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Simulation of Reactive Transport in Porous Media: A Benchmark for a COMSOL-PHREEQC-Interface

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Introduction:

- In Aquifer Thermal Energy Storage (ATES), aquifer porosity and permeability have a strong impact on the system's performance and reliability. These parameters can change due to interactions between rock matrix and pore fluid. Reactive transport simulations help understand these processes to optimize the operational mode of the overall system.
- The reactive transport simulation interface COMSOL_PHREEQC (Wissmeier & Barry 2011) couples COMSOL Multiphysics for flow and heat transport simulations with PHREEQC as a geochemical batch reaction simulator.
- COMSOL_PHREEQC is tested using the "calcite" example as a benchmark (Shao et al. 2011). The results are compared to OpenGeoSys (OGS), coupled with PHREEQC.

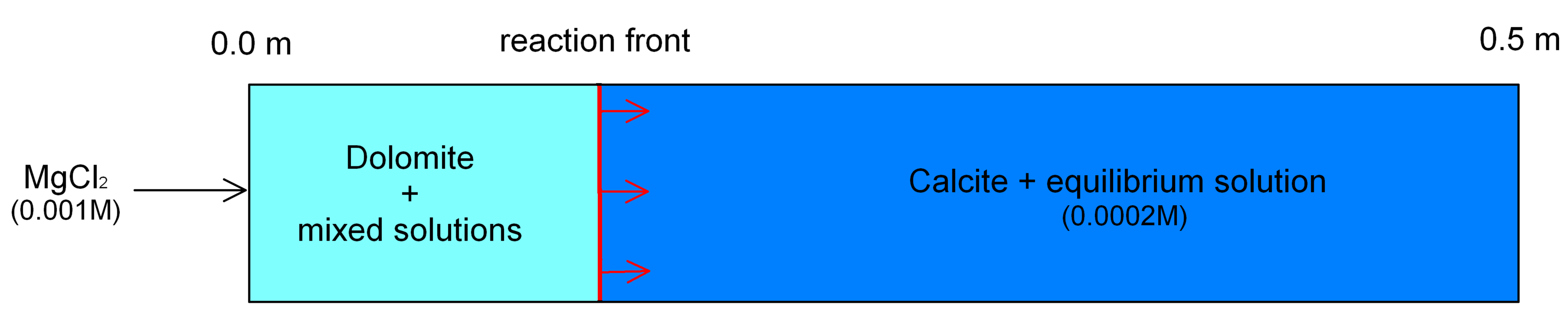


Figure 1. Model geometry and solution properties.

Computational Methods:

- In the "calcite" example, a column initially contains calcite and water. During the experiment, the column is flushed with a $MgCl_2$ solution. Calcite is dissolved and dolomite precipitates temporarily. Cl serves as a non-reactive tracer.
- Two test runs with different porosities were performed. The model properties are displayed in Figure 1 and Table 1.

Material Properties			Model Properties		
Column length	0.5	m	Nodes	101	-
Effective porosity	0.32 / 0.99	-	Cells	100	-
Bulk density	1800 / 1010	kg/m^3	Cell length	0.005	m
Longitudinal dispersivity	0.0067	m	Dimensions	1d	-
Darcy velocity	$3{\cdot}10^{-6}$	m/s	Time steps	42	
Permeability	$1.157{\cdot}10^{-12}$	m^2	Time step length	500	s

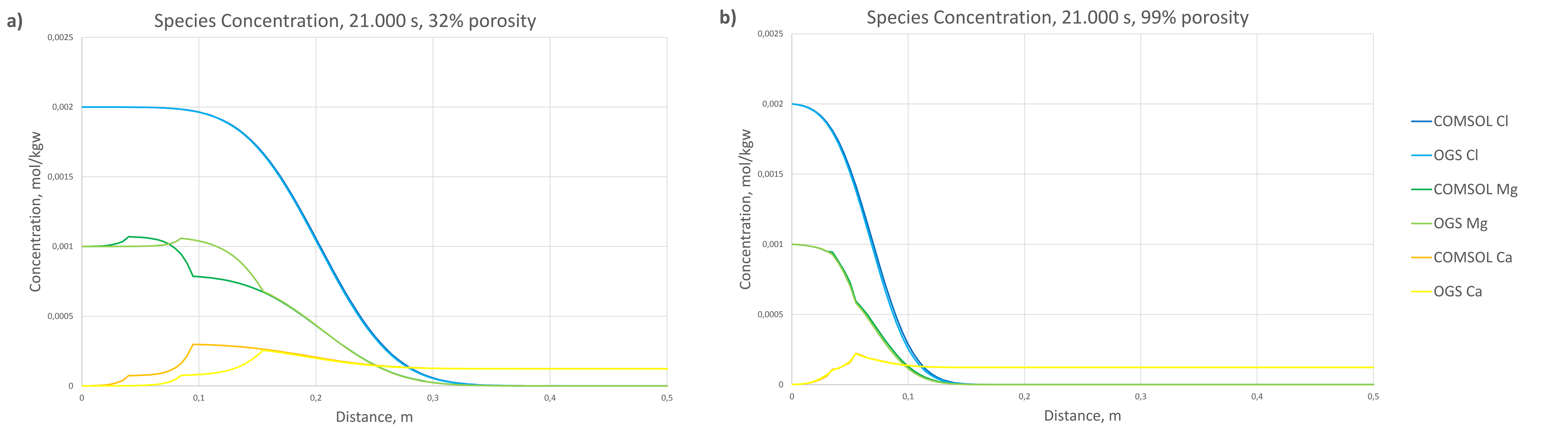
Table 1. Material and model properties.

- Constraints for both COMSOL and OGS:
  - A sequential non-iterative split-operator approach separates flow, solute transport and reaction calculations.
  - Density and porosity are assumed to be independent of chemical reactions.
  - Transport is calculated for master species only.
  - Kinetics is not considered.
- COMSOL Modules and Interfaces:
  - Flow simulation: Darcy's Law interface (Subsurface Flow Module)
  - Species transport: Species Transport in Porous Media interface (Chemical Reaction Engineering Module)
  - COMSOL_PHREEQC coupling/controlling application: LiveLink for Matlab

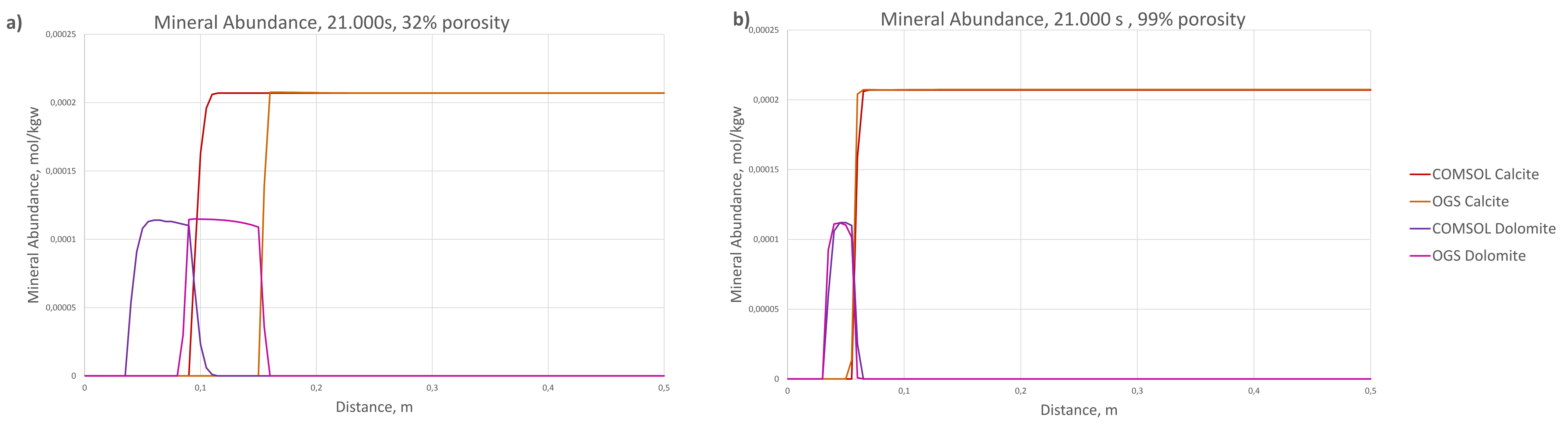
Results:

- The flow distance decreases with increasing porosity, as the Cl curve shows. Results are similar for COMSOL and OGS (Figs. 2 and 3).
- The element and mineral concentrations resulting from reactive transport calculations are similar for OpenGeoSys-PHREEQC and COMSOL_PHREEQC at 99% porosity. At 32% porosity, the position of the reaction front, where calcite is dissolved and dolomite precipitates, is shifted (Figs. 2 and 3).

Figures 2a and 2b. Species concentration of chloride (Cl), magnesium (Mg) and calcium (Ca) vs. distance after 21.000s, a) 32% porosity, b) 99% porosity.



Figures 3a and 3b. Mineral abundance of calcite and dolomite vs. distance after 21.000s, a) 32% porosity, b) 99% porosity.



Conclusions:

- Flow calculation and non-reactive element transport results are consistent for OpenGeoSys and COMSOL.
- Reactive transport yields similar results only when porosity is not considered (i.e. in a capillary). In porous media, the reaction front positions calculated by COMSOL_PHREEQC and OpenGeoSys-PHREEQC differ from each other.

References:

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2. L. Wissmeier & D.A. Barry, Simulation tool for variably saturated flow with comprehensive geochemical reactions in two- and three-dimensional domains, Environmental Modelling & Software, 26, 210-218 (2011)

Acknowledgments:

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