

Phast4Windows: A 3D Graphical User Interface for the Reactive-Transport Simulator PHAST

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Abstract

Phast4Windows is a Windows® program for developing and running groundwater-flow and reactive-transport models with the PHAST simulator. This graphical user interface allows definition of grid-independent spatial distributions of model properties—the porous media properties, the initial head and chemistry conditions, boundary conditions, and locations of wells, rivers, drains, and accounting zones—and other parameters necessary for a simulation. Spatial data can be defined without reference to a grid 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 (3D). PHAST simulates single phase,

constant density, saturated groundwater flow under confined or unconfined conditions. Reactions among multiple solutes include mineral equilibria, cation exchange, surface complexation, solid solutions, and general kinetic reactions. 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 column experiments, and for development of field-scale simulations of geochemical processes and contaminant transport.

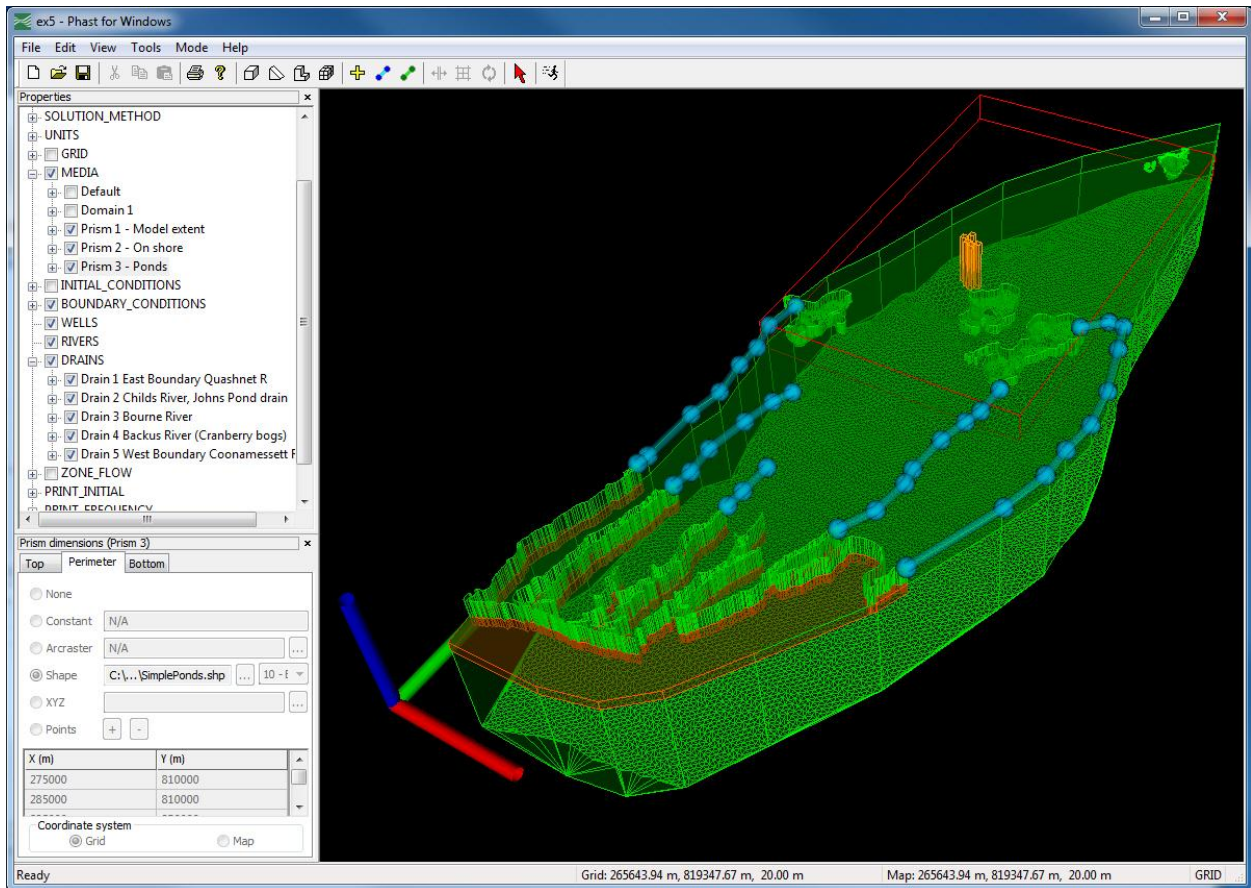


Figure 1. Phast4Windows screen capture of example 5 from the PHAST manual (Parkhurst et al. 2010), a simulation of nitrogen transport at Cape Cod, Massachusetts. Colors have the following definitions: red, specified-head boundaries for the ocean; light blue, drain boundaries for rivers; orange, flux boundary for sewage infiltration beds; and green, media properties. ArcInfo® coverages define the top of bedrock (bottom of the model) and four ponds at the upper right (red box indicates the pond zone has been selected).

Introduction

Phast4Windows (P4W) is a graphical user interface for the three-dimensional (3D), multicomponent, reactive-transport model, PHAST (Parkhurst et al. 2004, 2010). The interface can be used to develop and run pure groundwater-flow simulations, or reactive-transport simulations that combine solute transport with simultaneous geochemical reactions. P4W provides the capability to define data for simulations, including porous-media properties, initial head and chemistry conditions, boundary conditions, accounting zones for which the fluxes of water and solutes are summed, and locations of wells, rivers, and drains, and other parameters, such as time stepping and print control. The interface is intuitive and allows simple controls to define model features, to adjust the viewing perspective, and to select model features to visualize. The 3D visualization in the interface makes it much easier to see relationships among model definitions than interfaces with more limited 2D perspectives. All model features are defined spatially and are independent of a specific grid. The interface can easily define or refine a grid and then launch a serial or parallel simulation. Alternatively, the user can export a model-definition file that can be run with a batch version of PHAST.

PHAST is based on the solute transport model HST3D (Kipp 1987, 1997) and the geochemical model PHREEQC (Parkhurst and Appelo 1999). Flow capabilities are for saturated, confined or unconfined flow of a constant-density aqueous phase. Flow and transport simulations may include flux, leaky (head-dependent), specified-head, river, and drain boundary conditions and pumping and injection wells. 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. However, the lack of gas-phase transport limits the utility of a variable composition gas phase assigned to an individual grid cell.

P4W (Figure 1) is implemented for Windows® operating systems in C++ by using the VTK (Visualization Toolkit 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 file. The chemistry input file can be generated with the

graphical user interface PhreeqcI (Charlton and Parkhurst 2002) or Phreeqc for Windows (Post 2011). The thermodynamic database file can be specified from a set of thermodynamic database files that are distributed with P4W, PHAST, and PHREEQC programs. Additional thermodynamic database files also can be generated with PhreeqcI or Phreeqc for Windows.

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

Category	Function
TITLE	Sets the title for the simulation
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: hydraulic conductivity, porosity, specific storage, dispersivity, and tortuosity
INITIAL_CONDITIONS	Initial head and chemistry conditions
BOUNDARY_CONDITIONS	Flux, leaky, and specified-head boundary conditions
WELLS	Location, open intervals, and pumping rates for a well
RIVERS	River boundary conditions
DRAINS	Drain boundary conditions
ZONE_FLOW	Flow rates of water and solutes in and out of a zone; flux through boundary nodes in the zone; time series of heads and solution composition for nodes in the zone
PRINT_INITIAL	Selection of initial conditions to write to output files
PRINT_FREQUENCY	Selection of print intervals for writing data to output files
TIME_CONTROL	Time step, start time, and ends of simulation periods

P4W saves model definitions in an HDF (hierarchical data format) file (*.p4w*), which includes all of the data and files necessary to repeat a PHAST simulation. In addition, P4W can export or import an ASCII flow and transport file in the format defined by the PHAST documentation (Parkhurst et al. 2010). PHAST runs produce another HDF file (*.h5*), which can be used with the Model Viewer software (Hsieh and Winston 2002) to visualize input data and simulation results in 3D.

P4W has three main panels (Figure 1): a display panel that shows model features in 3D, a data-definition tree (upper left) that contains a list of all model definitions (Table 1), and a spatial-details panel (lower left) 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, the data-entry screen provides a detailed explanation of 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 use a second, local coordinate system that is based on the origin of the grid, which may be offset and at an angle relative to the map coordinate system.

ModelMuse (Winston, 2009) is another graphical user interface available for PHAST. The ModelMuse interface has even more features than P4W for defining spatial data for groundwater and reactive-transport flow models. ModelMuse also displays interpolated property

values at grid nodes, whereas the interpolated values for P4W are determined at runtime and are stored in the *.h5* file. The clear distinction between the two interfaces is that ModelMuse relies on three 2D planes and a 3D representation of the exterior of the model for viewing and defining model features, whereas P4W provides a full 3D visualization. The 3D approach has the advantage that the spatial relationships among zones are readily apparent, whereas the user must mentally construct a 3D view from multiple 2D planes with ModelMuse. However, the 3D approach is more difficult to implement because many 3D linear transforms are necessary to produce the correct scaling and viewpoint of the model features and it can be CPU intensive to triangulate and display prism surfaces. Further, the graphics rendering can be slow if many complex shape files are viewed simultaneously. Considerable effort was required to produce 3D images in P4W that are readily comprehended and can be manipulated quickly.

Building a Reactive-Transport Model with P4W


All model data are accessible through the 17 first-level items in the data tree (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.

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, a preliminary 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.

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 delineated by a rectangular box, a right-triangular wedge, an irregularly shaped volume called a prism, or a box that contains the entire model domain (regardless of the grid definition). These four types of zones correspond to icons on the toolbar at the top of the interface (, Figure 1). 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 that define a polygon, or by ArcInfo® shape files. Similarly, the top and bottom of a prism can be defined by horizontal planes, by a set of X-Y-Z points, or by ArcInfo® shape and raster files. Once a zone is defined, it may be used to define media properties, head initial conditions, chemistry initial conditions, or flux, leaky, 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 solutes through the zone boundaries and through any boundary-condition cells 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.

Properties defined with zones

Media properties (**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 (that is, whether a zone is active or inactive for water flow and reactive transport). If solute transport is modeled, then the additional media properties needed are longitudinal dispersivity, horizontal and vertical components of transverse dispersivity, and 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, as determined by the order in the data tree, 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.

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 steady-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. Head distributions from one model run (steady-flow or transient) may be saved and used as starting conditions for another model run, even if the models use different grids.

The initial chemistry condition defines the initial solution compositions in the model domain. A solution composition is identified by an integer that corresponds to a solution definition in the chemistry data file. Zones are used to distribute solutions (as identified by integers) to 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, like solutions, are identified by a user-assigned integer. A series of zones is used to spatially distribute these reactants. As a simple example, zone 1 could be initialized with exchange composition 10. The exchange composition of each cell in zone 1 would then be equal to exchange composition 10 at the beginning of the simulation, but once time stepping began, the exchange composition in each cell of the zone would evolve independently, according to the thermodynamic equilibrium calculations. Multiple zones, assigned different exchange compositions, could be used to assign heterogeneous initial exchange compositions through the domain. All reactants, except kinetic reactants, will react to equilibrium in the cells where they are present. Kinetic reactants will react as defined by a kinetic rate expression, which is usually a function of the solution composition and (or) mass of solid reactant in the cell.

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 any water entering the model domain through the boundary (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 through the boundary. Finally, a specified-head condition can be defined for cells within a zone, with either an associated solution for water that flows into the cells, or a fixed solution composition that is assigned to the cells.

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.

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 any of the four 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. This capability to report fluxes for zones is similar to the ZONEBUDGET capability of MODFLOW (Harbaugh 1990).

Wells, rivers, and drains

Wells, rivers, and drains (**WELLS**, **RIVERS**, and **DRAINS**, Table 1) are not defined with zone definitions, but by the three icons on the toolbar to the right of the zone icons

(, well, river, and drain, respectively, Figure 1). Wells are located by an X–Y point,

with additional definitions for 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 (which can be 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.

Printing and time stepping


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 HDF file (*.h5* file) is used to save selected model results in a binary format. The file can be used with the Model Viewer software (Hsieh and Winston 2002) to visualize results; in addition, data in the HDF file can be exported to ASCII files by using the utility PHASTHDF that is included in the PHAST distribution.

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, at which data are written to the output files. The print frequency for each file can be specified individually, and each print frequency may be specified to change at given times during the calculation. **PRINT_FREQUENCY** also can be used to write files with heads and solution compositions that can be used as initial conditions for subsequent submodel simulations.

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 series of time steps is 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. Optionally, printing at the end of simulation periods can be excluded. 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 in the toolbar (, Figure 1). Any errors in the input definitions will be identified, and once all errors are corrected, the simulation proceeds. 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 3D 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.

Data definitions of P4W can be saved in a binary, HDF file (*.p4w* file) at any point in the data definition process, and simulations can be launched from P4W. The *.p4w* file saves copies of all files that have been used in model definitions, including chemistry, ArcInfo®, XYZ, and XYZT files. Thus, the *.p4w* file is a complete archive of the model and can be used to run the simulation on any computer on which P4W is installed. Data definitions also can be exported to a readable, ASCII text file (*.trans.dat*). Either the serial or parallel version of PHAST (Parkhurst

et al. 2010) can be run from P4W. Running the parallel version with P4W requires the installation of the MPICH version of MPI (Message Passing Interface). A *.trans.dat* file exported from P4W can be used with either the serial or parallel batch version on Windows or Linux. 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 3D interface for developing groundwater-flow and reactive-transport models for the PHAST simulator. Spatial data for media properties, initial conditions, boundary conditions, wells, rivers, drains, and accounting zones, as well as other settings and parameters needed to run PHAST, can be defined through the interface. Data from ArcInfo® shape and raster files can be used to delineate zones for definition of spatial properties. Zones are visualized in 3D and can be selectively viewed or hidden, edited, reordered, copied, or deleted. All spatial data are defined independently from the finite-difference grid. Thus, the grid can be refined or coarsened without changes to any of the other model definitions. 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. P4W can be used to develop and run simple or complex models, and is ideal for use in the classroom, for analysis of laboratory column experiments, and for development of field-scale simulations of geochemical processes and contaminant transport.

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Supporting Information

P4W and batch versions of PHAST are available at http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phast. An example using P4W and PHAST to

model simple nitrogen transport reactions at Cape Cod, Massachusetts also is available at the web site. The example contains a site map, Shape and .xyz files that are used to define the model features, and PowerPoint slides that describe the step-by-step development of the model with P4W. Also included in the example are ASCII input files and a .p4w file of the complete model definition.

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