PHAST – A program for simulating ground-water flow, solute transport, and multicomponent geochemical reactions

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PHAST is a three-dimensional reactive-transport simulator derived from coupling the geochemical model PHREEQC with the solute-transport capabilities of HST3D. The flow and transport model is restricted to constant density, constant temperature, saturated ground-water flow. Chemical reactions include mineral and gas equilibia, ion exchange, surface complexation, solid solutions, and kinetic reactions. The simulator uses a point-distributed finite-difference grid and fixed-size time steps. After operator splitting, a sequential noniterative approach is used to solve the flow, transport, and chemical equations.

The input and output features of the simulator were designed for ease of use. Data are input in a flexible, keyword-data-block format; data input for chemistry is identical to data input for PHREEQC. Model-output options are available to write any chemical property (for example, activity, concentration, numbers of moles of minerals) to ASCII files or a binary Hierchical Data Format (HDF) file. Data in the HDF file can be read by the plotting program Model Viewer for three-dimensional visualization and animation of heads, velocities, and chemical data.

Three-dimensional reactive-transport calculations often require long computer processing times. A parallel version of the simulator has been developed to use multiple processors to shorten processing times. The parallel version is implemented with the Message Passing Interface (MPI), and can be used on multiprocessor computers or on a cluster of networked computers.

PHAST has been used in several field-scale hydrologic studies. At Cape Cod, Massachusetts, simulatons indicate a diminishment of sewage-derived phosphorus to Ashumet Pond over a period of decades; in an Aquifer Storage Recovery (ASR) experiment in Charleston, South Carolina, simulations account for the changes in water chemistry caused by storage; and in Oklahoma, reactive-transport simulations were used to explain the chemical and transport processes that produce large dissolved arsenic concentrations in the Central Oklahoma Aquifer.

Geochemical modeling of decontamination solutions for building surfaces

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A threat exists that a terrorist group may detonate a radiological dispersal device (RDD), generating a cloud of radioactive particles that could contaminate important surfaces. Rapid decontamination is needed to minimize the impact of such a terrorist action. Selection and implementation of a decontamination technique requires use of a model to evaluate applicability to a wide range of building materials. We have applied the geochemical reactive transport model, PHREEQc, to this problem. Geochemical principles commonly used to investigate reactions between ground water and geologic media are adopted and applied to interactions between decontamination solutions and building materials. Modeling is divided into mass transfer, and chemical mass transport. Explicit inclusion of mass transport is important because imbibition may occur when wet solutions encounter dry building surfaces, and the overall rate of decontamination may be limited by the diffusive transport of the chemical from the surface into the decontamination solution. The model is implemented in a finite-difference grid that incorporates a dual porosity approach and allows variable water chemistry and variable distribution of solid phases. Grids can be defined to represent the pore space of building materials, the building surface, and the decontamination foam. The transport problem is simplified to a 1-D scenario that envisions rapid initial transport into the building material (imbibition) and slow diffusive transport out of the building material. Radionuclides are distributed on the building surface in a variety of chemical forms including dissolved salts and particulate oxides. Decontamination solutions parameters are assigned to nodes in the finite difference grid, and the effect of foam-bubbles on transport can be tested by altering the effective diffusion coefficient(s). Mass transport between the building surface and the decontamination solution is based on diffusion along a concentration gradient.

The model will be validated using data from laboratory experiments conducted on contaminated coupons of common building materials. Once validated, the model can be used to manipulate the chemical environment of decontamination solutions to evaluate alternative chemical recipes or to evaluate the effectiveness on different building materials.