CEN (Belgium)

Concerned infrastructures or facilities

Remove this entire field as well as every below infrastructure or facility that do not apply and add lines to specify other relevant infrastructures or facilities as appropriate

- Underground research laboratory
- Waste packages control facilities
- Labs on gas, water and solutes transport
- Other relevant infrastructure or facility to be specified: Novel experimental works on multi-gas diffusion/transport in expansive clay.

Concerned phases

Remove this entire field as well as every below phase that do not apply

- Phase 5: Post-closure

Themes and topics

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
- Cementitious-based backfills, plugs and seals
- Salt backfills
- EBS system understanding

Theme 4: Geoscience to understand rock properties, radionuclide transport and

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

Keywords

Nuclear waste repository; Boom Clay; gas mixture diffusion; numerical modelling; Comsol..

EXECUTIVE SUMMARY

In a deep geological nuclear waste repository, the interaction of groundwater with barrier elements such as canisters, steel liners or waste packages can generate multiple gases. The accumulation of gases can adversely affect the integrity of an Engineered Barrier System (EBS) and host rock. Therefore, efficient repository modelling requires having a mechanistic understanding and predictive capabilities of these multi-gas interactions and transport processes.

Aalto, under WP6 Task 4.2 and milestone 61 (EURAD: Milestone 61 2021), is working on gas transport modelling in a generic nuclear waste repository using an in-house built Finite Element code Thebes. In the same framework, SCK CEN performs various experimental works on multi-gas diffusion in different materials including expansive clays, to study the gas transport behaviour.

The research internship under the EURAD mobility program brings a scientific collaboration between Aalto University and SCK CEN. The work primarily aims at validating recent developments in code Thebes, by employing a novel gas mixture experiment from SCK CEN. The enhancement in Thebes includes interaction between water vapour and two non-condensable inert gases, and transport (advection and diffusion) in porous materials under thermal, hydraulic and mechanical loading.

For validation of the formulation implemented into Thebes, we used two experiments by SCK CEN (EURAD: Milestone 173 2022): a) Diffusion of dissolved gas under controlled loading (CH4 and He), and b) Diffusive/advective gas flow (CH4 and He) by using a pure gas phase in the injection vessel (ongoing) in Boom Clay. The simulated results are further compared with the previously employed simplified Comsol model. The results show a good match against the experimental data while giving critical insight into diffusive gas flow mechanisms in expansive clays. Post-validation, other collaborative tasks are set where Aalto will provide computational insights on the ongoing and future experiments from SCK CEN.

1. MISSION BACKGROUND

This entire section shall be maximum two pages (remove this entire sentence).

1.1. R&D background

Aalto University, within the framework of EURAD Gas (WP6) Task 4.2 and as per milestone 61 (EURAD: Milestone 61 2021), is currently working on gas transport modelling in a generic nuclear waste repository using an in-house built Finite Element code Thebes.
The Finite Element Method code Thebes assumes a three-component representation of the material, consisting of a) air, b) soil (including salts), and c) water in 3 phases (gas, liquid and solid). The code is designed to model the response of unsaturated (expansive) materials to thermal, hydraulic and mechanical (THM) loading (Abed and Sołowski 2017, 2020).
Recent developments in the code include extending its capabilities to incorporate interaction of water vapour and two non-condensable inert gases and transport in porous materials under thermal, hydraulic and mechanical loading. The new unique formulation improves the Thebes code ability to model the Gas transport process, pressure build-ups and overall nuclear repository behaviour due to its ability to account for the interaction between air, vapour and hydrogen. The code has been verified before by comparing the results of several simplified 2D (1x1 m2 geometry) test cases simulated in Thebes and COMSOL. It is subsequently employed to model gas transport in a 2D tunnel section from Ondraf/Niras conceptual design under thermal and hydraulic conditions leading to some promising results in preliminary analysis (EURAD: Milestone 174 2022). However, to build more trust in the new formulation, a validation of the code Thebes is required. Hence, the objective of this study is to compare the modelled responses with the results of experiments on gas mixture flows and interaction.

1.2. Mission objectives

SCK CEN is a leading nuclear energy and waste management research centre in Europe. Within the EURAD framework and WP6, SCK CEN performs various novel experimental works on multi-gas diffusion in expansive clay. In particular, the long-term gas experiments (EURAD: Milestone 173 2022) Diffusion of dissolved gas under controlled loading (Ar and He) and b) Diffusive gas flow (CH4 and He) by using a pure gas phase in the injection vessel (ongoing), are of interest. The former experiment aims to quantify the dissolved diffusion of gas based on pure concentrations under constant pressures. SCK CEN utilises the latter test setup to study the behaviour of the Boom Clay (for example, dilatant pathways) when the gas pressure is close to the minimum principal stress, using very slow gas pressure increments.

Through this research internship, Aalto primarily aims at validating its new gas mixture formulation in code Thebes by numerically replicating experimental data from SCK CEN in the Thebes code. Additionally, the replication work compares the results with the previously employed simple diffusive model in COMSOL by SCK CEN.

Further, with the post-validation work, Thebes can perform predictive modelling to study the influence of changing initial and boundary conditions in the experiments, for instance, the effect of varying temperatures and confining pressure in gas transport. This task is in the interest of SCK CEN as they plan to expand their experimental setup to further their research on a better understanding of the gas transport process.

In addition, the planned research visit also serves as a secondary purpose of a technical visit to the underground laboratory setup HADES. It is a state-of-the-art facility that is a part of various research on nuclear waste management, such as thermo-, hydro-, mechanical-, chemical- and microbiological studies on clay and the interaction between radioactive waste and repository over packing materials. The visit gives an exciting opportunity to learn more about current research activities and experimental approaches.

1.3. Mission request

The research activity, with the aim of satisfying goals given in section xxx, was scheduled for one month and took place in September 2022. The requested mobility grant was 3000 euros. Table 1 shows the category-wise distribution of expenses during my research internship with SCK CEN. As the work is computational, there are no added expenses in the table specific to the research activity. The amount spent over 3000 euros was agreed to be covered by Aalto University.

Table 1. Expected costs for 1st to 30th September, 2022

Type	Details	Euros	Remarks
Travel	both ways Flight (Helsinki to Brussels)	360	Based on lower range of flight prices offered for a travel in August. Since I can only book tickets after the decision that will most likely means 1 month before the travel
	both ways train (Brussels to Mol)	40	Based on approx. Belgium train prices
Accommodation	Long term stays	1500	Based on average Airbnb prices
Daily allowance	for 30days	1500	Covers food, travel to office and other daily expenses, based on 50 euros/day allowance
Total Sum		**3400 ****	

1.4. Mission composition

Host organisation

SCK CEN, Mol Belgium.

Host facility

Department of Chemical engineering and associated gas experimentation laboratory.

Mission dates

1st September 2022 – 3 September 2022


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

The internship comprises two main activities: a) Observation of the techniques and tools to perform gas diffusion experiments and subsequent replication in code Thebes (see Sect. 2.1), and b) Learning about the various scientific research at HADES underground facility at SCK CEN (see, Sect. 2.2).

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

The major part of the internship involves understanding the workflow of two multi-gas transport experiments and their subsequent simulation for Thebes framework validation. The experiments are a) short-term Gas diffusion experiment under controlled loading (Jacops et. al., 2017), and b) Long term gas experiment diffusion/Advection experiment under Isostatic cell conditions (Jacops and Maes, 2021).

Description

A short-term gas diffusion experiment under controlled loading (Jacops et. al., 2017) features two gases, methane and helium, flowing through a fully saturated Boom Clay sample of 8 cm diameter and 3 cm height with 0.38 porosity. The test maintains roughly 1:1 volume ratio of gas and water in the cylinder of 1 litre and 10 bar pressure for 72 days. The diffusion coefficients obtained from the experiments for methane and helium are 2.54e-10 m2/s, and 1.23e-9 m2/s, respectively.

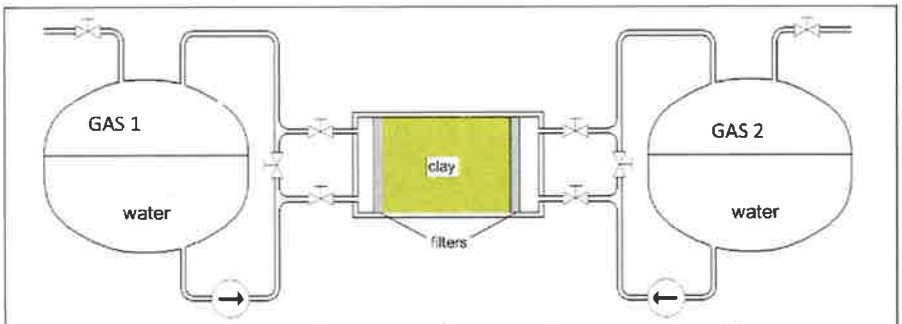

Fig. 1. Short-term gas diffusion experiment under controlled loading setup

Further, the ongoing long-term gas transport experiment (Jacops and Maes, 2021) works on a similar test setup where one chamber is pure gas (Helium). The experiment investigates the long-term effect of gas diffusion on Boom Clay (for example, dilatant pathways). Additionally, to monitor the transition in gas transport behaviour from diffusion to advection process, when the gas pressure is close to the minimum principal stress, using very slow gas pressure increments. The experiment uses an Iso-static cell pressure of 3 MPa, and the gas pressure increments at the helium side from 0.5 to 2.7 MPa while maintaining 0.5 MPa pressure at the dissolved methane chamber. The test achieves the 2nd loading cycle of 1 MPa during the internship.

Usage

The study utilises the derived Fick's law diffusion coefficient values from the experiments to regenerate the results computationally with Thebes. Further, to evaluate Thebes capabilities of handling multi-gas simulation by comparing the solution accuracy. Figure 2 depicts a few of the computed results from the internship showing a good agreement between the experiment and the simulation.

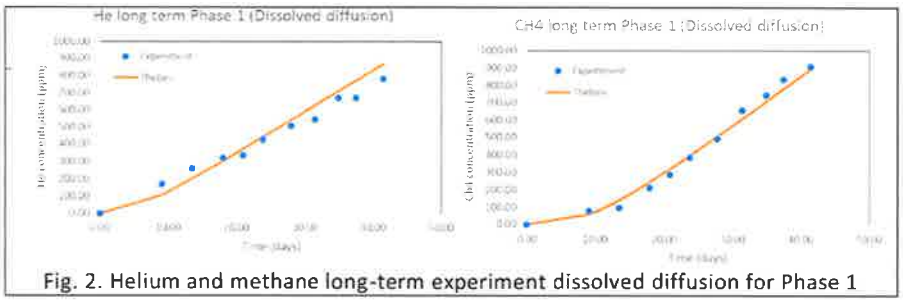

Fig. 2. Helium and methane long-term experiment dissolved diffusion for Phase 1

Benefits

Using the multi-gas flow experiments provides a partial validation for the extended framework of Thebes.

Limitations

Demonstrating and validating the full capability of Thebes framework, which can simulate multi-gas flow in a non-isothermal unsaturated medium, requires more experiments that can operate at highly coupled conditions. At present, building such experimental setups is a challenge due to equipment sensitivity toward gas and heat losses.

Applicability

In a broader application, Thebes can provide reliable predictive modelling for gas transport in a steady-state porous medium, such as for a nuclear waste repository. Additionally, Thebes can perform predictive modelling to study the influence of changing initial and boundary conditions for SCK CEN future experiments, for instance, the effect of varying temperatures and confining pressure in gas transport.

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

The other highlighting activity during the internship is touring the HADES lab. The visit helps to observe and learn about the various cutting-edge scientific research on nuclear waste management by SCK CEN.

Description

HADES is a world-class research facility that focuses on nuclear waste management. A 220 m deep structure built in Boom Clay provides real repository conditions that allow various studies on the transport behaviour of different types of radionuclides and gases, such as the effect of pore water pH, organic matter etc.

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

The technical tour of the lab gives an exciting opportunity to learn more about current research activities and experimental approaches.

Limitations

Replace this entire field with a description the limitations of this practice, technique, method, tool or system.

Applicability

The visit helps to identify the knowledge gap that can shape the future research plans at Aalto. For example, extending the numerical framework of Thebes to incorporate radionuclide transport under the influence of organic matter and variational pore water pH.

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

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3.1. Lessons learned and conclusions

The research outcomes are as follows:

1. Code Thebes – The research internship lead to the validation of a new and novel formulation of code Thebes. It increases the understanding of the physical process of gas transport in expansive soils. Additionally, building confidence in the predictive abilities of Thebes.

1. Joint publications – This research collaboration forms an exciting opportunity to produce joint publications. A conference paper on "Finite element modelling of multi-gas dissolved diffusion in expansive clay" at the Numerical Methods in Geotechnical Engineering 2023 conference in London is proposed (Abstract accepted).

2. EURAD – The research internship falls under the framework of EURAD gas WP 6 and Training WP13. The collaboration leads to scientific knowledge sharing between the experimental and computational teams. Therefore, increasing the reliability of gas transport phenomena in a nuclear repository.

SCK CEN plans to perform more gas transport experiments in future. The visit can initiate more prospective collaboration work and increase scientific contribution to the EURAD programme.

The code Thebes following the validation work will be applied to a final repository modelling of Ondraf/Niras conceptual design as per EURAD milestone 61, under full THM-G conditions, which will lead to added publications.

3. Personal Training Benefits – The internship is well-oriented with the research and publication requirements to fulfil my PhD studies at Aalto University. Besides an improved mechanistic understanding of the gas transport process, the visit will help familiarise me with the experimental approach to studying gas transport in clays. Further, it will provide hands-on experience in dealing with experimental and computational collaborative work strategies and expectations.

3.2. Relevant findings and conclusions for home organisation

This section is not mandatory but can be prepared with the mission supervisor or mentor from your home organisation. If applicable, replace this entire field with a description of about 200 words of findings and conclusions that are specifically relevant to your home organisation. If not applicable, remove the entire section.

3.3. Relevant findings and conclusions for host organisation

This section is not mandatory.

3.4. Relevant findings and conclusions for other organisations

This section is not mandatory.

4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

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

4.1. Generic potentials

This section is not mandatory.

4.2. Potentials for home organisation

This section is not mandatory

4.3. Potentials for host organisation

This section is not mandatory

APPENDICES

Mission journal

Table 1. Mission Journal

Days (1- 30th September 2022)	Activity
1st week	• Reading research papers and reports on gas experiments. • Lab visits and learning about the experiments: equipment, sample preparations etc. • Amendments in code Thebes to accommodate two gas flow to simulate the experiment
2nd Week	Amendments in code Thebes and the replication of short-term gas experiment.
3rd Week	• Replication of long-term experiments Phase 1 and 2. • Code amendments for other experiments, such as the diffusion of 4 gases in an unsaturated medium.
4th Week	• Code amendments for other experiments such as diffusion of 4 gases in an unsaturated medium and investigation on phase 3 of a long-term experiment. • Hades and plutonium lab visits. • Internship presentation.

Mission bibliography

1. Abed AA, Sołowski WT (2017) A study on how to couple thermo-hydro-mechanical behaviour of unsaturated soils: Physical equations, numerical implementation and examples. Comput Geotech 92:132–155. https://doi.org/10.1016/j.compgeo.2017.07.021
2. Abed AA, Sołowski WT (2020) Applications of the new thermo-hydro-mechanical-chemical coupled code "Thebes." Environ Geotech 7:3–16. https://doi.org/10.1680/jenge.18.00083
3. EURAD: Milestone 61 (2021) Technical Note defining a generic repository configuration, sets of parameters, conditions and relevant indicators.
4. EURAD: Milestone 173 (2022) Task 2.2 Experimental progress report.
5. EURAD: Milestone 174 (2022) Task 4.2 progress report on modelling and evaluation approaches applied to the generic repository derived from the conceptualizations of gas migration through geological disposal systemsand related processes, at the scale of a repository.
6. Jacops E and Maes N (2021), Status report long term gas injection end 2021 .

MOBILITY MISSION REPORT

MISSION BENEFICIARY

Abhishek Gupta
PhD Candidate
Department of Civil Engineering
Aalto University Finland

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Dr. Elke Jacops –
  Research project leader, Belgian Nuclear Research Centre (SCK CEN), Mol, Belgium.
- Dr. Norbert Maes
  Unit Head, SCK CEN, Belgian Nuclear Research Centre (SCK CEN), Mol, Belgium.
- Adithya S Gowrishankar –
  PhD candidate, SCK CEN, Belgian Nuclear Research Centre (SCK CEN), Mol, Belgium.

Home organisation experts

- Dr. Ayman abed –
  Senior Lecturer, Department of Architecture and Civil Engineering, Chalmers University, Gothenburg, Sweden.
- Dr. Wojciech T. Solowski –
  Associate Professor, Department of Civil Engineering, Aalto University, Espoo, Finland.

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	Abhishek Gupta	Wojciech T. Solowski	Elke Jacops
16-12-2022	Visa 	Visa 	Visa 


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