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Cellular Automaton for Multispecies Reactive Transport Modelling in Porous media

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The physical processes and chemical reactions occurring in the ground water system are intricately connected at various scales of space, time, transport coefficients and molecular concentration. Usually the complex system with high degrees of freedom manifests only the macroscopic behaviour which can be modelled using a deterministic approach. Since deterministic models do not accurately account for the molecular fluctuations, it is not possible to capture the emergent phenomenon evolving out of randomness. Another limitation is that round off errors due to the truncation of real numbers occur while iterating the numerical algorithm of non-linear macroscopic equations. This leads to data overflow with instability. Cellular automata are the mesoscopic models where the complexity of the system can be fixed by the interaction of particles in the cells following simple rules instead of solving complex equations. The proposed and realized Probabilistic Cellular Automaton model (PCA) has been verified for one dimensional PCE transport & degradation and two dimensional contaminant transport. There exists good concordance between the analytical and numerical solution.

Keywords: Cellular automaton; mesoscopic approach; PCA

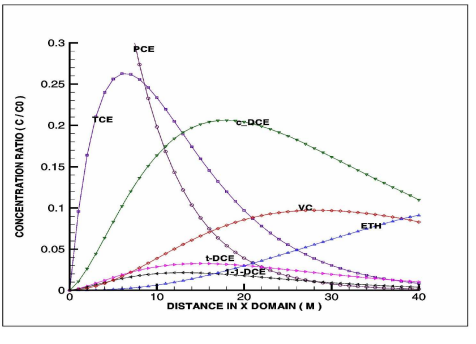

Figure 1: Comparison of PCE transport using probabilistic cellular automaton with analytical solution.

Reference

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