Modeling transport and biodegradation of BTX compounds in saturated sandy soil

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Abstract: Numerical models have been developed using finite difference and orthogonal collocation methods to simulate one dimensional transport with time-dependent pore water velocity. The modeling process includes sorption given by linear isotherm and biodegradation given by a variety of kinetics such as first-order, zero-order, Monod, non-growth associated Monod (Michaelis-Menten), Haldane and many other inhibitory and non-inhibitory kinetics. A number of initial and boundary conditions such as Dirichlet's, Neuman's, mixed, decaying, etc. have been modeled. The method of finite difference (for first order/zero order model only) and the method of orthogonal collocation (for all kinetics models) have been used to solve the governing transport equation. Numerical solutions have been verified with existing analytical solutions for special cases. Three models (first-order and/or zero-order, non growth associated Michaelis Menten, and Monod) have been inverted using a Gauss-Marquardt-Levenberg algorithm to assess the transport parameters. The models have been used to simulate one dimensional transport of BTX compounds in a pilot scale sand tank model. The data have been found to fit to all three kinetic models with acceptable coefficient of determination (R2) and parameter values. The high concentration data have been found to fit better to the Michaelis Menten and the Monod models than the first order/zero order model.