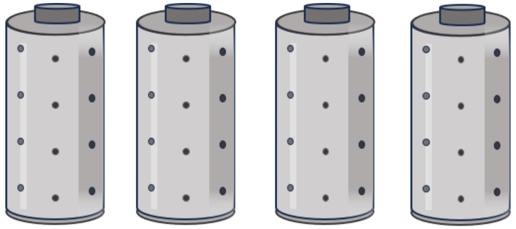
WP09 – INCOMAND MODELLING OF O_2 FLUXES AND FE CORROSION IN COMPACTED BENTONITE: THE EXAMPLE OF THE IC-A EXPERIMENT

Jin Ma, Mirjam Kiczka (UBERN) &
Natalia Jakus, Rizlan Bernier-Latmani (EPFL)

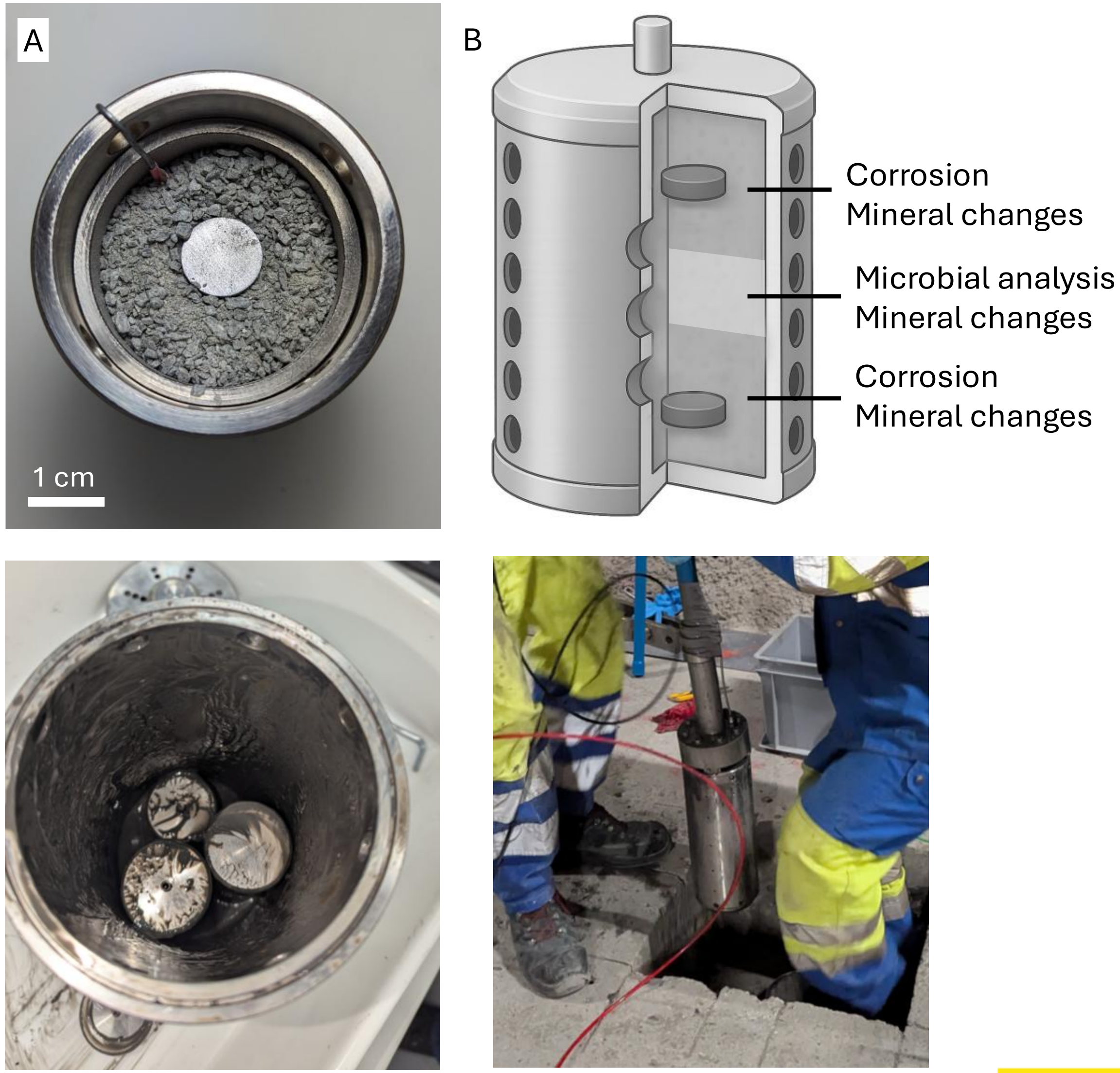
Co-funded by the European Union under Grant Agreement n° 101166718

THE IC-A EXPERIMENT

- **Long-term *in-situ* incubation experiment at Mont Terri, Switzerland**
- **Experimental study by EPFL & Nagra**
- **Studies the effect of O_2 in compacted MX-80 on**
    - **Corrosion**
    - **Microbial colonization**
    - **Bentonite mineralogy**

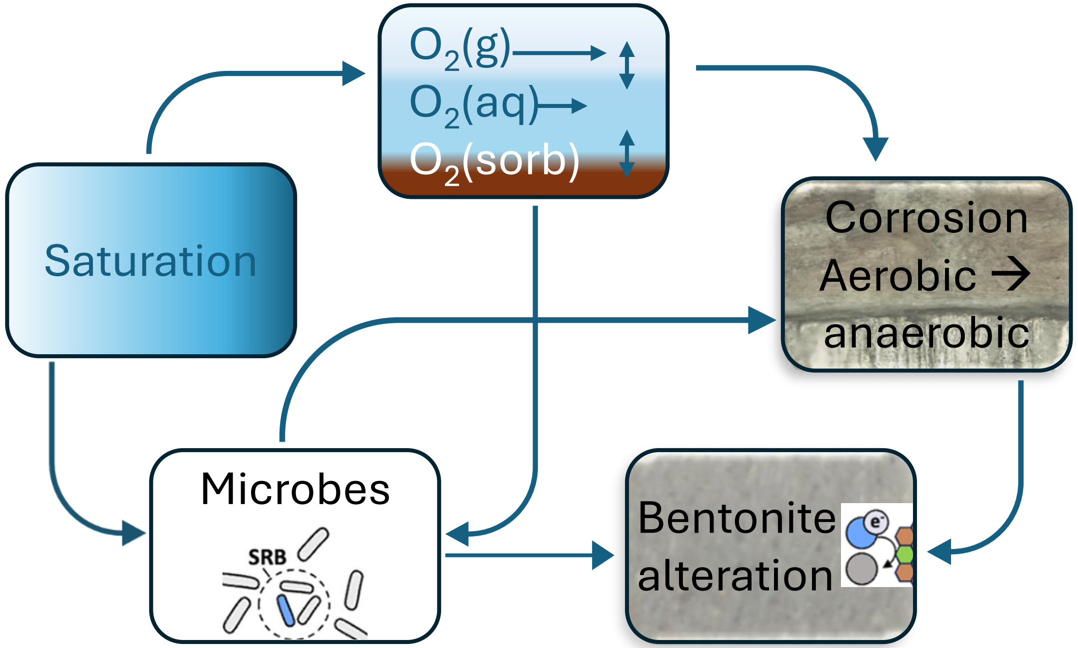


Bentonite: **0%** **21%** **21%-S** **100% O_2**
(γ-irradiated)



Jakus et al., 2025, Environ. Sci. Technol. 59, 25368-25379

THE IC-A EXPERIMENT – TRANSIENT CONDITIONS AND COUPLED PROCESSES



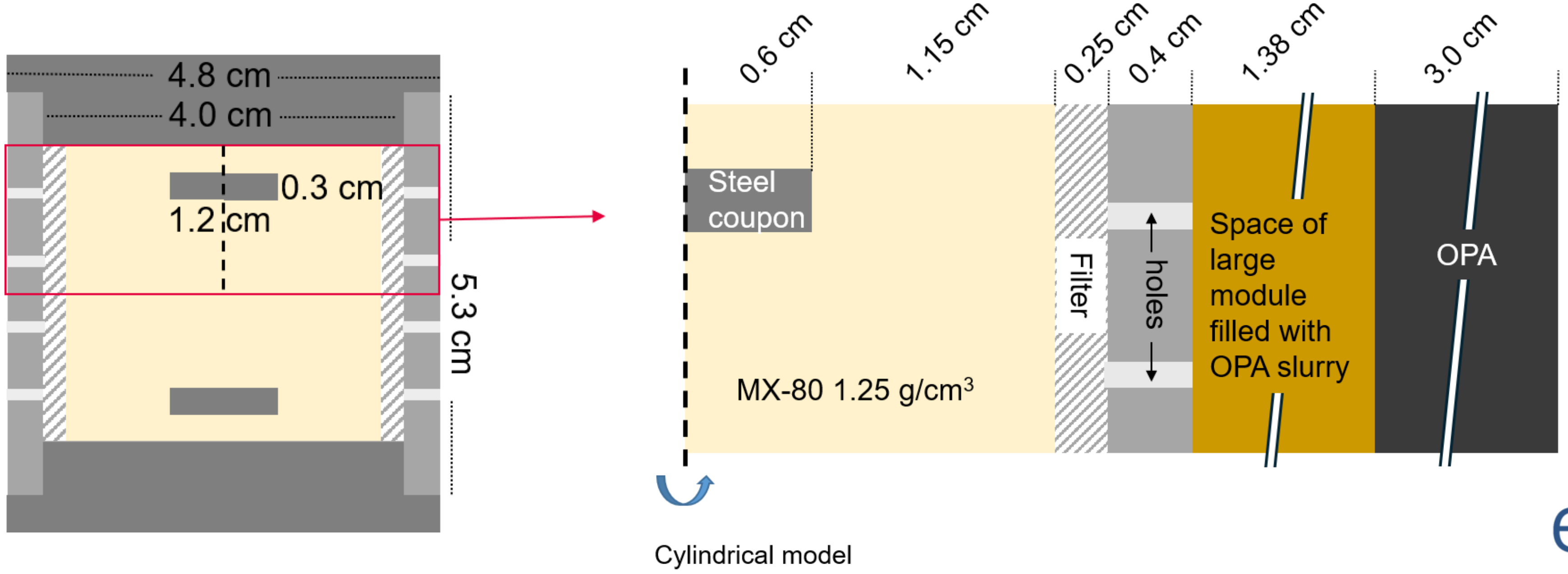
A reactive transport model for the IC-A experiment

- can contribute to the understanding of processes coupling in the experiment
- may serve as a validation tool for conceptual models for the early transient phase and their implementation in reactive transport model

MODEL DOMAIN

Model domain continously extended due to significant impact on saturation and O_2 fluxes

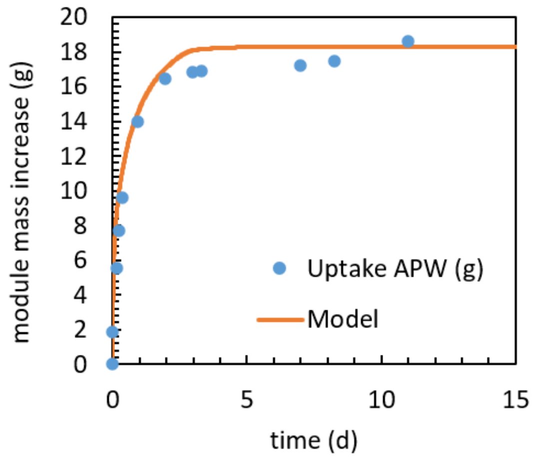
- Cylindrical model of half of a mini-module
- Void space in large module: proportion /mini-module included as ring, filled with OPA slurry (80% porosity)
- Boundary conditions:
    - Top and bottom: closed boundary, no flux
    - Mantle area: dirichlet boundary, Mont Terri porewater

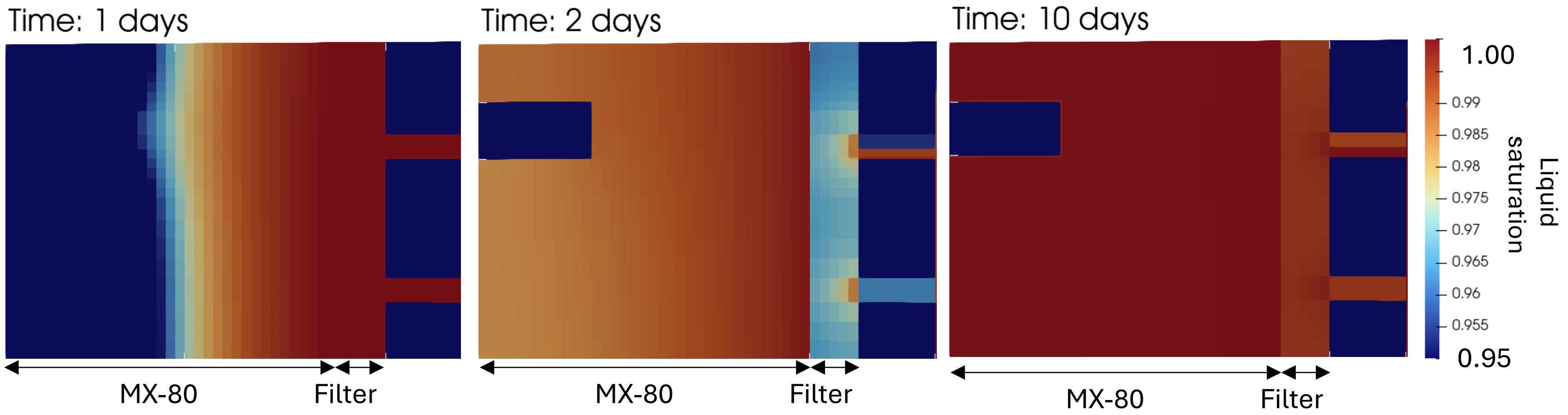


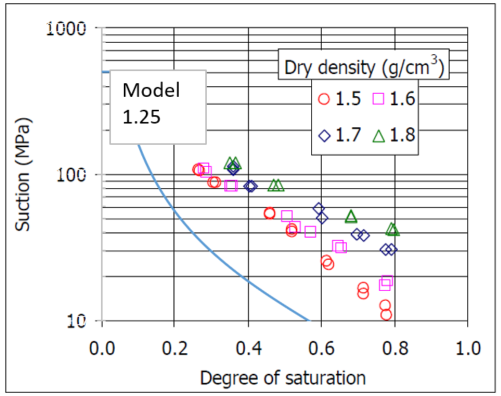
SATURATION PHASE

- Suction curve adjusted to align with experimentally determined water uptake of mini-module in OPA slurry

- > 99% saturation of mini-modul within days,
- some gas pressure remains till ~20-25 days

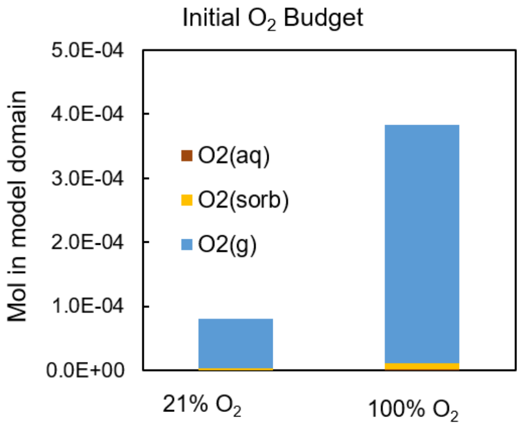


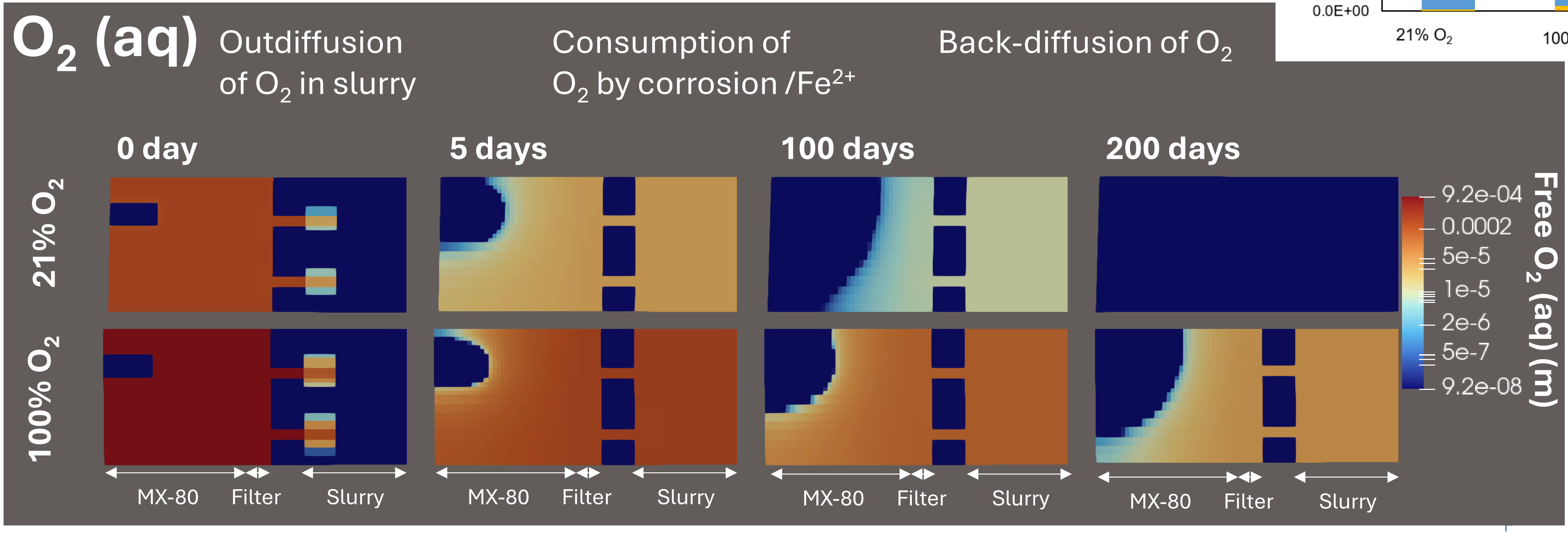




O_2 FLUXES

- Total initial O_2 budget dominated by O_2 in the gas phase
- O_2 (gas) rapidly depleted by corrosion and saturation ($O_2(g) \rightarrow O_2(aq)$)
- Slurry outside of modules acts as an intermediate O_2 storage (no aerobic microbes yet)

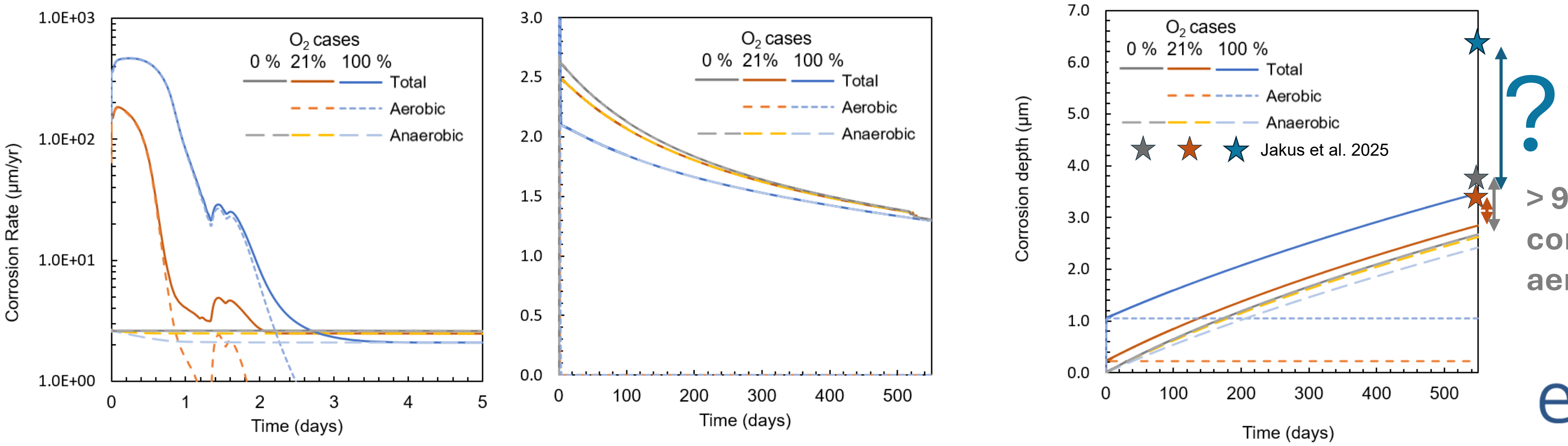




CORROSION RATES AND DEPTH

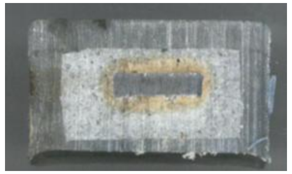
Evolution from aerobic to anaerobic corrosion

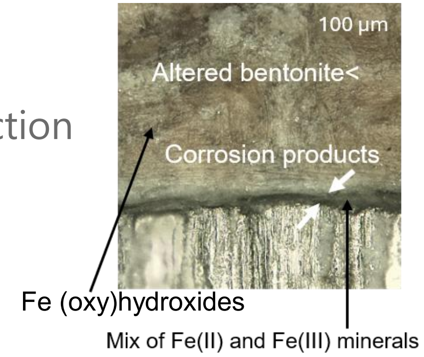
- Corrosion implemented as mineral reaction in a porous outer layer of the coupon
- **Aerobic corrosion**: half-order reaction kinetic with respect to O_2(aq) → stops within the first few days
- **Anaerobic corrosion:** initial corrosion rate of 2.5 µm/a → decreases as a function of porosity in the steel cell (blocking of the steel surface by corrosion products)



> 99 % of O_2 consumed by aerobic corrosion

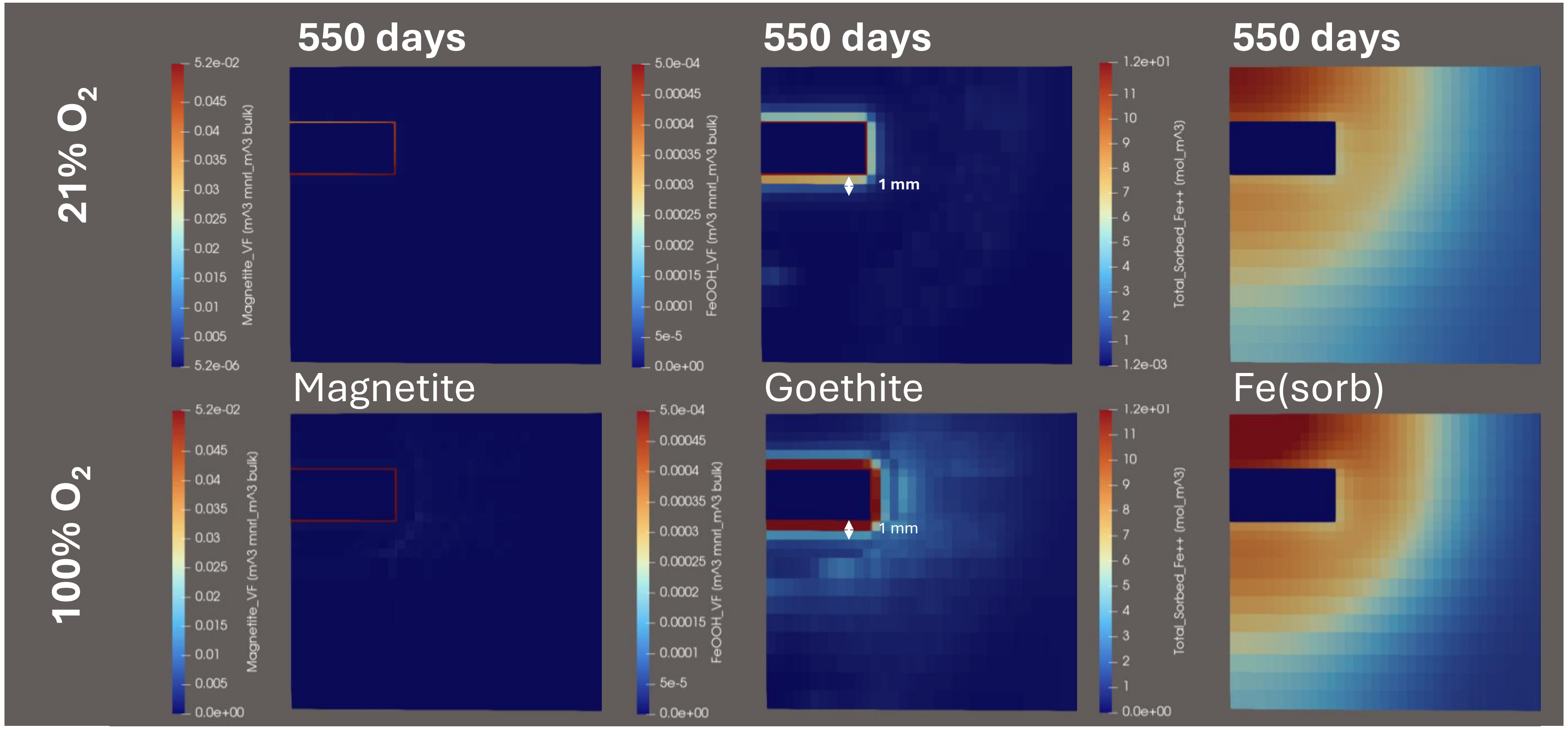
Jakus et al., 2025, Environ. Sci. Technol. 59, 25368-25379

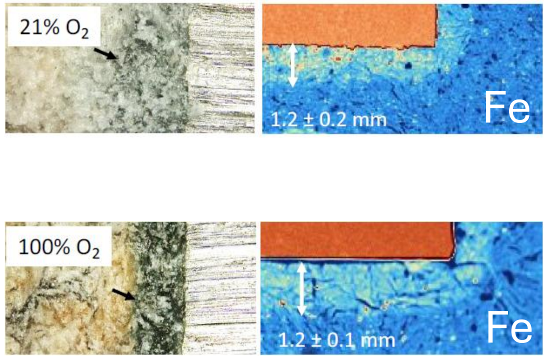




SECONDARY FE PHASES AND FE SORPTION

- Model reproduces small zone of corrosion products
- Larger rim of Fe(oxy)hydroxides due to Fe^{2+} diffusion and interaction with residual $O_2(aq)$
- Differences between O_2 cases mainly relates to the quantity not to spatial extent of the interaction





CONCLUSIONS

- The experimental observations in the IC-A experiments after 1.5 years are the results of several coupled processes relevant for the early transient phase of a repository
- A corrosion model accounting for abiotic, aerobic and anaerobic corrosion can reproduce phenomenological observations but not yet match all quantitively

- The further development of the model will:
  - Include microbial processes
    → How (much) do they contribute to O_2 depletion and corrosion
  - Re-evaluate the corrosion kinetics with data obtained after 3 years of incubation
  - Account for mineralogical changes due to interaction of sulfide and Fe(II) with montmorillonite