ASME
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Digitalization and Digital Twins in Long Term Management of Radioactive Waste

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Introduction

“Digital Twins” “Digitization” “AI/MR” “VR”

Advancements in data science, digitalization, digital twin concepts have large potential for all phases of long-term radioactive waste management.

EURAD-PREDIS discussion group

Objective

Present first examples related to digitalization/DT in the framework of EURAD & PREDIS.
EURAD and PREDIS

- European Joint programme on Radioactive Waste Management
- 2019-2024
- 17 WPs (incl. 10 R&D WPs)
- 115 partners from 20 Member States, 3 associated countries, 3 international partners
- 59,9 M€

- Pre-disposal management of radioactive waste
- 2020-2024
- 7 WPs
- 47 partners from 17 countries
- 23,7 M€
Example 1 Accelerating reactive transport models via machine learning

The geochemistry and machine learning benchmark, organized within EURAD-DONUT aims at providing a point of reference for testing codes and models and for addressing the challenges relevant to:

1) producing consistent high quality training datasets using the major geochemical codes, which will be usable by all available ML methods

2) using neural network, polynomial chaos expansion, Gaussian processes and other ML methods to learn from the generated data

3) measuring and assessing the accuracy (and speed) of predictions for geochemical calculations (and for reactive transport simulations.)
Geochemistry and machine learning benchmark

Input

<table>
<thead>
<tr>
<th>Variable heading</th>
<th>Description</th>
<th>Unit</th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaO</td>
<td>Amount of CaO</td>
<td>mole</td>
<td>0.1</td>
<td>1.8</td>
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<tr>
<td>SiO2</td>
<td>Amount of SiO2</td>
<td>mole</td>
<td>0.2</td>
<td>0.7</td>
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<tr>
<td>H2O</td>
<td>Mass of water</td>
<td>kg</td>
<td>0.05</td>
<td>0.15</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
<td>°C</td>
<td>25</td>
<td>25</td>
</tr>
</tbody>
</table>

Output

Blind test Machine learning model accuracy (MSE)

Preliminary results of surrogate model performance for the simplest case (Mean square error MSE of the output):
Each colour represents a different surrogate model
Example 1 Accelerating reactive transport models

• 1D RT in a Ca – Si cementitious system
• With portlandite and a solid-solution representation of the C-S-H phases
• Replacement of the geochemical solver in the HPx model by a trained emulator
  • DNN (parametric – careful training needed)
  • kNN (non-parametric – no actual training needed)
• Good emulation accuracy and speedup of about 5 (20) against 4-core (single-threaded) HPx
Concentration time series of at 3 observation nodes across the profile
Example 2 Digital decision platform for pre-disposal activities: geoml.eu

A collaborative digital tool development, educational and demonstration platform has been developed within EURAD-PREDIS, ready to accept hundreds of users.

https://digitaltwin.geoml.eu/

Digital Twin Demo relevant to waste package degradation
Example 2 Digital decision platform for pre-disposal activities
Outlook – Digital twins for a geological repository

<< Geological context

Model integration (CD-A) >>
Overview of all experiments (interactive), visual data base

<< Integration of small scale geological structures (fractures)

Sensor data integration (CD-A) >>
Outlook – Digital twins for a geological repository

Visual Digital Twin for the Underground Research Laboratory Mont Terri (in close collaboration with swisstopo and partners of the Mont Terri project)

Mixed and augmented Virtual Reality applications through (online) data and model integration, interactive navigation through the URL for research and educational purposes

Conclusion

• First steps taken for digitalization and digital twins
  • Acceleration for modelling of coupled multi-physic processes
  • Prototypes integrated environments

• Way forward
  • Uniform terminology
  • Identifying potential roles
  • Tackle scientific and technical challenges

Current discussion group
Special issue (next slide)

Integrated in proposal of EURAD-II in work packages or specific tasks
Topical Collection in Environmental Earth Sciences on Digitalisation

- Artificial intelligence and machine learning
- Extended reality (XR)
- Geological and building information models (BIM)
- Data processing
- High-performance computing
- Coupled processes: multi-physics and chemistry
- Knowledge management
- Roadmap: The way forward