A new CSMP++GEM reactive transport code

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Studies of reactive transport phenomena require simulations that combine versatile THM models with flexible chemical equilibrium speciation calculations. A successful SNIA coupling of CSMP++ and GEMS3K codes was performed, enabling simulations of non-isothermal single-phase multi-component transport through chemically reactive porous media. The CSMP++ framework [1], uses the finite element method to solve equations that describe diffusive processes, and the finite volume method - for advection processes. The GEMS3K Gibbs energy minimization code [2] computes (meta)stable chemical speciation in complex heterogeneous multi-phase systems. Our coupled code stands out as it combines the advantages of GEM over "classic" chemical speciation codes with the ability of CSMP++ to model THM processes on unstructured grids capturing complex flow geometries.

We have initially benchmarked CSMP++GEM against TOUGHREACT for a simple 1D model, representing a 10m rock column (10% of calcite), saturated and equilibrated with seawater. An aggressive solution (seawater equilibrated with $pCO2=10^{-2.2}$ bar) is injected on the column top at a rate $3 \cdot 10^{-8}$ m/s. Although the results after 300 years of injection (fig. 1) match almost perfectly, later the curves start to diverge gradually. This illustrates that even slight differences in the equations of state used for water and brine, as well as in aqueous activity models, can result in significant differences over geological time.

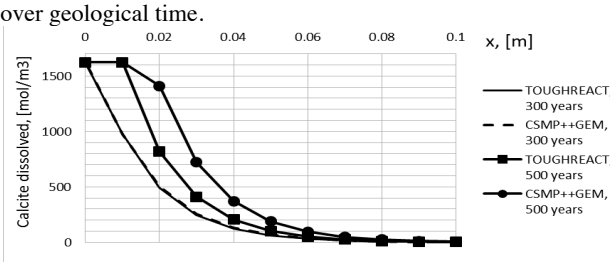

Figure 1: 1D calcite dissolution benchmark results.

1D reflux dolomitization benchmarks with dolomite kinetics and further simulations under more complex geometries are in progress.

[1] Geiger et al. (2004) *Geofluids* **4**, 284-299. [2] Kulik et al. (2013) *Computational Geosciences* **17**, 1-24.