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Particle tracking approach to model chemical reaction transport in 3D discrete fracture networks

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Fractures are major flow paths for solute transport in fractured rocks. Understanding the flow field in fractured rock is necessary to trace the transport of concentration plume including disposal of hazardous waste. However, reactive transport study with the detailed geometry of fracture is limited. Discrete fracture network (DFN) shows advantageous capability in representation natural fracture system because of its ability to explicitly model the individual fractures, moreover it allows us to obtain the detailed flow pathway of subsurface groundwater movement in fractured rock mass. The study mainly presents the concept of a framework that can simulate reactive transport in porous fractured media. The new technique coupled particle tracking (PT) and chemical reaction model is developed to simulate Tetrachloroethylene (PCE) degradation and transport in 3D discrete fracture networks. FracMan was employed to generate a stochastic DFN using fracture orientation, fracture size, and fracture intensity; and then particle tracking is performed with a view to obtain flow traces. The extracted particle traces can provide 1D flow paths for PHREEQC code to model reactive transport in complex fractured rocks. The study first uses a simple fracture system with three single fractures to evaluate and test the workflow with the new coupling FracMan & PHREEQC and develop the new module. Secondary, complex fracture network system with four realistic fracture sets obtained at a selected site is then simulated to implement the framework in order to model the reaction and transport of PCE in 3D DFN and the last case is point source injection is modeled with a view to demonstrates disposal of hazardous waste issue. The simulation results successfully show PCE reaction process along particle traces in both cases: simple fracture system and complex fracture system. Simple fracture network simulation shows good results for new technique of reactive transport model and also proves the work flow and the new module are correct. The results of complex fracture system simulation reflect the potential capability of this new model applying on complex situation which this new module can handle multi particles for PHREEQC simulation. Regarding disposal of hazardous waste phenomenon, the point source injection of contaminant simulation provides the understanding the fate of contaminant transport of subsurface flow with the specific geometry of fractures. For contaminant treatment problem, the new technique particle tracking – chemical reaction reflects a useful tool for fracture modeling and for predictions of flow and contaminant transport, furthermore, the safety time and distance also can be predicted for contamination treatment.