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PHREEQC for use in scripting and
programming languages.

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Abstract

The geochemical model PHREEQC is capable of simulating a wide range of equilibrium reactions between water and minerals, ion exchangers, surface complexes, solid solutions, and gases. It also has a general kinetic formulation that allows modeling of nonequilibrium mineral dissolution and precipitation, microbial reactions, decomposition of organic compounds, and other kinetic reactions. To facilitate use of these reaction capabilities in scripting languages and other models, PHREEQC has been implemented in modules that easily interface with other software. A Microsoft COM (component object model) has been implemented, which allows PHREEQC to be used by any software that can interface with a COM server—for example, Excel[®], Visual Basic[®], Python, or MATLAB[®]. PHREEQC has been converted to a C++ class, which can be included in programs written in C++. The class also has been compiled in libraries for Linux and

Windows that allow PHREEQC to be called from C++, C, and Fortran. A limited set of methods implements the full reaction capabilities of PHREEQC for each module. Input methods use strings or files to define reaction calculations in exactly the same formats used by PHREEQC. Output methods provide a table of user-selected model results, such as concentrations, activities, saturation indices, and densities. The PHREEQC module can add geochemical reaction capabilities to surface-water, groundwater, and watershed transport models. It is possible to store and manipulate solution compositions and reaction information for many cells within the module. In addition, the object-oriented nature of the PHREEQC modules simplifies implementation of parallel processing for reactive-transport models. The PHREEQC COM module may be used in scripting languages to fit parameters; to plot PHREEQC results for field, laboratory, or theoretical investigations; or to develop new models that include simple or complex geochemical calculations.



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Keywords

Geochemical modeling; PHREEQC; Reactive-transport modeling; COM; Component object model; C++; C; Fortran

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