PhreeqcRM: A reaction module for transport simulators based on the geochemical model PHREEQC

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With the release of IPhreeqc, a module that allows incorporation of PHREEQC reactions in other software, many groups have begun using it to couple geochemical reactions with groundwater transport simulation. While IPhreeqc provides a general interface, it relies heavily on string processing, and a substantial amount of code is necessary to provide a complete linkage with a transport model. PhreeqcRM is a reaction module, based on IPhreeqc, that designed specifically to perform geochemical equilibrium and kinetic reaction calculations for reactive transport simulators that use an operator splitting approach, that is, simulators that separate the transport simulation from the reaction simulations. The basic function of the reaction module is to take component concentrations for the model cells from the transport simulation, run geochemical reactions, and return revised concentrations. The reaction module maintains the composition of all of the reactants that react to equilibrium in each cell, which may include minerals, exchangers, surface complexers, a gas phase, and solid solutions, and reactants that react kinetically, which may simulate mineral dissolution and precipitation, biological transformations, bacterial cell growth, or any other kinetic process. The reaction capabilities are a complete implementation of the reaction capabilities of the PHREEQC geochemical model. Methods are available for assigning initial conditions and boundary conditions by use standard PHREEQC input (files or strings) for defining the chemical composition of solutions and reactants. Additional capabilities include methods to account for inactive grid cells, obtain selected results, print detailed reaction calculations for selected cells, and save the chemical state of a calculation. The reaction module uses parallel processing to speed the reaction calculations, either by multithreading on a single computer with OPENMP, or by multiprocessing on multiple computers with MPI (Message Passing Interface). PhreeqcRM is written in C++, but interfaces allow methods to be called from C or Fortran90. By using the PhreeqcRM reaction module, a wide range of geochemical reactions can be easily implemented for an existing multicomponent transport model.