MOBILITY MISSION REPORT

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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).

MISSION TITLE

Visit of conference of the International Association for Mathematical Geosciences (IAMG) 2022

DESCRIPTION

Concerned organisations

Research entities

Concerned infrastructures or facilities

Laboratories of research entities

Concerned phases

- Phase 1: Site evaluation and site selection
- Phase 2: Site characterisation

Themes and topics

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

Heterogeneities in host rock formation; measurement uncertainty; data-to-model workflow; sorption data on minerals; geostatistics

EXECUTIVE SUMMARY

Safety of nuclear waste repositories in crystalline host rocks depends on realistic predictions of radionuclide migration in undisturbed geologies beyond the geotechnical barrier. There, fluids will migrate - in absence of large scale connectivities like fissures, fault systems and joints - along weakzones like microcracks, alterations and grain boundaries. The retention potential of crystalline rocks is thus not only controlled by its modal mineralogy but also by the (heterogeneous) distribution of mineral grains and the contact area of different mineral surfaces to migration paths. Until now, reactive transport models assume homogeneous and isotropic distribution of minerals in the host rock. Including the spatial correlation of transport and mineralogy, especially the modal mineralogy along fluid migration paths in the various scales, would significantly improve the estimation of radionuclide retention potentials.

In the conference contribution we focused on the small scale correlation in the microstructure. We presented a workflow from (real) samples to microstructure aware retention models, and discussed challenges of input data uncertainties, how they affect the model, and whether these models can be used for upscaling. Our approach is based on the idea that models for heterogeneous distribution of mineral phases can be derived by estimating spatial co-occurrences from measured microstructures. The resulting variability of "accessible" mineral surfaces then allows to derive (by geochemical speciation codes) the variability of contaminant distribution coefficients based on sorption data and pore water composition. We suggested for this problem to use graphs with mineral grains as nodes and contacts as edges. Finally, the lithological results are applied in reactive transport models to calculate the effective radionuclide retention within a representative rock volume.

1. MISSION BACKGROUND

1.1. R&D background

Safety of nuclear waste repositories in crystalline host rocks depends on realistic predictions of radionuclide migration in the undisturbed host rock. Until now, reactive transport models assume homogeneous and isotropic geological bodies beyond the geotechnical barrier and EDZ.
But granitoids are characterized by heterogeneities, e.g. like (healed) microcracks, zones of alteration, different distribution of modal mineralogy, changes of grain sizes, etc. The fluids will migrate - in absence open joints - along these weakzones.

Figure 1: Granites with typical heterogeneities, e.g. sharp grain size boundaries (left), thin Biotite-veins (middle) or alteration zones along old fluid migration paths (right)

Macroscopically observed reactive transport rates are strongly related to the processes at the mineral scale. We aim to improve the estimation of radionuclide retention potentials of granitoid rocks by including the spatial correlation of transport and mineralogy, i.e. the contact area of different mineral surfaces along migration paths, instead of using the bulk modal mineralogy.

The heterogeneities can be described by graphs:

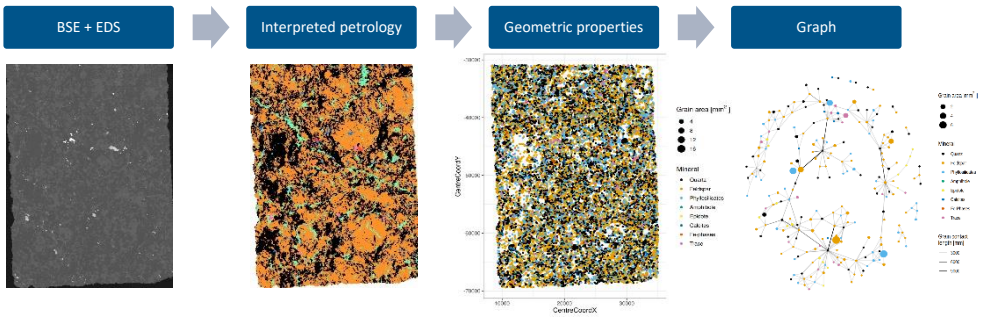

Figure 2: Workflow from measurement data to graph model.

1.2. Mission objectives

The International Association for Mathematical Geosciences IAMG is not yet involved in the research for nuclear waste repositories, but the members of the association are mainly concerned with modelling geological formations and elemental transport through geological bodies. As modelling the host rock is an important topic for the forthcoming of a deep seated nuclear waste repository exchange and cooperation of IAMG members with members of EURAD research entities might be fruitful. The conference visit aims at finding potential research cooperations for knowledge transfer into the EURAD community.

1.3. Mission request

The IAMG 2022 conference in Nancy, France, is an international conference in the field of geosciences organized by the International Association for Mathematical Geosciences IAMG (iamg.org), the Université de Lorraine and CNRS (GeoRessources laboratory, Centre de Recherches Pétrographiques et Géochimiques, Institut Elie Cartan de Lorraine, National Superior School of Geology). It aims to provide scientific exchange to researchers and students working on all subfields of mathematical geosciences and their applications, including classical and emerging subfields of statistics and geostatistics, artificial intelligence, machine learning, geoinformatics, geomodeling and computational methods.

The main themes of the conference include – among others - Compositional Data Analysis, Earth System Modeling, Geoinformatics, Geostatistics, Geotechnical Engineering, Geothermal Enginering, Hydrology and Hydrogeology, Inverse problems and data assimilation, Machine Learning, Natural risks and hazards, Optimization and Statistics..

1.4. Mission composition

Host organisation

Sending institution: Helmholtz-Zentrum Dresden-Rossendorf (HZDR)

Venue of conference: Nancy, France

Host facility

None

Mission dates

29.August – 3. September, 2022

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

Because this was a conference, no special practices, techniques or tools had been used during the mobility action.

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

Description

Usage

Benefits

Limitations

Applicability

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

Description

Usage

Benefits

Limitations

Applicability

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

Description

Usage

Benefits

Limitations

Applicability

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

Description

Usage

Benefits

Limitations

Applicability

3. MISSION FINDINGS AND CONCLUSIONS

3.1. Lessons learned and conclusions

IAMG conference provided a rich set of sessions with relevant content for the modelling the geological host rock for a nuclear waste repository. Several approaches presented at the IAMG conference have the potential to be transferred or translated into conceptual ideas for nuclear waste repositories. Especially concepts and workflows developed for resource estimations for future mines show a great potential to be transferred to the site selection and/or site planning, because the intial questions are similar. In my discussions with colleagues I also saw potential in translating methods for underground flow field analysis in combination with reactive transport for the requirements and settings of nuclear waste repositories, e.g. how to use graphs for element transport in porous or fractured rocks. Last but not least, the IAMG is leading in developing digital twins for geological settings and I had very fruitful discussions about this topic. I plan to incorporate selected ideas from the discussions as conceptual ideas in the report for the sub-task of DONUT.

3.2. Relevant findings and conclusions for home organisation

The IAMG could be a very interesting community of specialists for modelling host and cap rock formations. Especially if for future works digitalization and AI concepts are planned to be incorporated into models, IAMG conferences could also in future be a very interesting meeting option to forster new partnerships and develop new project ideas.

3.3. Relevant findings and conclusions for host organisation

None, because there was no host institution.

3.4. Relevant findings and conclusions for other organisations

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4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

4.1. Generic potentials

4.2. Potentials for home organisation

4.3. Potentials for host organisation

APPENDICES

Mission journal

28.8.: Travel to Nancy, France, from Dresden, Germany

29.8.: Planned conference trip to Meuse/Haute Marne Underground Research Laboratory (BURE) – skipped due to illness.

30.8.: Day1 of the conference

31.8.: Day2 of the conference, presenting own contribution

01.9.: Day3 of the conference, presenting own poster during poster session

02.9.: Day4 of the conference, networking about the contribution content

03.9.: Travel from Nancy, France, to Dresden, Germany

MISSION BENEFICIARY

Beneficiary requested his/her name not be published online
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PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- None, because this was a conference

Home organisation experts

- R. Tolosana-Delgado
- V. Brendler
- K. Bachmann
- J. Krause
- K. G. van den Boogaart
- F. Bok

Other organisations experts

- None

REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
Date of last signee	Name	Name	Name
	Visa	Visa	Visa