Abstract

The computer program PHAST (***PH*** REEQC ***A*** nd H ***ST*** 3D) simulates multicomponent, reactive solute transport in three-dimensional saturated groundwater flow systems. PHAST is a versatile groundwater flow and solute-transport simulator with capabilities to model a wide range of equilibrium and kinetic geochemical reactions. The flow and transport calculations are based on a modified version of HST3D that is restricted to constant fluid density and constant temperature. The geochemical reactions are simulated with the geochemical model PHREEQC, which is embedded in PHAST. Major enhancements in PHAST Version 2 allow spatial data to be defined in a combination of map and grid coordinate systems, independent of a specific model grid (without node-by-node input). At run time, aquifer properties are interpolated from the spatial data to the model grid; regridding requires only redefinition of the grid without modification of the spatial data.

PHAST is applicable to the study of natural and contaminated groundwater systems at a variety of scales ranging from laboratory experiments to local and regional field scales. PHAST can be used in studies of migration of nutrients, inorganic and organic contaminants, and radionuclides; in projects such as aquifer storage and recovery or engineered remediation; and in investigations of the natural rock/water interactions in aquifers. PHAST is not appropriate for unsaturated-zone flow, multiphase flow, or density-dependent flow.

A variety of boundary conditions are available in PHAST to simulate flow and transport, including specified-head, flux (specified-flux), and leaky (head-dependent) conditions, as well as the special cases of rivers, drains, and wells. Chemical reactions in PHAST include (1) homogeneous equilibria using an ion-association or Pitzer specific interaction thermodynamic model; (2) heterogeneous equilibria between the aqueous solution and minerals, ion exchange sites, surface complexation sites, solid solutions, and gases; and (3) kinetic reactions with rates that are a function of solution composition. The aqueous model (elements, chemical reactions, and equilibrium constants), minerals, exchangers, surfaces, gases, kinetic reactants, and rate expressions may be defined or modified by the user.

A number of options are available to save results of simulations to output files. The data may be saved in three formats: a format suitable for viewing with a text editor; a format suitable for exporting to spreadsheets and postprocessing programs; and in Hierarchical Data Format (HDF), which is a compressed binary format. Data in the HDF file can be visualized on Windows computers with the program Model Viewer and extracted with the utility program PHASTHDF; both programs are distributed with PHAST.

Operator splitting of the flow, transport, and geochemical equations is used to separate the three processes into three sequential calculations. No iterations between transport and reaction calculations are implemented. A three-dimensional Cartesian coordinate system and finite-difference techniques are used for the spatial and temporal discretization of the flow and transport equations. The nonlinear chemical equilibrium equations are solved by a Newton-Raphson method, and the kinetic reaction equations are solved by a Runge-Kutta or an implicit method for integrating ordinary differential equations.

The PHAST simulator may require large amounts of memory and long Central Processing Unit (CPU) times. To reduce the long CPU times, a parallel version of PHAST has been developed that runs on a multiprocessor computer or on a collection of computers that are networked. The parallel version requires Message Passing Interface, which is freely available. The parallel version is effective in reducing simulation times.

This report documents the use of the PHAST simulator, including running the simulator, preparing the input files, selecting the output files, and visualizing the results. It also presents six examples that verify the numerical method and demonstrate the capabilities of the simulator. PHAST requires three input files. Only the flow and transport file is described in detail in this report. The other two files, the chemistry data file and the database file, are identical to PHREEQC files, and a detailed description of these files is in the PHREEQC documentation.

PHAST Version 2 has a number of enhancements to allow simpler definition of spatial information and to avoid grid-dependent (node-by-node) input definitions. Formerly, all spatial data were defined with rectangular zones. Now wedge-shaped and irregularly shaped volumes may be used to specify the hydrologic and chemical properties of regions within the model domain. Spatial data can be imported from ArcInfo shape and ASCII raster files and from a simple X,Y, Z file format. To accommodate a grid that is not aligned with the coordinate system of the imported files, it is possible to define features in map and grid coordinate systems within the same input file.

The definition of leaky and flux boundary conditions has been modified to select only exterior faces within a specified volume of the model domain and to restrict the boundary conditions to the area of definition, which may include fractions of cell faces. Previously, flux and leaky boundary conditions were applied only to entire cell faces; thus, the area could vary as the model grid was refined and cell sizes changed.

New capabilities have been added to interpolate spatial data to the two- or three-dimensional locations of cells and elements. Two-dimensional interpolation is used to define surfaces for the tops and bottoms of three-dimensional regions within the model domain. Surfaces are created by two-dimensional interpolation of scattered X, Y points with associated elevation data. Within the bounds of the scattered points (the convex hull), natural neighbor interpolation is implemented, which uses an area weighting scheme to assign an elevation to a target point based on elevations at the nearest of the scattered points; outside the convex hull, the elevation of the closest point is assigned to a target point.

Three-dimensional scattered data can be used to define porous-media properties, boundary condition properties, or initial conditions. Three-dimensional interpolation always assigns the value of the closest scattered point to a target point. The interpolation capabilities allow head and chemical data to be saved at the end of one run and used as initial conditions for a subsequent run, even if the grid spacing has been changed.

A new capability has been added to aggregate flows of water and solute into an arbitrarily shaped region and through the boundary-condition cells included in the region. Any number of flow aggregation regions may be defined. These regions need not be mutually exclusive, and regions can be combined to define larger, possibly noncontiguous regions. A facility exists to save heads as a function of time and space for these regions, which then can be used to specify boundary-condition heads in a subsequent run.

A drain boundary condition has been added. Drains function similarly to rivers, except they only discharge water from the aquifer. Drains are one-dimensional features with an associated width or diameter, which will accept water if the head in the aquifer is greater than the elevation of the drain. Drains have no time-dependent parameters.

Other changes implemented in PHAST Version 2 include a method for row scaling of the flow and transport equations to allow the definition of a single convergence tolerance for both flow and transport. Memory requirements for the chemistry processes in parallel processing have been minimized by elimination of most flow and transport storage. A start time other than zero may be defined. PHAST Version 2 includes many bug fixes and some other minor additions to the input files.