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Chromium Transport Simulation in sub surface media using a Stochastic Algorithm and Cellular Automata

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The numerical simulation of multicomponent reactive transport has become a dynamic field of subsurface hydrology. Efficient simulation models are necessary which are capable of representing a multitude of parameters influencing geochemical reactions. The reactive transport system has mutliscale behaviour in subsurface medium. The multiscale problem occurs in two aspects: (a) Time scale (b) Different magnitude in species population involved in the reaction. The chromium, a heavy metal which is available in small quanitity undergoes transformations through abiotic reactions such as precipitation, complexation, sorption, dissolution, reduction etc. in subsurface media. ?The continuous and deterministic methods for solving ordinary differential equations are appropriate for reactions involving species with high concentration. But when the reaction dynamics is governed by species with low concentration, then the molecular fluctuations are to be accounted at discrete level. The assumption that concentration varies continuously and continually over time is no more valid. So the problem is subjected to the study of the stochastic behaviour of the system. Such a reactive system can be represented by a master equation which is one of the mode of describing the state change of a reaction system. Based on the incoming and outgoing transitions per time step the state of the system is evolved. Since the master equation for the reaction system with complex and coupled trajectories is difficult to be solved analytically, the Stochastic Simulation Algorithm (SSA) is applied for better solution. Apart from numerical scheme such as Finite Difference (FD), the probabilistic cellular automaton,

a mesoscopic approach can be applied for the simulation of transport processes such as advection and dispersion. The spatial discretisation is fixed according to the stability criteria. The temporal discretization is based on the minimum of the time step lengths of all processes. This paper deals with the coupling of Cellular Automata (for transport simulation) and stochastic algorithm (for reaction simulation) for the simulation of transport of chromium which occurs at low concentration in ground water system taking into account all possible types of reactions such as sorption, reduction, bio-transformation on Cr (VI), iron (Fe), Mn and organic matter. The transport parameters that were determined through the experiment were used for the modelling of chromium reactive transport in one dimensional system using operator splitting approaches. Since Gillespie Algorithm (GA) and Cellular Automata (CA) are sensitive to spatial and temporal discretisation, the significance of transport and reaction time steps are brought out by running the simulation of different timesteps. When the reactive time step is 1 in the coupling scheme of FD_GA and 4 in CA_GA, the transport of Cr (VI) is faster using the coupling scheme of CA_GA, but at the same time for the value of 0.05, the formation of Fe (II) is rapid using coupling scheme of FD_GA. In the simulation of abiotic reactions of chromium with iron and organic matter, the stochastic algorithms are more suited for simulating the reduction of chromium. When the reaction time step assumes the value of one fifth of the transport step, the concentration profiles of chromium (VI) using the coupling schemes of FD_GA and CA_GA are approaching similar results. The computational results obtained from the simulation studies of the chromium transport in subsurface media will be presented and discussed.