eurad
European Joint Programme
on Radioactive Waste Management

DONUT

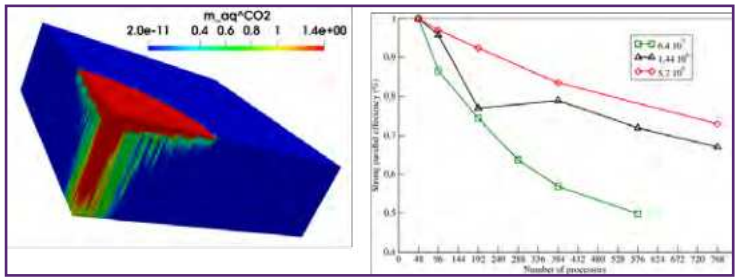
***D**evelopment and improvement **O**f **NU**merical methods and **T**ools for modelling coupled processes*

Eric Laloy & Diederik Jacques

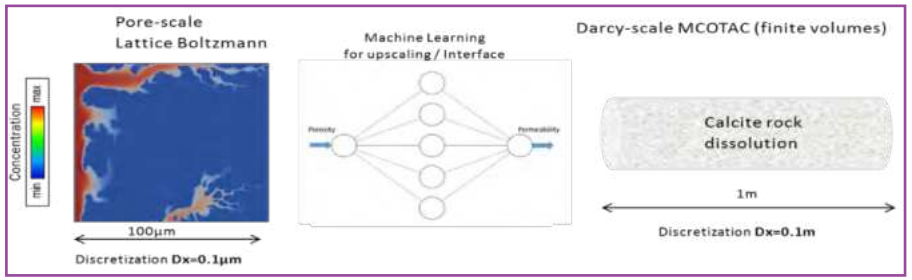
Exchange meeting EURAD 25/10/2024

DONUT AT A GLANCE

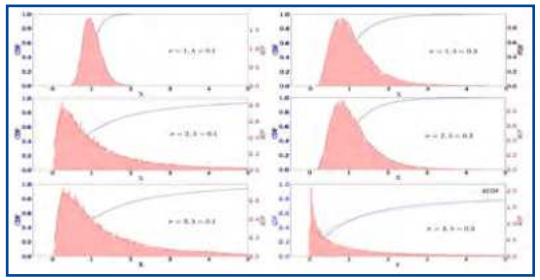
Task 1 Management (Leader F. Claret & G. Pepin)



Task 2 Numerical methods for high performance computing of coupled processes (Leader C. Cances)



Task 3 Scale transition schemes for coupled processes (Leader O. Kolditz & N. Prasianakis)



Task 4 Tools and methods to quantify/derive uncertainties induce by coupled processes (Leader A. Baksay)

Task 5 Benchmarks of methods and tools for coupled processes (Leader D. Lukin)

Benchmarks of methods and tools for coupled processes

Machine Learning and Geochemistry

ACED & FUTURE WPs

THM model evaluation

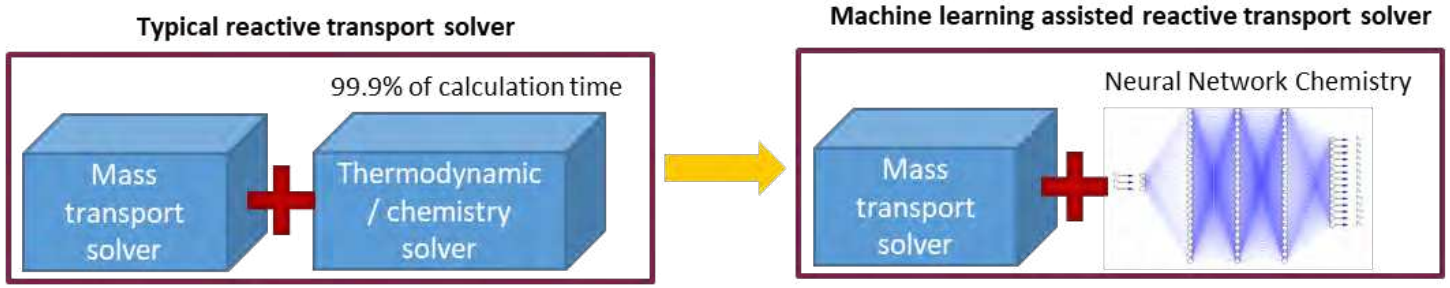
HITEC

Multiphase multicomponent reactive transport

ACED & GAS WPs

Machine learning & geochemistry

- RW disposal studies rely on reactive transport (RT) modelling to simulate, e.g.,
  - Cement and concrete degradation phenomena
  - The fate of radionuclides from drum matrix to the environment



- RT models can be computationally demanding
  - Transport component ~ 5-25% of CPU time
  - Geochemical component ~ 75 – 95% of CPU time

- RT model acceleration by replacing the geochemical solver by a trained ML regression algorithm → speedup of 4 to 20

GEOCHEMISTRY AND MACHINE LEARNING BENCHMARK WITHIN EURAD JOINT PROJECT

Participating teams

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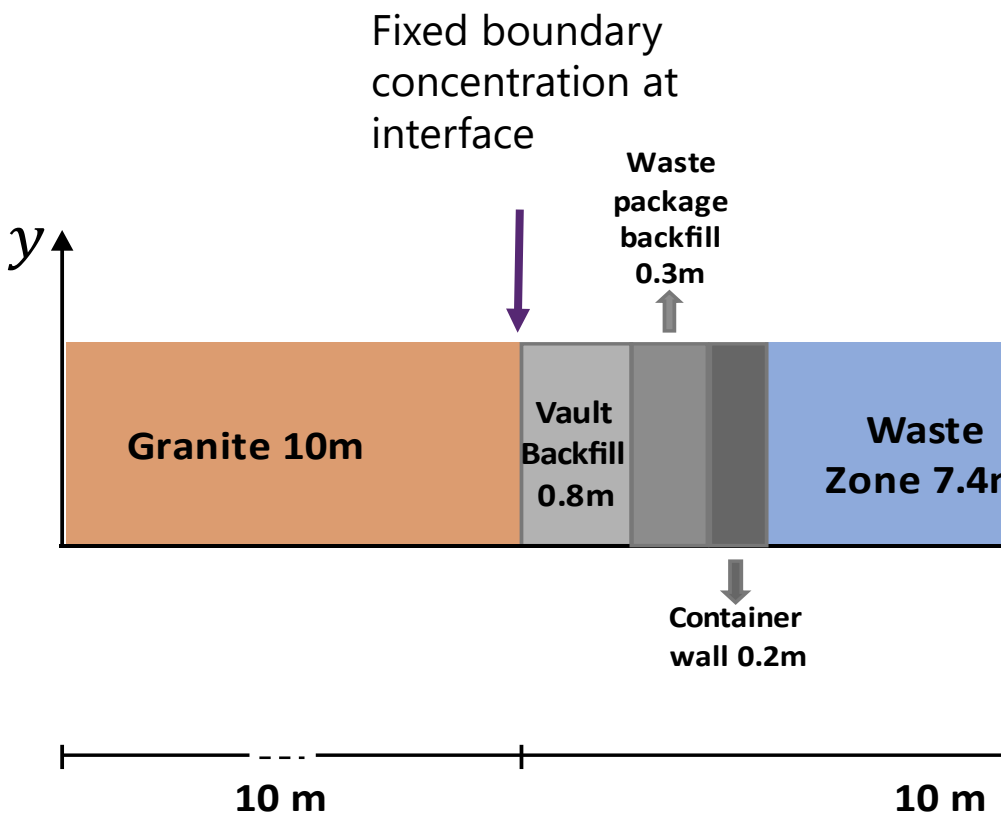
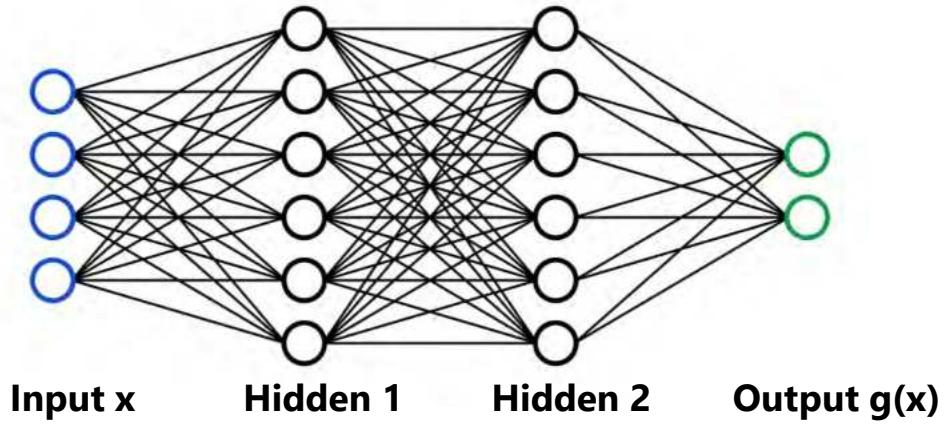
Application

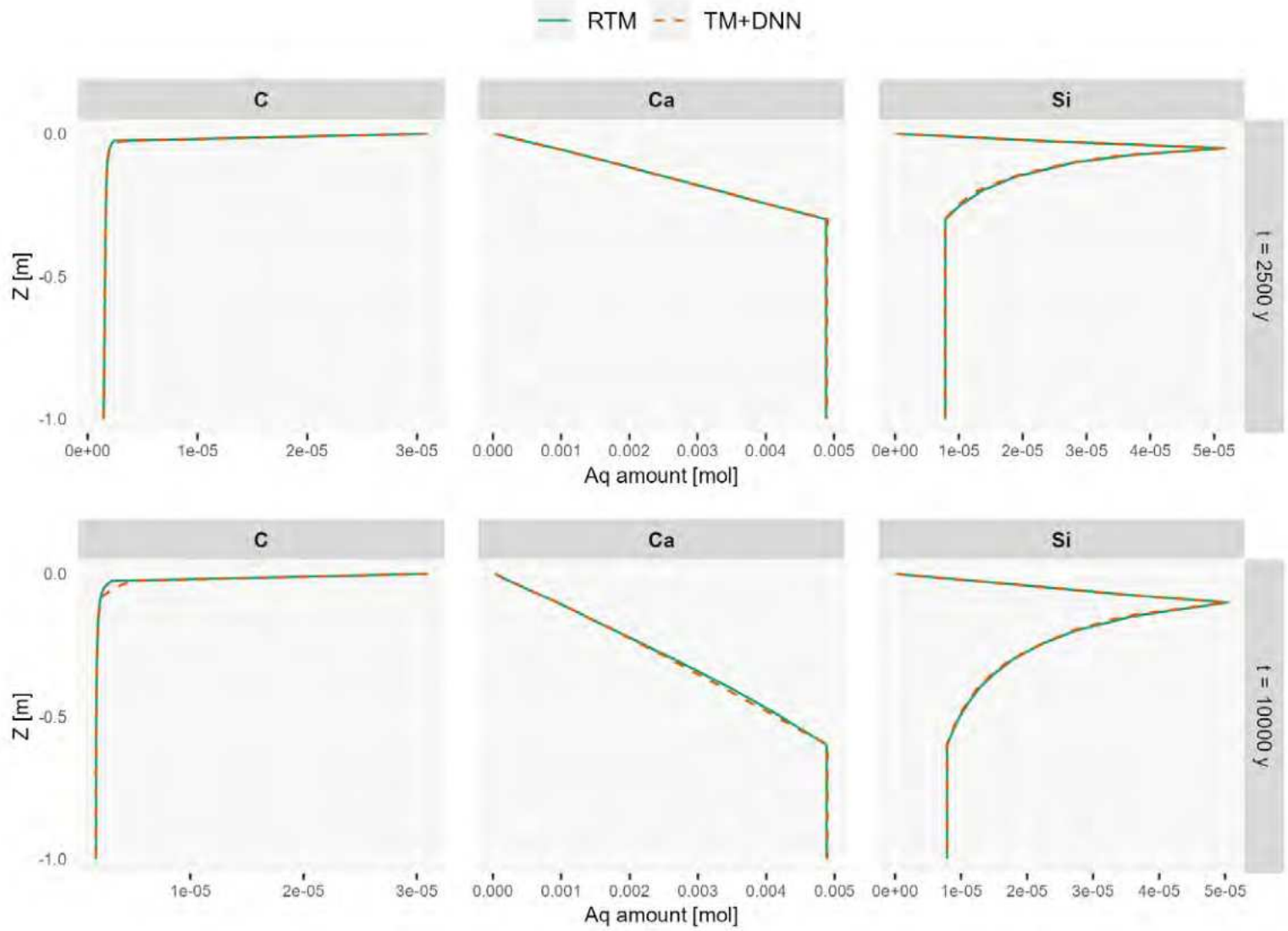


Simple cement: C, Ca, Si, O, H

- Portlandite, C-S-H
- Boundary solution is in equilibrium with Calcite
- Triggers leaching + calcite precipitation

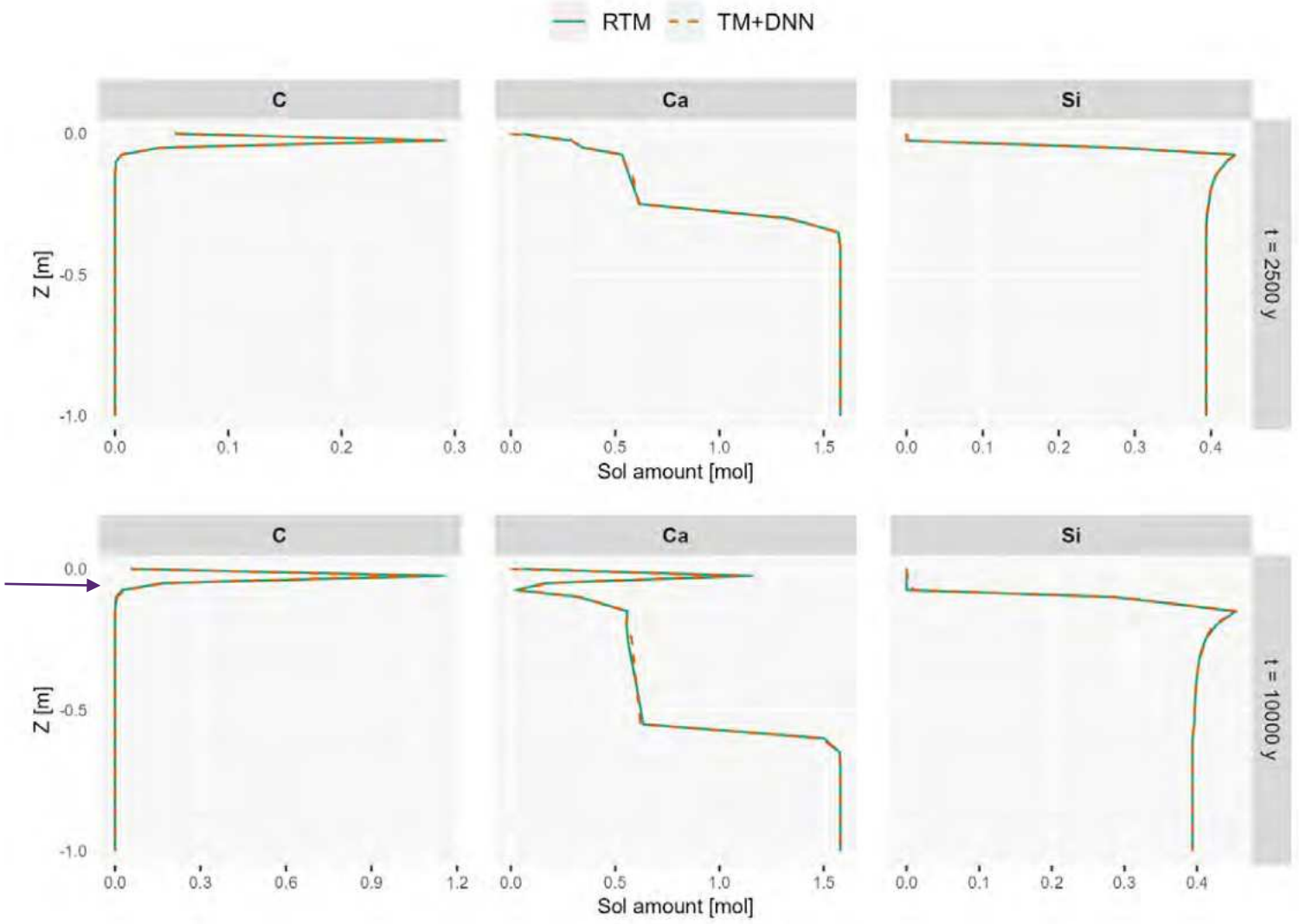


DNN, Case Pc (15) – Aqueous amount profiles at 2 times



DNN, Case Pc (15) – Solid amount profiles at 2 times

Calcite precipitation front



Conclusion

- Good accuracy and speedup of 5.5 (22) against HPx4C (HPx1C)
  - Close to “optimal” speedup ~ 85-90%

- Problem with more complex cement case (C-Ca-Si-Al-Cl-K-Na-Mg-S-O-H)
  - Limiting case for black-box DNNs?

- Follow-up in EURAD2 HERMES WP
  - Improve NN training set creation
  - Add physical constraints to NN training → physics-informed NNs (PINNs)
  - Accept/reject mechanism of ML predictions within the RT simulation
  - Apply to pore-scale RT simulation where geochemistry can take 99% of the CPU time