

MODELING SOLUTE TRANSPORT AND RETENTION IN SOILS

H. M. SELIM

Sturgis Hall, Louisiana State University, Baton Rouge, LA 70803, U.S.A.

ABSTRACT

This presentation summarizes several mathematical models used to describe sorption/desorption and transport of solutes in soils and their potential application for environmental monitoring of contaminants in soils. These models offer a mean for the assessment of potential mobility and prediction of long term movement of dissolved chemicals to the ground water. The models presented are empirical in nature and are based on the assumption that for a single species several reaction mechanisms govern its behavior and thus its potential mobility in the soil environment. These models range from the simple fully equilibrium type for one reaction to that for multisite or multireaction (kinetic and equilibrium) type models. Sorption properties based on quasi-equilibrium (Freundlich retention) for Co, Ni, Cu, Zn, Cd, Hg, V, Cr, Mo, B, Pb, P, As, S, and Se by a number of soil orders are discussed. The models are based on the classical convection-dispersion transport of solute in soil solution. Heavy metal retention processes considered include nonlinear kinetic mechanisms of the concurrent-consecutive reaction, second-order kinetic approach, diffusion and/or mass transfer of the mobile-immobile (two-region) concept, and irreversible reaction of the first order kinetic type. Availability of the necessary input parameters for each model and model sensitivities are addressed. Model validations based on selected studies are also presented.

Another class of models presented are those of the multi-component type where competitive adsorption, ion exchange, and complexation processes are considered. Unlike previous models which are empirical, multicomponent models are based on thermodynamic principles where the stoichiometry is explicitly con-

sidered. Several models that describe the transport of multiple ions in the soil profile are discussed. The transport models are of the convective-dispersive type and it is assumed that ion exchange is the retention reaction which governs the distribution of cations between solution and adsorbed phases. A commonly used model assumes that equilibrium reaction between solution and exchanger phases for any two cations is not influenced by other species present in solution. The necessary inputs are the cation exchange capacity and exchange selectivity coefficients for each cation pair. This classical approach has been modified by incorporating selectivity coefficients that vary with the fractional coverage on the exchanger phase. This approach more accurately represents the cation exchange reactions and has yielded improved description of Ca, Mg, and Na breakthroughs in effluent from soil columns. Nonequilibrium ion exchange behavior has been incorporated into the classical transport model using two different approaches. The first approach uses the two-region concept (mobile and immobile water) where it is postulated that physical nonequilibrium governs the ion transfer between mobile and immobile regions. The second nonequilibrium approach is based on the assumption that cation exchange reactions exhibit kinetic behavior. Depending on the type of clay and ions present in the soil, two types of cation exchange sites have been characterized; one which exhibits equilibrium and the other which shows kinetic behavior. Both nonequilibrium approaches require several additional input parameters, some of which are not easily attainable. The two-region approach has been successfully tested using several data sets from several transport studies, however, rigorous validation of the kinetic approach has not been performed. Other models requiring validation are those which account for the formation of complexes as well as ion exchange.