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GOLEM and PHREEQC: a novel THMC FEM simulator for assessment of ATES performance

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We present a novel open source reactive transport simulator based on the coupling of GOLEM, a finite element simulator for thermal-hydraulic- mechanical modeling based on the MOOSE multiphysics framework, with the PHREEQC geochemical solver. GOLEM solves coupled partial differential equations governing subsurface fluid flow, heat transfer, conservative mass transport, and mechanical deformation in complex heterogeneous geological environments. PHREEQC is an established geochemical solver widely adopted in the scientific community. Its coupling to GOLEM is achieved leveraging the convenient LITEPHREEQC library, an original wrapper extending the IPhreeqc module, and which also serves as basis for python and R packages. We showcase the capabilities of GOLEM-PHREEQC by validating its results with RTM benchmarks including equilibrium and kinetic mineral reactions and sorption processes, with feedbacks on porosity and permeability. Furthermore, we employ GOLEM-PHREEQC to both perform history matching of push-pull tests and to assess the potential impact of induced mineral scalings on the performance of an ATES (aquifer thermal energy storage) site in Berlin by means of 3D simulations in a heterogeneous setting.

[1] De Lucia, M., Frigo, S., Lübke, M., Cacace, M., Petrova, E., Hofmann, H., Scheck-Wenderoth, M., Blöcher, G. (2026): Towards fully coupled Thermo-Hydro-Mechanical-Chemical (THMC) modelling in advanced reservoir engineering: GOLEM-PHREEQC. Advances in Geosciences, 67, 117-127. https://doi.org/10.5194/adgeo-67-117-2026