Modelling two-phase flow and reactive transport with the CSMP++GEM coupled code

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The new CSMP++GEM reactive transport code, upgraded from its earlier version (Yapparova et al., 2017a,b), can now perform simulations of non-isothermal two-phase flow of aqueous liquid and steam with partitioning of chemical elements upon boiling and fluid-mineral reactions, including non-ideal mineral solid solutions.

Standard RTM codes often have restricted temperature and pressure range (e.g. temperature only up to 300ºC in TOUGHREACT), can model only incompressible single phase flow (e.g. OpenGeoSys-GEM), or cannot model solid solutions and gas mixture as separate phases (e.g. Geochemists Workbench, Bethke (2008)). In widely used LMA (Law of Mass Action) based reactive transport codes, solid solutions are modelled in one of two ways: either as kinetically controlled symmetric binary solid solution (TOUGHREACT) or as a discrete set of minerals with varying ratio of end-members. The latter approach is often used in PHREEQC, although PHREEQC can model non-ideal binary solid solutions.

The GEM-Selektor geochemical modeling package (http://gems.web.psi.ch), together with the GEMS3K kernel (Kulik et al., 2013) implementing the GEM (Gibbs Energy Minimization) method, can model complex multi- phase systems containing non-ideal mineral solid solutions, non-ideal gas mixtures, and aqueous phase, under varying temperature and pressure, over a wide range of conditions, in equilibrium or kinetically controlled partial equilibrium states.

The CSMP++ (Complex Systems Modelling Platform) is able to model two-phase liquid-vapour transport at hydrothermal conditions using the control volume finite element method (CVFEM) numerical scheme (Weis et al., 2014). In CSMP++, an equation of state for the H_2O-NaCl system from (Driesner and Heinrich, 2007; Driesner, 2007) is used, allowing simulations in the wide temperature-pressure-composition range from 0 to 1000ºC, 0 to 5000 bar, and 0 to 1 X_{NaCl}.

Two codes are coupled using Sequential Non-Iterative Approach (SNIA) (Steefel and MacQuarrie, 1996). Coupling of the CVFEM transport scheme with the GEMS3K kernel within the CSMP++GEM reactive transport code allows to accurately model water-rock interactions along with the partitioning of chemical species between fluid and vapour during boiling or condensation. This is due to the capability of CVFEM to perform the conservative enthalpy-based transport and the capability of GEMS3K to model gas mixtures in equilibrium with the aqueous electrolyte. As at any point on the boiling curve the chemical potentials of water liquid and vapour are equal, the total system enthalpy (Spycher and Reed, 1989) is used as an additional constraint for determining the amounts of liquid and vapour in the system in chemical equilibrium computations.

The CSMP++GEM reactive transport modelling code represents a powerful tool for studying complex natural systems, having access to state of the art heat flow and chemical models, and allows us to explore the interplay of chemical reactions and two-phase transport in ore forming and high-enthalpy hydrothermal systems. The capabilities of the code were benchmarked and tested against other available reactive transport codes such as TOUGHREACT and OpenGeoSys-GEM.

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