

MOBILITY MISSION REPORT

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KLIKNĚTE NEBO KLEPNĚTE SEM A ZADEJTE TEXT.

MISSION TITLE

Visit of the Goldschmidt2023 conference

DESCRIPTION

Concerned organisations

Research entities

Concerned infrastructures or facilities

Laboratories or 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

Europium; thermodynamic databases; aqueous speciation; radionuclide sorption on minerals; geochemical modeling

EXECUTIVE SUMMARY

Performance assessments of geological repositories for the underground disposal of high-level radioactive waste in deep geological formations require a deep understanding of the phenomena influencing the mobility of radionuclides, e.g. sorption, redox immobilization, surface precipitation, incorporation, etc. Reliable thermodynamic databases (TDB) are required in order to generate speciation calculations, surface complexation, and reactive transport models to predict the aforementioned mechanisms with the aim to achieve reliable and predictive safety assessments. Concerning europium, a lanthanide used as an analogue for trivalent actinides, there is currently no quality-assured and internationally recommended TDB such as the ones developed by Thermochemical Database Project of the Nuclear Energy Agency. Quality-assured refers to a transparent, internally consistent, and comprehensive thermodynamic database with recommended data derived from experimental measurements, with a clear selection procedure, a high traceability of data sources, as well as a transparent handling of uncertainties. The lack of such a collection of parameter sets severely hampers many modelling tasks concerning the application areas mentioned above.

In my contribution to the conference, I focused on the recommended data already published and on the selection procedure. I discussed with several attendees the current challenges and remaining data gaps, and could identify on which ligands (namely the hydroxide ion) to focus on for the next review paper. Furthermore, I could establish connections with several research groups also working on the complexation and solubility of f-elements in the low temperature regime to hydrothermal conditions. By combining my work with those of experimentalists (own work + that from scientific community), our team is convinced that it will be of benefit for the work package DONUT related to the development and improvement of numerical methods and tools for modelling of coupled processes.

1. MISSION BACKGROUND

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1.1. R&D background

In the work package DONUT (Development & Improvement Of NUmer-ical methods and Tools for modelling coupled processes), our team at HZDR contributes to topic 4 "Tools and methods to quantify/derive uncertainties induced by coupled processes". There, innovative numerical methods to treat uncertainty and sensitivity analysis on complex coupled representative cases (big systems, many media and input data) with strong non-linearities are being developed. All these efforts must be combined with the use of reliable thermodynamic databases.

I am working on developing a transparent, consistent, and robust thermodynamic database for europium (Eu), which can be used in aqueous speciation calculations, surface complexation, and reactive transport models. Eu is very commonly used as an analogue for trivalent actinides (Am, Cm), contributing considerably to the concern about the long-term safety of nuclear waste repositories. Currently, no international recommended thermodynamic databases as the ones developed by the Thermochemical Database Project of the Nuclear Energy Agency (NEA TDB) is available for europium.

Existing Eu thermodynamic databases have several drawbacks, a few of them being i) insufficient transparency about the selection procedure i.e. why certain data were selected and others not accepted ii) lack of systematic screening to gather primary literature sources, iii) too high reliance on the analogy with trivalent actinides iiiii) too high reliance on the charge analogy for the estimation of missing ion interaction coefficients when the Specific Ion Interaction Theory (SIT) was applied. Another important aspect concerns the lack of a proper consideration of the changes in the activity coefficients due to the replacement of up to 100 % of the background electrolyte anion (most often ClO₄⁻) by Cl⁻ or NO₃⁻ for weak complexes such as chloride and nitrate. Despite the significant number of investigations available, there are still some critical gaps in the europium thermodynamic database which need to be filled and which require the generation of new, consistent, and reliable thermodynamic data.

1.2. Mission objectives

My presentation at Goldschmidt2023 conference supports the transfer from geochemical and chemical thermodynamic aspects to the needs for nuclear waste management. Presenting our workflows and results as well as remaining open questions help to strengthen and foster contacts to a scientific community with extensive experience in geochemical modelling. The finalization of DONUT and the preparation of new activities within EURAD 2 will definitely profit from such a scientific exchange.

1.3. Mission request

The Goldschmidt2023 conference is an annual international conference on geochemistry and related subjects, organized by the European Association of Geochemistry and the Geochemical Society. Goldschmidt brings together scientists working on topics such as aqueous speciation of actinides/fission products/lanthanides and their retention at the solid/water interface, reactive transport modeling, uncertainty modelling, as well as the critical raw materials aspect (exploration, processing, recycling).

The main themes of the conference include – among others: Energy and resources, Environmental geochemistry and human health, Chemistry and physical processes of the oceans, Metals and nutrients in terrestrial and freshwater systems, Machine Learning and nanoscale techniques to big data, Vulcanology, Cosmochemistry..

1.4. Mission composition

Host organisation

Sending institution: Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR)

Venue of conference: Lyon, France

Host facility

None

Mission dates

9 July 2023 – 15 July 2023

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

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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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Applicability

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3. MISSION FINDINGS AND CONCLUSIONS

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3.1. Lessons learned and conclusions

The Goldschmidt2023 conference provided a rich set of sessions with relevant content for the modelling of the geological host rock for a nuclear waste repository. Several sessions were dedicated to the aqueous speciation/thermodynamics of lanthanides and actinides. It was very stimulating to discuss with colleagues working in the same field but on hydrothermal conditions. Since my work is related to low temperature data, both approaches are strongly complementary since the application of temperature-dependent equations such as the Helgeson-Kirkham-Flowers model strongly benefits from the accuracy of data at low temperature regime. I also observed that my first review paper about the thermodynamics of europium was of help for some colleagues working on the complexation of europium with sulphate ions in aqueous solutions as well as on the solubility of europium sulphate phases and that such an action for other ligands (with a priority for the hydroxide ion) is strongly required and expected by the scientific community. I will interact with these research groups on a regular basis in the future. Especially concepts and workflows developed for the handling of thermodynamic data from the raw data to the recommended values show a great potential to be transferred to other elements, since the needs and underlying questions are the same. This will definitely support the requirements for accurate and reliable surface complexation and reactive transport models in nuclear waste repositories. The analogy between trivalent lanthanides and actinides was also the topic of some discussions, for which some limitations were clearly revealed.

3.2. Relevant findings and conclusions for home organisation

The Goldschmidt conference is a very interesting community of specialists dealing with thermodynamic data for the modelling of radionuclides transport in the engineered and host rock formations. This conferences is 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

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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

APPENDICES

Mission journal

09.7.: Travel to Lyon, France from Dresden, Germany

09.7.: Day0 of the conference

10.7.: Day1 of the conference, presenting own poster during poster session

11.7.: Day2 of the conference, networking about the contribution content

12.7.: Day3 of the conference, networking about the contribution content

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

14.7.: Day5 of the conference, networking about the contribution content

15.7.: Travel from Lyon, France, to Dresden, Germany

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MISSION BENEFICIARY

Norbert JORDAN
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Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), Germany

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- None, because this was a conference

Home organisation experts

- Prof. Dr. Vinzenz Brendler
- Dr. Katharina Müller

Other organisations experts

- None

REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
Date of last signee	Norbert Jordan	Vinzenz Brendler	Name
	Visa	Visa	Visa