Geophysical Research Abstracts
Vol. 13, EGU2011-7625, 2011
EGU General Assembly 2011
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Random Walk Particle Tracking for reactive transport modelling

Luis Manuel de Vries (1,2,4), Albert Nardi (1,3), Luit Jan Slooten (1,2), Jesus Carrera (1,3)

(1) Energy City Foundation (CIUDEN), Spanish Government CO2 Geological Storage Programme, (2) GHS, Dept Geotechnical Engineering and Geosciences, Universitat Politecnica de Catalunya, UPC-BarcelonaTech, Barcelona, Spain, (3) GHS, Institute of Enviromental Assessment and Water Research (IDAEA), CSIC, Barcelona, Spain, (4) International Center for Numerical Methods in Engineering (CIMNE)

To simulate the transport of solutes in heterogeneous porous media, the Random Walk Particle Tracking (RWPT) method has proven to be an efficient method. Unlike classical Eulerian transport models, it does not suffer from numerical dispersion problems. This is crucial for accurate reactive transport simulation because artificial dispersion may lead to an overestimation of mixing and related reaction rates.

The objective of our current research is to implement a particle tracking method that incorporates reactive transport by applying a new type of particles using an accurate measure of mixing rate.

When modeling transport with classical RWPT methods the location of the particles is calculated at discrete time steps and after a discretization of the spatial domain, the number of particles at each element/cell/volume is converted into concentrations and/or concentration gradients. Other methods use kernel functions to reconstruct concentration gradients. With these methods each particle represents one mass of a specific solute.

Chemical reactions are incorporated in our proposed method using more sophisticated particles in the sense that each particle represents masses of different species and components which can change over time. The interchange of several masses of components and species between particles and their chemical reactions are determined iteratively. In this way reactive transport can be implemented with RWPT methods.

To demonstrate the benefits of the proposed method, a reactive transport problem will be solved by Eulerian FEM methods, classical RWPT methods and the new proposed method. To ensure a fair comparison, all algorithms used are implemented as extensions of the hydrogeological framework "Proost".