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Stochastic Algorithm for Reactive Transport simulation of Chromium in Palar River Basin, India

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The migration of species of chromium and their effective remediation in ground water system of palar river basin depends on the hydrogeological characteristics of the system, types of chromium species in soil, dissolution, sorption, immobility processes, and advective and dispersive characteristics of the contaminant. The mathematical structure of reactive transport problems in porous media is resolved by the decision in the chemical model part whether reactions are kinetically controlled or whether a local equilibrium assumption is made between various species involved in the geochemical reactions. At lower concentration of the contaminant species, the molecular fluctuations dominate the reaction dynamics. In these cases modeling of reactions as continuous fluxes of matter is no longer correct. So the stochastic behaviour of the system has to be studied. The main goal of this article is to illustrate the applicability of stochastic algorithms (Gillespie algorithms) which have been widely used as a tool for solving various natural science issues so far, to simulate the chromium reactive transport which includes the reactions such as redox reactions, sorption and degradation of chromium in palar river basin.

Keywords: Gillespie stochastic algorithm chromium transport; palar basin

Figure 1: Palar study area

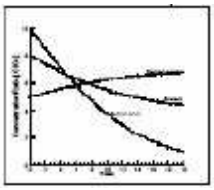

Figure 2: Chromium degradation simulation

References

[1] D. T. Gillespie, *Jour.Phy. Chemistry.* **81 (25)** (1977).
[2] M. Thangarajan, *Environmental Geology.* **38 (3)** (1999).