

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

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## **Abstract**

Fractures are one of the major paths for solute transport in rocks. Contaminant transport and fate is fundamentally different in fractured rock than in unconsolidated aquifers. Understanding the flow field in fractured rock is necessary to trace the transport of concentration plume. This study developed a coupled particle tracking (PT) and chemical reaction model to simulate Tetrachloroethylene (PCE) degradation and transport in 3D discrete fracture networks. FracMan was employed to generate stochastic discrete fracture network (DFN) and conducted PT in DFNs. The extracted particle traces can provide 1D flow paths for PHREEQC code to model reactive transport in complex fractured rocks. The study first uses simple fracture connection to evaluate the developed model. Complex case was then simulated to illustrate the reaction of PCE in the DFN with the fracture sets obtained at a realistic site. The simulation results successfully show PCE reaction process along particle traces.

**KEY WORDS:** *Discrete fracture network, particle tracking, PCE degradation*