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Reactive Transport Modeling of Hydrothermal Systems with Reaktoro and OpenFOAM

MR. JASPER ENGELMANN AND LARS RUEPKE
GEOMAR Helmholtz Centre for Ocean Research Kiel

Seafloor hydrothermal vent systems are of great geological, oceanographical, biological and potentially economical interest. By nature, they are difficult to access and observe directly, and long-time observation on the scale of their lifespans (10s of ka) is impossible. Outside of preservation in the rock record, numerical models have proven very capable in investigating the subseafloor processes involved.

Fluid dynamic models have revealed much, including an explanation for the observed upper limit of vent temperatures around 400°C. Yet, these models often exclude changes to the system induced by fluid rock interaction. On the other hand, many studies of the thermodynamics of hydrothermal systems exclude the effects of physical processes (e.g., chemical transport).

Our newly developed model joins one with the other, resulting in a widely applicable toolbox for reactive transport modeling in a hydrothermal context. It is based on two open-source libraries:

1. HydrothermalFOAM, an implementation of porous (Darcy) flow within the finite volume CFD-toolbox OpenFOAM (openfoam.org), expanded with an equation to model chemical species transport
2. Reaktoro (reaktoro.org) to model chemical reactions through Gibbs Energy Minimization, using the MINES thermodynamic database

OpenFOAM allows for easy creation, adaption and refinement of computational meshes (in 1D, 2D, and 3D), and includes a wide variety of customizable initial and boundary conditions. It also includes a range of modern, efficient and versatile solution algorithms for partial differential equations, allows for parallelization and runs on high performance computers.

Reaktoro on the other hand provides access to a number of widely used thermodynamic databases and an easy-to-use API in both C++ and python. Through the GEM method, chemical systems can quickly and easily be adapted to different settings, without the need to parametrize each reaction.

We employ our coupled solver in the exploration of feedback mechanisms between mineral precipitation, subseafloor permeability and the hydrological regime below black smoker systems.