PROJECT SUMMARY

Title: Groundwater Modeling: Semi-Analytical Approaches for Heterogeneity and Reaction Networks

Project I.D.: R/UW-CTP-002

Investigator(s): Dr. Gerald R. Eykholt, formerly Assistant Professor, Department of Civil and Environmental Engineering; Dr. Craig H. Benson, Professor, Department of Civil and Environmental Engineering; Lin Li, Graduate Research Assistant, Department of Civil and Environmental Engineering, University of Wisconsin-Madison.

Period of Contract: July 1, 2000 - June 30, 2001

Background/Need: Reactive transport modeling for heterogeneous aquifers is challenging and computationally intensive. While numerical packages allow simulation of multiple species transport with aquifer heterogeneity, run times on high speed PCs and workstations make many jobs impractical. Stream tube approaches, such as that used in this study, are computationally efficient numerical methods, and offer significant advantages in run time over more numerical methods.

Objectives: The objectives of this study include testing the performance of linear operator methods for simulation of first-order decay reactions in heterogeneous aquifers, and how to extend the solutions to assess how irregular sources and mixed-order kinetics processes affect the contaminant transport. Accuracy of the proposed numerical approach solutions and run times is compared with predictions made with RT3D and analytical solutions.

Methods: A new stream tube model was developed for multiple species reactive transport in a heterogeneous aquifer. The model is based on the primary hypothesis that reactive transport in heterogeneous aquifers can be approximated with linear transforms, where reactivity and flow distributions are not coupled. For many cases, the method provides good accuracy and significant computational advantages, especially for complex reaction networks and more heterogeneous aquifers.

Realistic heterogeneous synthetic aquifers were created using a stochastic turning bands procedure. MODFLOW was been used to solve the head solutions and provide steady state flow for reactive transport. Path3D or MT3D were modified to generate residence time distributions from a tracer source. Distributed and multiple point sources were considered, and residence time distributions were found through superposition. The kinetic response function for each species in the reaction network was analytically expressed. Convolution and other linear operator methods were used to generate responses from irregular source loading and to determine transient concentrations over the aquifer domain.

Results and Discussion: Comparisons between the new modeling approach, other analytical models and numerical models showed that the hypothesis is correct. Reasonable agreement was obtained for all of the cases that were tested. Significant computational time was saved using the method. For a 2D-aquifer simulation, the new approach was found to be 1500 times faster than RT3D, a popular numerical application. Parameter sensitivity analysis includes mean of log-normal hydraulic conductivity, standard deviation of log-normal hydraulic conductivity, correlation length, retardation coefficients and first order reaction rate constants.

Conclusions/Implications: A new stream tube modeling approach was developed for multiple species reactive transport in heterogeneous aquifers. The method can handle complex flow and reaction networks. The approach has been extensively tested and compared with a full numerical model. For heterogeneous hydraulic conductivity and homogeneous reaction rate, the results indicate that reactive transport can be de-coupled into flow and reaction processes. This de-coupling significantly decrease the simulation time and ensures an acceptable level of accuracy.

Related Publications: None to date.

Key Words: Reactive transport, multi-species, heterogeneous aquifer, stream tube approach, retardation coefficients, numerical model

Funding: University of Wisconsin System