

# EURAD2 Annual Event 2025

Digital Transformation  
DITICO2o3o and HERMES

## Model-Hub

Bologna – 09-11.09.2025



*Co-funded by the European Union under Grant Agreement n° 101166718*

# Agenda

## HERMES Model-Hub Preface

- ▶ Lessons learned from EURAD1 [4]
- ▶ Opinion Papers [6, 3]
- ▶ ↪ Modelling strategy for EURAD2
  - ▶ Automated workflows (data and model integration)
  - ▶ Computational efficiency (HPC)
  - ▶ Machine Learning (Task 4)
- ▶ Model-Hub

**eurad**  
European Joint Programme  
on Radioactive Waste Management

**Frontiers in Nuclear Engineering**

**EURAD state-of-the-art report: development and improvement of numerical methods and tools for modeling coupled processes in the field of nuclear waste disposal**

E. Cerletti<sup>1</sup>, N.L. Prassanakis<sup>2</sup>, A. Balog<sup>3</sup>, D. Lukic<sup>4</sup>, G. Pagan<sup>5</sup>,  
D. Rosner<sup>6</sup>, M. Ammel<sup>7</sup>, G. Rizzo<sup>8</sup>, S. Boulton<sup>9</sup>,  
F. Bouchard<sup>10</sup>, J. Bourrel<sup>11</sup>, V. Bruneau<sup>12</sup>, B. Rzewuska<sup>13</sup>,  
O. Chaves<sup>14</sup>, S. V. Chubarov<sup>15</sup>, M. Hohen<sup>16</sup>, D. Horst<sup>17</sup>,  
J. Kaczmarek<sup>18</sup>, T. Krivoluta<sup>19</sup>,  
B. Lallemand<sup>20</sup>, J. Llorente<sup>21</sup>, J. Lutz<sup>22</sup>, E. Logunov<sup>23</sup>,  
I. Lopez-Villaseca<sup>24</sup>, R. Marquart<sup>25</sup>,  
A. M. Molinari<sup>26</sup>, A. P. Novotny<sup>27</sup>, S. S. Park<sup>28</sup>,  
A. Puchala<sup>29</sup>, S. Sannino<sup>30</sup>, X. Wang<sup>31</sup>,  
Y. Yang<sup>32</sup>, H. Zura<sup>33</sup>

**Environmental Earth Sciences (2022) 60:8420**  
<https://doi.org/10.1007/s00167-022-09674-4>

**EDITORIAL**

**Digitalisation for nuclear waste management: predisposal and disposal**

Olaf Kolditz<sup>1,2\*</sup>, Dominik Jacques<sup>3</sup>, Frédéric Cérelle<sup>4</sup>, Jérôme Bertaud<sup>5</sup>, Sergey V. Chubarov<sup>6</sup>, Christophe Delaey<sup>7</sup>, Sébastien Deville<sup>8</sup>, Sébastien Galli<sup>9</sup>, Jean-Michel Guiguer<sup>10</sup>, Christophe Leterrier<sup>11</sup>, Dominique Létolle<sup>12</sup>, Bertrand Lévesque<sup>13</sup>, Bertrand Louiset<sup>14</sup>, Bruno Mathieu<sup>15</sup>, Nikolaj L. Prassanakis<sup>16</sup>, Karsten Röhl<sup>17</sup>, Jeanne Samper<sup>18</sup>, Ingrid Scherzer<sup>19</sup>, François Valente<sup>20</sup>, Jérôme Witten<sup>21</sup>

Published online: 1 January 2022  
© The Author(s) 2022

**Abstract**

This science digitalization and a artificial intelligence (AI)-based model approach were coined as well as industry and in changing the way sciences were viewed to be well suited, especially for data intensive application, etc. In the recent past, particularly, data-driven and physics inspired AI models have been applied for many scientific fields, including nuclear waste management cycle. In addition to process-based approaches for creating safety methods and high performance computing are leveraging the potential of high-fidelity simulation and digital twin. In this respect, AI processes, multi-scale and probabilistic approaches in Digital Twins of complex systems can be considered as a major challenge. However, the general problem is how to use AI methods for the predictive challenge for DTR in radioactive waste management in the continuation of EURAD1. In this context, the main target of EURAD2 is to provide the challenge for DTR in radioactive waste management in the continuation of EURAD1. In this context, the main target of EURAD2 is to provide the challenge for DTR in radioactive waste management in the continuation of EURAD1. In this context, the main target of EURAD2 is to provide the challenge for DTR in radioactive waste management in the continuation of EURAD1. In this context, the main target of EURAD2 is to provide the challenge for DTR in radioactive waste management in the continuation of EURAD1. In this context, the main target of EURAD2 is to provide the challenge for DTR in radioactive waste management in the continuation of EURAD1. In this context, the main target of EURAD2 is to provide the challenge for DTR in radioactive waste management in the continuation of EURAD1. In this context, the main target of EURAD2 is to provide the challenge for DTR in radioactive waste management in the continuation of EURAD1.

**Keywords** Environment • Nuclear energy • Artificial intelligence • Data science • Machine learning • Geochimistry • Numerical methods

**Environmental Earth Sciences (2022) 60:8419**  
<https://doi.org/10.1007/s00167-022-09669-7>

**ORIGINAL ARTICLE**

**Paper on high fidelity simulations for coupled multiphysics and chemistry in geological disposa**

S.V. Chubarov<sup>1\*</sup>, E. Cerletti<sup>2</sup>, A. Iltan<sup>3</sup>, D. Jacques<sup>4</sup>, J. Gorisetti<sup>5</sup>, O. Kolditz<sup>6</sup>

Received: 1 July 2021 / Accepted: 22 August 2021 / Published online: 29 August 2021  
© The Author(s) 2021

**Abstract**

This option paper describes the major applied F10M in hydrogeochemical and geochemical simulation system and the history of related model development. Several approaches and open research questions with respect to the further development of hydrogeochemical and geochemical models are discussed. The focus is given to the application of hydrogeochemical models for coupled multiphysics and chemistry in geological disposal systems. These include the use of micro-simulation and mesoscale models for the description of multi-phase flow and solute mixing in porous media and flow modelling for model development.

**Keywords** F10M-C processes • Reactive transport • High fidelity simulation

**Introduction**

The purpose of this editorial is to abridge the scope of the Topic Collection on "Topical Collection for Nuclear Waste Management Cycle: Predisposal and Disposal". We look at waste treatment, waste disposal as well as surface and groundwater protection. This is to be done by different methods, processes, algorithms and systems to reduce or eliminate risks to the environment and humans. Moreover, this is an important indicator for future decision making and is revolutionizing the way of research already to a large extent (von der Ahe 2020). Originally, data science was

\* To whom the correspondence should be addressed.  
✉ olaf.kolditz@tu-dresden.de

**Environmental Earth Sciences**  
Published online: 22 October 2021  
© Springer Nature Limited 2021  
This article is licensed under a Creative Commons  
Attribution 4.0 International License, which permits  
use, sharing, adaptation, distribution and  
reproduction in other formats, without prior permission or  
authorization, subject to the terms and conditions  
outlined in the Terms of Use agreement. Further  
distribution of this version is not permitted.  
The original publication is available at  
<https://doi.org/10.1007/s00167-021-01049-2>

**Introduction**

Geochanical and reactive transport modelling in a necessary tool need to investigate subsurface processes (Kolditz et al. 2012, 2021; Buelens et al. 2016; Huang et al. 2018). Numerical simulation models have been developed for stable hydro-chemical geo-reactive conditions and to understand reaction pathways and associated processes. These coupled hydro-chemical reactions in the subsurface environment provide the best solution to predict the behavior of the natural system (Kolditz et al. 2022). Some of the mechanisms investigated are listed in Table 1.

**What are coupled geohydrochemical models?**

Based on its philosophy, a coupled model consists of two parts: Level 1 models (L1) and Level 2 models (L2). The

in al. 2009; Patel et al. 2019). Reactive transport models couple fluid flow, heat transfer and solute transport with chemical reactions and physical processes operating under nearly controlled conditions. The results of such models can be used to design and assess the long-term performance of the repository and its ability to contain the radionuclides over time (Suzuki and Hyodo 2009).

© Springer Nature Switzerland AG 2021  
This article is licensed under a Creative Commons  
Attribution 4.0 International License, which permits  
use, sharing, adaptation, distribution and  
reproduction in other formats, without prior permission or  
authorization, subject to the terms and conditions  
outlined in the Terms of Use agreement. Further  
distribution of this version is not permitted.  
The original publication is available at  
<https://doi.org/10.1007/s00167-021-01049-2>

**Environmental Earth Sciences**  
Published online: 22 October 2021  
© Springer Nature Limited 2021  
This article is licensed under a Creative Commons  
Attribution 4.0 International License, which permits  
use, sharing, adaptation, distribution and  
reproduction in other formats, without prior permission or  
authorization, subject to the terms and conditions  
outlined in the Terms of Use agreement. Further  
distribution of this version is not permitted.  
The original publication is available at  
<https://doi.org/10.1007/s00167-021-01049-2>

**Topic Collection on Digitalisation**

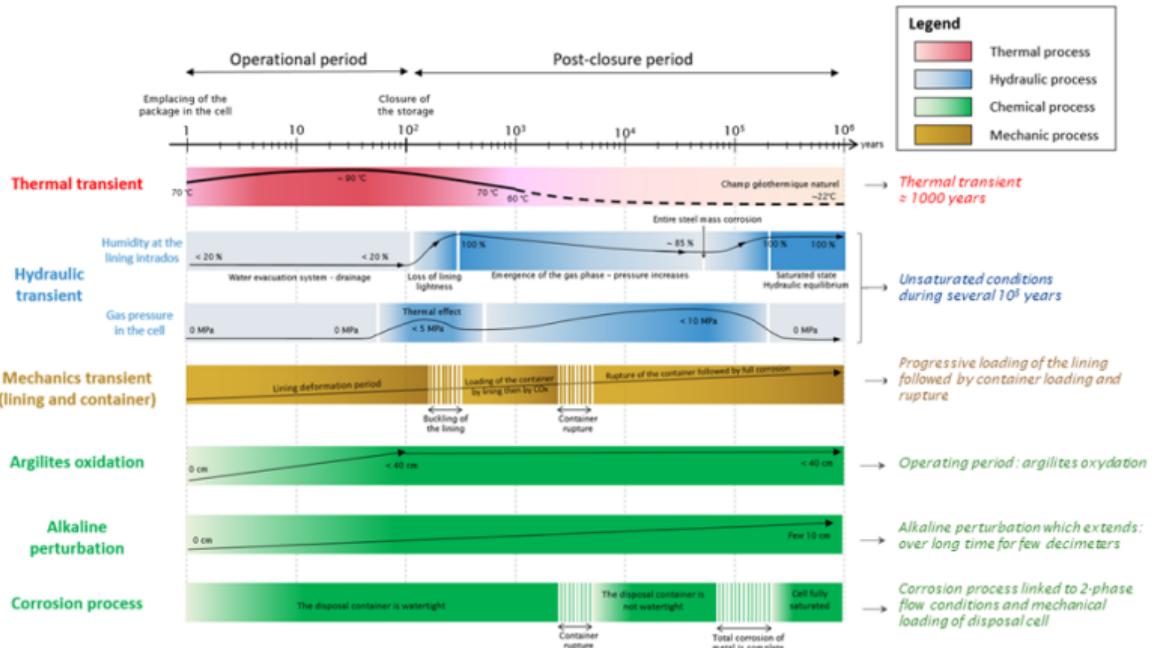
Springer

Top 1

# Introduction

# THMC Processes

## EURAD HERMES Task 3



Collaborative platform  
for code development  
and data management

ST2.3

Data and Model Integration

ST3.3

HERMÈS

ST3.1

Benchmarking  
Coupled Processes  
Computational Performance

ST3.2

Inverse Modelling  
Sensitivity Analysis  
Upscaling

Churakov et al. (2024) Position paper on THMC processes and modeling [3]

Top 2

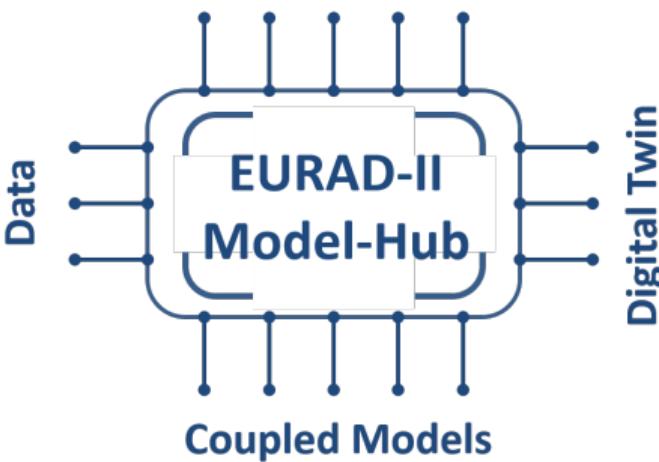
# Model-Hub

# Collaborative platform for data and model integration

Model-Hub (HERMES Kick-Off (11/2024))

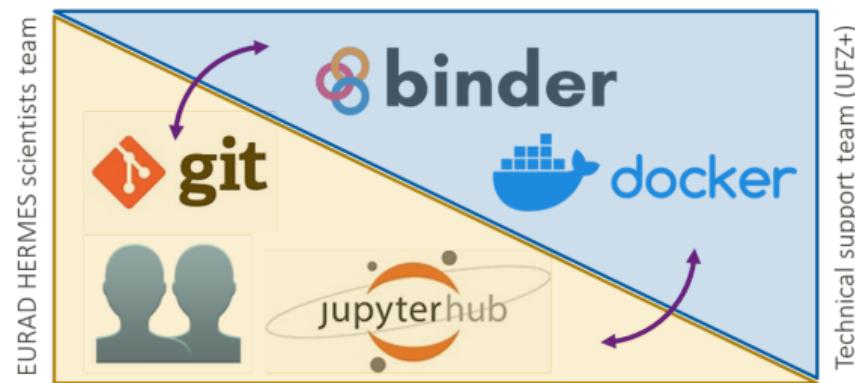
Idea

## Process- and data-driven models



Implementation concept

binder: providing the computational web-platform  
docker: providing the software environment (Python et al.)

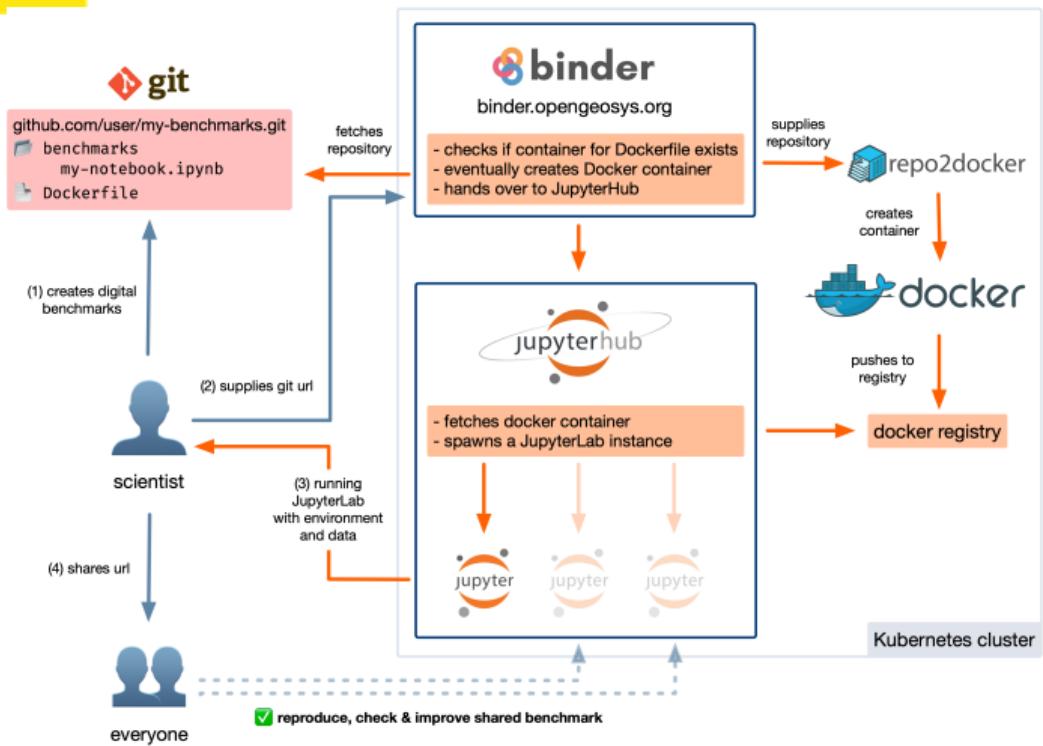


git: version-management for repos (scientists + hermes)  
jupyterhub: working environment for scientists

eurad

# Collaborative platform for data and model integration

Model-Hub: Infrastructure development (available 09/2025)



## Admin side (UFZ server)

- ▶ hard- and software
- ▶ OGSTools
- ▶ container technology
- ▶ git version management

## User side

- ▶ interesting examples
- ▶ Jupyter notebooks
- ▶ GitLab skills

eurad

# Collaborative platform for data and model integration

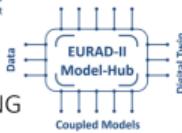
Model-Hub: Thematic Web-Interface (available 09/2025)

**eurad<sup>2</sup>**  
European Partnership  
on Radioactive Waste Management

Process- and data-driven models

DIGITAL BENCHMARKING

Data → EURAD-II Model-Hub → Coupled Models → Digital Twin



CLASSIC BENCHMARKS ANALYTICAL SOLUTIONS



**DECOVALEX 2027**

MODEL COMPARISON AGAINST EXPERIMENTS

MATERIALS

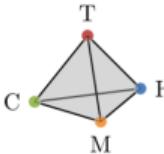


SOURCE: BGE

CLAY – SALT - CRYSTALLINE

DIGBEN & EURAD#HERMES MODEL-HUB SOFTWARE-FRAMEWORK

PROCESSES AND SCALES

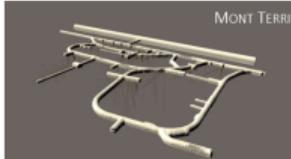


LAB SCALE



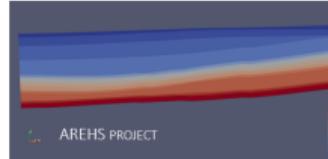
GREAT HALL (EDINBURGH)

URL SCALE



MONT TERRI

FIELD SCALE



AREHS PROJECT

# Collaborative platform for data and model integration

## Model-Hub: Layer-Structure



### WebLayer

structured user-web-interface organized by thematic areas:  
materials, processes, scales > projects

### InfoLayer

specific information about thematic areas including literature links  
> list of current benchmarks and examples (extending)

### JupyterLab

interactive Jupyter Notebooks of benchmarks and examples < coding area for interactive work



Top 3

## Model-Hub Demo

<https://www.opengeosys.org/hub/>



eurad



Top 4

# Synthesis and Next

# Synthesis

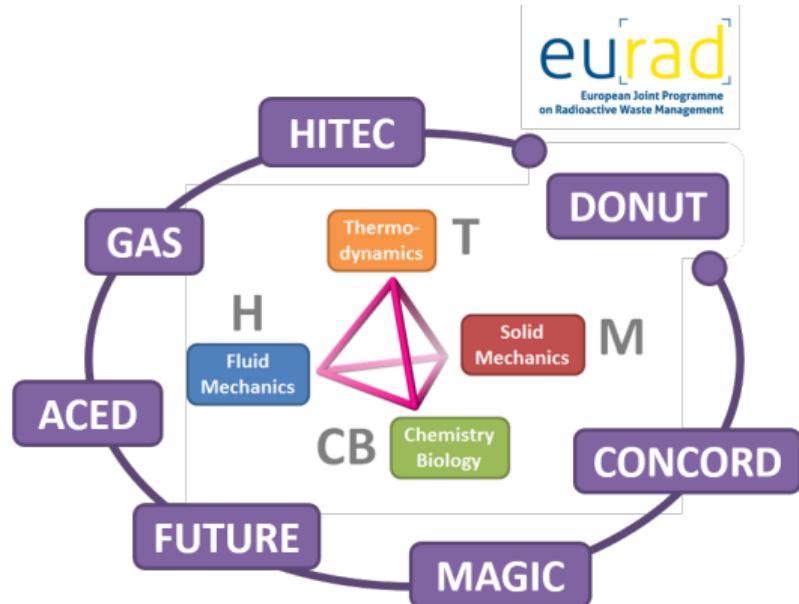
added value

What added value does the Model Hub bring?

- ▶ fosters networking on strategic AND technical levels, Claret et al. (2024) [4]
- ▶ contribution to KM
- ▶ contribution to FAIR

Workflows and Automation are prerequisites for Digital Twins (DITOCO)

EURAD Digi-Session on safeND 2025 (next week in Berlin)



eurad

# Next →

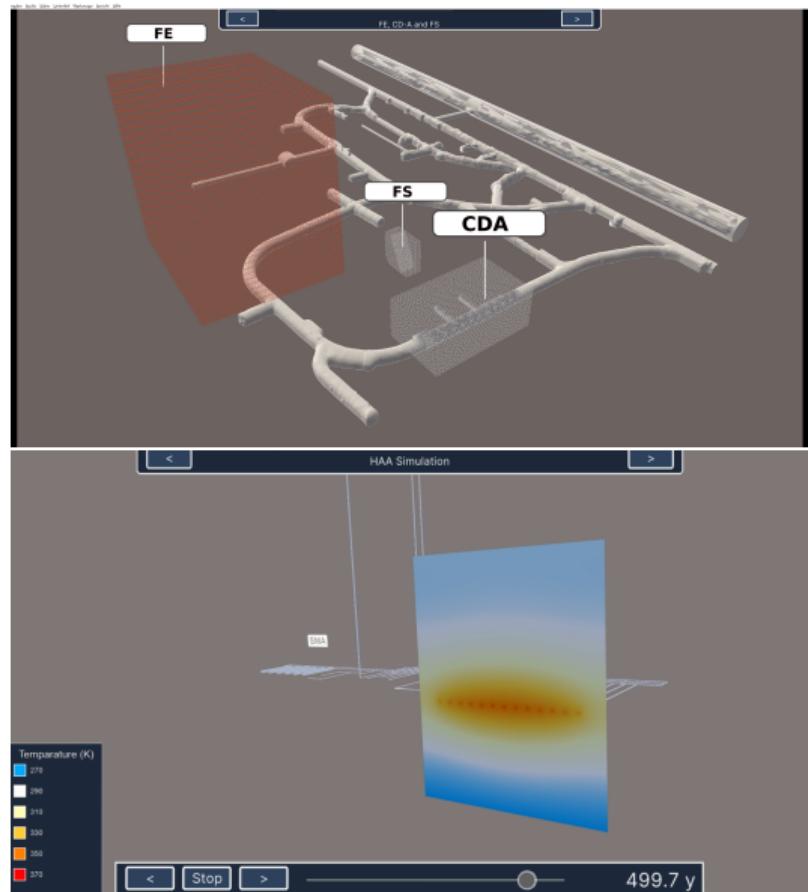
With Jupyter Notebooks (ipynb)  
to Workflows (snakemake/aiida)

## Benchmarking

- ▶ ANCHORS benchmarking exercises
- ▶ HERMES Annual Meeting (24-25.11.2025 Leipzig) hackathon for integration
- ▶ DECOVALEX links

## Workflows for complex applications

- ▶ ipynb's can be fully integrated (e.g. tools for performance/safety indicators)
- ▶ Data and model integration in Mont Terri, Graebling et al. (2024) [5]
- ▶ Workflows for safety cases (snakemake, aiida), Bilke et al. (2025) [1]



# Acknowledgements and Partners



European Partnership  
on Radioactive Waste Management



DigBen    OpenWorkflow



# References |

- [1] Lars Bilke et al. "Reproducible HPC software deployments, simulations, and workflows – a case study for far-field deep geological repository assessment". In: [Environmental Earth Sciences](#) 84.16 (2025). DOI: [10.1007/s12665-025-12501-z](https://doi.org/10.1007/s12665-025-12501-z).
- [2] Jens T. Birkholzer et al. "DECOVALEX-2023: An international collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems". In: [Geomechanics for Energy and the Environment](#) 42 (2025). Cited by: 0. DOI: [10.1016/j.gete.2025.100685](https://doi.org/10.1016/j.gete.2025.100685). URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-105006976962&doi=10.1016%2fj.gete.2025.100685&partnerID=40&md5=a79e864363093548fd3a6cf19bb5c941>.
- [3] S.V. Churakov et al. "Position paper on high fidelity simulations for coupled processes, multi-physics and chemistry in geological disposal of nuclear waste". In: [Environmental Earth Sciences](#) 83.17 (2024). Cited by: 4; All Open Access, Hybrid Gold Open Access. DOI: [10.1007/s12665-024-11832-7](https://doi.org/10.1007/s12665-024-11832-7). URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-85202876737&doi=10.1007%2fs12665-024-11832-7&partnerID=40&md5=ae5b196c808b7ccb8fa1cee7d93d3ad8>.
- [4] F. Claret et al. "EURAD state-of-the-art report: development and improvement of numerical methods and tools for modeling coupled processes in the field of nuclear waste disposal". In: [Frontiers in Nuclear Engineering](#) 3 (2024). Cited by: 7; All Open Access, Gold Open Access. DOI: [10.3389/fnuen.2024.1437714](https://doi.org/10.3389/fnuen.2024.1437714). URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-85214023365&doi=10.3389%2ffnuen.2024.1437714&partnerID=40&md5=428a4b7fb55008122a93bd29437c6235>.
- [5] Nico Graebling et al. "VR-EX – An immersive virtual reality serious game for science communication about the electrical resistivity tomography measurements in the Mont Terri Rock Laboratory, Switzerland". In: [Environmental Earth Sciences](#) 83.10 (2024). DOI: [10.1007/s12665-024-11613-2](https://doi.org/10.1007/s12665-024-11613-2). URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-85192849857&doi=10.1007%2fs12665-024-11613-2&partnerID=40&md5=a13e5cea164158ca515437db59187d5f>.
- [6] Olaf Kolditz et al. "Digitalisation for nuclear waste management: predisposal and disposal". In: [Environmental Earth Sciences](#) 82.1 (2023). Cited by: 19; All Open Access, Green Open Access, Hybrid Gold Open Access. DOI: [10.1007/s12665-022-10675-4](https://doi.org/10.1007/s12665-022-10675-4). URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-85145415563&doi=10.1007%2fs12665-022-10675-4&partnerID=40&md5=b25a80bca286c383d6353e25cfa85002>.
- [7] Christoph Lehmann et al. "OpenWorkFlow—Development of an open-source synthesis-platform for safety investigations in the site selection process; [OpenWorkFlow – Entwicklung einer Open-Source-Synthese-Plattform für Sicherheitsuntersuchungen im Standortauswahlverfahren]". In: [Grundwasser](#) 29.1 (2024). Cited by: 9; All Open Access, Hybrid Gold Open Access, pp. 31–47. DOI: [10.1007/s00767-024-00566-9](https://doi.org/10.1007/s00767-024-00566-9). URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-85183908802&doi=10.1007%2fs00767-024-00566-9&partnerID=40&md5=22e95b5f3b269dfe6c4d398cba8f39c1>.

# References II

- [8] N.I. Prasianakis et al. "Geochemistry and machine learning: methods and benchmarking". In: [Environmental Earth Sciences](#) 84.5 (2025).  
Cited by: 0; All Open Access, Hybrid Gold Open Access. DOI: [10.1007/s12665-024-12066-3](https://doi.org/10.1007/s12665-024-12066-3). URL:  
<https://www.scopus.com/inward/record.uri?eid=2-s2.0-85218421007&doi=10.1007%2fs12665-024-12066-3&partnerID=40&md5=97db00b959521194f3a8534ef57a6d51>.