Experimental characterizations of 30-year-old radioactive waste packages and its use for the development of digital twins

RAINER DÄHN, PAUL SCHERRER INSTITUT

25th of October 2023
Pre-disposal management of radioactive waste

WP7: Innovations in cemented waste handling and pre-disposal storage

T7.1 Management

T7.2 State of the art

T7.3 Testing and monitoring

T7.4 Digital Twin

T7.5 Data and Decision

T7.6 Demonstration

T7.7 Reporting

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 945098.
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Background T7.4 Digital Twin

Input data:
- Composition (cement, aggregates, waste, ...)
- Design, geometry
- Storage conditions (Monitoring data)

Digital twin
User Interaction (choosing recipes, models, etc)

Digital twin
(summary computer model of waste package integrity evolution, surrogate models)

Predicted integrity evolution
- Gas production
- Volume expansion
- Package corrosion
- ...

Output:
- Gas production
- Volume expansion
- Package corrosion
- ...

Decision framework (dashboard), decisions for the user

Calibration, validation
Data from characterization of old cemented waste packages, old cement samples, ...

Numerical, geochemical and chemo-mechanical models for: moisture evolution, carbonation, ASR, gas generation, metal corrosion, swelling reactions etc.

Sensing and monitoring
Background – 200l drums with waste

- Steel reinforcement
- Pressed waste
- Empty space
- Mortar
- Steel casing of the 200 l drum (0.135 cm)
Background – Swiss Federal Interim Storage Facility (BZL)

Swiss Federal Interim Storage Facility on the PSI campus was built for the interim storage of all radioactive waste from medicine, industry, and research and went in operation in 1992. Capacity for interim storage is expected to be needed up to 2065.
# Material inventory

<table>
<thead>
<tr>
<th>Drum Nr.</th>
<th>Date conditioning</th>
<th>Bulk mass</th>
<th>Al</th>
<th>ORGANICA</th>
<th>PVC</th>
<th>Steel</th>
<th>Na-22</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Tara</td>
<td>kg</td>
<td>kg</td>
<td>kg</td>
<td>kg</td>
<td>kg</td>
</tr>
<tr>
<td>1303</td>
<td>24.06.1994</td>
<td>25</td>
<td>4.5</td>
<td>101.1</td>
<td>38.5</td>
<td>329</td>
<td>101.1</td>
</tr>
<tr>
<td>1312</td>
<td>18.07.1994</td>
<td>25</td>
<td>4.5</td>
<td>125.1</td>
<td>38.5</td>
<td>353</td>
<td>100.1</td>
</tr>
</tbody>
</table>
Activity inventory according to gamma spectrometry measurements in January 2022 (initial nuclide Na-22)

<table>
<thead>
<tr>
<th>Nr.</th>
<th>Date conditioning</th>
<th>Mass of the raw waste</th>
<th>K-40</th>
<th>Cs-137</th>
<th>Pb-214</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>kg</td>
<td>Bq</td>
<td>Bq/kg</td>
<td>Bq</td>
</tr>
<tr>
<td></td>
<td>Exemption limit</td>
<td>1000</td>
<td>100</td>
<td>1E+05</td>
<td></td>
</tr>
<tr>
<td>1303</td>
<td>24.06.1994</td>
<td>101.1</td>
<td>7E+04</td>
<td>692</td>
<td></td>
</tr>
<tr>
<td>1312</td>
<td>18.07.1994</td>
<td>125.1</td>
<td>3E+04</td>
<td>240</td>
<td>400</td>
</tr>
</tbody>
</table>

Inventory data together with the sampling concept were submitted to the Swiss Federal Nuclear Safety Inspectorate (ENSI), and approved within 6 weeks.
Sampling of two cement drums created in 1994
Sampling of cement drums created in 1994
### Reconditioning

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<table>
<thead>
<tr>
<th>Number of the drum</th>
<th>Material</th>
<th>Mass [kg]</th>
<th>Date of the clearance measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-1303, P-1312</td>
<td>Steel 200-l-drums</td>
<td>57</td>
<td>26.08.2022</td>
</tr>
<tr>
<td>P-1312</td>
<td>Steel of the waste drums</td>
<td>42</td>
<td>25.10.2022</td>
</tr>
<tr>
<td>P-1303, P-1312</td>
<td>Inactive mortar</td>
<td>406.5</td>
<td>16.11.2022</td>
</tr>
<tr>
<td>P-1303</td>
<td>Steel of the waste drums</td>
<td>48.5</td>
<td>24.11.2022</td>
</tr>
<tr>
<td>P-1303</td>
<td>Rubber, paper/wood, plastic, PVC</td>
<td>62.1</td>
<td>Conditioned as burnable waste</td>
</tr>
<tr>
<td>P-1312</td>
<td>Aluminum, paper/wood, plastic, PVC</td>
<td>54.5</td>
<td></td>
</tr>
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</table>
Characterization of cemented waste at KIT provided by PSI (from Swiss interim storage facility)

Methods foreseen in the characterization at KIT

- XRD: phase identification
- TG-DTA: phase identification, water content
- mycro-CT: spacial distribution
- Alkaline dissolution + ICP OES/MS analyses: elemental analysis
- XRF: elemental analysis
- SEM-EDS: morphology and elemental analysis (surface technique)
- XPS: elemental analysis, oxidation state analysis
- Others …
X-ray microtomography

- Identification of two well-defined regions, characterized by two different porosities.
X-ray microtomography

- Identification of two well-defined regions, characterized by two different porosities.

Pore size distribution determined for one of the samples in the upper drum position
Fe particle interlinked with SiO$_2$, with background dominated by portlandite.
XRD

- XRD characterization completed for selected samples.
- Calcite identified in all samples
- Evaluation of XRD patterns on-going.
XPS

- XPS analysis completed for upper / middle / bottom samples.
- Preliminary evaluation suggests decreased Ca:Si ratio of cement in upper layers of the drum.

![Graph showing XPS analysis results]

PSI-CSH.2.spe: 1.P15-Deckel OBCR 1312
PSI-CSH.3.spe: 2.P10-OBEN Rechts 1303
PSI-CSH.4.spe: 3.P12-MITTE Rechts 1303
PSI-CSH.5.spe: 4.P15-UNTEN Rechts 1302
TG-DTA (thermogravimetric analysis)

- TG-DTA characterization completed for selected samples.
- Evaluation of TG-DTA on-going. Information on cement phases, e.g. calcite.
SCK-CEN: Drum-scale Alkali Silica Reaction (ASR) experiment - design

- 2 mixes
  - Reactive RCA – recycled aggregate
  - Non-reactive SIB – Sibelco sand
- 2 temperatures
- Duration: 2 years

Mortar samples
w/c ratio = 0.47
Sand/cement = 2
Sensors and placement

- Inside concrete
  - Vibrating strain gauge (8)
  - Temperature (8)
- Lid of the barrel
  - Pressure
- Ambient
  - Temperature
  - Humidity
- Acoustic Emission
  (top of concrete, circumference of the barrel)
This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 945098.

Vibrating strain wire
Temperature sensor

Placement based on a digital twin model
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Temperature, Humidity, Pressure

Heating belts
Digital twin workflow

Industrial scale experiments → Sensing

Sensing → Compare with measurements → Update the model

Laboratory data → Constitutive law → Additional lab data

Improved understanding of in situ performance

Digital twin
Digital TWIN 1.0 a toolkit of models

- A collection of models (simplified) that predict the evolution.
- Ability to run processes on different compositions / input waste package properties.
- Assess different waste package compositions for possible problems in chemical evolution.
- Predict the normal evolution and identify exceptional cases using monitoring.
Technical implementation / user interaction

- Use of Jupyter notebook development environment to run the models based on user input
- Can call GEMS/Orchestra/other codes/ for doing geochemical calculations
- Different models can be added, input/output can be developed
- Can be run on an online platform (e.g., GeoML.eu, google colab, binder, setup on Azure) or installed and run on a local machine (use of sensitive data)
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Ongoing work

• Implement additional models
• Refine the input and output – user interaction
• Would need access to a database of waste composition (to provide relevant input for users)
Digital TWIN 2.0 – real time monitoring/evolution

- Data cycle between package – sensors and database
- Data cycle between the Digital Twin and the database
- data formats / interfaces to connect and queries to retrieve data
Work on ASR example

• Laboratory experiments – accelerated alkali-silica-reaction
• Analytical model for expansion and strain evolution
• Monitoring at the waste package level – used to actively optimize a model that then can make predictions
• Simple geochemical / kinetic model for aggregate dissolution and ASR product formation could also be tested
• In principle the model can also be used in DT 1.0
Github (actions) and metadata

- **https://github.com/predis-h2020** (public) - everybody is welcomed – can be also transferred to other solutions
- Develop a consistent solution from the minimal example – works / tested / can be referred by everyone
- github actions a “free” solution that can be used in the demonstrator to trigger the DT workflow.
- Can run on Azure or locally (private data)
VLJ-luola and Swiss repository for LLW and ILW

Finland 60–100 m in bedrock

Switzerland ~800 m in Opalinus clay

nagra.ch/en/downloads/report-the-site-for-the-deep-geological-repository-nagras-proposal/

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.
Conclusions

- Experiments under enhanced conditions (e.g. in temperature) are suitable to get an in-situ understanding of reactions ongoing in the waste forms (like SCK-CEN is performing). The use of real scale waste forms avoid problems with upscaling of laboratory based experiments.

- Even simple mechanical models implemented in a digital twin (DT) are sufficient to predict the long-term behavior of waste forms. If chemical reactions are expected to occur, additionally geochemical models can be implemented in the DT.

- If the drums are stored under controlled humidity (e.g. in predisposal), and the solidification of the waste was well thought through, these drums are expected to be safe for the next 30-50 years.

- At the time the disposal site goes operational it should be considered to check if the radioactivity in the waste packages is below the exemption limit.
Acknowledgements

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Suresh Seetharam
Quoc Tri Phung
2024 Final Conference

3 – 7 June 2024 at Novotel Avignon Center, Avignon, France
20 Bd Saint-Roch, 84000 Avignon - https://all.accor.com - 15 min from Avignon TGV Rail station

Welcome to:
- learn the outcomes of the 4-year project on technology innovation & developments in predisposal of radioactive waste management
- connect with the pre-disposal community and end users

Restricted to consortium partners 3-4 June, public open to all 5-7 June

Registration is Now Open! https://www.lyyti.in/PREDIS_Final_Conference_03070624
More details at tuned https://predis-h2020.eu/

Also included: Technical visits in Marcoule CEA Center

This project has received funding from the Euratom research and training programme 2019-2020 under grant agreement No 945098.
# First preliminary agenda

**PREDIS Final Conference 3-7.6.2024, Avignon, France**

<table>
<thead>
<tr>
<th><strong>Monday 3.6.2024 13 – 18 CET</strong></th>
<th><strong>Wednesday 5.6.2024 - Public</strong></th>
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<tbody>
<tr>
<td><strong>WP1 Management Team meeting + dinner</strong>&lt;br&gt;• Restricted only to PREDIS Management Team</td>
<td><strong>Scientific presentations from all WPs</strong>&lt;br&gt;• incl. Student presentations</td>
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<tr>
<td><strong>WP3 Students session</strong>&lt;br&gt;• Only for PREDIS Students</td>
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<thead>
<tr>
<th><strong>Tuesday 4.6.2024 9 – 17 CET</strong></th>
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<tbody>
<tr>
<td><strong>All PREDIS Partners</strong></td>
<td><strong>Thursday 6.6.2024 - Public</strong>&lt;br&gt;<strong>Main results and impacts</strong>&lt;br&gt;• Presentations and two panel discussions <strong>Conference dinner</strong></td>
</tr>
<tr>
<td><strong>9-10 WP1 – WP3 specific issues</strong></td>
<td></td>
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<tr>
<td><strong>10-15 WP4-7 Own parallel sessions</strong>&lt;br&gt;• Feedback, lessons learnt, final reporting, budgetting</td>
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<tr>
<td><strong>15-17 General Assembly, other issues</strong></td>
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<td><strong>17.30-19.30 Guided city/palace tour (optional)</strong></td>
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</table>

<table>
<thead>
<tr>
<th><strong>Friday 7.6.2024 9-13 (optional)</strong></th>
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</thead>
<tbody>
<tr>
<td><strong>All PREDIS Partners (and EUG, if spaces allows)</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Technical visit to CEA Marcoule (max 50 p)</strong></td>
<td></td>
</tr>
</tbody>
</table>