MTHP: coupling PHREEQC to MT3D-USGS for reactive transport

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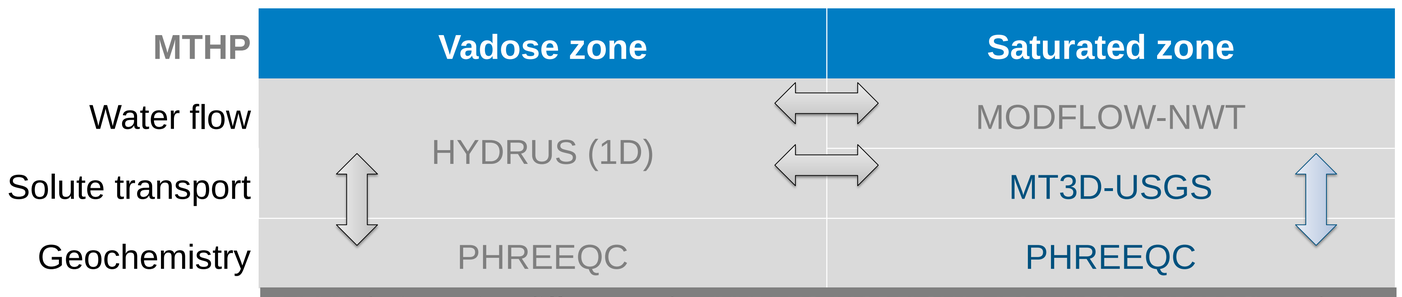
Introduction

A simulation tool is presented for three-dimensional reactive transport in saturated porous media. The code couples the geochemical code **PHREEQC** (Parkhurst and Appelo, 2013) to the existing **MT3D-USGS** (Bedekar et al., 2016). This tool is similar to PHT3D (Prommer and Post, 2010), but eventually the resulting code **MTHP** (**M**odflow **T**ransport **H**ydrus **P**hreeqc) will include reactive transport in the unsaturated zone.



MTHP design, using different codes (HYDRUS, MODFLOW, MT3D-USGS, PHREEQC) to obtain a reactive transport model coupling the vadose zone to the saturated zone. The focus of this poster is on the coupling of PHREEQC with MT3D-USGS.

Methods

MCP package

A new package ("MCP") is added to MT3D-USGS. Initial and boundary solutions are defined similarly to the structure of HPx (Jacques and Simunek, 2005; Jacques et al., 2018) A geochemical model can then be defined using the standard PHREEQC utilities (*exchange*, *surface*, *equilibrium phases*, *kinetics*…).

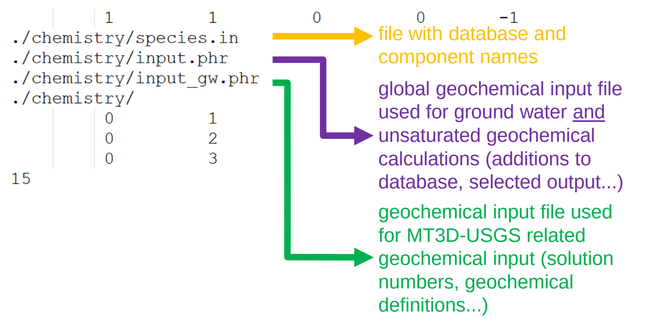


Fig. 1. Snapshot of an MCP file and links to other input files for the geochemical calculations.

User-defined model outputs can be added to the default MT3D-USGS outputs, including time series at observation points and concentration profiles across the domain.

BTN and SSM packages

A few flags and options were added to BTN. The modified SSM package allows PHREEQC solution numbers be applied to sources and sinks.

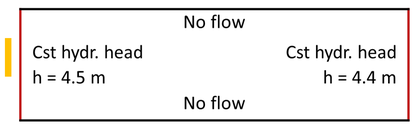
Results

Benchmarking against HPx

2D simulation of a cation exchange problem:

4.4 × 12 m (45 layers, 240 columns in MTHP), 100 days

mmol / kgw	Initial	Source
pH	5.5	2.9 charge
Cl	0.0001	10
Ca	0.0001	5
Mg	0.75	1
Na	6	-
K	2	-
Al	0.5	0.1
Cd	0.09	-
Zn	0.25	-
Pb	0.1	-
Br	11.9 charge	3.7



x exchange sites 0.0011 mol/kgw

Discussion

PHREEQC was successfully coupled to MT3D-USGS for simulating geochemical reactions in saturated media. Benchmark examples showed a small discrepancy between MTHP and HPx. This is probably the result of a different dispersion caused by the coarser grid resolution of MTHP (to be investigated ; cf. Cl inert tracer in Fig. 2).

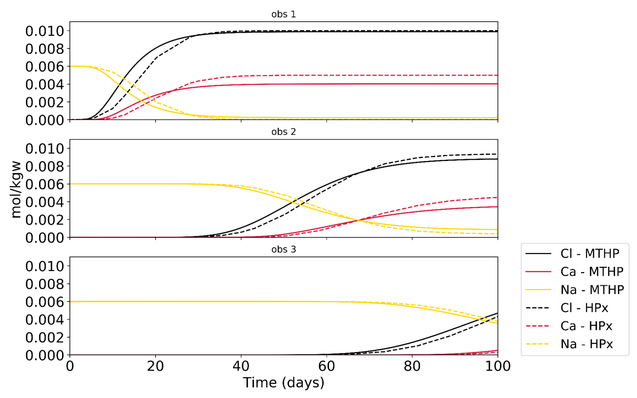
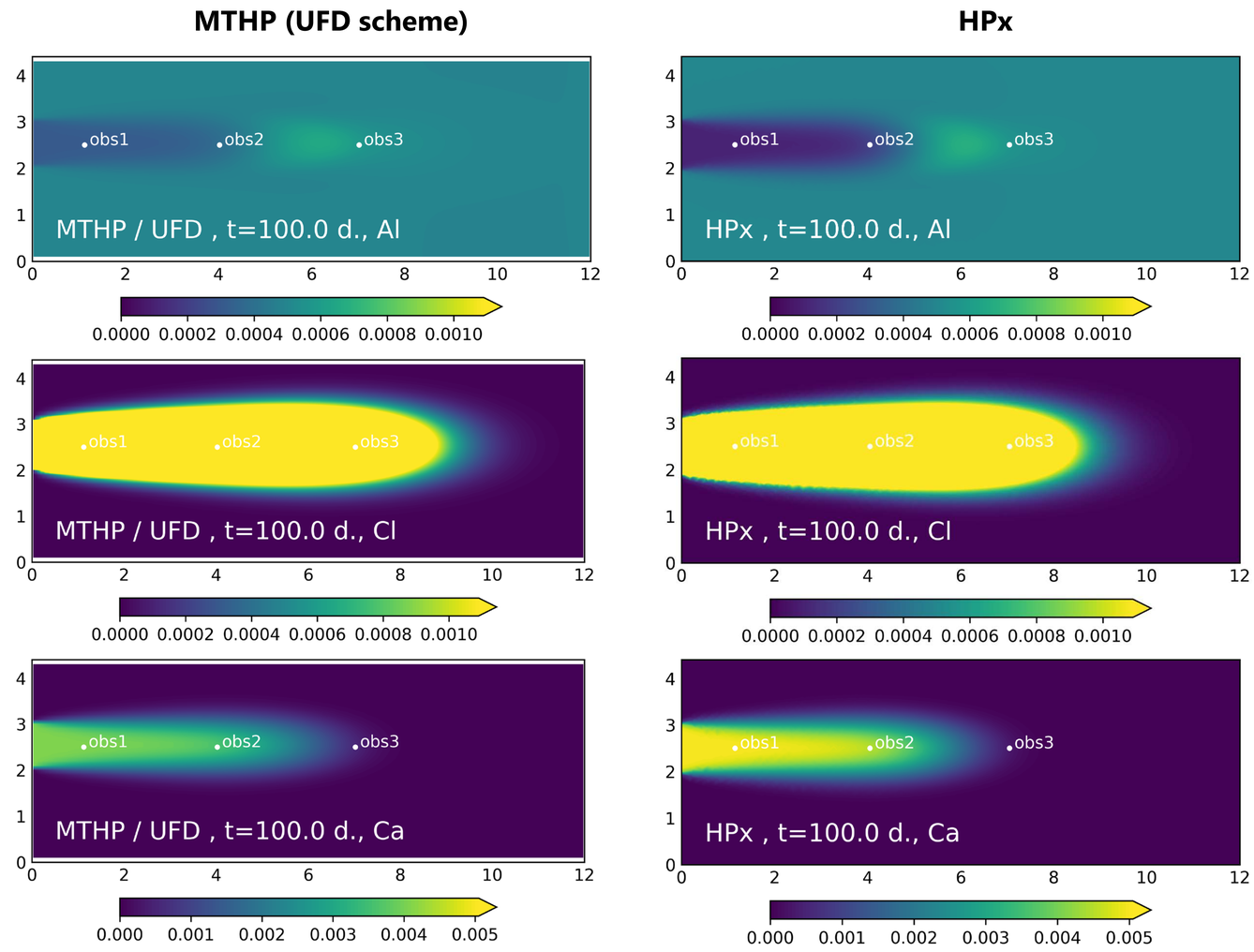


Fig. 2. Cl, Ca and Na concentrations over time at three observation points, MTHP *vs.* HPx.

Al, Cl and Ca concentrations (mol/kgw) after 100 days



Perspectives

Further benchmarking examples will be performed to test other geochemical models (precipitation, kinetics…). MTHP will also be compared to PHT3D in order to have identical spatial and temporal discretization.

References

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