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HPx - a tool for simulating interactive biohydrogeochemical processes in soil systems

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During the last two decades, different numerical codes have been developed capable of simulating interactive physical, hydrological, biological, and geochemical processes in porous media. The simulator HPx, which couples the HYDRUS codes with PHREEQC, is one of the state-of-the-art models, which specializes in variably-saturated soil systems and explicitly accounts for atmospheric boundary conditions (precipitation and potential evapotranspiration) and root water uptake. It combines most of the advanced features of the two individual codes (Jacques et al., 2008). The versatility of the HPx code is illustrated in this presentation using several examples. An overview of different physical and geochemical conceptual models is also provided. The first example shows the results of a benchmark test, in which combined effects of mineral dissolution and precipitation on changes in physical properties during both porosity increase and clogging were simulated. The second example illustrates the flexibility of the model to include a soil organic matter submodel when simultaneously simulating organic matter degradation and CO_2 diffusion in a variably-saturated soil. Since the HPx codes also simulate heat transport in the soil, they can account for fluctuations of kinetic parameters throughout the year due to their temperature dependency. Global seasonal variations in soil pCO_2 and soil organic pools followed expected behavior, whereas daily values of soil pCO_2 clearly exhibited the effects of daily and spatially variable temperatures and water contents on the biologically-controlled kinetic parameters. The last example illustrates the inclusion of various conceptual models for root solute uptake into the HPx modeling framework. Due to close link with the chemistry of pore water, parameters needed in the uptake equations may depend, in addition to their dependency on root system and ion uptake characteristics, also on the geochemistry of the system, resulting in time-dependency of solute uptake.

Jacques, D., Šimůnek, J., Mallants, D., van Genuchten, M.T., 2008. Modeling Coupled Hydrologic and Chemical Processes: Long-Term Uranium Transport following Phosphorus Fertilization. Vadose Zone Journal 7, 698–711.