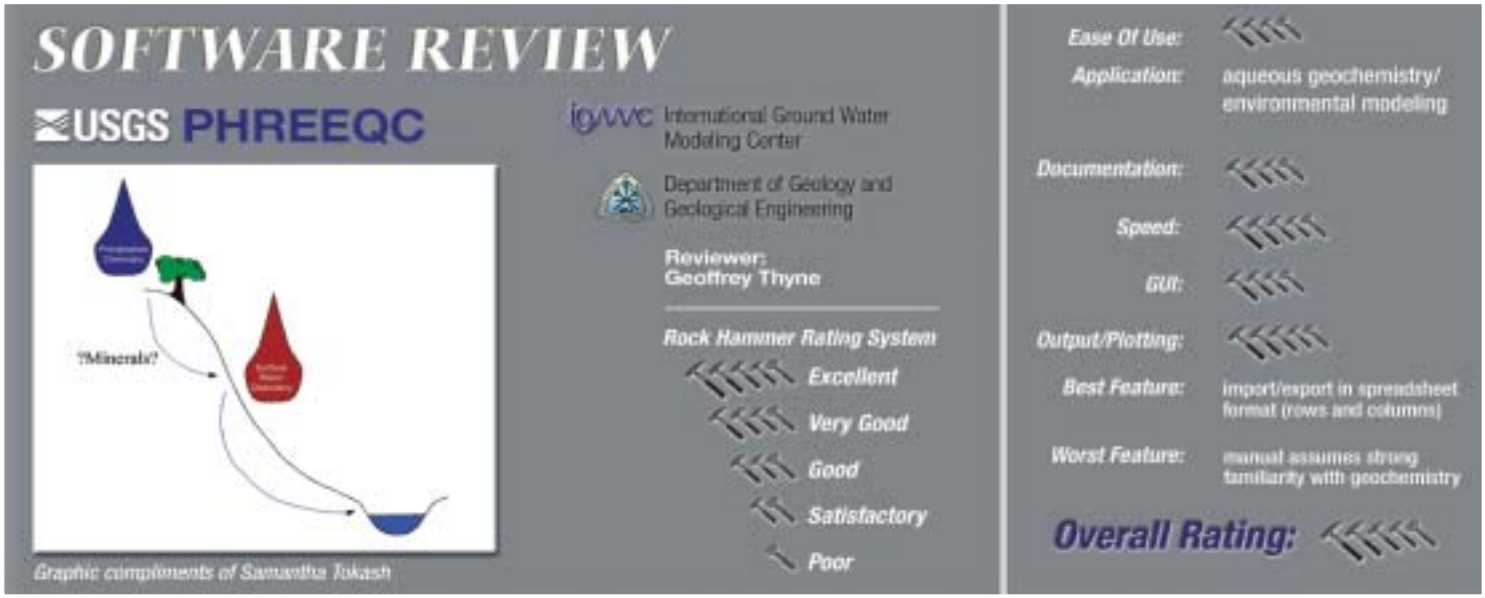

Review of PHREEQC

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PHREEQC is a geochemical modeling program for low-temperature (less than 100°C) aqueous solutions. The model has a variety of capabilities and is written in C programming language with format-free input. It is a public-domain code that performs speciation and saturation index calculations, pH, redox, batch reactions and simple 1-D advective/reaction transport simulations (advection, dispersion, and various options for dual porosity models). The code simulates a variety of reversible reactions in a system that can include gas, aqueous and solid phases, equilibrium with surfaces (sorption reactions using the Dzombak and Morel double layer formulation), and ion-exchange. The code also will perform irreversible reactions that include adding reactants such as minerals or gases to solutions, kinetically controlled reactions, mixing of solutions and changing temperature. A unique feature is an inverse modeling package, which calculates sets of mineral and gas transfers that account for changes between two solutions.

The input files can be edited with a standard text processor, and any number of simple operations can be strung together to produce complex simulations comprised of sequential steps. The code structure is efficient, with short computation time, on the order of minutes for complex simulations. Input files can be edited to include new species and phases on a trial basis, rather than modifying the databases. Features of the code that make it easy to use include the ability to choose between several databases (all supplied), data input from single files or spreadsheets, generation of custom output files that can be exported to spreadsheets, and a window-based interactive interface that is intuitive and easy to use. The code is developed and maintained by Dr. David Parkhurst at the U.S. Geological Survey in Denver, who regularly increases its capabilities.

The code is available at wwwbrr.cr.usgs.gov/projects/GWC _coupled/phreeqc/, where downloadable PC, Unix, and Mac versions (batch and interactive versions) are available, along with answers to frequently asked questions, full documentation, and training course notes. The download comes with 17 example input and output files. The manual includes detailed explanations of these examples, as well as good documentation for the code and descriptions of the keywords with examples of their use.

Visit www.mines.edu/igwmc , wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc