European Partnership on Radioactive Waste Management

EURAD-2 Spotlight on Cutting Edge Science

10th September 2026

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

Moderators

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on Radioactive Waste Management

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

Work In the Framework of
Eurad-2 WP6 STREAM

European Partnership
on Radioactive Waste Management

Corrosion of Magnesium alloy in geopolymer: In situ corrosion and mechanical alteration monitoring

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Plan

1. Context
2. Magnesium Corrosion: Key Concepts
3. Experimental Study
4. Numerical Study
5. Conclusion

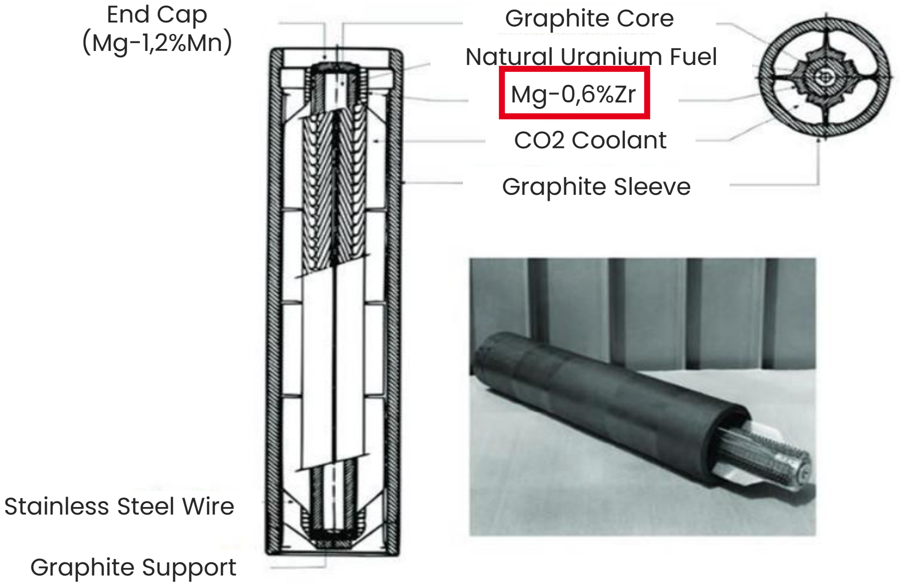
Context

Uranium Natural Graphite Gaz UNGG Reactors

- ***Fuel:* Natural Uranium**
- ***Moderator:* Graphite**
- ***Coolant:* CO2**

UNGG Assemblies

- **Metallic Uranium Rod**
- **MgZr alloy Cladding**
- ***Two MgMn alloy end caps***
- ***Tubular Graphite Sleeves***

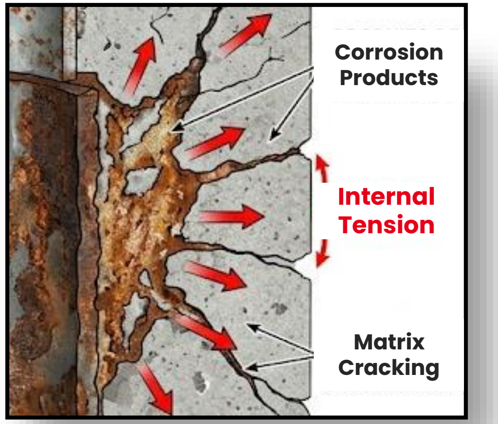


UNGG Fuel Element

Generation of Reactive Nuclear Waste →

Mg-Zr alloy cladding embedded in a geopolymer matrix [ANDRA-DECIMAL]

⚠ **If poor binder formulation: Metal corrosion** →



Context

Phenomenon

Generation of expansive products due to corrosion

Risk

Degradation of the mechanical properties of the waste package

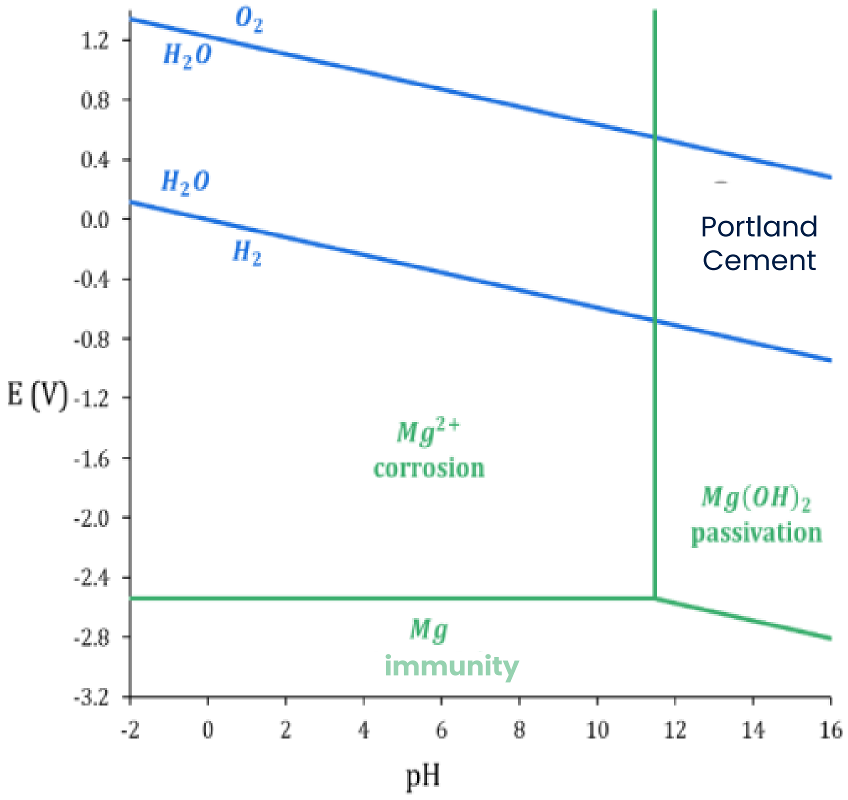
Challenge

Experimentally reproduce and model the hydro-chemo-mechanical interactions between the metal and its binder to ensure storage safety

Outline

- State of the art on Magnesium Corrosion and its monitoring in nuclear waste conditioning matrices
- Experimental Study of Magnesium Corrosion in Geopolymer Matrices
- Development of a First, Simplified Hydro-Chemo-Mechanical Model Based on Experimental Results

Magnesium Corrosion: Key Concepts



Pourbaix's Diagram

➡ $A\ pH < 11{,}5 : Mg + 2H^+ \rightarrow Mg^{2+} + H_2$

➡ $A\ pH > 11{,}5 : Mg + 2H_2O \rightarrow Mg(OH)_2 + H_2$

Galvanic Corrosion of Magnesium

$$Mg + 2H_2O \rightarrow Mg^{2+} + H_2 + 2HO^- \rightarrow Mg(OH)_2 + H_2$$

Formation of expansive corrosion products

Hydrogen gas generation

What is a Geopolymer?

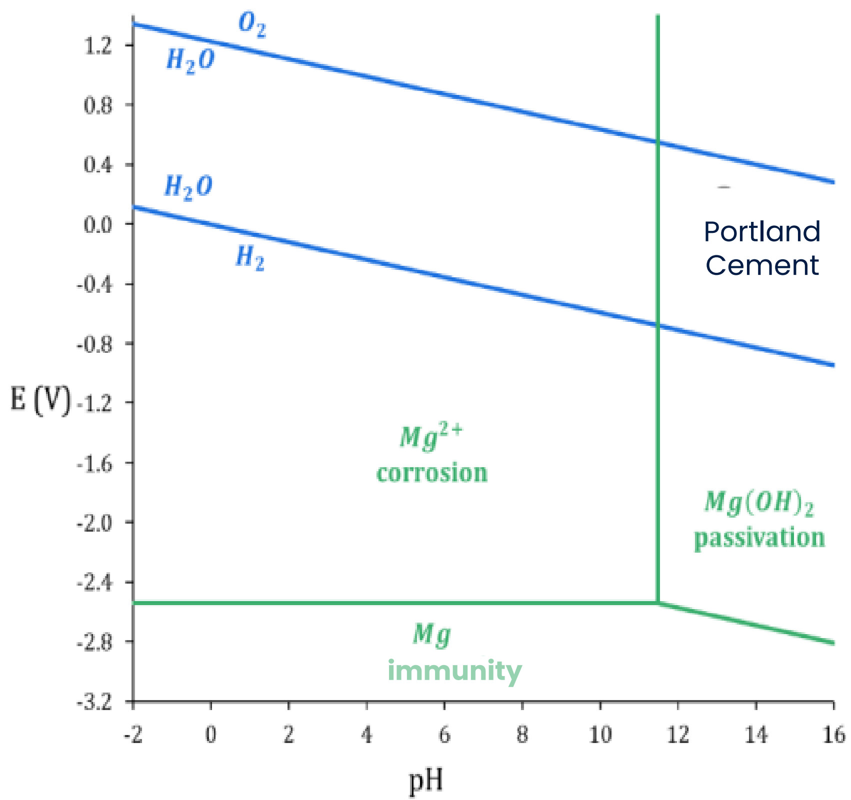
$$M_n\{-(SiO_2)_z - AlO_2\}_n.wH_2O$$

- Cation (Na, K, Cs)
- Degree of polycondensation
- Si/Al Ratio (1-3)
- Water Molecules

Aluminosilicate-based material activated with alkaline solutions

$1Na_2O\text{-}3{,}96SiO_2\text{-}1Al_2O_3\text{-}12{,}5H_2O$

Magnesium Corrosion: Key Concepts



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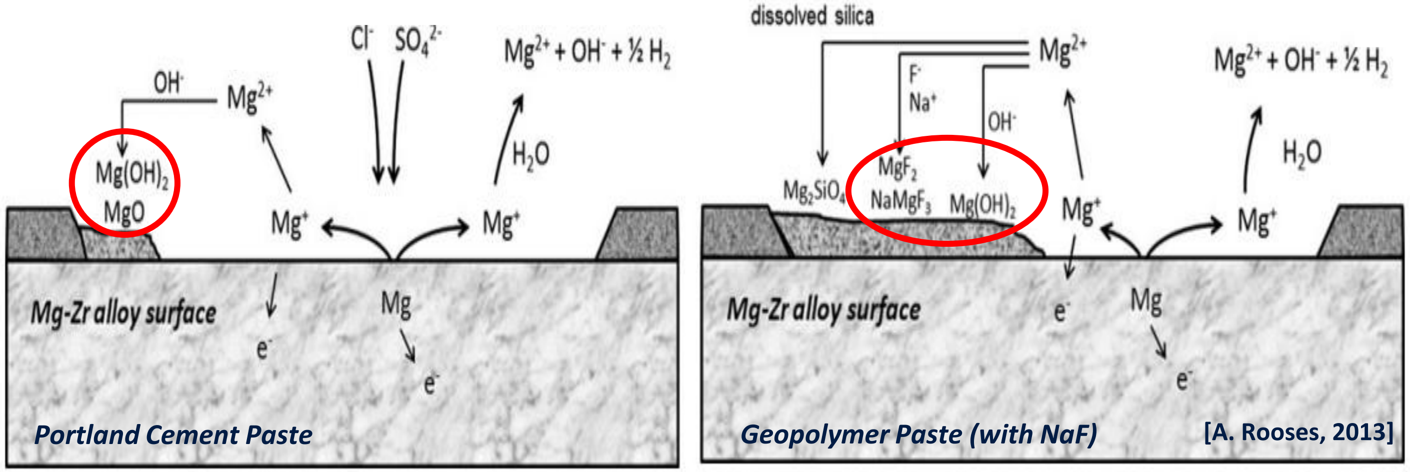
Formation of expansive corrosion products

Hydrogen gas generation

Why The Geopolymer?

- ph>11 → Passivation domain
- NaF → More protective layers than $Mg(OH)_2$

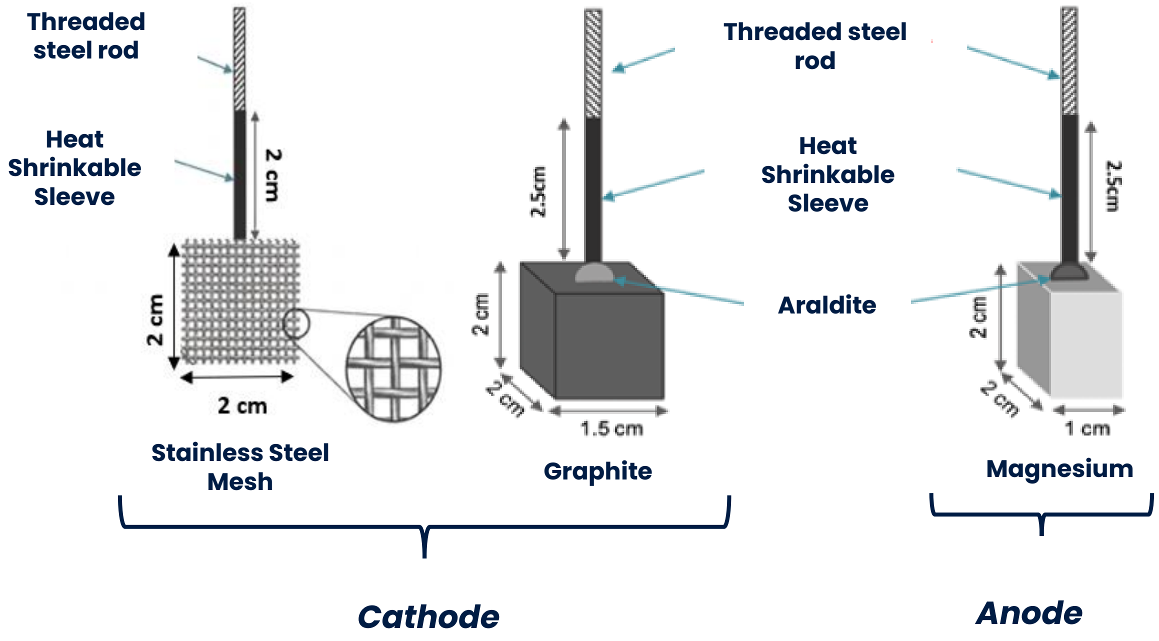


Experimental Study

Study of Mg–graphite or Mg–stainless steel galvanic couples in geopolymers for future electrochemical testing

More Significant Corrosion – Easier To Measure

Electrodes



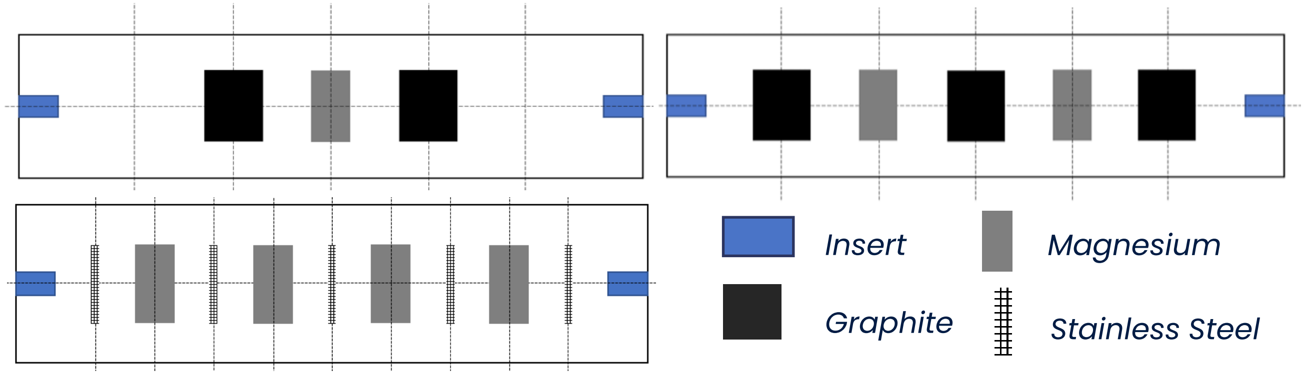
Choice Of Geometry

Mechanical + Corrosion

Displacements Measurements

Electrochemical tests

4*4*16cm Specimen



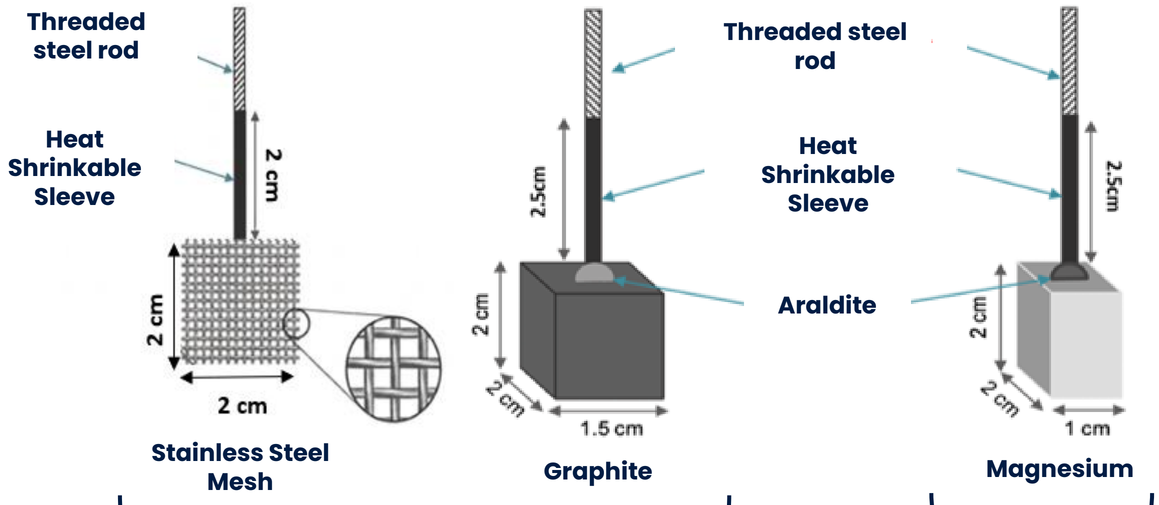
Configurations proposed to optimize specimen displacement based on numerical simulations

Experimental Study

Study of Mg–graphite or Mg–stainless steel galvanic couples in geopolymers for future electrochemical testing

More Significant Corrosion – Easier To Measure

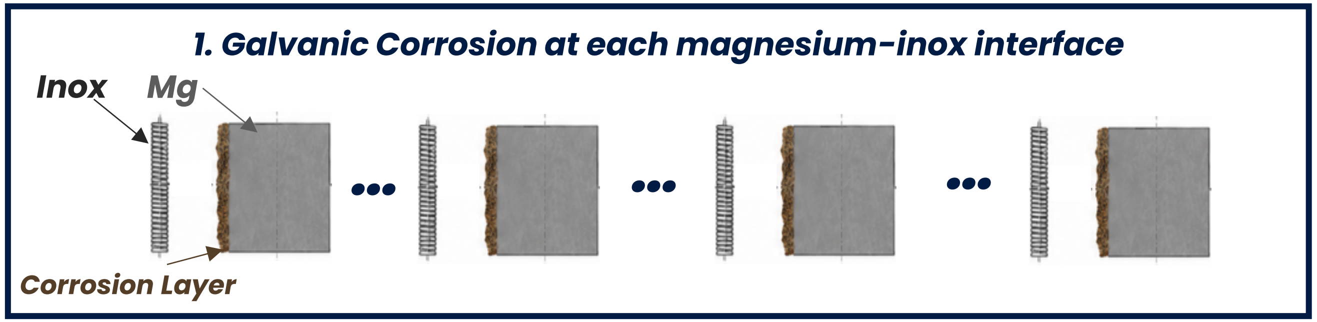
Electrodes



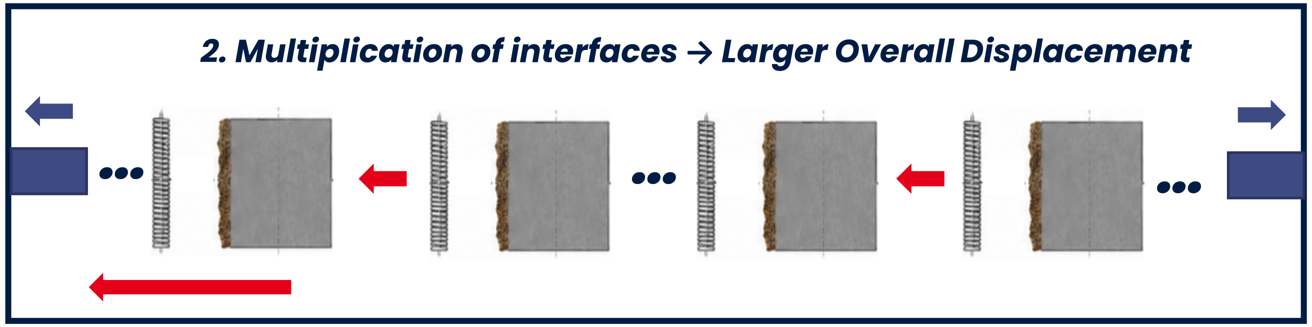
Cathode

Anode

Choice Of Geometry



Each Mg-Inox interface corrodes → Local material degradation & displacement



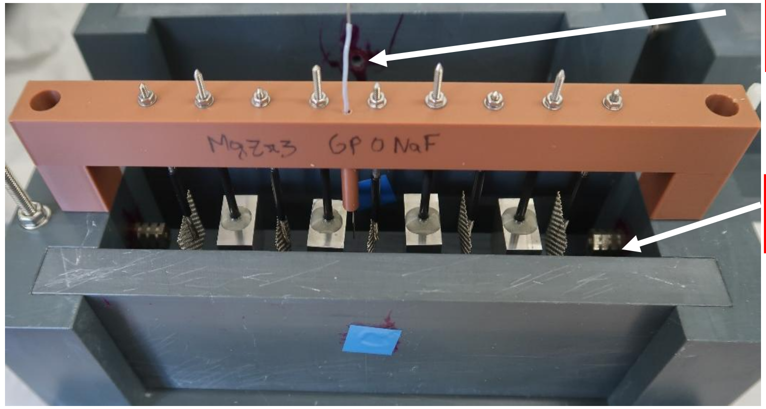
Corrosion at multiple interfaces accumulates → Larger displacement

Cumulative expansion across many interfaces

Experimental Study

Methodology for all configurations

Custom-designed standardized molds



Platinum wire as reference

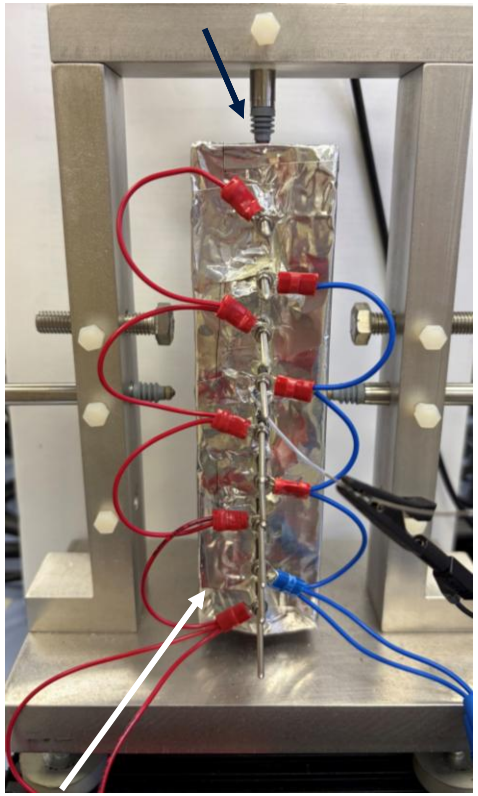
Inserts for LVDTs

LVDT: Linear Variable Differential Transformer (Displacement Sensor)

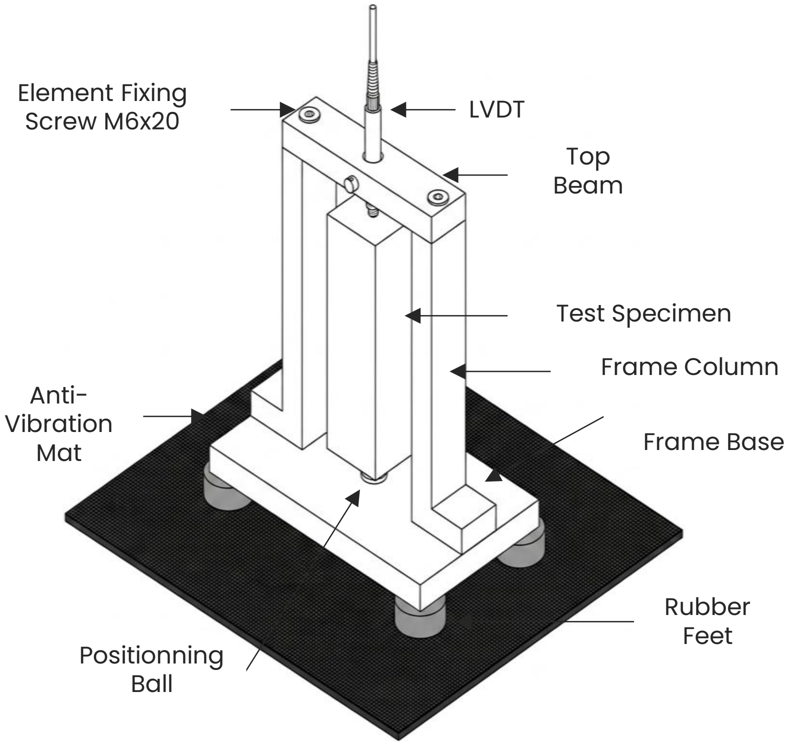
4 × 4 × 16 cm specimens for electrochemical tests

Reference Specimens (Mg_Mn covered with varnish)

LVDT



Potentiostat-linked connectors

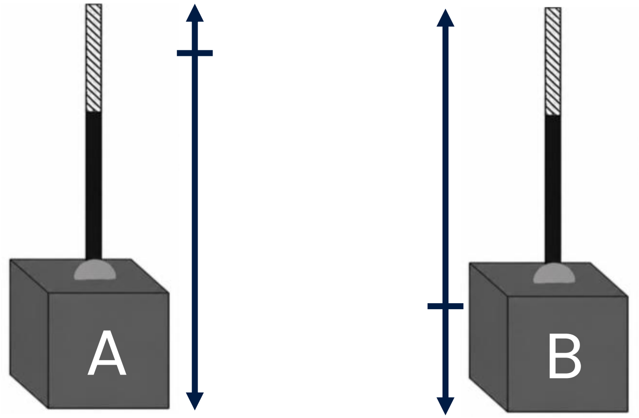


Specimen placement in a custom-designed frame for electrochemical tests and displacement measurements

Experimental Study

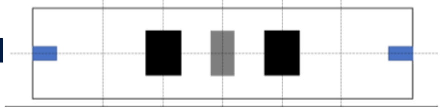
Electrochemical Method:
Zero Resistance Ammeter (ZRA)

Potential A **Potential B**



Experimental Study

Configuration 1



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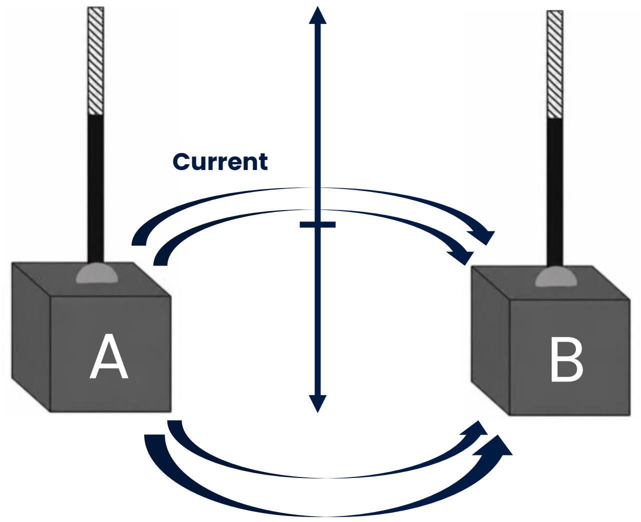
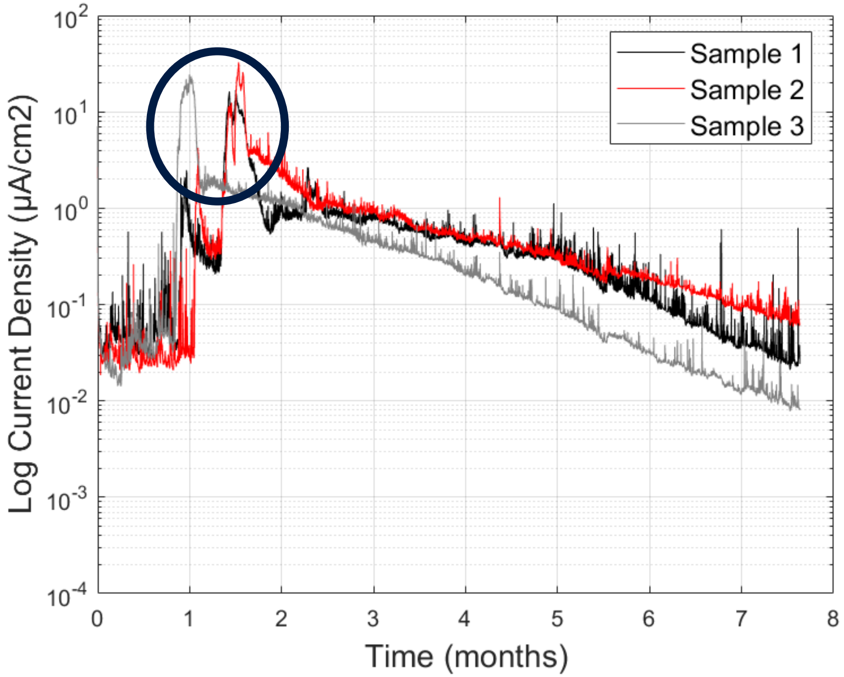
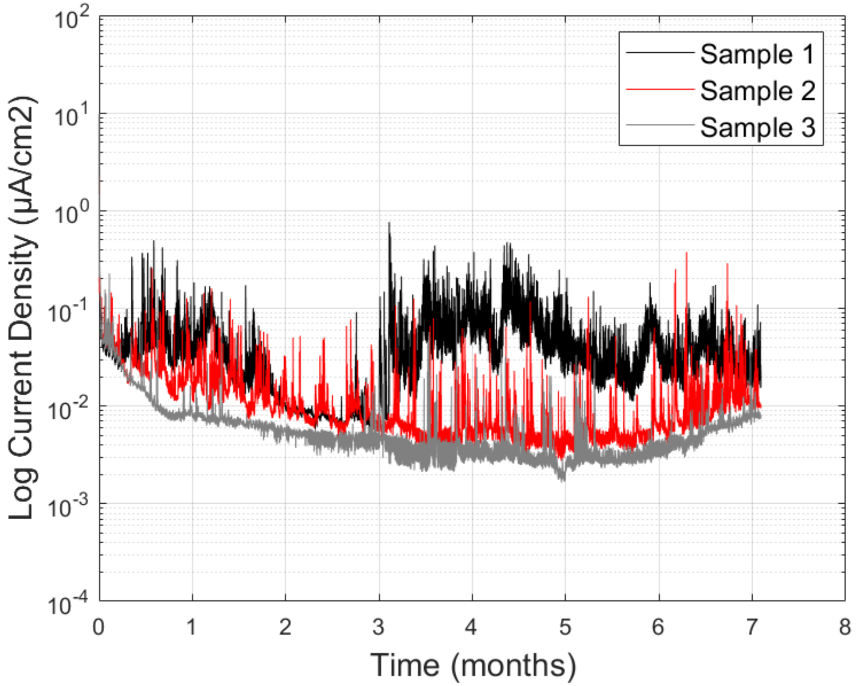


Without NaF



With NaF



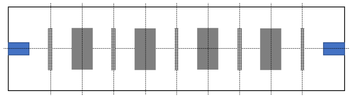
Calculated quantities	GP 0 NaF			GP 1,25 NaF		
	Sample 1	Sample 2	Sample 3	Sample 1	Sample 2	Sample 3
Charge (Coulombs)	222	295	236	10,5	3,75	2,57
Mass of corrosion products (mg)	27,9	37,2	29,7	1,3	0,47	0,32
Equivalent thickness of corroded metal (μm)	10	13,4	10,7	0,48	0,17	0,12
Average corrosion rate (μm/year)	16	21,4	17,1	0,81	0,29	0,2

For 7 months

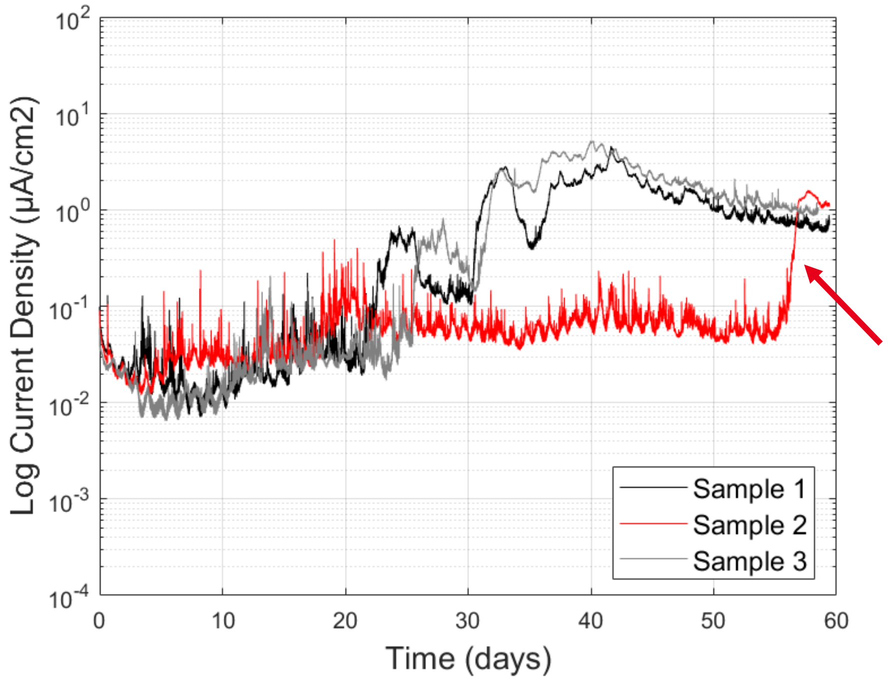
→ **NaF shows corrosion-inhibiting behavior**

Experimental Study

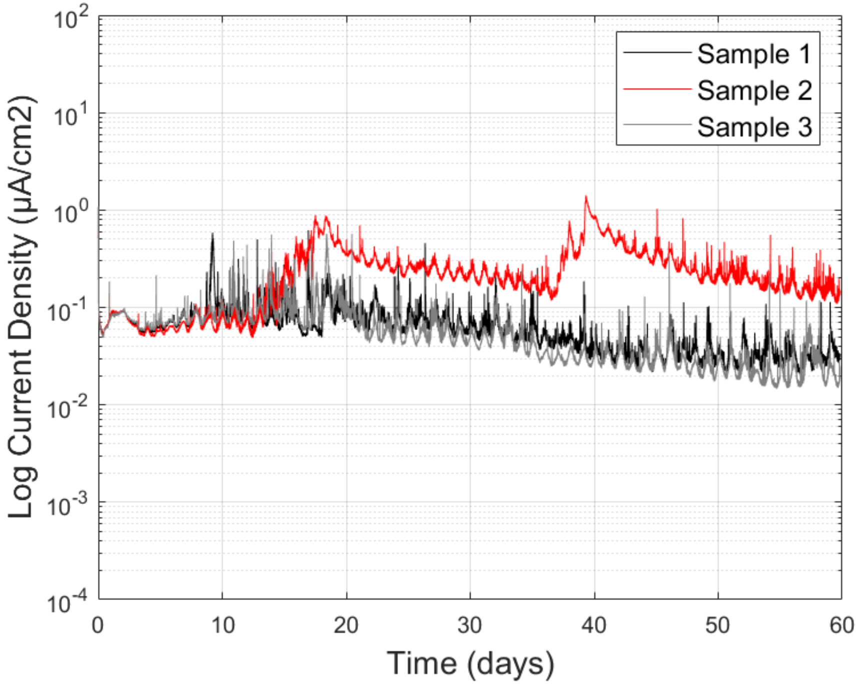
Configuration 2



Without NaF



With NaF



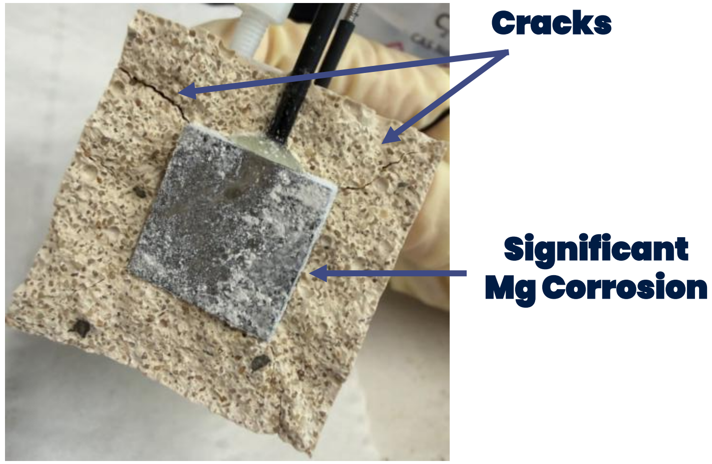
Calculated quantities	GP 0 NaF			GP 1,25 NaF		
	Sample 1	Sample 2	Sample 3	Sample 1	Sample 2	Sample 3
Charge (Coulombs)	244	36,84	342,37	20,19	78,15	18,13
Mass of corrosion products (mg)	3,07	0,46	4,31	0,25	0,98	0,23
Equivalent thickness of corroded metal (µm)	1,10	0,17	1,55	0,09	0,35	0,08
Average corrosion rate (µm/year)	6,79	1,02	9,52	0,56	2,15	0,50

For 2 months

→ NaF shows corrosion-inhibiting behavior (Further monitoring is required, as corrosion is a slow process)

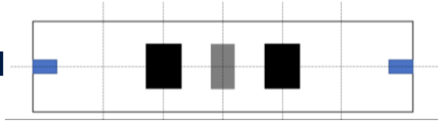
Experimental Study

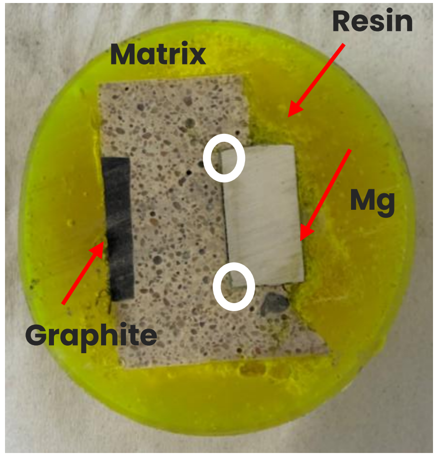
Without NaF : Specimen Fractured in two pieces

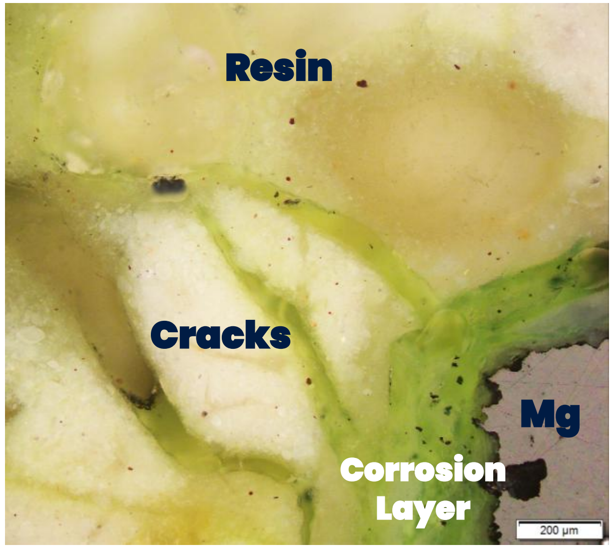


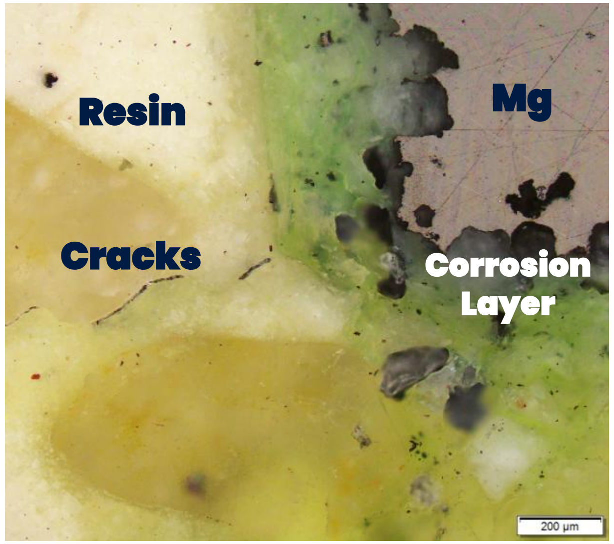
With NaF : Specimen remained intact

Configuration 1





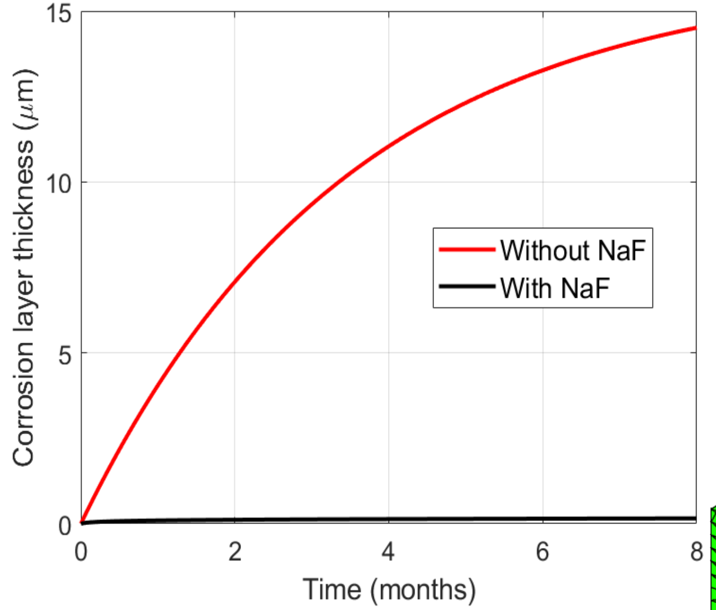




Corroded magnesium surface in GP without NaF – optical microscopy

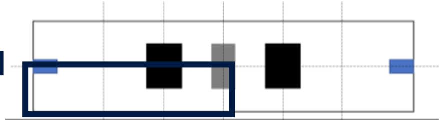
Numerical Study

Loading: Evolution of corrosion layer thickness



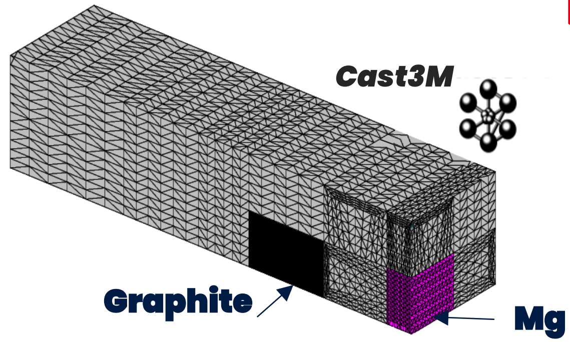
Mechanical Properties / Material	Young's Modulus (GPa)	Poisson's Coefficient
Magnesium	44	0,35
Graphite	20	0,2
Geopolymer	18	0,2

Configuration 1



Algorithm 1 Numerical modeling of corrosion by equivalent expansion

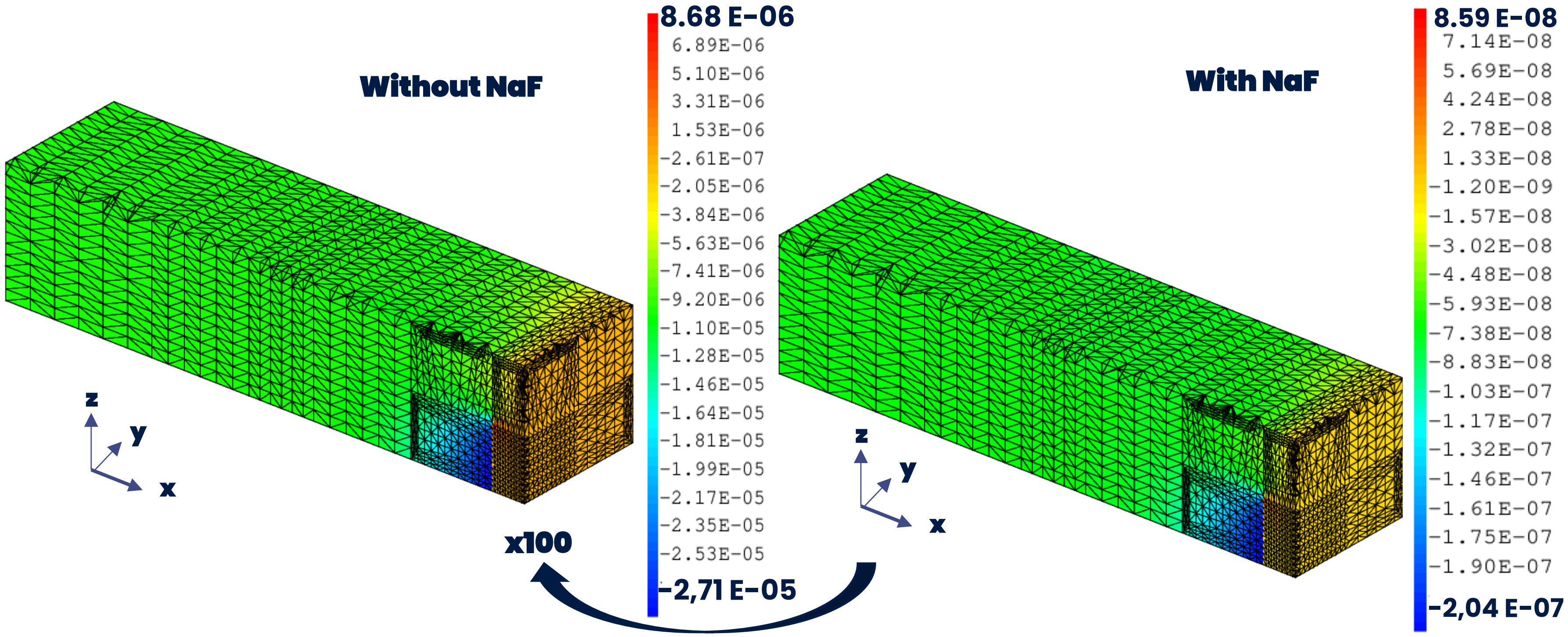
1: Generate the mesh of the study domain
2: Create interface elements between magnesium and matrix
3: Assign an elastic model and mechanical properties to each element
4: Apply boundary conditions related to symmetry
5: Model corrosion by equivalent expansion at the interface
6: Display the results



$$\tilde{k}_n = \frac{2\tilde{\mu}_c(1-\tilde{\nu}_c)}{h(1-2\tilde{\nu}_c)}$$

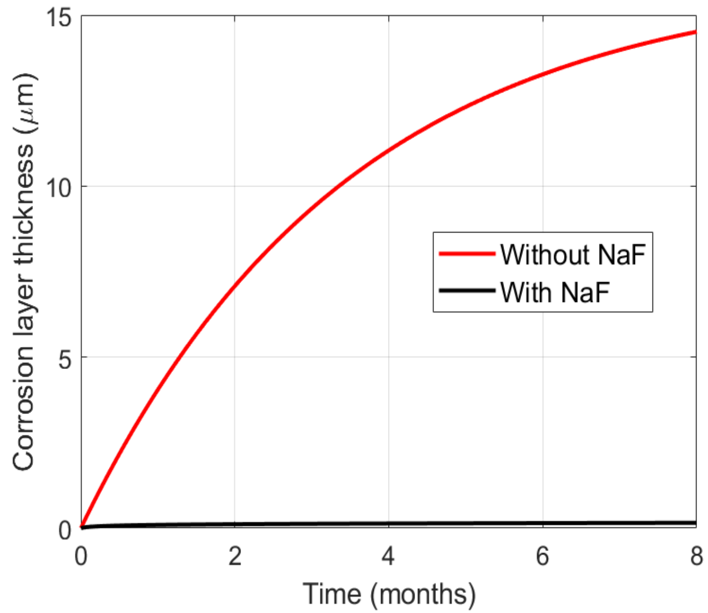
$$\tilde{k}_t = \frac{\tilde{\mu}_c}{h}$$

Displacements Ux of the 4 x 4 x 16 cm specimen



Numerical Study

Loading: Evolution of corrosion layer thickness



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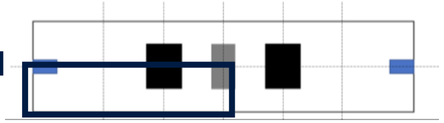

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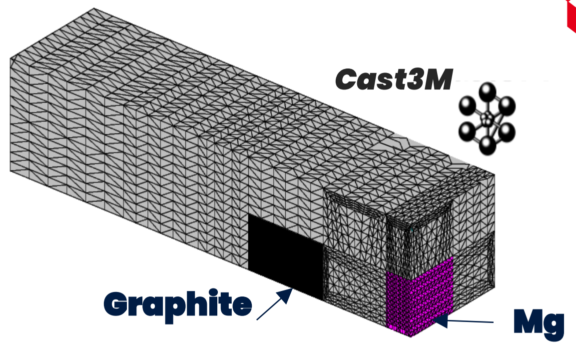

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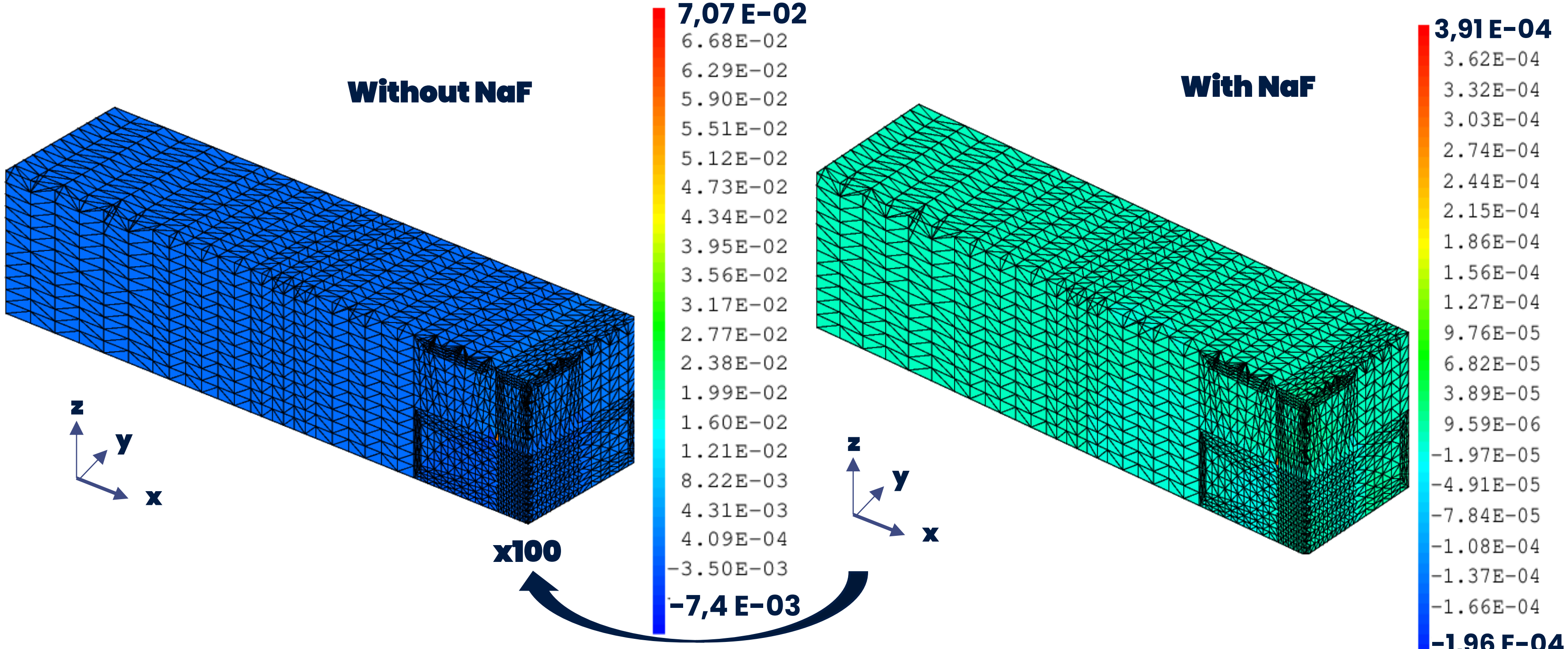
Deformations Ux of the 4 x 4 x 16 cm specimen



Conclusion

- Different experimental configurations were investigated to improve corrosion monitoring.
- NaF addition significantly reduces Mg corrosion in the geopolymer matrix.
- The coupling between experimental measurements and numerical modelling is key to better understanding and predicting Mg corrosion and the resulting material response.

Future Work

- Incorporate drying shrinkage, creep, and a damage variable into the numerical model.
- Use Portland cement as the encapsulation matrix to achieve a greater corrosion layer thickness.
- Characterize the corrosion products using nanoindentation measurements.

Thank you !

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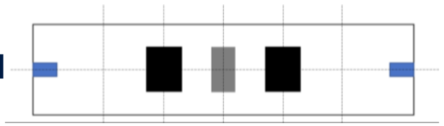
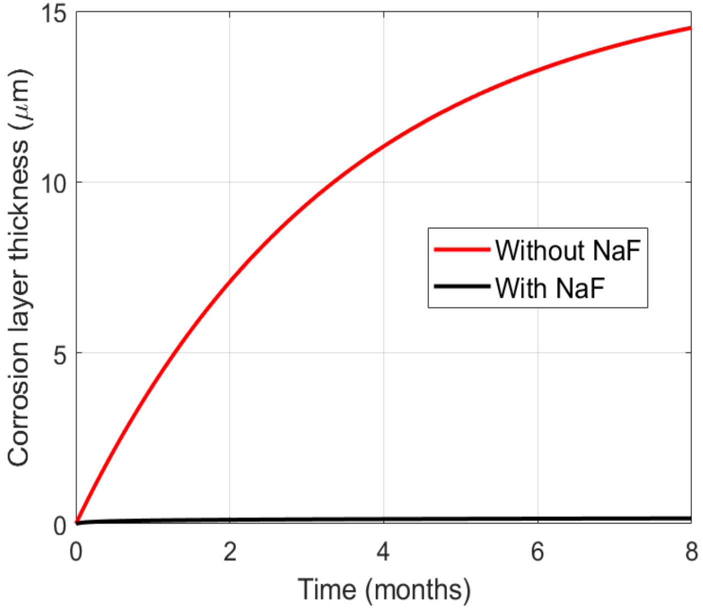
Numerical Study

Configuration 1



Loading: Evolution of corrosion layer thickness



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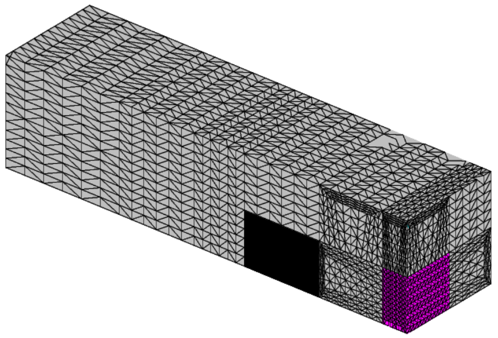

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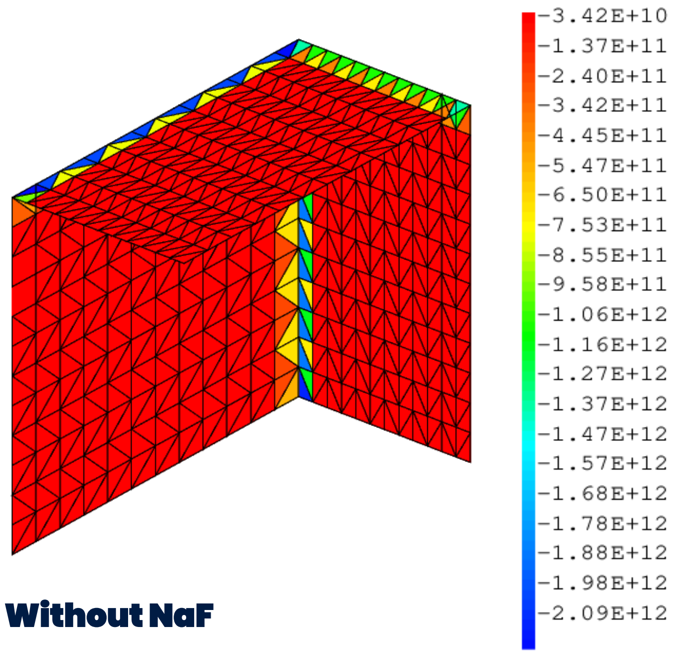
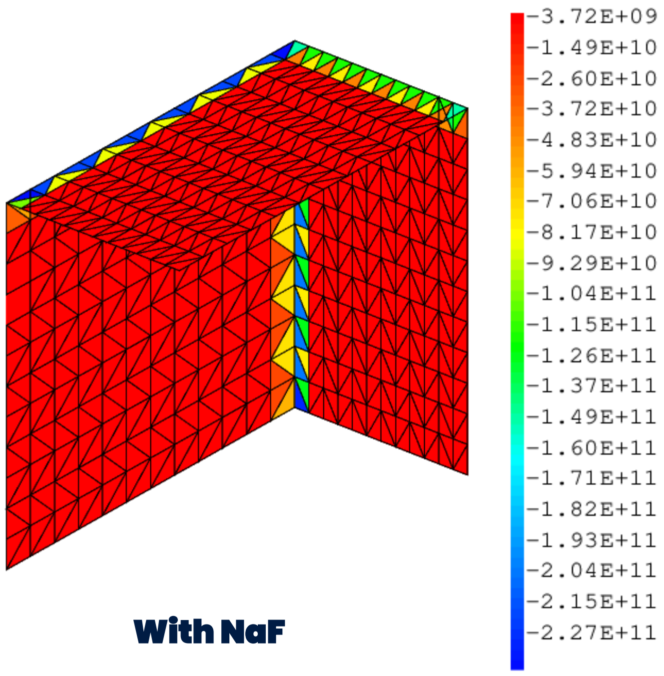
$$\tilde{k}_t = \frac{\tilde{\mu}_c}{h}$$

Normal Stress Field on interface elements



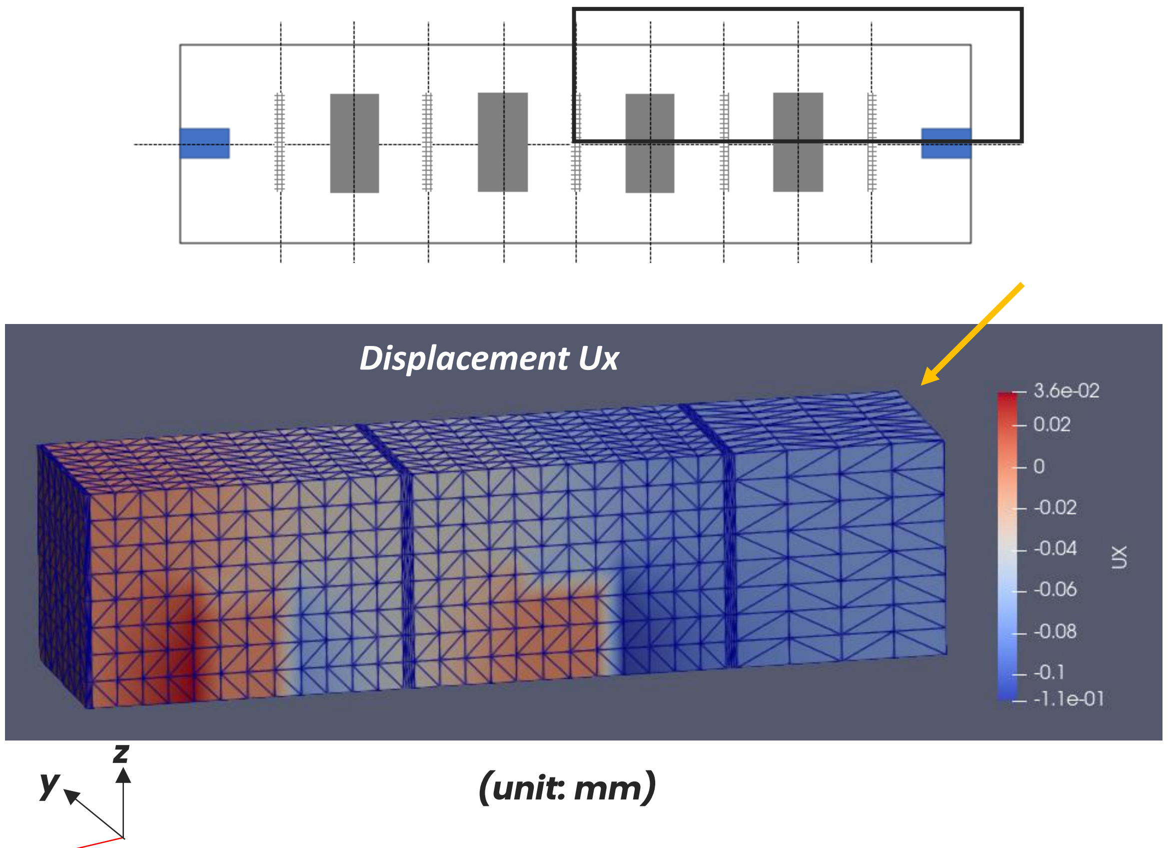
Without NaF



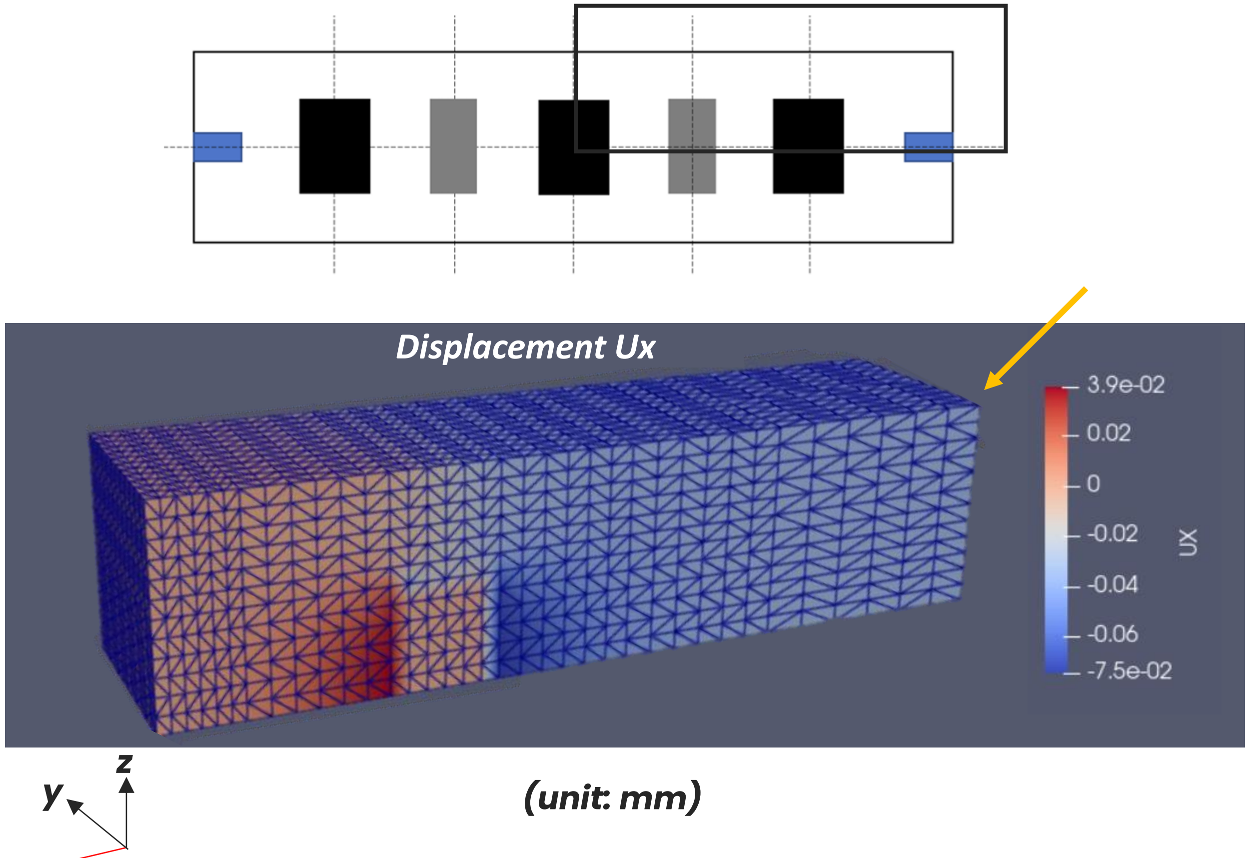
With NaF

Numerical Study

Numerical optimization of the configuration to improve LVDT measurements (Cast3M)
(For the same applied load)



~ 80 µm after 2 months



~ 40 µm after 2 months

European Partnership
on Radioactive Waste Management

EURAD-2 Spotlight on Cutting Edge Science

Post-Closure Criticality Safety:
Studying and Modelling Aspects of the DGR Long-Term Evolution

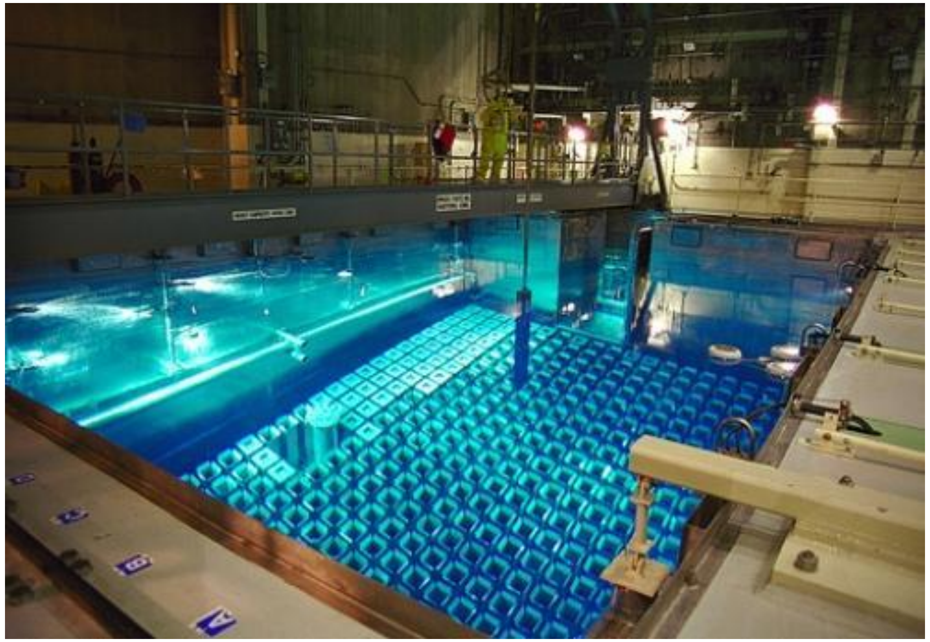
10th September 2026

A. de Aragao (EPFL/Nagra)
M. Wittel (Nagra)

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

INTRODUCTION

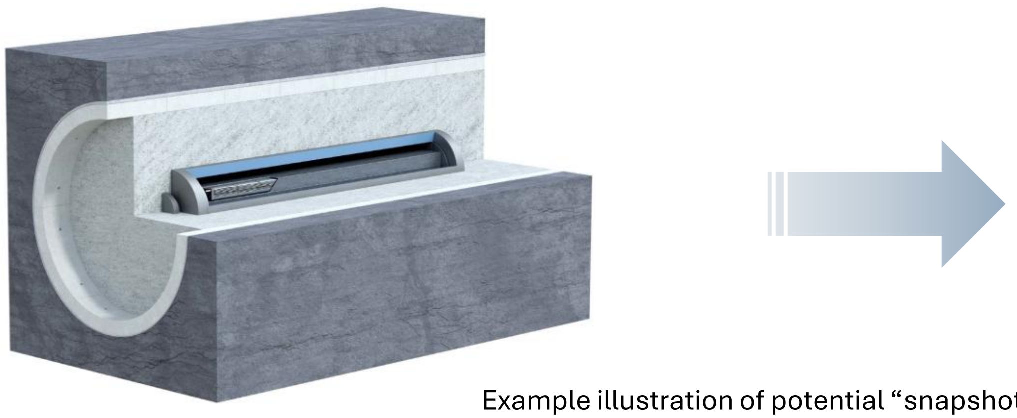
- **Deep geological repositories (DGR) are designed and built to ensure the safe disposal of radioactive waste for very long timescales.**
  - High-level radioactive waste such as spent nuclear fuel still contains certain amounts of fissile material.
  - Under very specific circumstances, this could theoretically lead to new fission chain reactions (criticality) ocurring in the DGR.
  - ➢ **Criticality safety is a safety requirement in all national programmes that must dispose of high-level waste.**



- **WP-17 "CSFD" addresses the unique challenges posed by the very long time frames by**:
  - Identifying & exploring the optimisation potential of **measures for ensuring** post-closure criticality safety.
  - Developing & improving **methods to demonstrate** post-closure criticality safety.

WHERE CUTTING-EDGE SCIENCE IS KEY

- Demonstrating post-closure criticality safety is a unique challenge: we are **assessing a system that is evolving continuously over** timeframes of **thousands of years**.
    - Over such large timescales, the system changes through a multitude of processes such as material degradation (e.g. corrosion), geometrical deformation, radioactive decay, etc.



Example illustration of potential “snapshots“ in the system evolution.
Graphics: courtesy of Nagra.

- WP-17 “CSFD” is carrying out innovative R&D work to develop a holistic framework to address these challenges and contribute to demonstrating post-closure criticality safety.

THE INNOVATIVE R&D WORK IN WP-17 “CSFD” [SELECTION]

- WP-17 is developing & consolidating the scientific basis to bring the understanding of the post-closure system evolution to a new level of detail and **for the first time with a specific focus on criticality safety:**
  - **Task 3** is developing a catalogue of post-closure features, events and processes that are specifically relevant for post-closure criticality
- WP-17 is investigating modelling approaches for post-closure criticality safety assessments that address both the need for detailed computational models and the extremely large parameter space
  - **Task 4** is creating a detailed understanding of various modelling methods and aims at producing, for the first time, a systematic evaluation of the impact of unavoidable model assumptions and simplifications.
- WP-17 is exploring the potential of assessing the effects of potential post-closure criticality events with a view to improving the system understanding and demonstrating the robustness of the disposal concept
  - **Task 7**: is investigating various approaches to modelling and assessing the effects of potential post-closure criticality events.

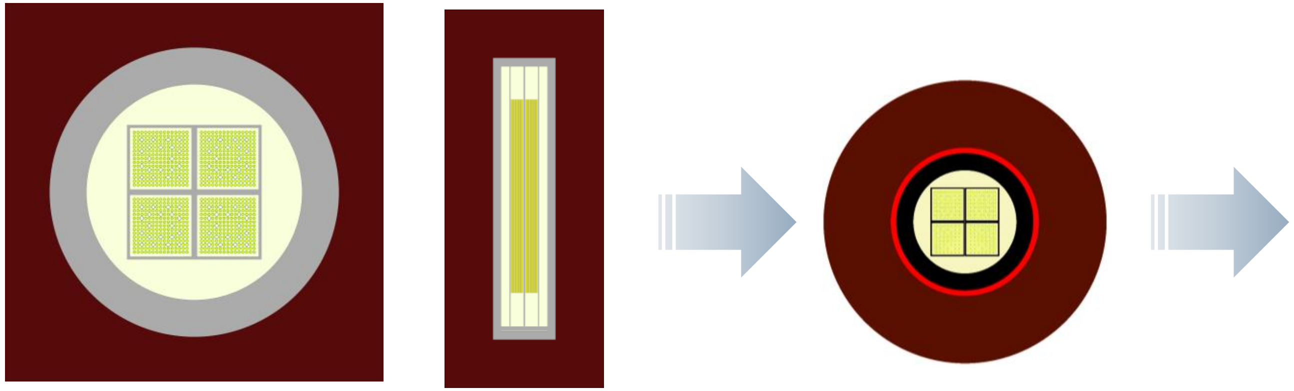
WP-17 SPOTLIGHT ON CUTTING EDGE R&D WORK

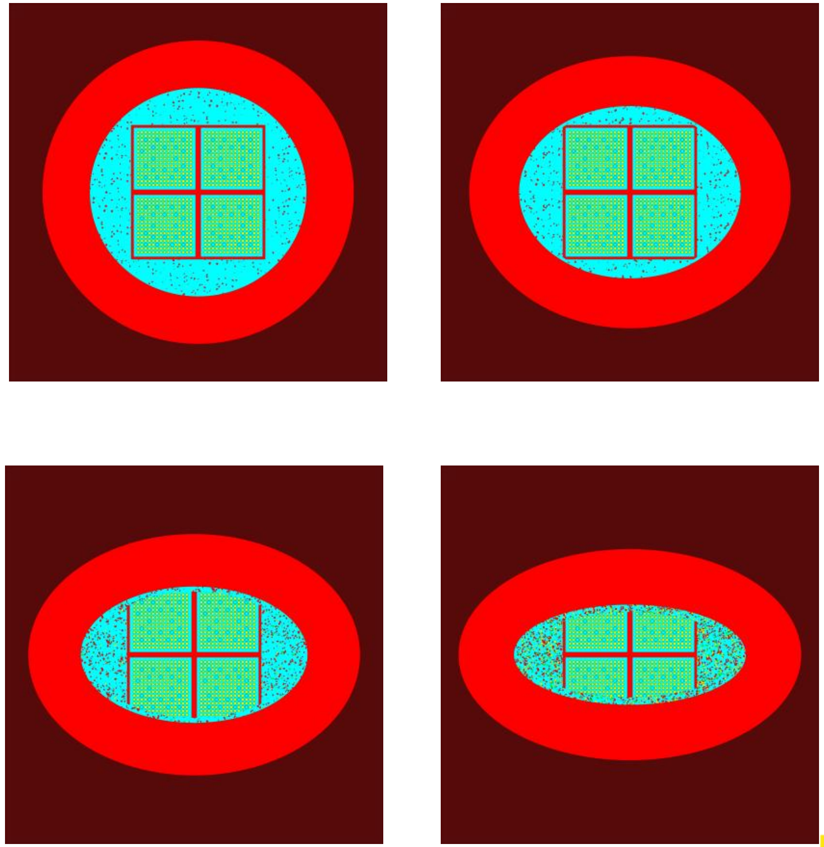
- **Example illustration of the innovative R&D work carried out in WP-17**
  - Research carried out in a joint **EPFL – Nagra PhD thesis project**
  - Defined at the interface of **WP-17 Tasks 3,4 and 7**
  - Aims at addressing **key questions** such as:
    (example focused on the Swiss DGR concept)
    - What are the post-closure processes that matter most for post-closure criticality safety?
    - Developing & implementing new modelling techniques to reach unprecedented level of realism
    - What is the impact of modelling decisions, assumptions and simplifications?
      How can this be quantified?
    - How can neutronics aspects be coupled with the nearfield modelling?
    - What are the relevant feedback mechanisms?
    - Etc.

WP-17 SPOTLIGHT ON CUTTING EDGE R&D WORK II

nagra EPFL

- No individual process determines post-closure criticality safety: This R&D work contributes to improving the understanding of the impact that the coupled evolution of material composition and geometrical changes has on the system reactivity:





A container filled with 4 PWR UO_2 fuel assemblies was modelled surrounded by a layer of bentonite.
Assumptions: corrosion rate of 0.3 μm/yr & Pilling-Bedworth ratio of 2.

- A **completely new approach** was developed to model the evolution & assumed degradation of the spent fuel elements and internal support structures.

eurad 2

SUMMARY

- **Demonstrating post-closure criticality safety is a unique challenge due to the very long timeframes required for assessment.**
- **WP-17 is addressing the challenges by developing & improving methods to demonstrate post-closure criticality safety, e.g. by:**
  - Identifying the post-closure processes relevant specifically for criticality safety
  - Investigating new approaches to modelling the long-term evolution considering both the need for detailed computational models and the large variations due to an almost infinite parameter space.
  - Developing new methods to assess the impact of modeling assumptions and sytem uncertainties.
  - etc.
- **The deepened understanding achieved will support and strengthen the confidence in DGR as a robust and safe solution for final disposal.**
- **This represents only a “spotlight” selection of the innovative work carried out in WP-17.**

THANK YOU


Javier Samper


Alba Mon


Brais Sobral


Luis Montenegro

REACTIVE TRANSPORT MODELS AND METAMODELS FOR THE GEOCHEMICAL EVOLUTION IN A HLW REPOSITORY

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8-10th September 2026

OUTLINE

- **Introduction**
- **High-fidelity reactive transport models for lab corrosion tests**
- **CORE code improvements applied to HLW repository**
- **Geochemical machine learning benchmark:**
  - Metamodel for a corrosion reactive transport model
  - Metamodel for a uranium system
- **Conclusions & Future work**

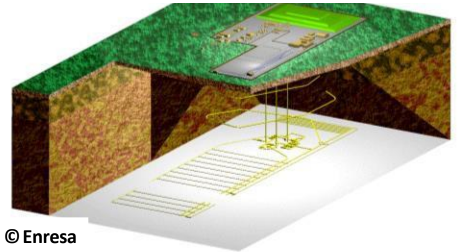
INTRODUCTION

- **This work is developed by the UDC within EURAD2 project-WP HERMES:**
  - **High-Fidelity models**: Enhance Thermal-Hydraulic-Chemical (THC) models for key iron/bentonite interfaces.
  - **Machine Learning Surrogates:** Develop fast ML metamodels to replace computationally heavy geochemical solvers.
  - **Repository scale simulation:** Model long-term geochemical evolution in granite disposal cells over thousands of years.

Laboratory FeMo test

HLW repository

Deep geological repository



© Enresa

Multibarrier concept:

- Waste
- Fe canister
- Bentonite buffer
- Granite

Chemical barrier

© ENRESA

Engineered barrier

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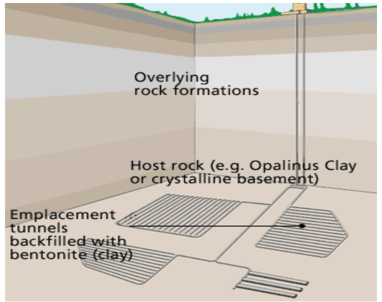
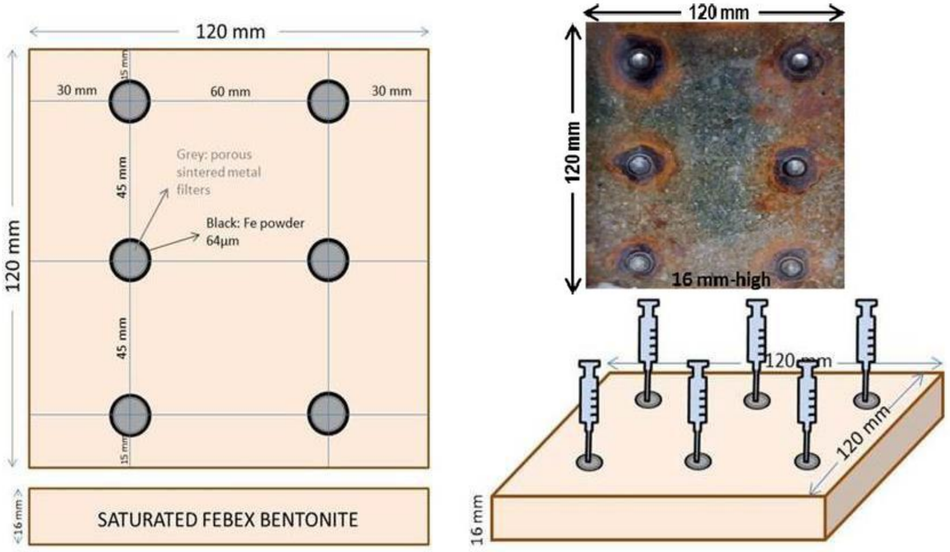
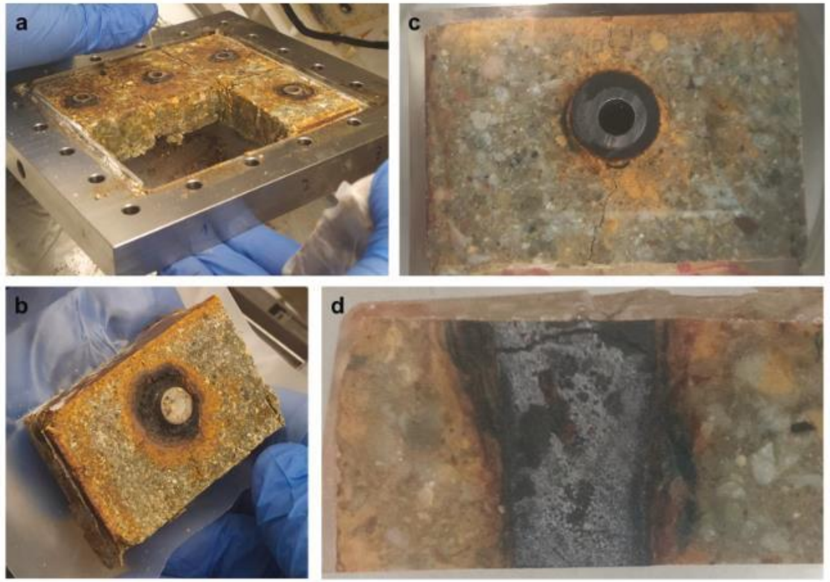
Geological barrier



FEMO CORROSION TEST

- **Laboratory FeMo test description (Turrero et al., 2026)**
  - Compacted bentonite block (120 mm × 120 mm × 16 mm) performed by CIEMAT/UAM
  - Stainless-steel sinter surrounded by iron powder
  - Fe powder particle size of 64 and 240 µm
  - Compacted FEBEX bentonite
  - Hydrated with granite-type water ($CaHCO_3$) through the sinters
  - Corrosion under saturated and ambient conditions
  - Duration of 15 years
  - Experimental data shows magnetite, goethite and siderite precipitation in the iron powder and iron/bentonite interface (Turrero et al., 2026)

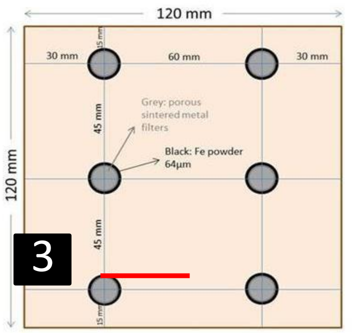


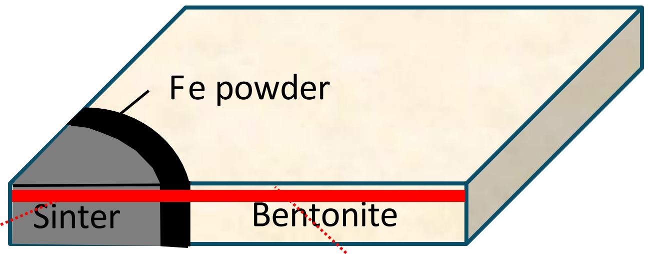


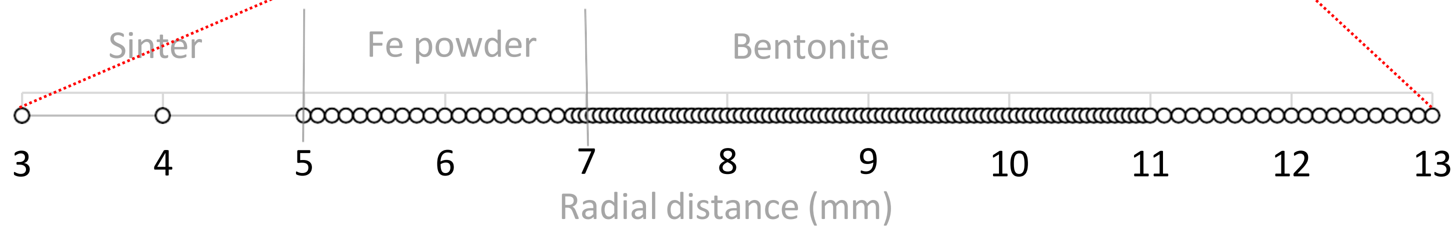
Turrero, M.J., Torres, E., Martín, P.L., Fernández, R., Ruiz, A.I., Ortega, A., Garralón, A., Notario, B., Mota, C., Cuevas, J.F. (2026). Long-term iron-bentonite interaction in a water-saturated room-temperature environment: Advancing for safety of metal waste containment in the geosphere. Surfaces and Interfaces 82, 108466.

FEMO CORROSION TEST

- **Numerical model description**
  - Model of the section 3 (64 µm iron powder grain size)
  - Isothermal and saturated conditions
  - 1D mesh porous media: sinter, Fe powder and bentonite
  - Geochemical reactions:
    - Aqueous complexation
    - Acid-base
    - Redox
    - Cation exchange
    - Surface complexation
    - Mineral dissolution/precipitation
  - Anaerobic corrosion rate.
    - Sinter: very low corrosion (0.02 µm/year)
    - Fe powder: 0.35 µm/year
    - Fe powder/bentonite interface: 0.45 µm/year
  - Calibration of the specific surface areas of the minerals to fit the laboratory observations

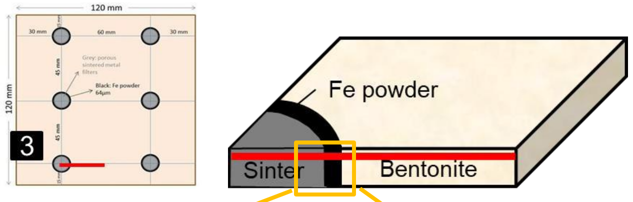


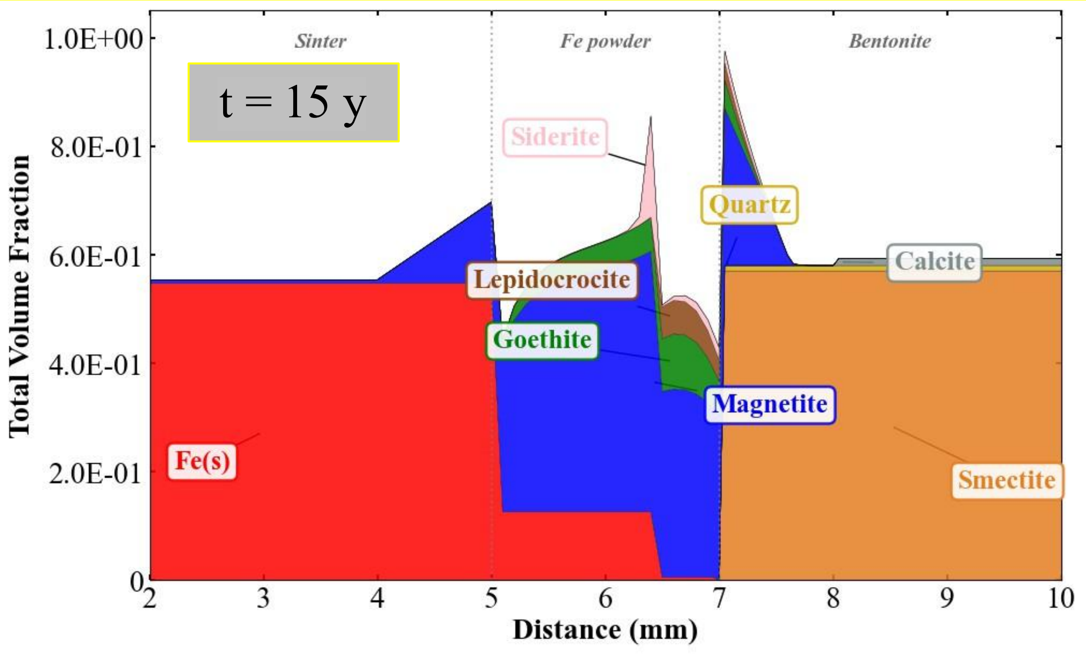


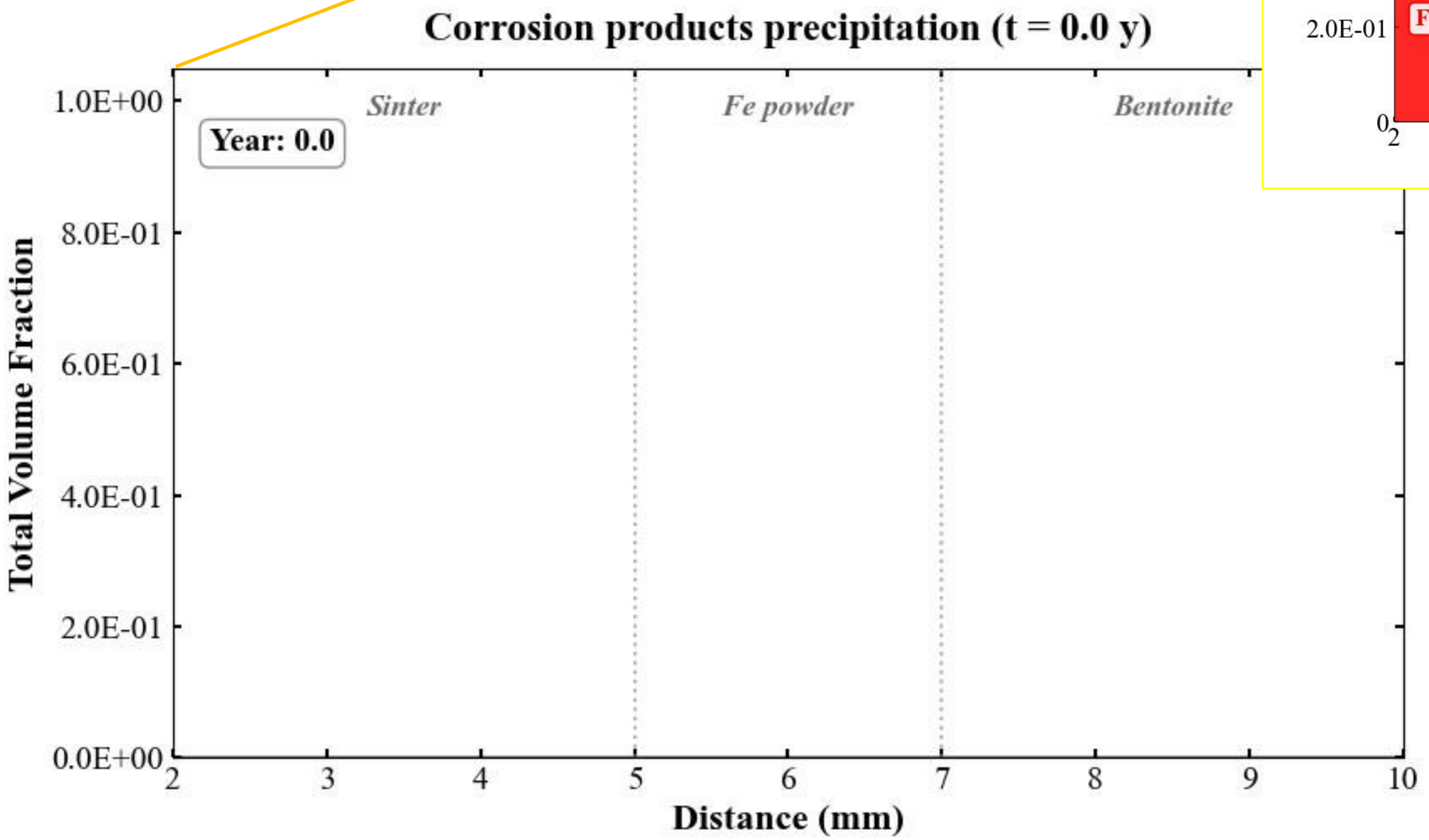


FEMO CORROSION TEST

- Numerical model results: Mineral volume fraction



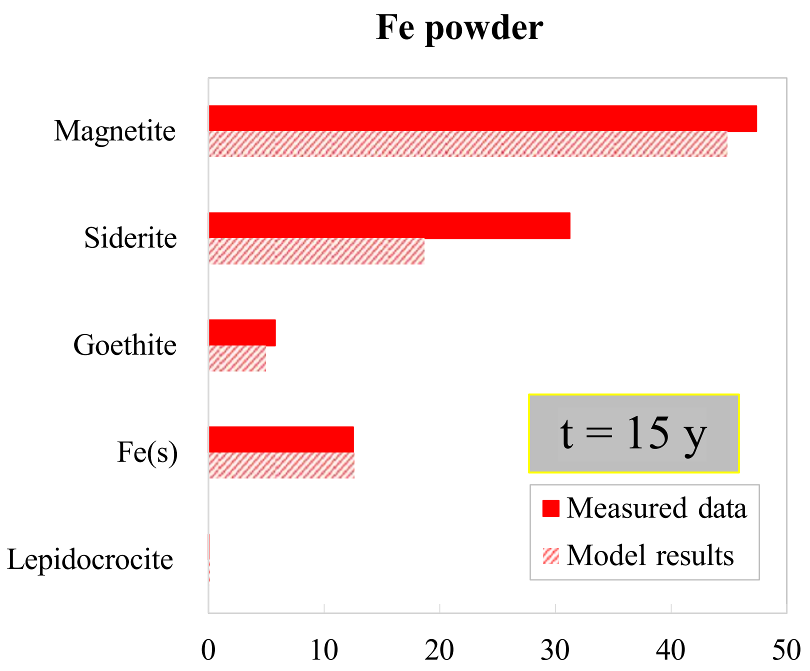


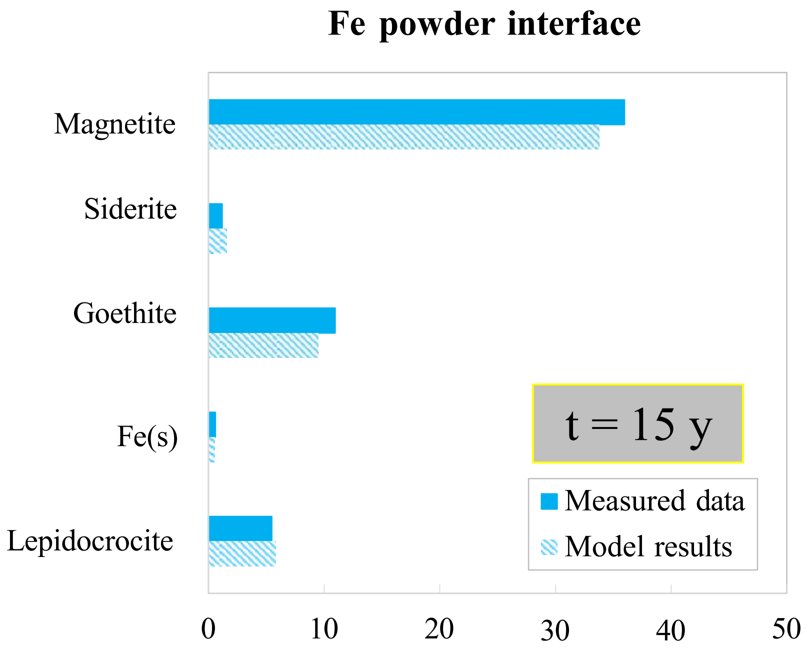


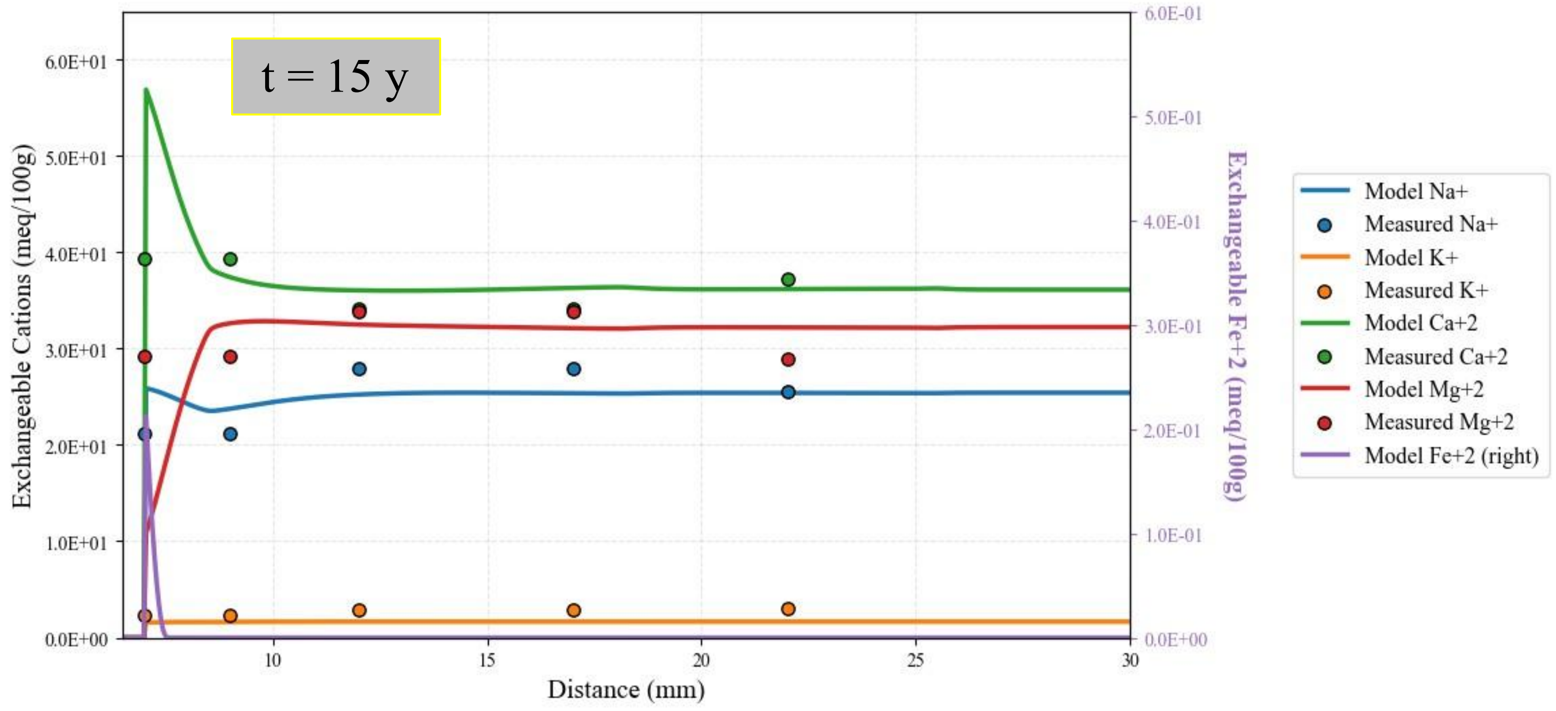
- Fe(s) dissolves in Fe powder and more in the interface
- Magnetite:
  - The main corrosion product
  - Precipitates more in the inner Fe powder
- Goethite and lepidocrocite precipitates more in the interface
- Siderite precipitates in the Fe powder when the HCO_3 arrives

FEMO CORROSION TEST

- **Numerical model results: Comparison with the measured data**
  - Model results fit the volume fraction measured data
  - Model results fit the trend of cation exchange, except at the interface

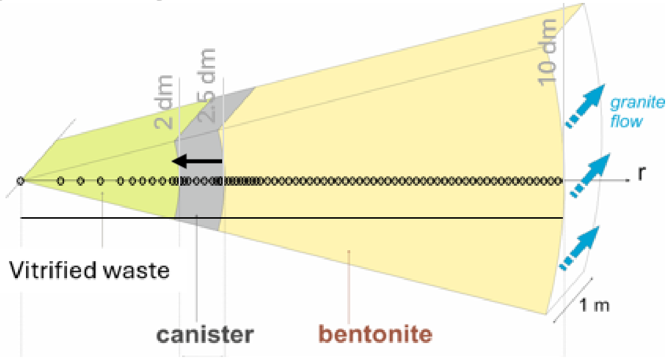


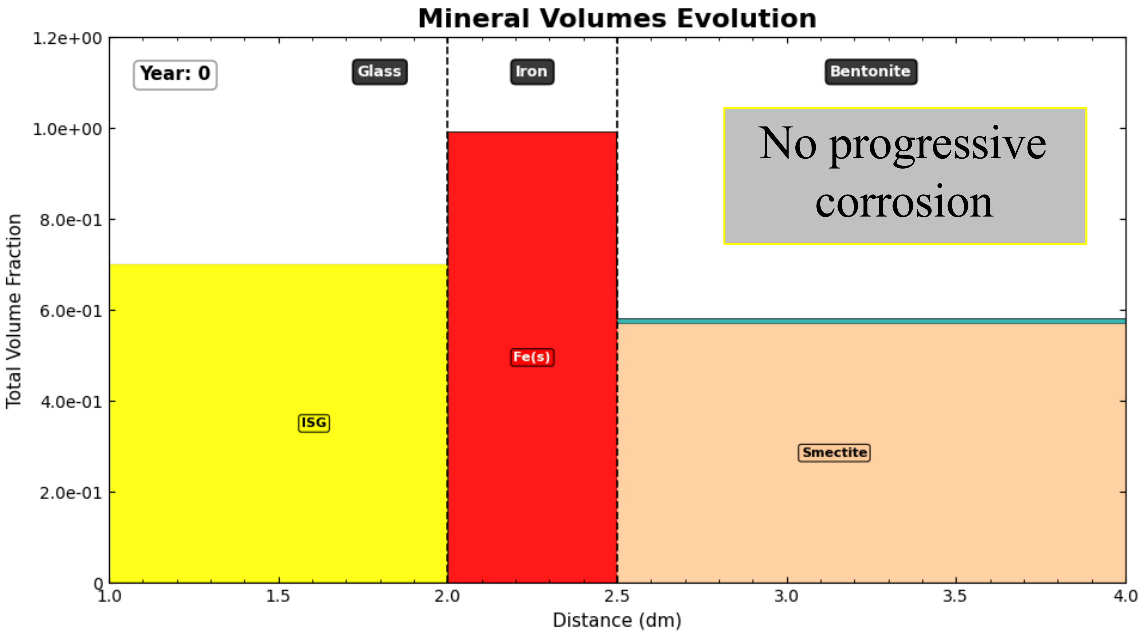


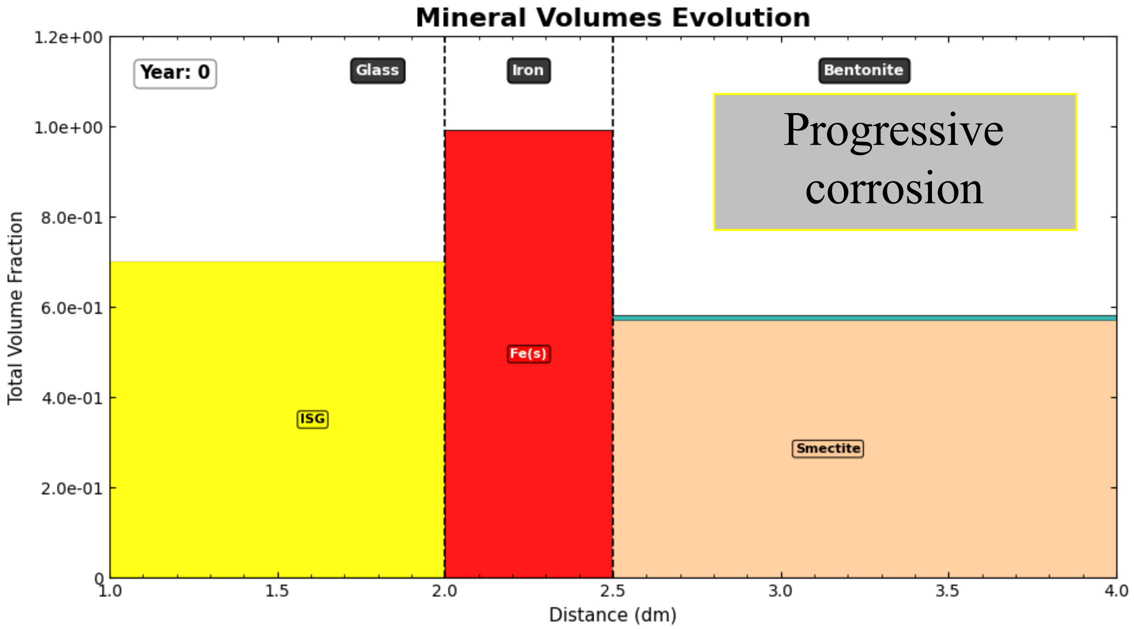


CORE^{2D}V5 CODE IMPROVEMENTS: PROGRESSIVE CORROSION AND PASSIVATION LAYER

- **Progressive corrosion:**
  - Iron corrodes node-by-node rather than all at once, providing realistic spatial front propagation in disposal cells.
- **Magnetite passivation film:**
  - The thickness of the magnetite film is calculated on the assumption that the magnetite precipitates uniformly across the entire surface
  - We calculates uniform magnetite film growth thickness, updating effective diffusion and retarding corrosion rates over time.
- **Application to a HLW repository**
  - Integrated into EURAD-ACED model to simulate long-term geochemical evolution at disposal cell scale.





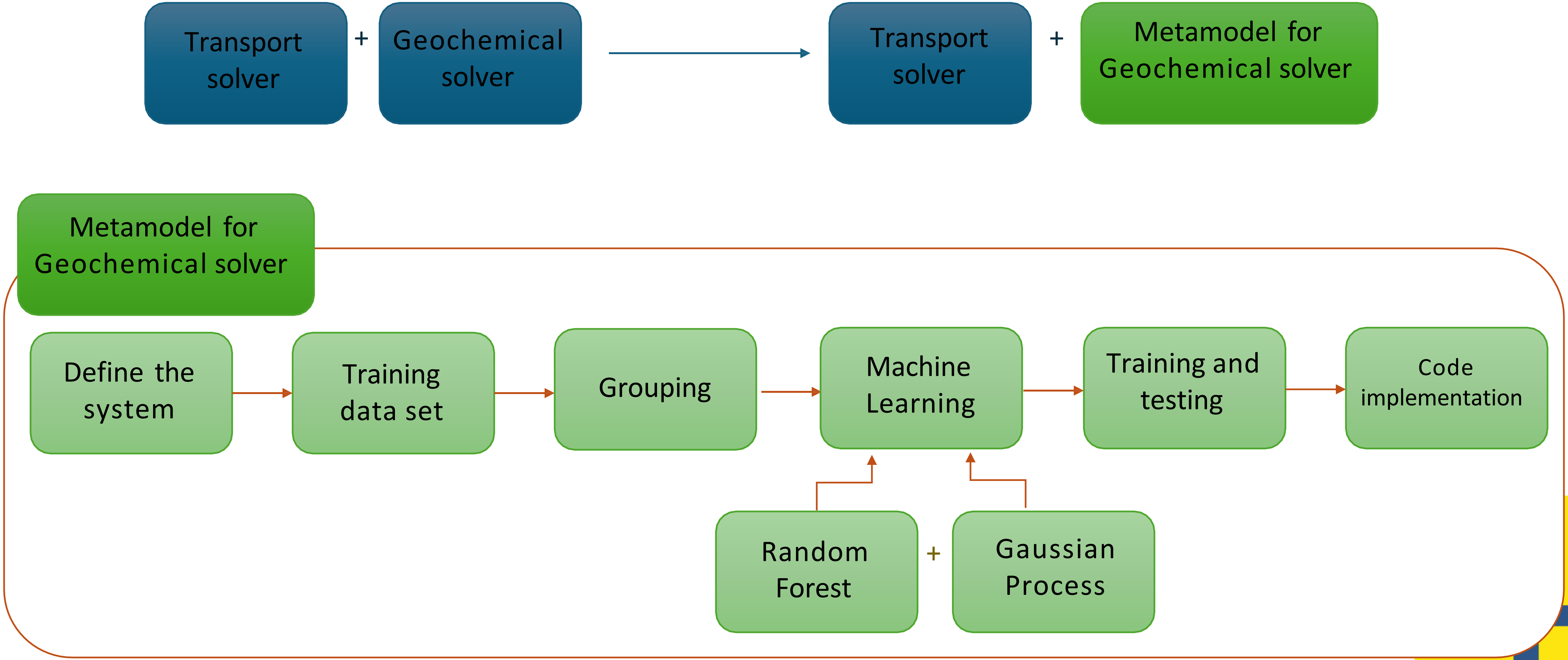


METAMODELS FOR REACTIVE TRANSPORT

- **Motivation:**
  - Reactive transport models require a lot of CPU time mostly for solving the geochemical reactions
    - 24 hours for the FeMo corrosion test
    - More than 10 days for the full long term HLW repository
  - Metamodels and surrogate models provide:
    - Approximate very efficient solutions
    - Emulate the high-fidelity reactive transport simulations
    - Reduce significantly the CPU times
  - Here we present metamodels which could replace the geochemical solver for a chemical system involving canister corrosion and interactions with clay buffer
  - On going work within HERMES WP GEOML benchmark initiative

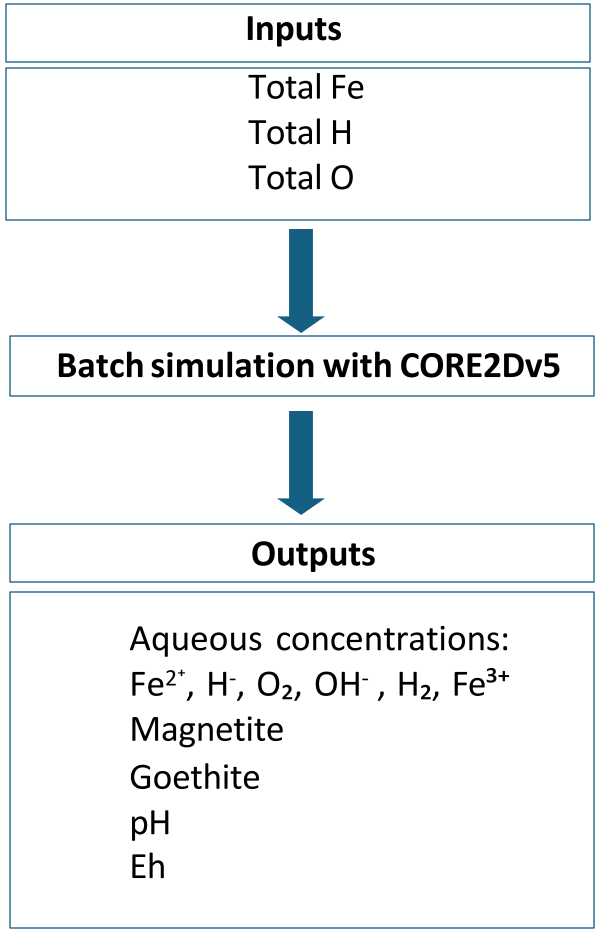
METAMODELS FOR REACTIVE TRANSPORT

- **Strategy for the metamodel:**



METAMODELS FOR CORROSION

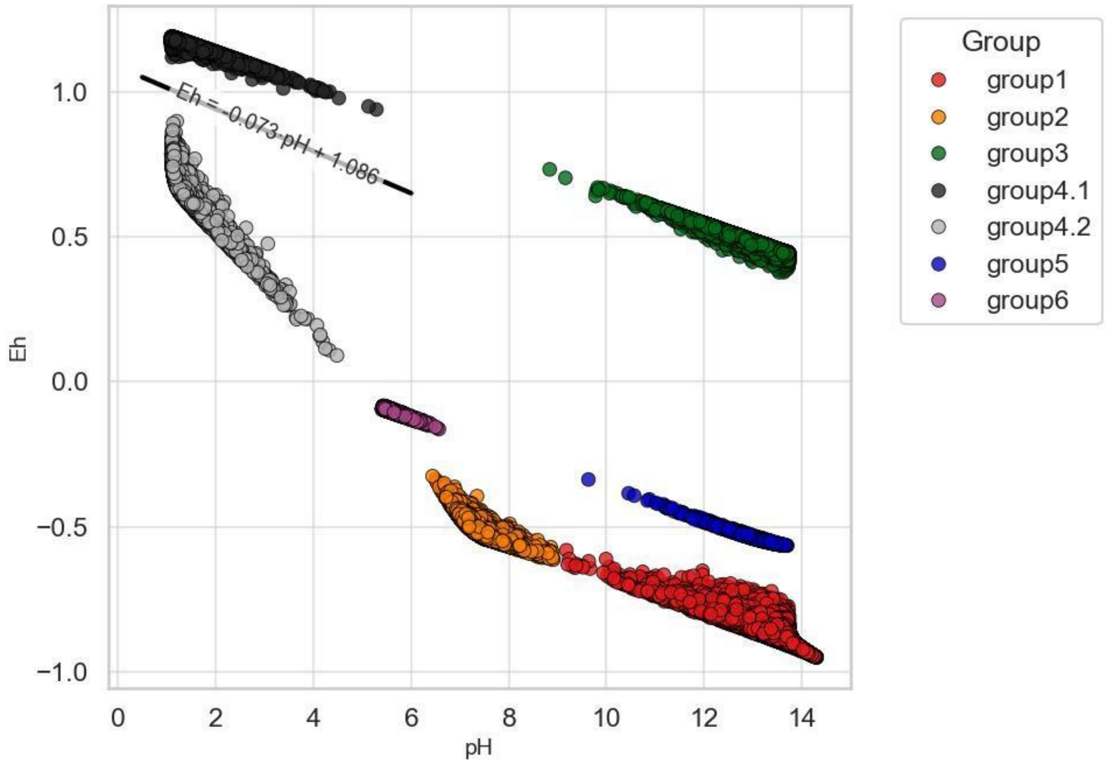
- **Sampling data test**
  - 500,000 sampling data
  - 3 inputs variables:
    - Total Fe, H and O
    - Sampling with LHC
    - Ranges taken from long term RT simulations
  - 8 output variables:
    - The valuable output variables for a RT code:
      - Total dissolved Fe, H and O
      - Total precipitated Fe, H and O
      - pH
      - Eh



METAMODELS FOR CORROSION

- Grouping criteria
  - Group 1: If Cmag > 0; Cgoethite = 0 & pH > 9
  - Group 2: If Cmag > 0; Cgoethite = 0 & pH <= 9
  - Group 3: If Cgoethite > 0; Cmag = 0 & pH > 9
  - Group 4.1: If Cgoethite > 0; Cmag = 0; pH <= 9 & [Eh > −0.12·pH + 1.16]
  - Group 4.2: If Cgoethite > 0; Cmag = 0; pH <= 9 & [Eh < −0.12·pH + 1.16]
  - Group 5: If Cmag > 0; Cgoethite > 0 & pH > 9
  - Group 6: If Cmag > 0; Cgoethite > 0 & pH <= 9

Groups	500 000 data set
1	285 774
2	53 538
3	138 576
4.1	8125
4.2	11 026
5	993
6	1968

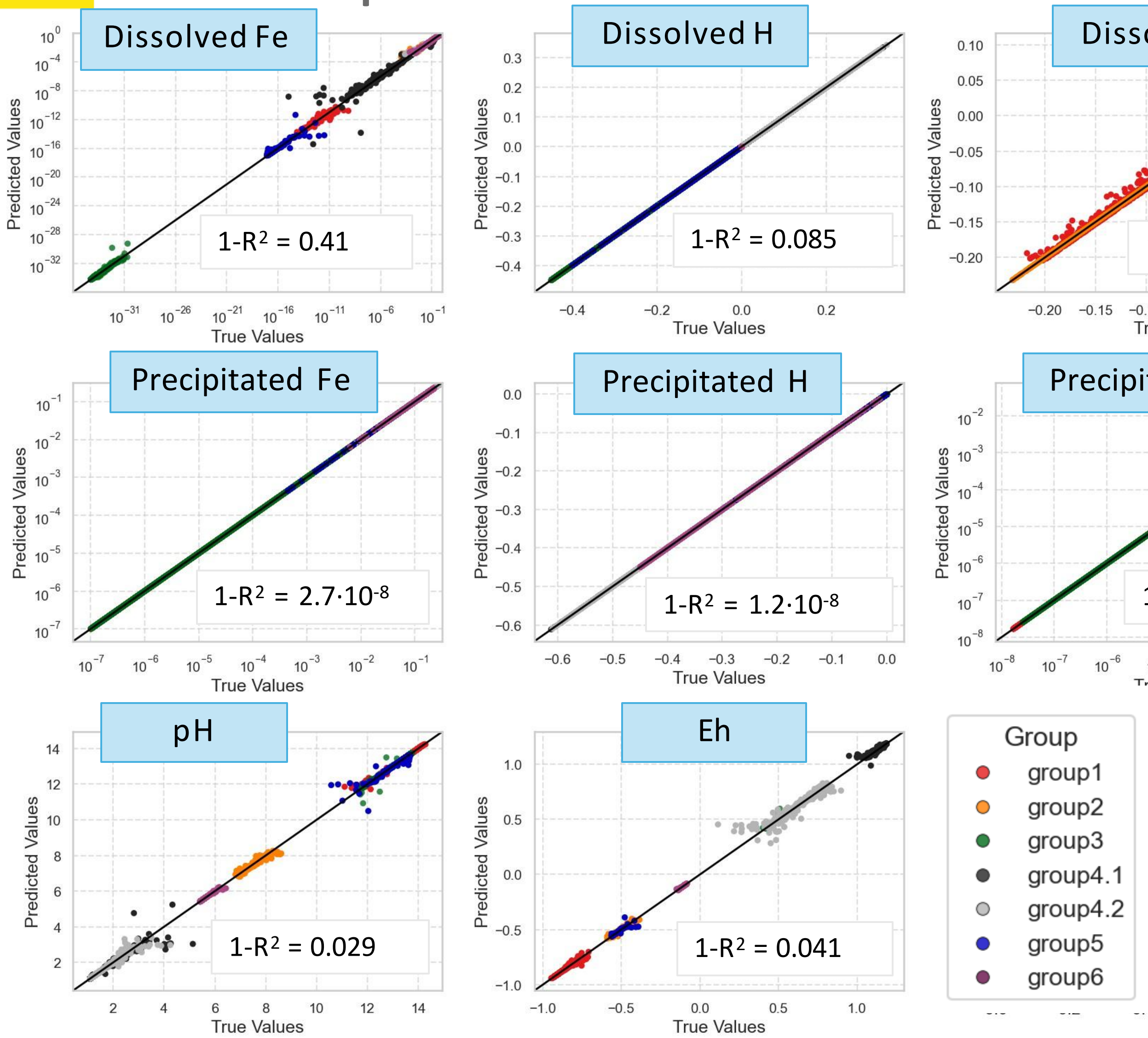


METAMODELS FOR CORROSION

- **Hybrid metamodel: RF + GP**
  - Random forest
    - 2,000 decision trees
    - Train-test split = 80 % - 20 %
    - Random shuffle before splitting
    - Accuracy of the RF model = 0.998
    - Better results were obtained in the groups with the largest number of samples
  - Gaussian Process
    - Trained with actual groups to evaluate the performance of the GP without considering RF miss groupings
    - Train-test split:
      - 80 % - 20 % for groups 5 and 6
      - 5,000 samples for the rest of the groups
    - Models trained for each variable and each group

METAMODELS FOR CORROSION

- **Metamodel performance**



Group 1: If Cmag > 0; Cgoethite = 0 & pH > 9
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Group 4.2: If Cgoethite > 0; Cmag = 0; pH <= 9 & [Eh < −0.12·pH + 1.16]
Group 5: If Cmag > 0; Cgoethite > 0 & pH > 9
Group 6: If Cmag > 0; Cgoethite > 0 & pH <= 9

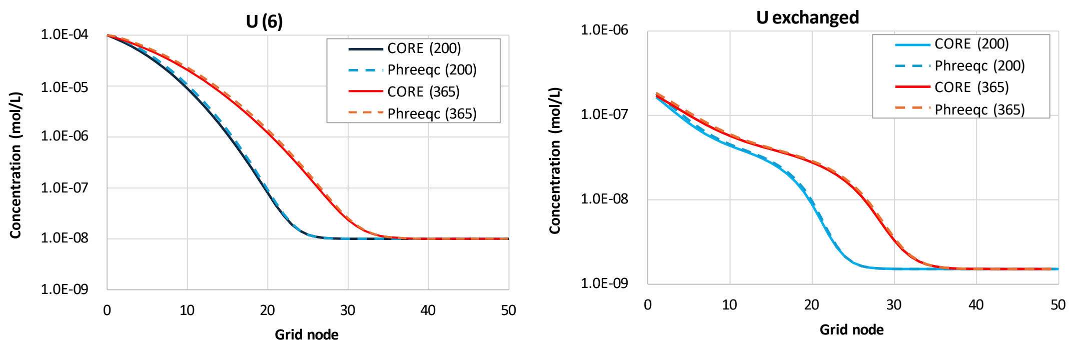
- Results:
  - Good performance metric in most groups and variables
  - Some bad performance metrics for:
    - Dissolved Fe in group 4.1 and 5
    - Dissolved O in group 1

METAMODELS FOR A URANIUM SYSTEM

- **Migration of U in a clayey host rock based on ML benchmarks in EURAD1- WP DONUT**
- **Uranium sampling cases:**
  - U exchange
    - 30,000 sampling data
    - Sampling with a real 1D RT model for diffusion and advection
    - Inputs: Total U, H, O and Na
    - Outputs: Dissolve U, O, and Na, Exchange U and Na
  - U sorption
    - 30,000 sampling data
    - Sampling with a real 1D RT model for diffusion and advection
    - Inputs: Total U, H and O
    - Outputs: Dissolved U and H, Sorbed U and H
- **Uranium metamodels:**
  - Gaussian process:
    - Train/test split = 80/20 %
    - Other parameters: like those of the corrosion case

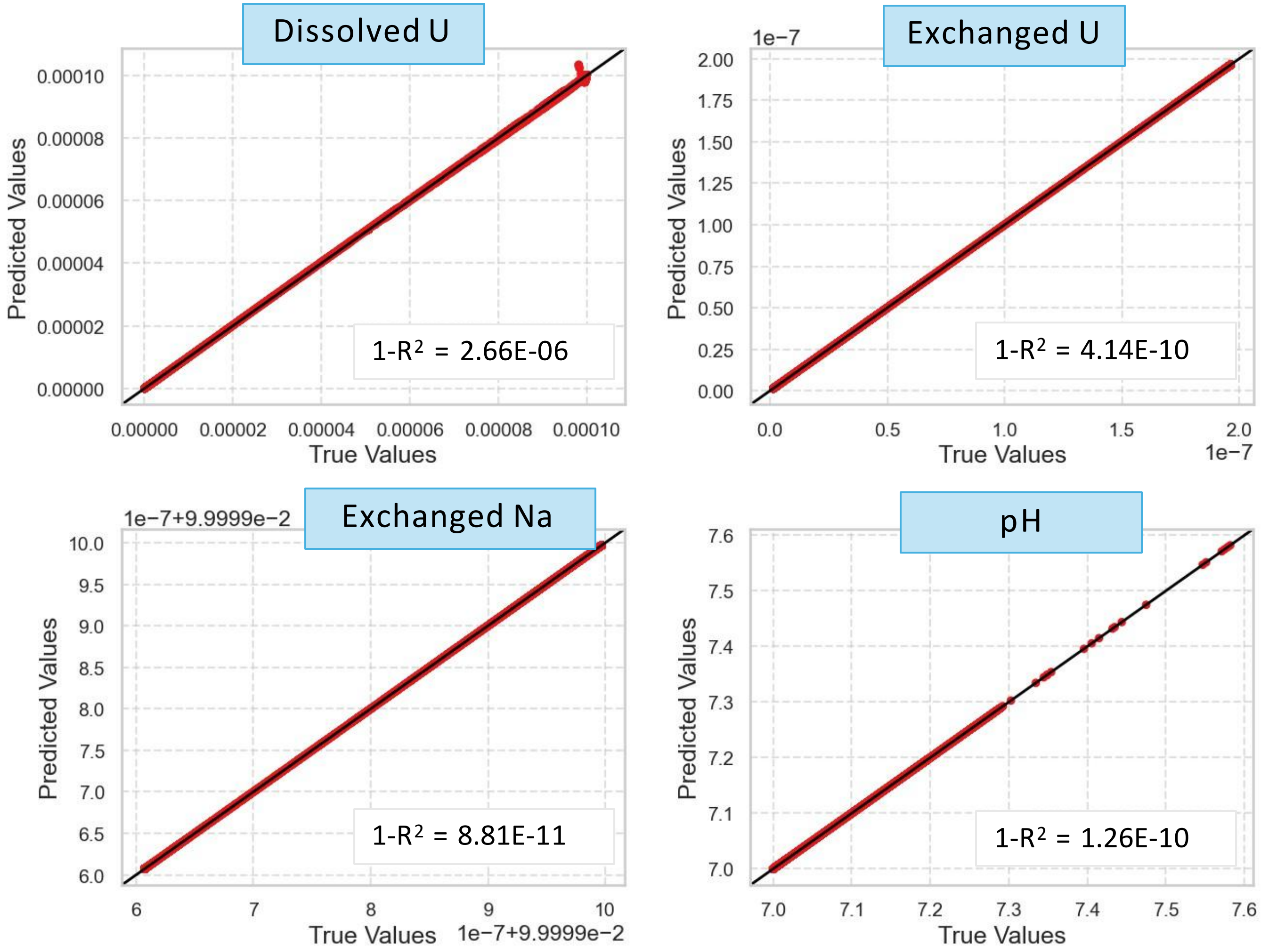
Chemistry: U-Na-Cl system
Processes: Cation Exchange – Surface Complexation
Transport: Diffusive – Advective – Advective-dispersive

Results of the 1D RT model



METAMODELS FOR A URANIUM SYSTEM

- **Performance of the metamodel for Exchanged U case:**



- Results:
  - Good performance metrics for the outputs
  - Scatter plots show good adjustment to the 1:1 line

CONCLUSIONS

- **The high-fidelity THC model of the FeMo corrosion test**
  - The RT model successfully reproduces the long-term laboratory observations of mineral precipitation at the iron-bentonite interface
- **Code improvements for RT simulation**
  - Progressive corrosion and magnetite passivation layer successfully capture corrosion retarding phenomena
- **Performance of the metamodels:**
  - Corrosion case
    - The hybrid Random Forest (RF) and Gaussian Process (GP) surrogate models demonstrate high accuracy (NRMSE<0.02) in predicting geochemical evolution
    - The performance is excellent for the precipitated
  - Uranium case
    - Good performance for the metamodel for most species
    - On progress the improvements of pH of the sorbed U case
  - The use of ML metamodels significantly addresses the CPU-intensive nature of geochemical solvers, enabling faster and more complex simulations

FUTURE WORK

- **Code Integration:**
  - Implementation of the trained RF and GP metamodels into the CORE2Dv5 reactive transport code
  - Metamodel performance and evaluation of the CPU time saving
- **Large-Scale Application:**
  - Global Sensitivity Analysis:
    - Perform large-scale GSA (>5,000 runs) for long-term granite repositories.
  - Dataset Expansion:
    - Expand geochemical training space for repository safety assessments.

ACKNOWLEDGEMENT

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  - ENRESA within WP ACED of EURAD (Grant Agreement nº 847593) and WP HERMES of EURAD-2 (Grant Agreement nº 101166718)
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THANK YOU FOR YOUR ATTENTION