Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.19362

P^3R, a graphical user interface for PhreeqC model fits to geochemical data

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P^3R stands for Python-PhreeqC-Parameter-Refinement. P^3R is a Phython 2.7 based software, which allows the adjustment of geochemical parameters to match geochemical data sets on the basis of PhreeqC models. Geochemical parameters in that sense may be almost any parameter that could be part of a PhreeqC database: thermodynamic constants, ion-exchange or surface complexation model parameters, parameters for activity or temperature corrections... The graphical user interface allows import of various datasets along with a corresponding PhreeqC-like model and definitions of adjustable parameters. PhreeqC calculations are performed via the PhreeqPy python wrapper around PhreeqC (https://phreeqpy.com). Plots of data and modelling results are permanently visible and updated, so the impact of certain parameter variations on the model fit can be directly experienced. Two algorithms are implemented for least square optimization of adjustable parameters, a Levenberg-Marquardt and a Downhill-Simplex routine. Parameter statistics calculations for the estimation of parameter variances and co-variances follow largely the procedures used in the USGS optimization software UCODE (Poeter and Hill, 1998). For the estimation of model uncertainties, a Monte-Carlo routine is implemented, which allows to calculate the model standard deviation either on the basis of parameter standard deviations alone, or on the basis of full co-variance matrices for the optimized parameters. The importance of employing co-variances for such tasks will be highlighted in the presentation. P^3R is certainly not (yet) a fully developed user-friendly and bug-free software, but it has been developed with the aim to provide a generally applicable optimization tool for geochemists. The code has been successfully employed during the development of our latest surface complexation model for calcite (Heberling et al., 2021), and is currently in use for further model developments. The source code is available on github: https://github.com/FHe/P3R, and potential users or co-developers are always welcome.

References:

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Poeter, E.P. and Hill, M.C. (1998) Documentation of UCODE, a computer code for universal inverse modeling. US Geological Survey.