PHREEQC: A Geochemical Code for Calculating Aqueous Speciation, Mineral Solubility, Mass Transfer, and Advective Reactive Transport Over a Range of Temperature and Pressure

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PHREEQC is a geochemical coded developed by David Parkhurst, Niel Plummer, and Donald Thorstenson of the USGS and C.A.J. Appelo, consultant, that computes a wide range of multi-component water-gas-solid reactions and processes:

- speciation of aqueous solutions
- mass transfer between solutes and solids including precipitation/dissolution reactions, sorption reactions, ion-exchange reactions, and ingassing/degassing reactions
- simulates chemical evolution during temperature increases or decreases, pressure changes, and evaporation
- simulates advective-dispersive reactive transport
- includes inverse modeling, i.e. considers changes in fluid composition along a flow-path due to mineral precipitation, dissolution, or sorption
- includes 2 types of ion-association models, the Pitzer model, the SIT model, the Lawrence Livermore model, and others or custom-made
- includes solution mixing with reaction
- includes kinetics and irreversible reactions
- includes molal volume data for electrolytes to calculate density and molality from other concentration terms
- includes some isotopic fractionation capability
- includes graphing and spreadsheet capability for output

Developed over the last 40 years for interpreting groundwater chemistry, it has many additional uses for aqueous systems. Several publications are readily available at the US Geological Survey and the code is free.

References

1. Parkhurst, D.L., and Appelo, C.A.J., 2013, Description of input and examples for PHREEQC version 3—A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations *: U.S. Geological Survey Techniques and Methods*, book 6, chap. A43, 497 p., https://doi.org/10.3133/tm6A43