



Stochastic Particle Tracking in Fractured Sedimentary Formations

Matthias Willmann and Wolfgang Kinzelbach

ETH Zurich, Institute of Environmental Engineering, Zurich, Switzerland (willmann@ifu.baug.ethz.ch)

Particle tracking simulations are very useful tools to assess transport behavior in deep subsurface formations. Unfortunately, those formations are often fractured. And particle tracking accounting for fracture and matrix transport simultaneously are conceptually complex and difficult to implement. Major problems are that particles moved within the matrix might jump over fractures, and the unclear nature of exchange between fractures and matrix. Due to these difficulties transport simulations are most often reduced to pure fracture transport. The matrix contribution is either ignored or approximated by using a retention mechanism like matrix diffusion. In crystalline rocks this appears to be a reasonable assumption, but in sedimentary rocks should be studied without any a priori assumption on the type of matrix transport. For sedimentary rocks advective transport within the matrix is expected to influence strongly the overall transport behavior.

We developed a stochastic particle tracking method that models transport explicitly in both fractures and matrix. Similar to most flow simulators we conceptualize transport as a superposition of two separate domains, the fracture and the matrix domain, which exchange particles between them. But in our case this exchange is possible at each position within the fractures and not only at the nodes of the fracture. We restrict ourselves to an orthogonal grid for the matrix and here we allow only that fractures lay on the sides of individual matrix cells. This leads to step-like fractures with an enlarged path length inside the fractures. But it also enables us to use the Pollock method without major modifications. Now we calculate the position where a particle leaves an individual matrix cell. At a cell face a check is performed whether a fracture is present. This avoids a time consuming search for fractures at each point of the particle path. The time a particle stays in a fracture before being released again to the matrix depends only on the (hydraulic) fracture aperture and the matrix flux perpendicular to the fracture as well as a molecular diffusion component. A flux-weighted random choice at fracture intersection makes the method essentially stochastic.

Finally, we apply the method to a fractured sedimentary formation in Northern Switzerland which is currently under investigation as a host rock formation for nuclear waste. It is a 3D data set with about 15 Mio. nodes and 3 stochastically distributed fracture systems. In our particle tracking analysis we find a markedly different transport behavior at the lower permeable parts of the formation than at the more permeable ones. Overall, we find this particle tracking method very useful to investigate fractured sedimentary formations.