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

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# Abstract

Phast4Windows is a Windows® program for developing and running flow and reactive-transport models for the PHAST simulator. This graphical user interface allows definition of spatial distributions of model properties—the porous media properties, the initial 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 single phase, constant density, saturated groundwater flow under confined or unconfined conditions. 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 and run simple or complex models, and is ideal for use in the classroom, for analysis of laboratory experiments, and for development of field-scale simulations of geochemical processes and contaminant transport.

# Introduction

PHAST is a three-dimensional (3D), multicomponent, reactive-transport model (Parkhurst and others, 2004, 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 aqueous phase. Flow and transport simulations may include wells and flux, leaky (head-dependent), constant-head, 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 for the Windows® operating system 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).

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.

Model features are defined spatially, without reference to a particular grid. Thus, the grid can be refined or coarsened without changes to any of the other model definitions. P4W allows two coordinate systems for defining model features, referred to as "map" and "grid" coordinate systems. It is expected that data imported from ArcInfo® will be in a coordinate system such as UTM (Universal Transverse Mercator) or state plane, which will be the map coordinate system. 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, which may be at an angle relative to the map coordinate system. A linear transform is defined to allow model features to be converted from one coordinate system to the other.

# Building a Reactive-Transport Model with PHAST4WINDOWS

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 or when New is selected from the File menu. 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, an optional 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 by using the data tree of 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 constant parameters and initial conditions and no flows across the model boundaries. To complete the model, spatial definitions are needed to supply the appropriate heterogeneity in media properties and initial conditions, and to define the boundary conditions that describe the flow and transport system. Most 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 contains 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 horizontal planes, or can be defined by a set of points, or by ArcInfo® shape and 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 (figure 1).

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. A zone also may be used to define a volume over which flow and solute fluxes are calculated, including the flux of water and solute through the zone boundaries and through any boundary-condition cells that fall within the zone.

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 or linearly varying in a coordinate direction. A set of points or file with X–Y–Z–V data (where V is a property value) can be used to define the spatial distribution of any media or boundary condition property and files with X-Y-Z-T-V (where T is time) can be used to define spatially distributed and time-varying boundary condition properties.

## 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 single zone can be used to define one or more of these properties. The order of the zone definitions is important because each zone overlays the previous zones, such that, if two zones define the same property for the same location, then the latter definition of the property takes precedence over the former. This order of precedence—later definitions superseding previous property definitions 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 and initial chemistry conditions (**INITIAL\_CONDITIONS**, table 1) are 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 a 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 chemical condition in the simulation is more than just the initial condition because it defines not only the initial solution compositions in the model domain, but also the types of chemical reactions 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 also is possible to spatially distribute mixtures of the solutions.

In addition to the initial solution composition, any combination of reactants can be distributed by zones 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 are identified by a user-assigned integer. A series of zones is used to spatially distribute these reactants; as a simple example, exchange composition 10 could be assigned to zone 1 and exchange composition 20 could be assigned to zone 2. All reactants except the kinetic reactants will react to equilibrium in the cells where they are present. The kinetic reactants will react as defined by a kinetic rate expression, which is usually a function of the solution composition and (or) mass of solids in the cell.

## 5. Boundary conditions

Three types of boundary conditions can be defined with zones: flux, leaky, and specified-head boundary conditions (**BOUNDARY\_CONDITIONS**, table 1). Flux boundaries define a flux of water (L/T) through the set of cell faces defined by the zone 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 selected by the zone definition and assigned a head external to the model domain, 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 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, and drains

Wells, rivers, and drains are model features that are not defined with zone definitions (**WELLS**, **RIVERS**, and **DRAINS**, table 1, and the three icons to the right of the zone icons). Wells are located by an X–Y point, with additional definitions to define the open intervals of the well and the pumping (or injection) rate, which can be a time series.

Rivers are defined by drawing a series of X–Y points. At each point a river width is defined, which is used to calculate the area influenced by the river. Other parameters needed in a river definition are the elevation, thickness, and hydraulic conductivity of the riverbed, the head of the river, and the composition of the river water. The head and river-water composition may be time series. The flux of water to or from the aquifer is calculated from the hydraulic conductivity of the riverbed and the head gradient through the riverbed. All parameters must be defined for the first and last point of a river, but interpolation can be used to specify parameters at intermediate points.

Drains are similar to rivers, except that drains can only accept water from the aquifer and cannot supply water to the aquifer. Drains are defined by drawing a series of X–Y points. Width, thickness, and hydraulic conductivity are defined as with rivers, and the flux of water to the drain is calculated analogously to rivers. However, a time-invariant elevation is assigned to each point of a drain, rather than the head (possibly time-varying) that is defined for a river, and no water composition is needed because water never enters the aquifer from the drain. Water and solutes entering a drain are removed from the system and cannot be reintroduced to the model domain.

## 7. Zone flows

For flow and solute transport models, it frequently is useful to know the fluxes of water and solute through particular locations or boundary cells of the model. Accounting zones (**ZONE\_FLOW**, table 1) can be defined in P4W by using the standard zone definitions. For each accounting zone, the fluxes of water and solutes into and out of the zone boundaries are calculated. In addition, for the set of cells within the zone with each boundary-condition (source/sink) type—flux, leaky, specified-head, well, river, and drain—the fluxes of water and solutes into and out of the cells are calculated.

## 8. Printing

Nearly twenty output files of different data, including descriptions of the problem definition, heads, velocities, chemical data, and log information, can be written during the course of a PHAST simulation. 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. A Hierarchical Data Format (HDF) file (*.h5* file) is used to save most model results in a binary format. The file can be used with the Model Viewer software (Hsieh and Winston, 2002) to visualize data input and results or data in the HDF file can be exported to ASCII files.

The **PRINT\_INITIAL** item in the data tree specifies whether initial conditions are written to output files. The **PRINT\_FREQUENCY** item in the data tree is used to specify print frequencies, in terms of time steps or elapsed time, when data are written to the output files. The print frequency for each file can be specified individually, and, in addition, each print frequency may be specified to change at given times during the calculation. **PRINT\_FREQUENCY** also can be used to write a file of heads that can be used as initial conditions for subsequent simulations.

## 9. Time stepping and simulation periods

The **TIME\_CONTROL** item of the data tree (table 1) allows definition of the time interval used for time-stepping through the calculation. The time step may vary through the calculation, in which case a time series of time steps can be defined. A time to begin the simulation also may be defined, which makes it easy to begin time-stepping from a particular time, a given year for example. One or more simulation periods may be defined, which may affect printing of results; by default, most data are printed at a specified frequency and at the end of each simulation period. The last time for a simulation period defines the end of the simulation.

# 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 run. Spatial distributions of heads, velocities, and chemical constituents are written to files at the specified frequencies. Model Viewer can be used with the HDF output file (.*h5*) to produce solid rendering, isosurface contours, and time-series animations of the model results. It also is possible to use Model Viewer 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. Reactive-transport calculations can be computer intensive, in which case the parallel version offers a way to reduce calculation time if multiple computer processors are available. 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 intuitive interface for developing simple or complex groundwater models and reactive-transport models for the PHAST simulator. Spatial data for media properties, initial conditions, boundary conditions, wells, rivers, drains, and accounting zones can be defined through the interface, as well as all other settings and parameters needed to run PHAST. Data from ArcInfo® shape and raster files can be used to define zones for definition of spatial properties. All spatial data are defined independently from the finite difference grid. Chemical reaction capabilities include all of the reaction capabilities from the geochemical model PHREEQC. Simulations can be run through the interface, or the input files necessary to run a batch version of PHAST can be exported. The interface is an excellent tool for a variety of uses including classroom instruction, analysis of laboratory experiments, and field-scale simulations of geochemical processes and contaminant transport.

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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 |
| **WELLS** | 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 |