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CORE: A general purpose code for groundwater flow, heat and solute transport, chemical reactions and biological processes in porous and fractured media

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Understanding natural groundwater quality patterns, quantifying groundwater pollution and assessing the effects of waste disposal, require modeling tools accounting for water flow, and transport of heat and dissolved species as well as their complex interactions with solid and gasses phases. Here we present CORE, a COde for modeling saturated and unsaturated water flow, heat transport and multicomponent REactive solute transport under both local chemical equilibrium and kinetic conditions. COREuses the sequential iteration approach to solve the coupled hydrological transport processes and hydrochemical reactions. The finite element method is used for spatial discretization, while general finite difference schemes are used for time discretization. CORE can cope with heterogeneous systems having irregular internal and external boundaries. The code can handle heterogeneous and anisotropic media in 1-, 2- and 3-D dimensions. Both steady-state and transient flow regimes can be simulated. Prescribed head and water flux as well as mixed boundary conditions are included. Both point and areal fluid sources can be specified. In addition, free drainage boundary condition (unit gradient type) is allowed for variably saturated flow. Solute transport processes included in the code are: advection, molecular diffusion and mechanical dispersion. Solute transport boundary conditions include: (1) specified solute mass fluxes, (2) specified solute concentrations and (3) solute sources associated to fluid sources. The code can handle the following types of reactions under the local equilibrium assumption: acid-base, aqueous complexation, redox, mineral dissolution/precipitation, gas dissolution/exsolution, ion exchange (based on the constant charge model) and sorption via surface complexation (using the diffuse double

layer model). COREcan take into account any number of aqueous, exchanged and sorbed species, minerals and gases. Heat transport is solved at each time step. Computed temperatures are used for updating equilibrium constants and the constants for calculating activity coefficients. BIOCORE-2D is a version which copes with both thermodinamically-controlled abiotic geochemical reactions and subsurface microbial processes in 2-D while INVERSE-CORE solves the inverse problem of automatic estimation of flow, solute and chemical parameters. Finally, INVERSE- FADES-CORE allows the forwards and inverse problem of coupled nonisothermal multiphase flow and reactive transport.