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Simulating water flow, heat and solute transport and biogeochemistry in variably-saturated porous media using HP1

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Coupling physical and biogeochemical processes within one integrated numerical simulator provides a process-based tool for investigating the fate of contaminants as affected by changing hydrologic regimes and geochemical conditions. The numerical simulator HP1 attempts to bridge these two interactive processes. The code is especially geared for variably-saturated conditions, thus serving as a powerful tool for vadose zone research and engineering applications. HP1 extends the capabilities of HYDRUS-1D to simulate physical soil processes by including the capabilities of PHREEQC to account for biogeochemical processes, all embedded in a user-friendly windows interface. The HP1 reactive transport simulator was obtained by weak, non-iterative coupling of HYDRUS-1D and PHREEQC-2. HP1 is free software and can be obtained at http://www.pc-progress.com as part of HYDRUS-1D.

A detailed account is given of the new features and processes that were recently incorporated in HP1: (i) full implementation of HP1 into the graphical user interface of HYDRUS-1D, (ii) dynamic changes in porosity, permeability and tortuosity when minerals dissolve or precipitate, and (iii) diffusion of gas components in the gaseous phase. The implementation of the porosity-permeability-tortuosity changes was benchmarked against results from the MIN3P code. HP1 users can implement their own porosity-permeability and porosity-tortuosity relationships using BASIC statements in the input file. Additionally, hydraulic conductivity and pressure head scaling factors can now also vary with time depending upon the geochemical state variables.

An example is further presented in which HP1 is coupled with the model-independent optimization tool UCODE_2005 (Poeter et al., 2005) . The resulting software allows thermodynamic, kinetic and geochemical parameters to be estimated from experimental data. The optimization features are illustrated for an experimental data set involving transient water flow, solute transport and cation exchange processes.

References

Poeter, E.P., M.C. Hill, E.R. Banta, S. Mehl, and C. Steen, 2005. UCODE_2005 and six other computer codes for universal sensitivity analysis, calibration and uncertainty evaluation. U.S. Geological Survey Techniques and Methods 6-A11.