

THMC-Coupled Modelling of Muschelkalk Diagenesis and Reservoir Simulation in the NGB

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1. Introduction

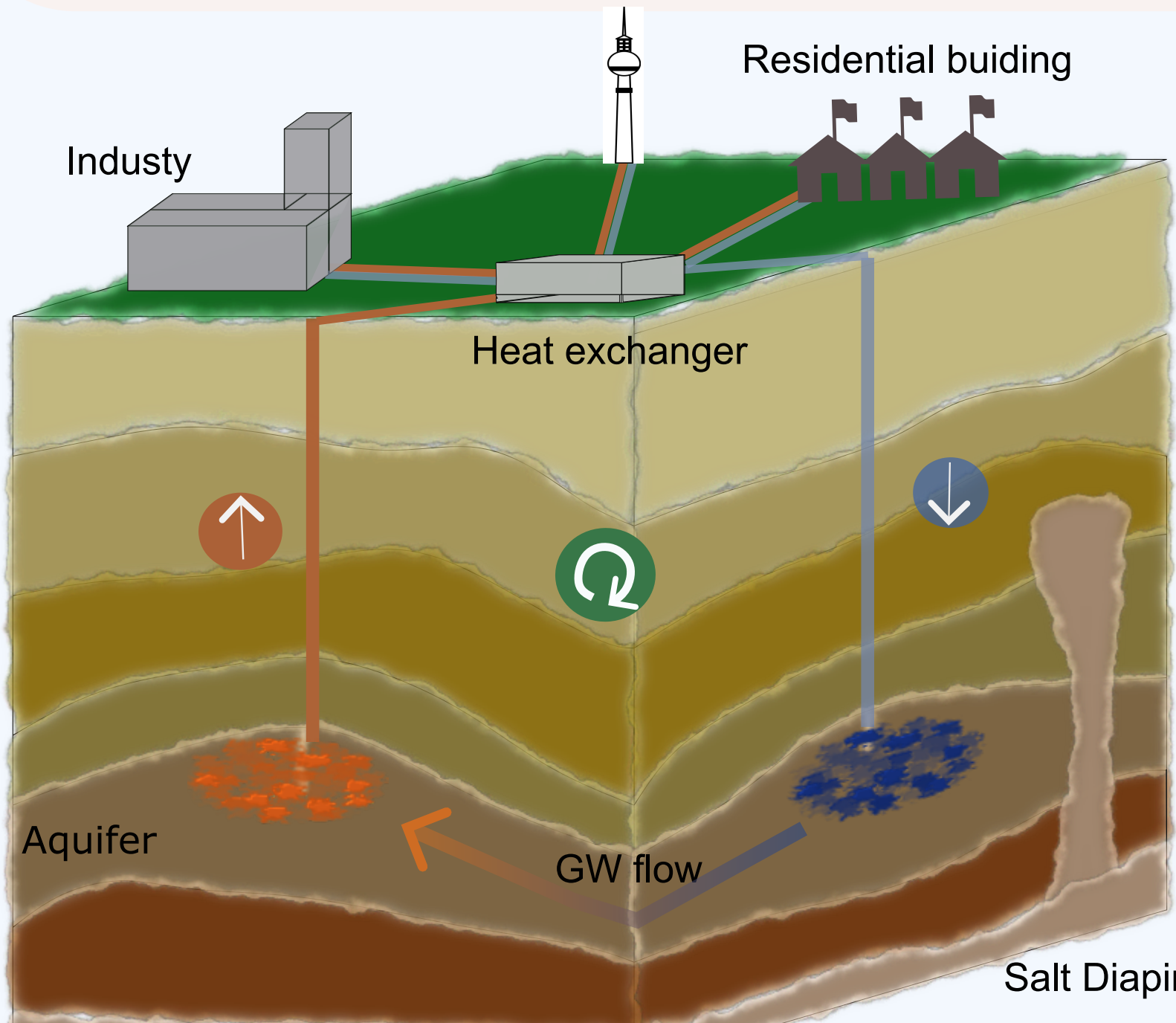
Motivation & Challenges

- Growing demand for **sustainable geothermal energy** in the Berlin-Brandenburg region.
- The **Muschelkalk** is a promising geothermal formation in Berlin-Brandenburg, providing potentials for **future site selection and doublet systems**.
- Integration of Thermal, Hydraulic, Mechanical, and Chemical (THMC) processes modelling (e.g., dolomitization, halokinesis) to better understand **diagenetic evolution** and **improve geothermal assessment**.

But **Complex coupling** between THMC-coupled process; Multiscale **heterogeneity**.
High computational demand and **parameter uncertainty**

2. Objectives

- Develop a **THMC-coupled modelling framework** to simulate **diagenetic and geothermal processes** in the Muschelkalk Formation.
- Quantify the impact of **THMC parameters and geochemical reactions** (e.g., dolomitization, dissolution) on porosity-permeability evolution.
- Perform **basin- to reservoir-scale simulations** with doublet systems to evaluate geothermal productivity and reservoir process behavior.



Continuous geothermal circulation
Goal: Test 100 doublet systems

Potential of the Muschelkalk Reservoir

- High porosity-permeability
- Favorable hydrochemistry
- Secondary porosity
- Existing well data

Fig.1: Schematic subsurface model of Berlin-Brandenburg showing a continuous operation geothermal doublet circulation system (carbonate aquifer).

3. Methods & Modelling Framework

THMC coupled Challenges

- Coupling multiphysics interactions (THMC) across **different time and spatial scales**.
- Ensuring **stable data exchange** between mechanical, flow, and geochemical solvers.
- Managing **high computational demand** of fully coupled THMC simulations.

How the THMC Coupling Works?

Solve thermal, hydraulic, and mechanical fields (T, p, σ) in porous media

GOLEM
MOOSE

Temperature, pressure, and species concentrations



Compute geochemical reactions (e.g., dolomitization, dissolution, precipitation)

Iterate data exchange at each time step for a fully coupled THMC simulation

Update porosity and permeability

Framework Validation

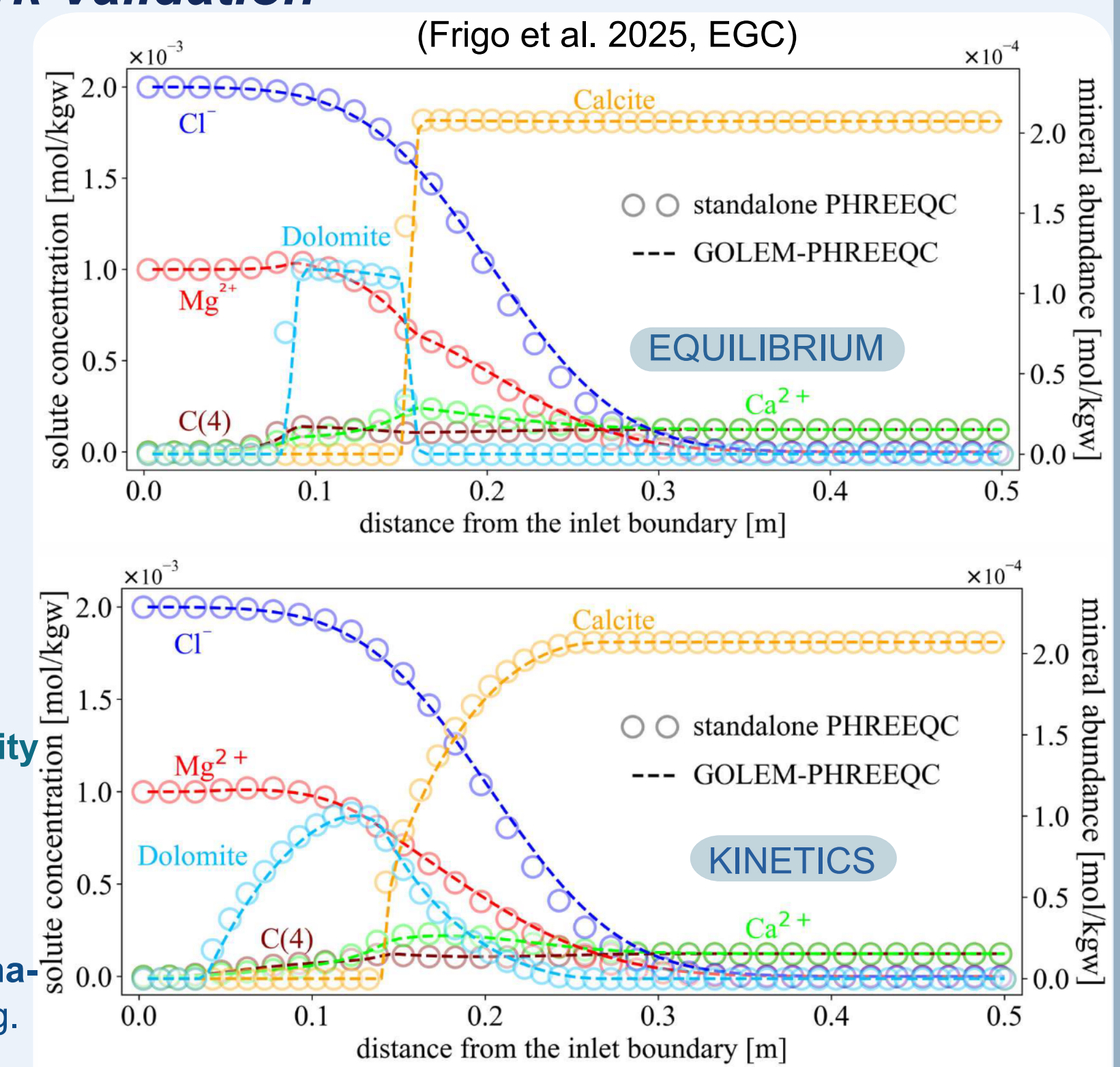
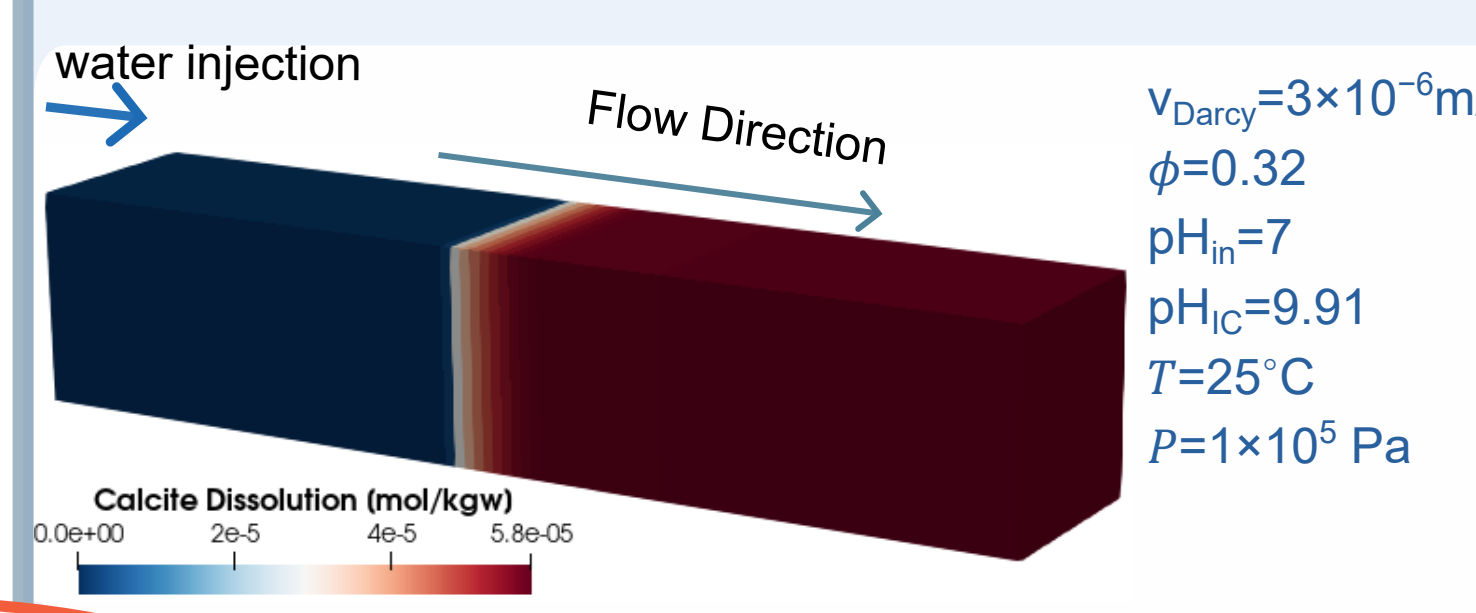
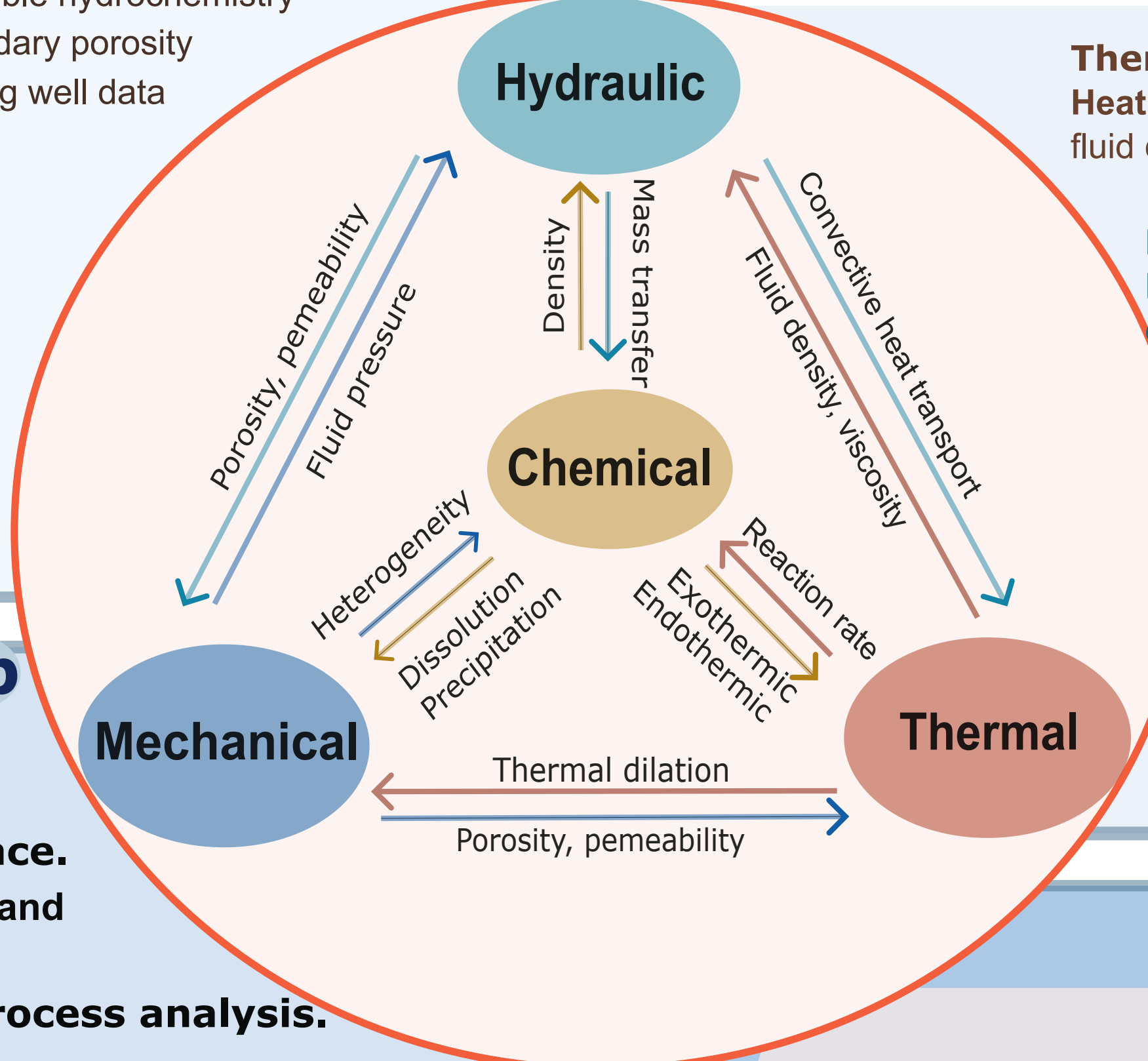


Fig.2: Code validation against PHREEQC. good agreement ($R^2 > 0.95$) under equilibrium and kinetic condition



4. Conceptual & Facies Model Setup

Geological Context

- Muschelkalk formation within the **Berlin-Brandenburg subsurface**.
- The basin-scale model with multiple subsurface facies, e.g. **dolomitic and limestone**
- Data derived from **regional stratigraphic and 8 boreholes process analysis**.

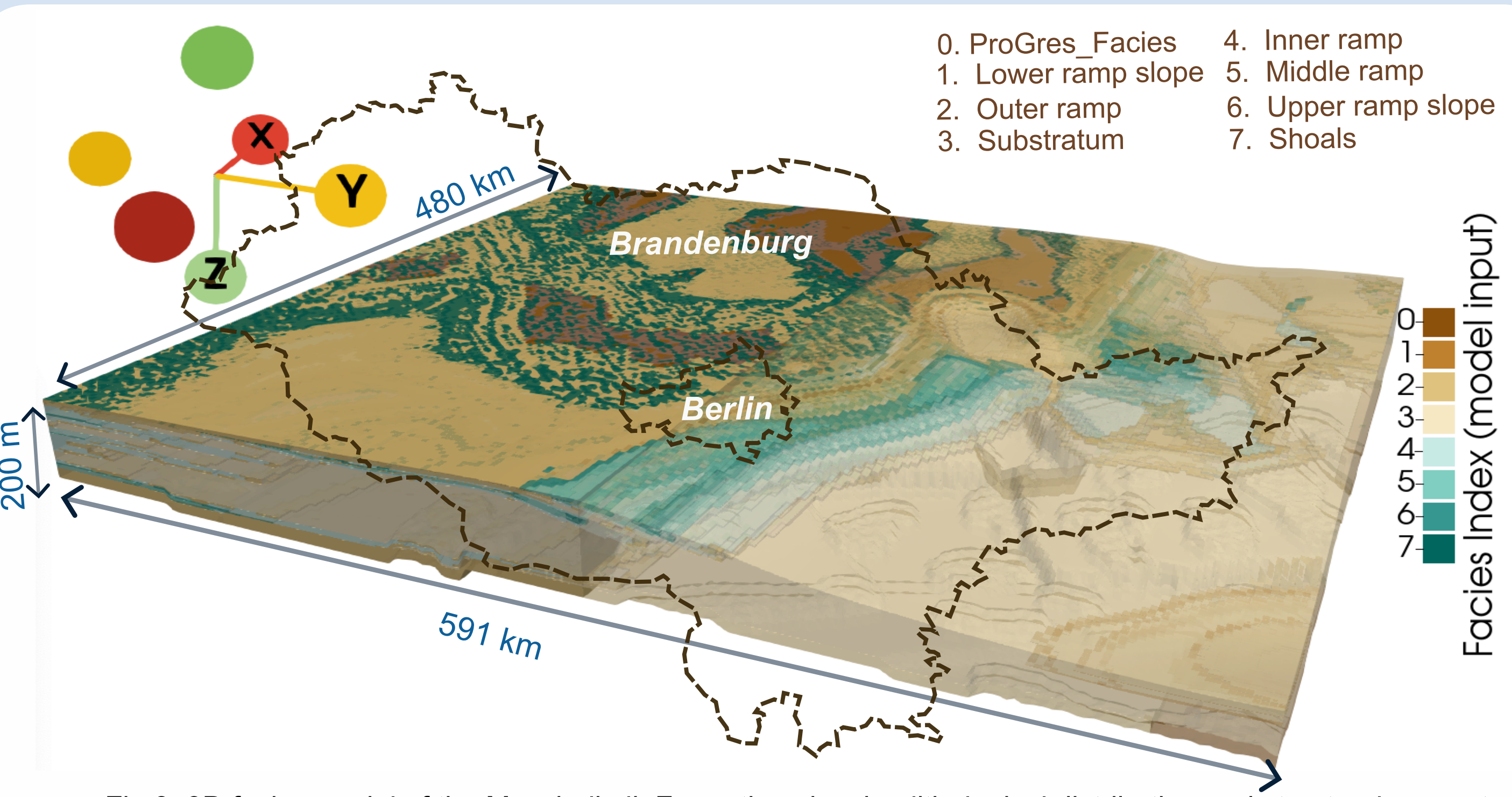


Fig.3: 3D facies model of the Muschelkalk Formation showing lithological distribution and structural geometry

Facies Model Description

- 3D facies distribution created from **stratigraphic layering and depositional patterns**.
- Each facies assigned **distinct petrophysical properties** (porosity, permeability).
- **Corner-point grid to hexahedral mesh conversion**
- Model imported into **GOLEM** for mesh generation and property mapping.

Property Type	Parameter	Symbol	Range / Value	Unit
Thermal	Thermal conductivity	λ	2.7 - 5.8	$\text{W m}^{-1} \text{K}^{-1}$
	Volumetric heat capacity	c_s	2.2 - 2.5	$\text{MJ m}^{-3} \text{K}^{-1}$
Hydraulic	Porosity	ϕ	0.10 - 0.27	-
	Permeability	k	$1 \times 10^{-14} - 1 \times 10^{-12}$	m^2
Mechanical	Bulk density	ρ	2000 - 2700	kg m^{-3}
	Young's modulus	E	9 - 40	GPa
	Poisson's ratio	ν	0.20 - 0.30	-
Chemical	Thermal expansion coeff.	α_T	$1 \times 10^{-5} - 3 \times 10^{-5}$	K^{-1}
	Calcite dissolution rate	k_c	$1 \times 10^{-7} - 1 \times 10^{-6}$	$\text{mol m}^{-2} \text{s}^{-1}$
	Dolomite dissolution rate	k_d	$1 \times 10^{-10} - 1 \times 10^{-9}$	$\text{mol m}^{-2} \text{s}^{-1}$

Table 1. Representative THMC Properties of the Muschelkalk Formation, Berlin Region

5. Model Analysis (Ongoing)

Key Research Focus

- **THMC-coupled effects** on porosity, permeability, and **related uncertainties** driven by diagenetic evolution.
- **Diagenetic processes** (e.g., dolomitization, dissolution) controlling reservoir quality and **heterogeneity**.
- **Sensitivity analysis** of coupled parameters and **injection-extraction** on reservoir performance.
- **Basin-scale simulation** and assessment of **doublet system** in the Muschelkalk Formation.

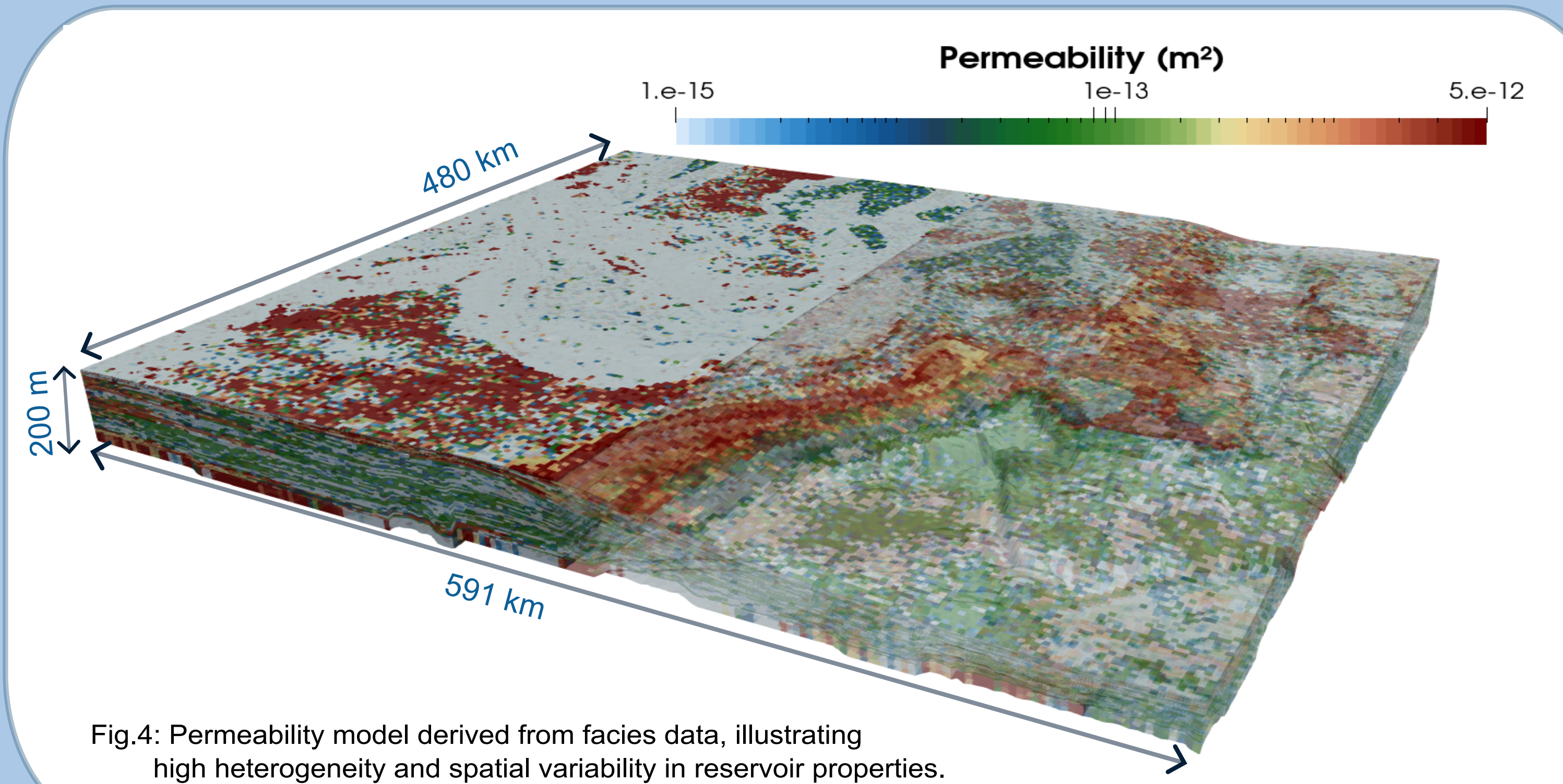


Fig.4: Permeability model derived from facies data, illustrating high heterogeneity and spatial variability in reservoir properties.

6. Summary & Outlook

- **THMC-coupled workflow** reproduces key diagenetic processes and property evolution.
- Demonstrates **process-based integration** of THMC-coupled **mechanisms**.
- Evaluate **porosity-permeability evaluation** and reservoir doublet systems.

Next:

- Apply model to **regional-scale Muschelkalk reservoir** (Berlin-Brandenburg).
- Extend to **doublet well simulation** for long-term production assessment.
- Implement **uncertainty quantification** to evaluate model sensitivity and reliability.



Reference

Frigo et al. (2025). Coupling GOLEM, PHREEQC, and Reaktoro for enhanced simulation of reactive processes in geothermal systems.
De Lucia et al. (2021). POET (v0.1): speedup of manycore parallel reactive transport simulations with fast DHT lookups. Geosci. Model Dev., 14, 7391-7409.

Acknowledgement

Funded by the Federal Ministry of Education and Research (BMBF) - **Project ProGRes** ("Development of a **Diagenetic Process Model of the Muschelkalk and Numerical Simulation of Reservoir** and Extraction Performance"), 03V01892; 01.2025-12.2027.



Expertise Highlights:

- Multi-scale, coupled thermo-hydro-mechanical-chemical (**THMC**) modelling of subsurface processes
- **Numerical simulation and constitutive modelling** using FEM (**MOOSE Framework, Golem**)
- High-performance computing (**HPC**) for **multi-scale** geoscientific simulations