
Groundwater modelling meets geochemistry: Building the bridge between FEFLOW and PHREEQC with IFMPHreeqc

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Abstract

A FEFLOW plug-in (IFMPHreeqc) has been developed in order to couple the multi-component reactive capabilities of PHREEQC-2 (Parkhurst and Appelo, 1999) and the advanced three-dimensional flow and transport features of FEFLOW (Diersch, 2002). This development aims to add geochemical modelling capabilities to FEFLOW, potentially opening a wide range of applications such as heap leaching and acid mine drainage simulation.

IFMPHreeqc has been benchmarked against other multi-component reactive transport codes. Two benchmarks are presented, the first regarding migration of precipitation/dissolution fronts, while the second benchmark addresses multiple cation exchange. Benchmark results indicate a good correlation between IFMPHreeqc and other codes, with a minor numerical dispersion related to the mass transport process.

The development of IFMPHreeqc enabled the coupling of PHREEQC-2 with FEFLOW, breaking the barrier between groundwater and geochemistry models. Additional benchmarking for remaining PHREEQC-2 capabilities such as kinetics and surface complexation, field scale and complex applications using variable density and saturation is currently in progress.

Keywords: reactive transport, groundwater modelling, hydrogeochemistry, FEFLOW, PHREEQC-2

Introduction

FEFLOW is a finite element computer program for simulation of groundwater flow, mass and heat transfer in porous and fractured media and has become the standard groundwater modeling software in the mining industry. PHREEQC-2 (Parkhurst and Appelo, 1999) is a program designed to perform a wide variety of low-temperature aqueous geochemical calculations and is currently one of the most used platforms for evaluation and modeling of acid drainage processes.

The modeling of groundwater flow and geochemistry systems of high complexity is often constrained by software capabilities. From a hydrogeological perspective, while FEFLOW can easily calculate three dimensional groundwater flow and advective/dispersive solute transport, the representation of geochemical aspects such as speciation, equilibrium and cation exchange is not featured in FEFLOW. From a geochemistry perspective, the calculation of complex geochemical processes can be implemented easily in PHREEQC-2, however, advective-dispersive transport is restricted to one dimension.

The development of a tool capable of simulating both complex groundwater flow fields and geochemical processes is therefore highly valuable, with potential to be

used in a wide variety of mining-related applications such as heap leaching, in-situ leaching and acid mine drainage.

This paper presents IFMPHreeqc, a FEFLOW plug-in developed to couple PHREEQC-2 to FEFLOW. The following sections summarize its design and preliminary benchmarking of two examples involving processes of precipitation/dissolution and multiple cation exchange.

Methods

Coupling of FEFLOW and PHREEQC was made possible with the implementation of a FEFLOW plug-in (IFMPHreeqc). This plug-in was developed using the FEFLOW Interface Manager API, which allows user-built code to be executed during run-time, when simulation results and parameters can be interrogated and modified.

The design of IFMPHreeqc was inspired by and based on the PHT3D reactive transport code (Prommer and Post, 2010), which couples PHREEQC to MT3DMS (Zheng, 1999) and is largely used in MODFLOW based models. A split-operator technique was adopted, where the geochemical calculations of PHREEQC are performed at the end of transport steps or at specific reaction steps defined by the user.

After every transport time-step (or specific times specified by the user), IFMPHreeqc collects the concentrations for all species from FEFLOW, and performs PHREEQC-2 calculations for every node in the model domain. Once PHREEQC-2 calculations are finished, IFMPHreeqc retrieves the calculated values and reassigns them to the FEFLOW model, proceeding to the next step. The basic workflow performed by the plugin is illustrated in figure 1.

In order to validate IFMPHreeqc, two benchmark exercises have been conducted to date. The first benchmark is intended to evaluate transport and mineral precipitation/dissolution capabilities of IFMPHreeqc. It consists of a LEA (local equilibrium assumption) model used by Engeesgard and Kipp (1992) and later by Prommer and Post (2010) for benchmarking of MST1D and PHT3D, respectively. The experiment consists of a one-dimensional model where water is in equilibrium with calcite. This water is continuously flushed by lower pH water, resulting in multiple precipitation and dissolution fronts. Details of model parameters, boundary conditions and initial conditions are presented in figure 2.

The model domain is 0.5 m in length. Its mesh was developed in quadrilateral mode so that square elements, equivalent to the cell size used in the PHT3D model, could be defined. A total of 50 square elements of 0.001 m length by 0.001 m width were created. In terms of temporal discretization, the total simulation time is 0.243 days. The time step distribution for flow and transport are defined by the automated time stepping mechanism of FEFLOW. Initially, reaction calculations were defined to each flow/transport time. Further modelling assigned the user defined reaction step of 0.001157 seconds, matching the 210 time steps used in the PHT3D simulation.

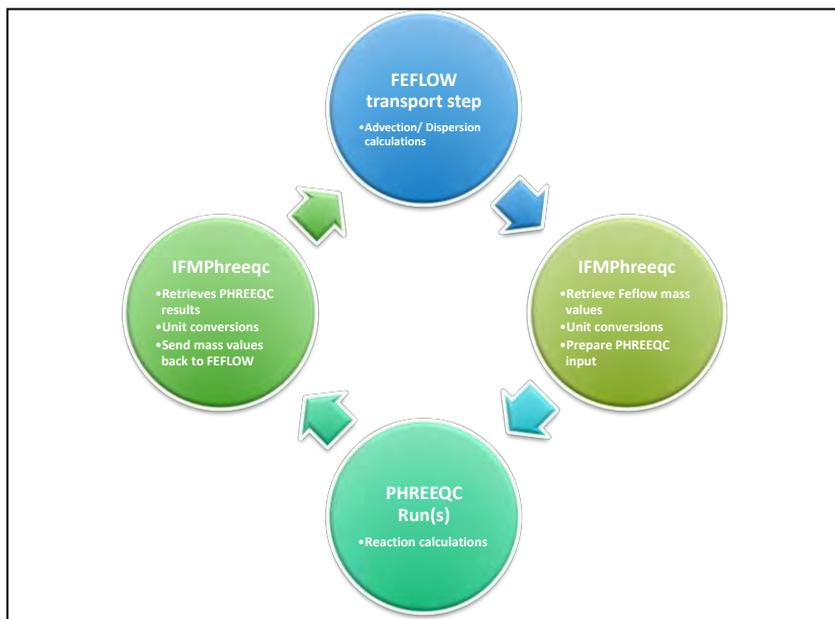


Figure 1 Schematic view of IFMPhreeqc workflow.

Groundwater flow throughout the model domain was defined as constant (steady-state) throughout the simulation, parallel to the X-Axis with a pore velocity of 0.81 m/d using a darcy velocity of 0.259 m/d and porosity of 0.32. This flow field was defined using constant flux boundaries at the source points and constant heads at the ends of the model domain (outflow area).

Transport parameters for the benchmark were applied according to those presented by Engesgaard and Kipp (1992). The chemistry of the system is defined by 4 mobile (subject to dispersion and advection) components, namely carbonate (C(4)), calcium(Ca), magnesium(Mg) and chloride(Cl) and three immobile phases, pH, calcite and dolomite. The component pH is considered immobile as it is controlled by charge balance.

Initial and injected concentrations for all components are presented in Table 1. The thermodynamic database used for the PHREEQC-2 calculations is the same used in PHT3D benchmark, which is a subset of the standard PHREEQC-2 database. Since this benchmark does not involve redox changes and reactions, pe was not included in the simulation and a default value of 4 is adopted. Inflow concentrations were specified using constant concentration boundaries at the nodes where constant flux boundaries were assigned.

The second benchmark involves multiple cation exchange reactions in a flow-through system. This example was firstly used as a test case for PHREEQM (Nienhius et al., 1994), being further included in PHREEQC documentation (Parkhurst and Appelo, 1999) and PHT3D (Prommer and Post, 2010).

The example describes a hypothetical one-dimensional column experiment where the pore water, initially containing sodium, potassium and nitrate in equilibrium with exchangeable cations. This pore water is progressively replaced by a solution containing calcium chloride (CaCl_2). The model setup is summarized in figure 3.

The model domain was setup to represent a column experiment with length of 0.08 m. The model mesh was defined in quadrilateral mode in order to create a reasonable geometric match with the PHT3D example. A node spacing of 0.002 m was used, creating 40 elements and matching the 40 grid-cells from the PHT3D example. The majority of flow and transport parameters used in this benchmark were taken from example 4 of the PHT3D user's manual. Tables 2 and 3 summarize the parameters used in this benchmarking.

Pore water flow along the column is steady-state throughout the simulated period and was implemented using constant flux boundaries at the inflow side and constant head boundaries at the outflow side. A darcy flow of 0.1 m/d was assigned together with porosity of 0.1, equating to a pore velocity of 1 m/d.

Temporal discretization for flow and transport steps was defined by FEFLOW automatic time-step control, with a total simulated period of 0.24 days.

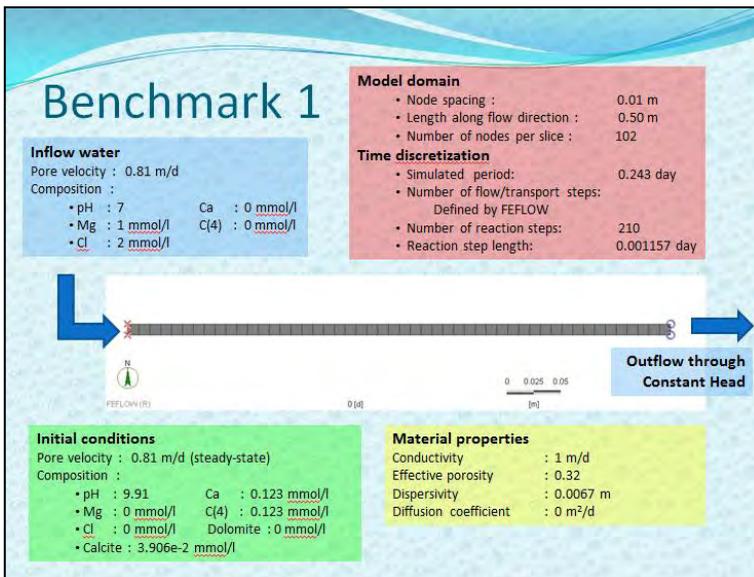


Figure 2 Parameters, boundary conditions and initial conditions used in benchmark 1.

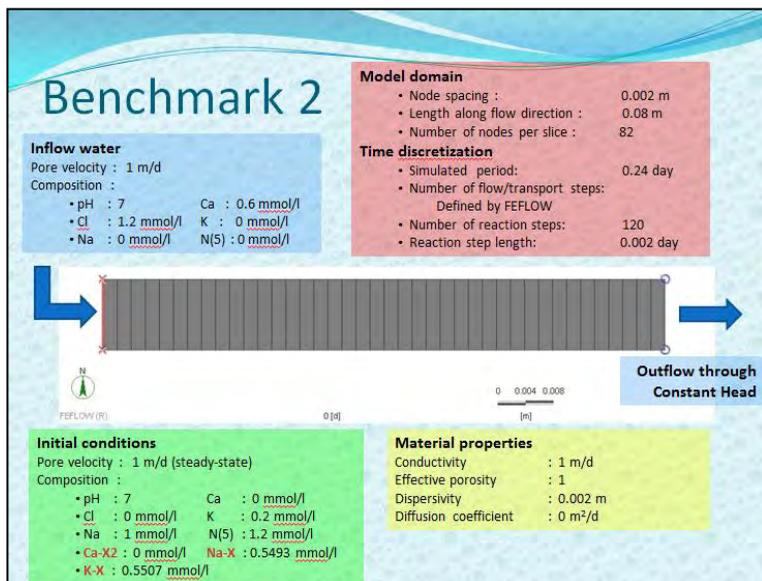


Figure 3 Parameters, boundary conditions and initial conditions used in benchmark 2.

Considering the column length of 0.08 m and pore velocity of 1 m/d, the simulated period equates to the flushing of the column by three pore-volumes. Reaction time-steps had to be controlled by IfmPhreeqc in order to match those from the PHT3D example. The simulated period was divided into 210 time steps with uniform length of 0.002 days.

System chemistry was defined by 6 mobile components, namely pH, calcium (Ca), chloride (Cl), potassium (K), sodium (Na) and nitrate (N(5)). Three additional immobile components were added to represent calcium, sodium and potassium exchangers (Ca-X2, Na-X, K-X, respectively). Initial and inflow concentrations of these components are presented in Table 2.

Results and Discussion

A comparison between results generated by FEFLOW/IFMPHreeqc and PHT3d is presented in figure 4, where concentrations along the model domain at the end of simulation are displayed. Results from FEFLOW/IFMPHreeqc present a good correlation to those generated by PHT3D for both mobile (chloride, pH, magnesium, and calcium) and immobile (calcite and dolomite) phases. Chloride results, used as a conservative tracer, indicated a minor numerical dispersion in relation to PHT3D.

Results for benchmark 2 are illustrated in figure 5 in terms of calcium, sodium, potassium, nitrate and chloride concentrations. A comparison between results obtained using FEFLOW/IFMPHreeqc and PHT3D, in general, show a good correlation. It can be observed towards the end of the simulation (>1.5 pore volumes) that the simulated transport from FEFLOW/IFMPHreeqc is slightly faster

than results provided by PHT3D. Reasons for this remain unclear, although the author speculates that it might be related to numerical dispersion.

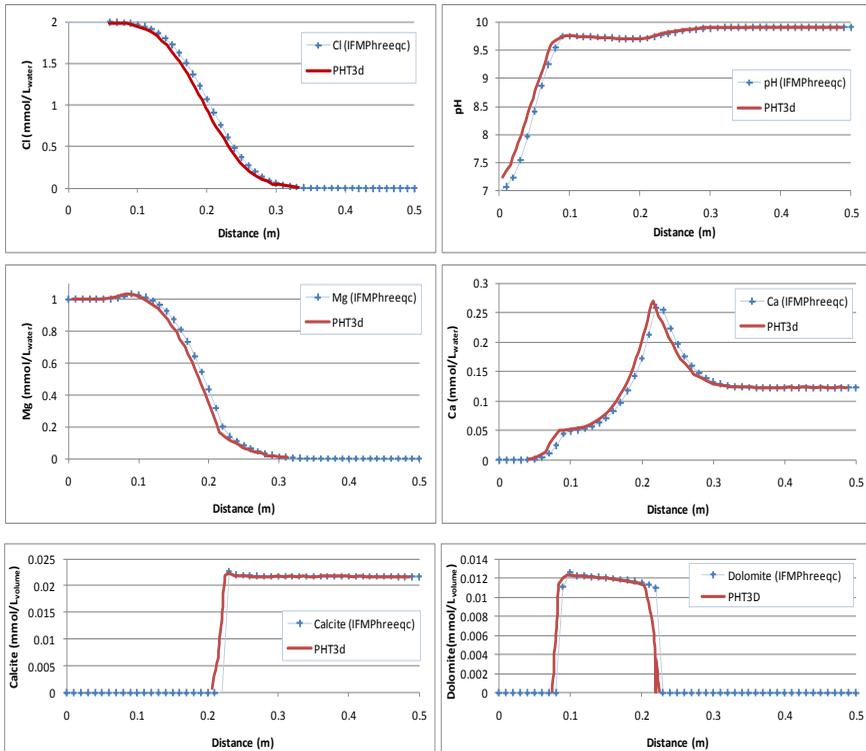


Figure 4 Comparison between results from IFMPHreeqc and PHT3d for benchmark 1.

Conclusions

The development of IFMPHreeqc enabled FEFLOW to include geochemical capabilities from PHREEQC, breaking the barrier between groundwater and geochemistry models.

Initial benchmarking for LEA and multiple cation exchange has been carried out, comparing results from IFMPHreeqc and other reactive transport codes. Additional benchmarks for remaining PHREEQC capabilities such as kinetics and surface complexation, field scale and complex applications using variable density and saturation are currently being developed.

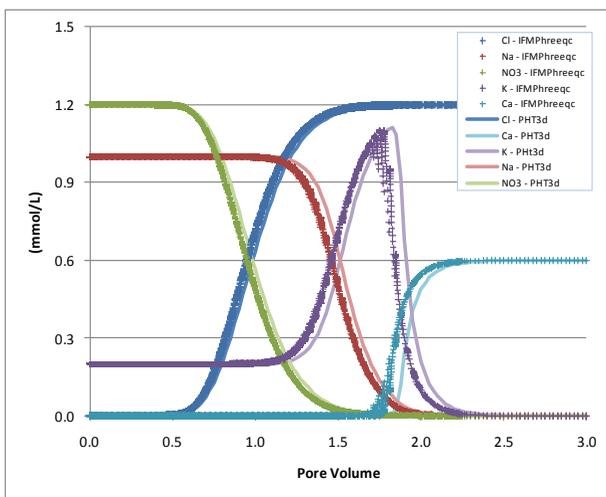


Figure 5 Comparison between results from IFMPhreeqc and PHT3D for benchmark 2.

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