Geophysical Research Abstracts
Vol. 14, EGU2012-7724, 2012
EGU General Assembly 2012

Serial reaction modeling using random walk particles tracking methods

C. Henri and D. Fernàndez-Garcia
Department of Geotechnical Engineering and Geosciences, Technical University of Catalonia, Barcelona, Spain

Since the middle of the previous century, DNAPL contamination is a clear identified problem for the management of urban and suburban groundwater resources quality. Random walk particles tracking methods showed their legitimacy and efficiency for modeling reactive transport especially thanks to the absence of numerical dispersion and computational efficiency. We present a new method to efficiently simulate a serial reaction, i.e. the natural degradation of chlorinated solvents, into a trustable 3D random walk particle-tracking model (RW3D). The chemical specie is defined as a particle property (state of the particle). Results of the zeroth spatial moment of the mass transfer equation derivation in the Fourier domain are used as particle state transition probabilities. We obtain thereby the state of a particle after a given time i.e. the mass evolution of the different species involved into the serial reaction. The particle tracking approach is successfully compared to the well- known finite difference code RT3D. We apply this approach to model the behavior of chlorinated compounds resulting from the sequential degradation of tetrachloroethylene (PCE) in highly randomly heterogeneous porous media.