Phast4Windows: A Three-Dimensional Graphical User Interface for the Reactive-Transport Simulator PHAST

By Scott R. Charlton and David L. Parkhurst

Ground Water: Methods Note or Rapid Communication

PHAST is a three-dimensional, multicomponent, reactive-transport model (Parkhurst and others, 2010) that is based on the solute transport model HST3D (Kipp, 1987, 1997) and the geochemical model PHREEQC (Parkhurst and Appelo, 1999, 2011). Flow capabilities are for saturated, confined or unconfined flow of a constant-density, isothermal aqueous phase. Flow and transport simulations may include wells and constant-head, flux, leaky (head-dependent), river, and drain boundary conditions. PHAST can be used purely as a flow model or as a multicomponent reactive-transport model. All of the reaction capabilities of PHREEQC are available in PHAST, including mineral and gas equilibria, cation exchange, surface complexation, solid solutions, and general kinetic reactions.

Phast for Windows (P4W) is a graphical user interface for PHAST (figure 1). P4W is implemented in Visualization Toolkit (VTK, 2011) and allows model features to be defined and displayed in 3D. The view of model features may be adjusted with zoom, pan, and three-dimensional rotation by the use of mouse buttons and mouse movements. A tree at the left (by default) of the screen contains all of the model definitions (Table 1). The tree can be expanded or collapsed to adjust the level of detail of model definitions that are shown. All features (including the perimeter, bottom, and top of prisms) may be made visible or invisible by clicking check boxes in the tree. Features may be made visible by category (for example, media properties or boundary conditions) or individually within each category.

At least three files are necessary to run a reactive-transport PHAST simulation: the flow and tranport file, which defines all spatial distributions of media properties, initial conditions, and boundary conditions; the chemistry input file, which defines a set of chemical reactions and solution compositions that are used as chemical initial and boundary conditions; and a thermodynamic database file. Phast for Windows (P4W) is a graphical user interface for the flow and transport file. [The two chemistry files can be generated with the graphical user interface PhreeqcI (Charlton and Parkhurst, 2002) or Phreeqc for Windows (Post, 2011).] With P4W it is possible to define all features of the flow and tranport data file; save the definitions in a binary file ( *.wphast*), which is an HDF (hierarchical data format) file; and run the simulation (provided chemistry files are available, if needed). P4W also can export or import an ASCII flow and transport file in the format defined by the PHAST documentation (Parkhurst and others, 2010). P4W allows use of additional files that contain spatial data at X-Y or X-Y-Z points as part of the definition of the model features. ArcInfo shape files can be used for definition of the perimeter, bottom, or top of a prism. A file with X-Y-Z-value can be used to define the spatial distribution of any media or boundary condition property and files with X-Y-Z-T-value (where T is time) can be used to define spatially distributed and time-varying boundary condition properties.

PHAST allows model properties to be defined by zones, which include rectangular boxes, right-angle wedges (aligned with a coordinate direction), and prisms. A prism is defined laterally by a polygonal perimeter and vertically by bounding surfaces at the bottom and top. Within a zone, properties are defined to be constant, linearly varying in a coordinate direction, or by interpolation from a set of three-dimensional (3D) points with associated property values.

Table 1. Items in the data-definition tree

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| --- | --- |
| Category | Function |
| SOLUTE\_TRANSPORT | Selects between flow-only and reactive-transport simulations |
| STEADY\_FLOW | Selects steady or transient flow conditions |
| FREE\_SURFACE | Selects presence or absence of a free-surface boundary condition |
| SOLUTION\_METHOD | Parameters for numerical method for solving finite-difference equations |
| UNITS | Units for input data |
| GRID | Definitions for finite-difference grid |
| MEDIA | Porous-media properties: porosity, hydraulic conductivity, specific storage, dispersivity, and tortuosity |
| INITIAL\_CONDITIONS | Initial head and chemistry conditions |
| BOUNDARY\_CONDITIONS | Constant-head, flux, and leaky boundary conditions |
| WELL | Location, open intervals, and pumping rates for a well |
| RIVERS | River boundary condition |
| DRAINS | Drain boundary condition |
| ZONE\_FLOW | Flow rates of water and solutes in and out of a zone; time series of heads for nodes in the zone |
| PRINT\_INITIAL | Selection of initial conditions to write to output files |
| PRINT\_FREQUENCY | Selection of print intervals to write data to output files |
| TIME\_CONTROL | Time step, start time, and ends of simulation periods |

Within the tree, items within the categories can be removed or copied by clicking the right mouse. Items can be reordered within a category by drag and drop.

Model features can be defined in either of two coordinate systems, grid or map. It is expected that GIS data will be in a common X-Y map coordinate system, such as UTM. In addition to the map coordinate system, it is possible to have a second, local coordinate system that is based on the origin of the grid. Coordinates of both systems are shown as the cursor is moved over the model-display window.

P4W runs on Windows operating systems.

Provides help for each input item.

Wizard guides initial units and media properties.

P4W is an excellent tool for developing simple or complex groundwater models. The added capability to simulate reactive transport

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