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PHREEQCI—A Graphical User Interface to the Geochemical Model PHREEQC

PHREEQCI Version 2 is a complete Windows-based graphical user interface to the geochemical computer program PHREEQC (Version 2). PHREEQCI can be used interactively to perform all the modeling capabilities of PHREEQC—speciation, batch-reaction, one-dimensional (1D) reactive-transport, and inverse modeling.

Applications:

- Mine drainage
- Radioactive-waste isolation
- Contaminant migration
- Natural and engineered aquifer remediation
- Aquifer storage and recovery
- Water treatment
- Natural systems
- Laboratory experiments

Features of the interface:

- Compatible with Windows 95 and 98, Windows NT 4.0, Windows ME, Windows 2000, and Windows XP
- Automated installation using InstallShield
- Interactive access to all of the capabilities of PHREEQC—create and modify input data files, run simulations, and display results

Modeling capabilities:

- Aqueous, mineral, gas, surface, ion-exchange, and solid-solution equilibria
- Kinetic reactions
- 1D diffusion or advection and dispersion with dual-porosity medium
- A powerful inverse modeling capability allows identification of reactions that account for the chemical evolution in observed water compositions
- Extensive geochemical databases

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PHREEQCI Version 2

PHREEQCI Version 2 is a computer program for simulating chemical reactions and transport processes in natural or contaminated water. PHREEQCI provides all of the capabilities of the geochemical model PHREEQC (Parkhurst and Appelo, 1999), including speciation, batch-reaction, 1D reactive-transport, and inverse modeling.

Data for PHREEQC are entered through a series of keyword data blocks, each of which provides a specific type of information. For example, the SOLUTION keyword data block defines the chemical composition of a solution. PHREEQCI provides tabbed dialog boxes for each PHREEQC keyword. Figure 1 shows the main screen of PHREEQCI and the SOLUTION keyword dialog box.

Speciation Modeling

Applications—Speciation modeling is useful in situations where the possibility of mineral dissolution or precipitation needs to be known, as in water treatment, aquifer storage and recovery, artificial recharge, and well injection.

Description—Speciation modeling uses a chemical analysis of a water to calculate the distribution of aqueous species by using an ion-association aqueous model. The most important results of speciation calculations are saturation indices for minerals, which indicate whether a mineral should dissolve or precipitate.

Keyword data blocks used in speciation modeling include:

SOLUTION—define the chemical composition of a solution.

SOLUTION_SPREAD—define the chemical composition of multiple solutions in a spreadsheet format.

Batch-Reaction Modeling

Applications—Batch-reaction modeling can be applied to problems in laboratory, natural, or contaminated systems. The reaction capabilities of PHREEQC have been used frequently in the study of mine drainage, radioactive-

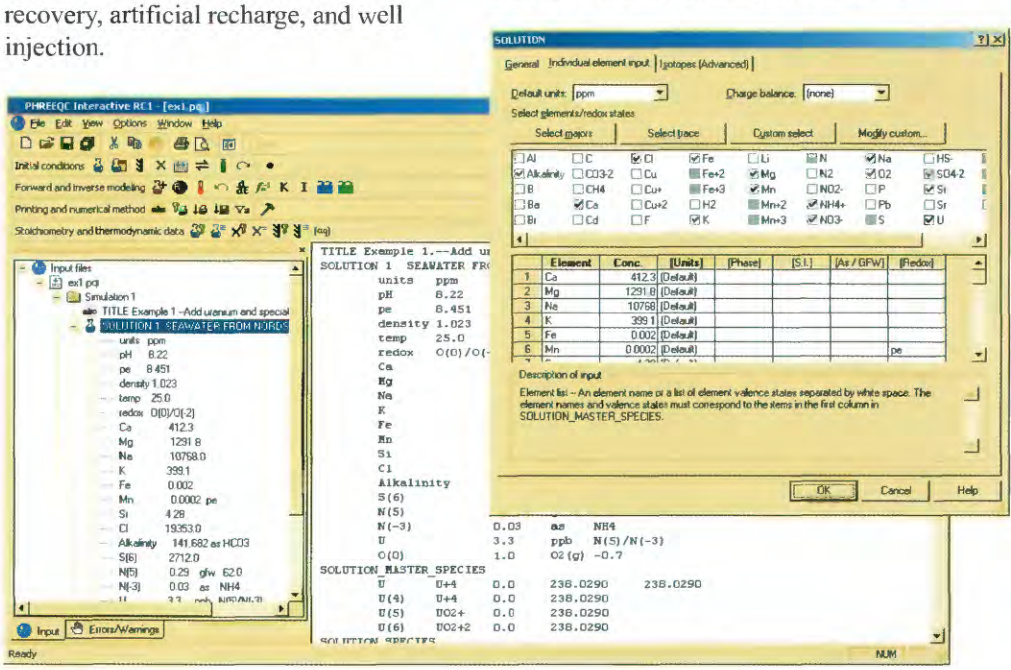

Figure 1. Main screen of PHREEQCI, with the SOLUTION keyword dialog box open.

waste disposal, degradation of organic matter, and microbially mediated reactions.

Description—Batch reactions can be divided into equilibrium and nonequilibrium reactions. Equilibrium reactions include equilibration of a solution with an assemblage of minerals and specified-pressure gases, ion-exchange sites, surface-complexation sites, a finite gas phase, and (or) solid solutions. Nonequilibrium reactions include kinetic reactions, addition or removal of elements from solution, mixing, and changing temperature.

Keyword data blocks used in batch-reaction modeling include:

EQUILIBRIUM_PHASES—an assemblage of minerals and gases that react to equilibrium (or until exhausted).

EXCHANGE—one or more sets of reaction sites for exchangeable ions, an important reaction for major cations.

SURFACE—one or more sets of sites that react by surface complexation, a major reaction for phosphorus, arsenic, and other trace elements.

GAS_PHASE—a finite reservoir of gas that reacts with a solution.

SOLID_SOLUTIONS—solids that precipitate as mixtures of minerals, an important reaction for radionuclides and other trace metals.

KINETICS—any nonequilibrium reaction, for which a rate expression can be formulated.

RATES—BASIC language statements define rate expressions for kinetic reactions.

REACTION—addition and removal of specified elements from solution.

MIX—mixing together specified fractions of solutions.

REACTION_TEMPERATURE—changing the temperature of the reaction system.

USE—use the composition of previously defined or saved (SAVE keyword) SOLUTION, EQUILIBRIUM_PHASES, EXCHANGE, SURFACE, GAS_PHASE, SOLID_SOLUTION, or a previously defined KINETICS, REACTION, MIX, or REACTION_TEMPERATURE data block.

SAVE—save the composition following the batch reaction of the SOLUTION, EQUILIBRIUM_PHASES, EXCHANGE, SURFACE, GAS_PHASE, or SOLID_SOLUTION for use in subsequent reactions.

Transport Modeling

Applications—The reactive transport capabilities can be used to study contaminant migration of nutrients, metals, radionuclides, and organic compounds; natural and engineered aquifer remediation; diffusion in sediment pore water; the chemical evolution of natural systems; and laboratory column experiments.

Description—Reactive-transport modeling simulates advection, dispersion, and chemical reactions as water moves through a 1D column. The column is divided into a number of cells, and reactant compositions and nonequilibrium reactions can be defined for each cell. All of the reactants and reactions described for batch reactions can be applied to the cells for transport modeling. The TRANSPORT keyword data block is used to simulate advection and dispersion, or pure diffusion, in the column. The TRANSPORT data block also can be used to simulate a dual-porosity medium, where water flows through the column but simultaneously allows for diffusion into stagnant side pores. The ADVECTION keyword data block is used to simulate purely advective transport.

Keyword data blocks for transport calculations:

TRANSPORT—1D advection, dispersion, and reaction modeling.

ADVECTION—1D advection and reaction modeling.

Inverse Modeling

Applications—Inverse modeling can be used to deduce geochemical reactions and mixing in local and regional aquifer systems, and in aquifer storage and recovery studies.

Description—Inverse modeling calculates geochemical reactions that account for the change in chemical composition of water along a flow path. For inverse modeling, at least two chemical analyses of water are needed at different points along the flow path, as well as a set of minerals and gases that are potentially reactive. Mole transfers of phases are calculated that account for the change in water composition along the flow path. The numerical method accounts for uncertainties in analytical data.

Keyword data block for inverse modeling:

INVERSE_MODELING—deduce mixing, mineral, and gas reactions that account for the chemical evolution of waters.

How to Obtain PHREEQCI, PHREEQC, and Additional Information

Versions of PHREEQCI and PHREEQC may be obtained at no cost from the USGS at World Wide Web address http://water.usgs.gov/software. Many other hydrologic computer models are also available from this site.

Reports documenting USGS model programs can be purchased from the following address:

U.S. Geological Survey
Branch of Information Services
Box 25286
Denver, CO 80225-0286

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References

Parkhurst, D.L. and Appelo, C.A.J., 1999, User's guide to PHREEQC (Version 2)—A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations: U.S. Geological Survey Water-Resources Investigations Report 99-4259, 310 p.