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

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# Abstract

Phast4Windows is a tool for developing and running flow amd reactive-transport models with the PHAST simulator. This graphical user interface allows definition and visualization of heterogeneous, three-dimensional spatial data-- the porous media properties, the inital head and chemical conditions, boundary conditions, and locations of wells, rivers, and drains--and all other parameters and data necessary for a simulation. Spatial data can be defined by drawing, by point-by-point definitions, or by importing files, including ArcInfo shape and raster files. All definitions can be inspected, edited, deleted, moved, copied, and switched from hidden to visible through the data tree of the interface. Model features are visualized in the main panel of the interface, so that it is possible to zoom, pan, and rotate features in three dimensions. PHAST simulates saturated groundwater flow under confined or unconfined conditions for constant-density water. Reactions among multiple transport components include mineral equilibria, cation exchange, surface complexation, solid solutions, general kinetic reactions, and water-gas equilibria. The interface can be used to develop simple or complex models, and is ideal for use in the classroom, for analysis of experiments, and for development of field-scale models.

# Introduction

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 equilibria, cation exchange, surface complexation, solid solutions, general kinetic reactions, and gas-water equilibria.

Phast4Windows (P4W) is a graphical user interface for PHAST (figure 1) implemented in C++ by using the Visualization Toolkit (VTK, 2011). At least three files are necessary to run a reactive-transport PHAST simulation: (1) the flow and transport file, which defines all spatial distributions of media properties, initial conditions, and boundary conditions; (2) the chemistry input file, which defines a set of chemical reactants and solution compositions that are used as chemical initial and boundary conditions; and (3) a thermodynamic database file. With P4W, it is possible to define all features of the flow and transport 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). The two chemistry files are PHREEQC files and can be generated with the graphical user interface PhreeqcI (Charlton and Parkhurst, 2002) or Phreeqc for Windows (Post, 2011).

# Building a Reactive-Transport Model with PHAST4WINDOWS

P4W has three main panels: a display panel that shows model features in 3D, a data-definition tree that contains a list of all model definitions (Table 1), and a spatial-details panel that allows definition and editing of the locations of zones that define model features. The display of model features may be adjusted with zoom, pan, and three-dimensional rotation by the use of mouse buttons and mouse movements. The data-definition tree (at the left of the screen by default) can be expanded or collapsed to adjust the level of detail of model definitions that are shown. All model features may be made visible or invisible in the display panel by clicking check boxes in the tree or by View menu selections. Features may be made visible by category (for example, media properties or boundary conditions) or individually within each category. In addition, data can be selected from the tree to be edited by double clicking, deleted or copied by right clicking, and moved by dragging and dropping. When defining or editing model parameters, detailed explanations are available for each data item. An undo/redo capability exists for all changes to model definitions.

All model data are accessible through the 16 first-level items in the data tree, which are listed in table 1. A new-model wizard may be used to define the basic data for a model, after which the first-level items in the tree can be used to modify or extend the definitions. Data for the first-level items may be defined in any order, but the order listed in the tree and in this section is a reasonable sequence in which to develop a groundwater or reactive-transport model.

## 1. New-model wizard

The new-model wizard can be selected when P4W is started. The wizard is used to define the type of model that is to be developed--flow-only or solute-transport, transient or steady-state flow, and confined or unconfined flow. In addition, the wizard sets the units of data input, a site bitmap, the finite-difference grid, default media properties, initial head condition, initial chemistry condition, and simulation time parameters. All of these data (except the site map registration) can be changed in the interface after completing the wizard.

## 2. Zones and properties

The wizard provides enough information to make a model run, although it will not be very interesting with essentially constant parameters and initial conditions and no boundary conditions. To complete the model, spatial definitions are needed to supply the appropriate heterogeneity in media properties and initial conditions, and the boundary conditions that describe the flow and transport system. All spatial properties are defined with zones, which are volumes of space defined by a rectangular box, a right-triangular wedge, an irregularly shaped volume called a prism, or a box that is equal to the entire model domain. A prism is defined by a polygonal perimeter, a top surface, and a bottom surface. Perimeters can be defined by drawing, by a set of points, or by ArcInfo shape files. Similarly the top and bottom can be defined by a set of points, or by shape files or raster files. Zones are defined with the four icons to the right of the question mark in the line of icons near the top of the interface screen.

Once a zone is defined, it may be used to define media properties, head initial conditions, chemistry initial conditions, flux boundary conditions, leaky boundary conditions, or specified head boundary conditions. The volume within a zone can be assigned properties--such as porosity, a head distribution, or a boundary condition parameter--in a variety of ways. A property can be constant, linearly varying in a coordinate direction, or interpolated from the values of the property at a set of 3D points (either listed in the input file or read from a file). A zone also may be used to define a volume over which flow and solute budgets are calculated, including the flux of water and solute through the boundary-condition nodes that fall within the zone.

## 3. Media properites

Media properites (**MEDIA**, table 1) include the hydraulic conductivity in each coordinate direction, porosity, specific storage, and whether or not a zone is included within the model domain. If solute transport is modeled, then additional media properties are needed, including the longitudinal dispersivity, the horizontal and vertical components of transverse dispersivity, and the tortuosity. The spatial distributions of these properties are defined with a series of zones. A zone can be used to define one or more of these properties. The order of the zone definitions is important in that each zone overlays the previous zones, such that if two zones define a property for the same location, then the latter definition takes precedence over the former. This order of precedence--later definitions superseding a previous property definition for the same location--applies not only to media properties, but to initial and boundary condition definitions as well.

## 4. Head and chemistry initial conditions

The initial head condition is defined through a series of zones. For steady-flow simulations, the initial head distribution is not too important because the heads will be adjusted to obtain as state-state flow condition. For transient flow, the initial head condition is important because the simulated flow and corresponding solute transport will begin from the defined initial head condition. It is possible to calculate a steady-flow head condition and use it to begin a subsequent simulation of transient flow.

The initial chemical condition in the simulation is really more than just an initial condition because it defines not only the initial solution compositions in the model domain, but also the types of chemistry that will be present in each zone throughout the duration of the simulation. Each solution composition is identified by an integer and corresponds to a solution definition in the chemistry data file. The zones are used to distribute these solutions (as identified by integers) throughout the model domain; it is also possible to distribute spatially mixtures of the solutions.

In addition to the initial solution composition, any combination of reactants can be distributed by zone throughout the model domain. Reactants include minerals, cation exchangers, complexation surfaces, solid solutions, general kinetic reactions, and gas phases. Reactants of each type may be defined in the chemistry data file and an integer is assigned to each reactant composition in the chemistry data file. A series of zones are used to distribute these reactants, as identified by integers, throughout the model domain.

## 5. Boundary conditions

Three types of boundary conditions can be defined with zones: flux, leaky, and specified-head boundary conditions. Flux boundaries define a flux of water (L/T) through a specified set of cell faces and an associated solution composition for water entering the model domain; water leaving the model domain has the composition determined by the composition in the boundary cell. Leaky, or head-dependent, boundary conditions are defined by a head external to the model, a thickness, and a hydraulic conductivity. The flux of water depends on the hydraulic conductivity times the gradient between the external head and the boundary-cell head using the thickness as the distance between the two heads. As with flux boundaries, a specified solution composition is associated with any water that flows into the model domain. Finally, a specified-head boundary condition can be defined for cells within a zone, with either an associated solution for water that flows into the cell, or a fixed chemical composition assigned to the cell.

Flux and leaky boundaries can coexist on one or more faces of a boundary cell, but are applied only to cell faces that are on the exterior of the model domain. A specified-head boundary condition can be applied to any cell in the model domain, but cannot coexist with a flux or leaky boundary condition. Fluxes, heads, or solution compositions associated with boundary conditions need not be constant, but can be defined with time series of values.

## 6. Wells, rivers, drains

In addition t

## 7. Zone flows

In addition t

## 8. Printing

In addition t

HDF, Ascii, Model Viewer

## 9. Time Stepping and Simulation Time

In addition t

# Running Simulations

Once the model features have been defined, the model can be run from P4W by clicking on the running-man icon. Any errors in the input definitions will be identified and once no errors are found, the model will be run. Spatial distributions of heads, velocities, and chemical constituents are written to files at specified frequencies. Some of the output files are intended to be viewed by a text editor (*.txt* files), some are tab-separated values files (*.tsv* files), which are suitable for post-processing or spreadsheets. Input distributions of model parameters and model results also may be written to a Hierarchical Data Format (HDF) file (*.h5* file), which can be visualized with the ModelViewer software (Hsieh and Winston, 2002). ModelViewer provides 3D views of data from the HDF file and produces solid rendering, isosurfaces contours, and time-series animations of the model results. It also is possible to view the locations of model features, including boundary conditions, wells, rivers, and drains, and the spatial distribution of media properties.

All data definitions of P4W are stored in a binary, HDF file (*.wphast* file), which can be reloaded and run with P4W. Data definitions also can be exported to an intuitive, ASCII text file (*.trans.dat*), which can be used as input for the sequential or parallel batch versions of PHAST. The *.trans.dat* file also can be edited to add or modify model definitions, and then imported back into P4W.

# Summary and conclusions

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

visualize (including the perimeter, bottom, and top of prisms)

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.

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.

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Table 1. First-level items in the data-definition tree of Phast4Windows

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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** | Flux, leaky and constant-head 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; flux through boundary nodes in 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 |