



MCPhreeqc: Extending geochemical modelling with automatic stochastic simulations

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Geochemical processes can be modelled with many different types of software. These processes all have in common the uncertainty about the exact value of the used parameters. The classical approach is to do direct modelling combined with calibration to find the “correct” parameter values. A limited manual sensitivity analysis is often applied afterwards. The approach applied in our work is the stochastic modelling method using Monte-Carlo simulations. A probability distribution is chosen for each parameter. Combinations of random values are generated from these distributions and the modelling software is run taking each of these combinations as input. The stochastic approach is a well-known and commonly applied method. In this work we present a framework, called MCPhreeqc, to apply Monte-Carlo simulations automatically. The framework consists of an engine, written using the Python programming language, which takes care of all functionality and a graphical user interface to provide the Monte-Carlo configuration to make the software more accessible. In addition it can automatically generate histograms and scatter plots from the results. The software, released as open source software, is set up in such a way that it is easily extendible to different types of software. The first release of the software, which includes coupling with the geochemistry software PHREEQC, will be used to present an example application.