

PHREEQC

Model Uses	PHREEQC is a computer program used to perform a variety of low-temperature aqueous geochemical reactions.	
Major Categories	Hydrology and Water Use; Water Quality	<u>Subject Knowledge Level</u> Advanced
Minor Categories	Temperature; Chemical	<u>Technical Difficulty Level</u> Intermediate
Model Type	Data Analysis Package	<u>Geographic in Nature?</u> No

Abstract

PHREEQC is a computer program written in the C programming language that is designed to perform a wide variety of low-temperature aqueous geochemical calculations. PHREEQC is based on an ion-association aqueous model and has capabilities for (1) speciation and saturation-index calculations; (2) batch-reaction and one-dimensional (1D) transport calculations involving reversible reactions, which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibria, and irreversible reactions, which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes; and (3) inverse modeling, which finds sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainty limits.

Future Developments

Unknown

Model Limitations

Unknown

Model Features

- Speciation and saturation-index calculations
- Batch-reaction and one-dimensional transport calculations with reversible reactions
- Inverse modeling capabilities

Required Data Types

Input is arranged in keyword data blocks, which can appear in any order. Data fields for a keyword are read in a free format, thus they are not column dependent.

Model Outputs

Unknown

For speciation modeling, analytical data for a solution composition (SOLUTION keyword) are needed.

For batch-reaction modeling, the initial solution composition is required (SOLUTION or MIX data block). Other equilibrium reactants may be defined with EQUILIBRIUM_PHASES, EXCHANGE, SURFACE, GAS_PHASE, and SOLID_SOLUTION data blocks. Nonequilibrium reactions may be defined with KINETICS and RATES, REACTION, and REACTION_TEMPERATURE data blocks.

For 1D transport modeling, the data for batch-reaction modeling are needed for each cell in the modeled system. In addition, physical information is needed about column dimensions, time steps, boundary conditions, and dispersivity.

For inverse modeling, the solution composition of the final solution and one or more initial solutions are needed (SOLUTION data block). Uncertainty limits must be defined explicitly or by default for each element and

element redox state in the solutions. In addition, the identity and composition of a set of plausible reactants and products are needed.

Three default databases are included that contain the definition of aqueous species, exchange species, surface species, and mineral and phases for a set of elements.

Hardware Requirements
At least 100mhz processor

Software Requirements
None noted

Cost, Licensing and Availability
Free - available from link below.

Source
US Geological Survey

Source URL
[http://water.usgs.gov/cgi-bin/man_wrdapp?phreeqc\(1\)](http://water.usgs.gov/cgi-bin/man_wrdapp?phreeqc(1))

Supported Platforms			
DOS	<input checked="" type="checkbox"/>	UNIX	<input checked="" type="checkbox"/>
Windows	<input type="checkbox"/>	Macintosh	<input type="checkbox"/>