Analytical Model for 3-D Solute Transport of Sequentially Decaying Species with Dual Porosity, Sorption, and Time-Varying Source

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Background/Objectives. U.S. Environmental Protection Agency (EPA) and its contractors performing oversight at Superfund Sites review numerical models developed to simulate contaminant transport and often could use an analytical solute transport model to perform checks on the numerical model results. An analytical transport model does not require spatial and temporal discretization of the model domain and a separate groundwater flow model, is not affected by numerical dispersion, and is easy to set up. The role of an analytical model in Superfund oversight is to simulate the general plume behavior and guide the development of, and provide a check for, a more detailed and complex numerical solute transport model. However, a practical modeling tool based on 3-D analytical solute transport model is not publicly available. EPA tasked APTIM to develop an analytical model for solute transport in a three-dimensional aquifer of finite thickness with uniform flow, dual porosity, sorption, sequential decay, and finite-extent source with specified time-variable concentration.

Approach/Activities. APTIM derived new solutions for 3-D solute transport for single or sequentially decaying species with a vertical patch source represented by the first or third type boundary condition, and for single species with a point or volumetric mass generation term. The models include dual porosity with sorption coefficients different for the mobile and immobile domain, and decay coefficients different for the dissolved and sorbed mass in each domain. The mass transfer between the two domains is represented by a first order coefficient. The analytical solutions were derived using integral transform techniques and a numerical Laplace transform algorithm is used to obtain a time domain result. The model is coded as a standalone executable that uses text input and output files.

Results/Lessons Learned. Verification simulations included comparison of the new model against existing time-domain models for special cases and against numerical models MT3DMS and RT3D. The numerical models require fine discretization in both lateral and vertical dimensions to provide accurate results. Simulations of perchlorate plume at the Stringfellow Superfund Site used a range of transport parameters and suggest that the plume has achieved steady state. The model functionality is shown using simulations for single or double porosity, range of mass exchange rate coefficient values, different sorption and decay coefficients, and various time-dependency of the source term including instantaneous pulse, constant, oscillatory, series of steps, and piece-wise linear interpolation between a set of time-concentration pairs. The new analytical model is suitable for simulating the general behavior of contaminant plumes, and guide the selection of solute transport parameters and provide a check on accuracy for more detailed numerical solute transport models. The executable and its documentation will be available on EPA's website.