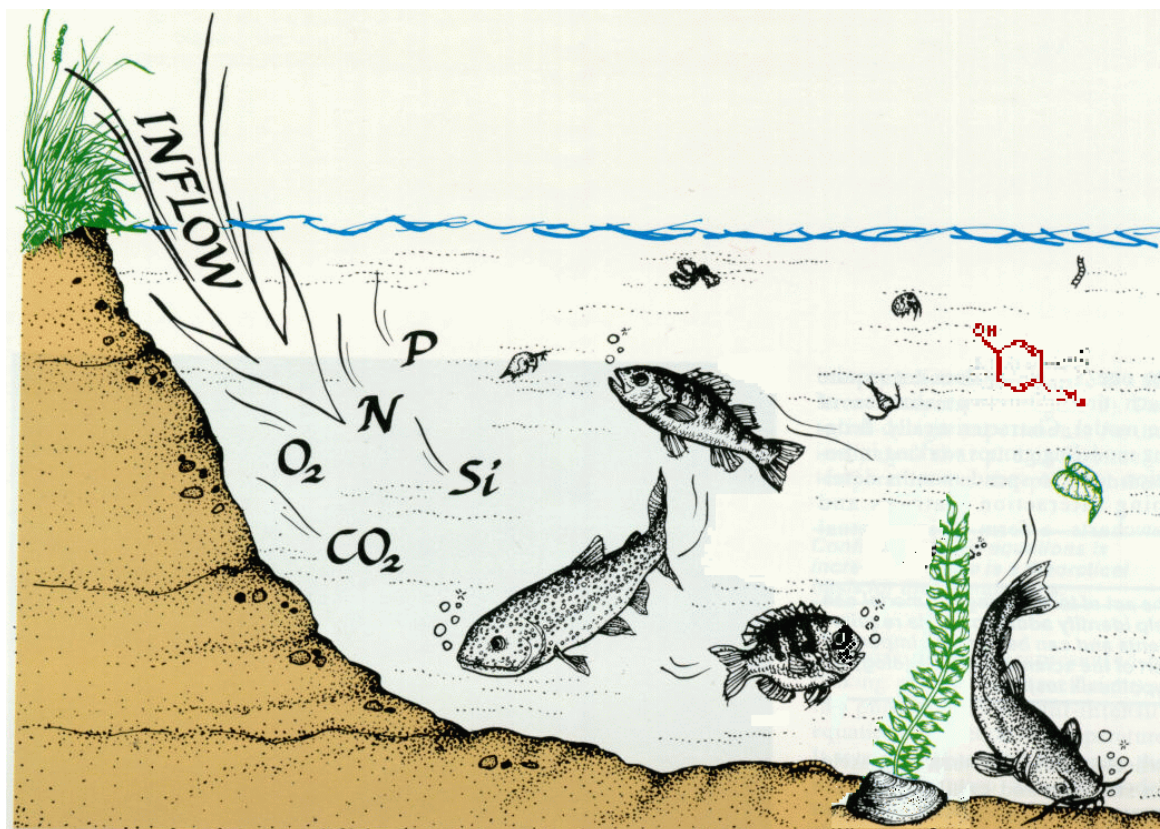




AQUATOX (RELEASE 2.1)

MODELING ENVIRONMENTAL FATE AND ECOLOGICAL EFFECTS IN AQUATIC ECOSYSTEMS

VOLUME 3: USER'S MANUAL FOR THE BASINS (VERSION 3.1) EXTENSION TO AQUATOX RELEASE 2.1



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AND ECOLOGICAL EFFECTS
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**VOLUME 3: User's Manual for the BASINS (Version 3.1)
Extension to AQUATOX Release 2.1**

Jonathan S. Clough

OCTOBER 2005

**U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF WATER
OFFICE OF SCIENCE AND TECHNOLOGY (MAIL CODE 4305T)
WASHINGTON DC 20460**

DISCLAIMER

This document has been approved for publication by the Office of Science and Technology, Office of Water, U.S. Environmental Protection Agency. Mention of trade names, commercial products or organizations does not imply endorsement or recommendation for use.

This document describes an enhanced version of an ecosystem simulation model. It is not intended to serve as guidance or regulation, nor is the use of this model in any way required. This document cannot impose legally binding requirements on EPA, States, Tribes, or the regulated community.

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The assistance, advice, and comments of the EPA work assignment manager, Marjorie Coombs Wellman of the Exposure Assessment Branch, Office of Science and Technology have been of great value in developing this extension and preparing this report.

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1 INTRODUCTION TO THE BASINS AQUATOX EXTENSION

1.1 Overview and Background

It has become increasingly apparent that methods and tools are needed to analyze the combined fate and effects of all stressors on aquatic ecosystems from all sources. Stressors may include nutrients, organic loading, toxic organic compounds, sediments and habitat alteration; sources include point and non point source loadings and atmospheric deposition. Stressors may affect water clarity, algae populations, dissolved oxygen levels, fish and invertebrate communities, levels of contaminants in fish tissue, and many other important environmental conditions. Management approaches that focus on one stressor at a time may miss important interactions that could determine whether overall environmental goals, such as restoration of a more natural aquatic ecosystem, are met. Environmental management programs and activities that could benefit from additional tools for an integrated approach include water quality criteria and standards, Total Maximum Daily Loads (TMDLs), identification of the cause(s) of biological impairment where there are multiple stressors, and ecological risk assessments.

AQUATOX is a time-variable ecological risk assessment model that simulates the fate and effects of various environmental stressors in aquatic ecosystems. It simulates the fate and transfer of pollutants from loads to the water, sediments, and biotic components, and transfer throughout the food web. Simultaneously it predicts the effects of the stressors on the ecosystem, by simulating the chemical, physical and biological processes that bind the ecosystem together. AQUATOX can predict the fate and ecological effects of nutrients, organic toxicants, and bioaccumulative compounds, as well as the expected ecosystem responses to pollution reductions. It considers several trophic levels, including attached and planktonic algae and submerged aquatic vegetation, invertebrates, and forage, bottom-feeding, and game fish; it also represents associated organic toxicants.

BASINS (Better Assessment Integrating Point and Nonpoint Sources) is a combined GIS/water quality modeling system that includes numerous national level environmental and cartographic data layers, analytical tools, watershed loading models, and instream water quality models. One of the main advantages of an integrated system such as BASINS is that the time consuming task of developing input data files for the various models is reduced: watershed characteristics necessary for the watershed models can be developed from the landscape data layers, and data can be converted into the proper formats for model input files. BASINS Version 3 changed the system architecture to a modularized system, and converted the models and many other functions to ArcView "extensions." The modular setup allows the models to run either as part of BASINS or stand alone. The modularity also makes it easier to add components, and for users to customize BASINS for their own purposes. This new software extension links the AQUATOX ecosystem model to the BASINS modeling system.

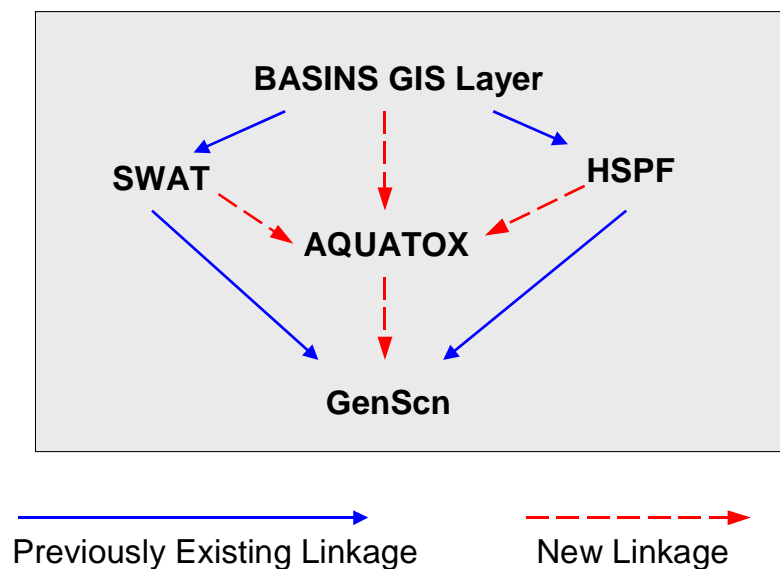
The extension has been developed to assist in comprehensive environmental analysis and prediction. When linked to BASINS, AQUATOX can be used to track ecological effects of point and non point source loadings of organic and nutrient loadings, organic chemicals and pesticides, and changes in hydrology. Specifically, the extension has been designed so that AQUATOX can be run with site characteristics and loadings input directly from the BASINS GIS data layers or from the HSPF and SWAT watershed models. The extension makes possible the direct linkage of the following types of data from BASINS to AQUATOX:

- Site Physical Characteristics (*source: GIS Layer, HSPF, SWAT*)
- Dynamic Water Volume Data (*source: HSPF, SWAT*)
- Nutrient & BOD time-series Loadings (*source: HSPF, SWAT*)
- Organic Chemical or Pesticide Loadings (*source: HSPF, SWAT*)
- Time Varying TSS Concentrations (*source: HSPF, SWAT*)

For each of the time-series that are linked, the extension converts units and integrates data to an appropriate time-step automatically. Additionally, the extension allows AQUATOX output to be linked to GenScn, the post-processor within BASINS. GenScn offers several statistical functions that are not available through the AQUATOX output screen such as comparison of predicted and observed time-series and duration analysis.

The following diagram illustrates how the BASINS AQUATOX extension integrates AQUATOX into the previously existing BASINS framework:

Linkages Between Models



1.2 System Requirements

The BASINS AQUATOX extension requires Microsoft Windows 98, NT, 2000, or XP. Because ArcView and the constituent models are resident in memory, 256 MB of RAM or higher is highly recommended. A user may be able to use the extension with less RAM by setting up a significant virtual memory file within the Windows control panel, although that will necessitate frequent disk access and increase simulation run times. See section 3 of the *BASINS 3.0 Users Manual* (EPA-823-B-01-001, or see the BASINS web site at <http://www.epa.gov/OST/BASINS/>) for more information about BASINS Hardware and software requirements. Within BASINS, ArcView's Spatial Analyst extension is required to run the SWAT model and to automatically delineate rivers within the BASINS modeling system.

2 WINHSPF TO AQUATOX LINKAGE

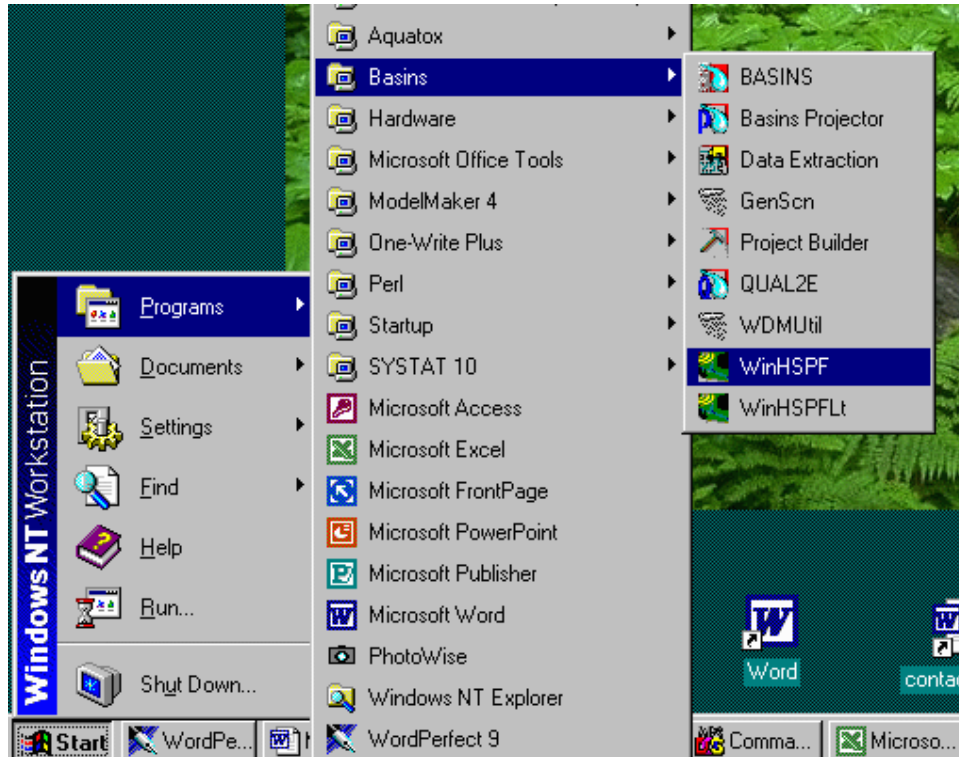
2.1 Introduction

Data from HSPF (Hydrological Simulation Program- FORTRAN) can be linked to the AQUATOX ecosystem model through the BASINS AQUATOX Extension. HSPF is a model that simulates the hydrologic processes, and associated water quality processes, on pervious and impervious land surfaces and in streams and well-mixed impoundments. AQUATOX accepts data from HSPF assuming that a single HSPF river reach is equivalent to a single AQUATOX riverine segment. Using the results of an HSPF simulation, AQUATOX accepts input for the water volume of the system, nutrient time-series loadings, organic chemical time-series loadings, and physical characteristics of the system.

To link HSPF data to AQUATOX the following steps are undertaken:

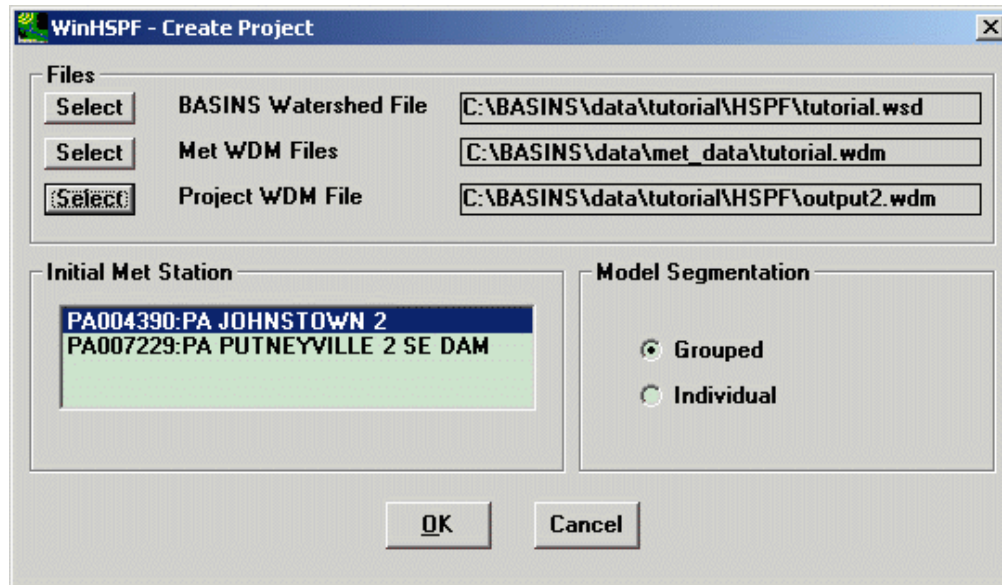
- WinHSPF is executed
- An HSPF simulation is loaded from disk (or using the BASINS interface)
- Appropriate pollutants for linkage to AQUATOX are selected within WinHSPF
- The WinHSPF software is told to produce specialized AQUATOX output files
- The HSPF simulation is executed
- AQUATOX is invoked from the WinHSPF interface, causing the linkage process to take place
- Additional parameters are specified within AQUATOX to complete the AQUATOX simulation
- The AQUATOX simulation is run

To link HSPF data to AQUATOX, the WinHSPF interface must be used. WinHSPF provides an interactive Windows interface for the HSPF model. WinHSPF assists the user in building UCI files from GIS data, especially data from the BASINS system. This program can be found under the BASINS Start menu as shown below.



As an illustrative example, this documentation will walk through the steps required to link the **tutorial.uci** file that comes with the BASINS installation set to AQUATOX. To ensure that this file has not changed during previous uses of WinHSPF, we will start by using the “Create” option to restore the tutorial.uci file to its original state. (*Note:* If you wish to retain your existing tutorial.uci file, please backup the file found in the /basins/data/tutorial/hspf directory to a different name.)

To open the create project window within WinHSPF go to the “File” menu and select “Create.” The Create Project window contains **Select** buttons for three types of files, a list for selecting a meteorological station (met station), and a set of radio buttons for choosing between two land surface segmentation options.



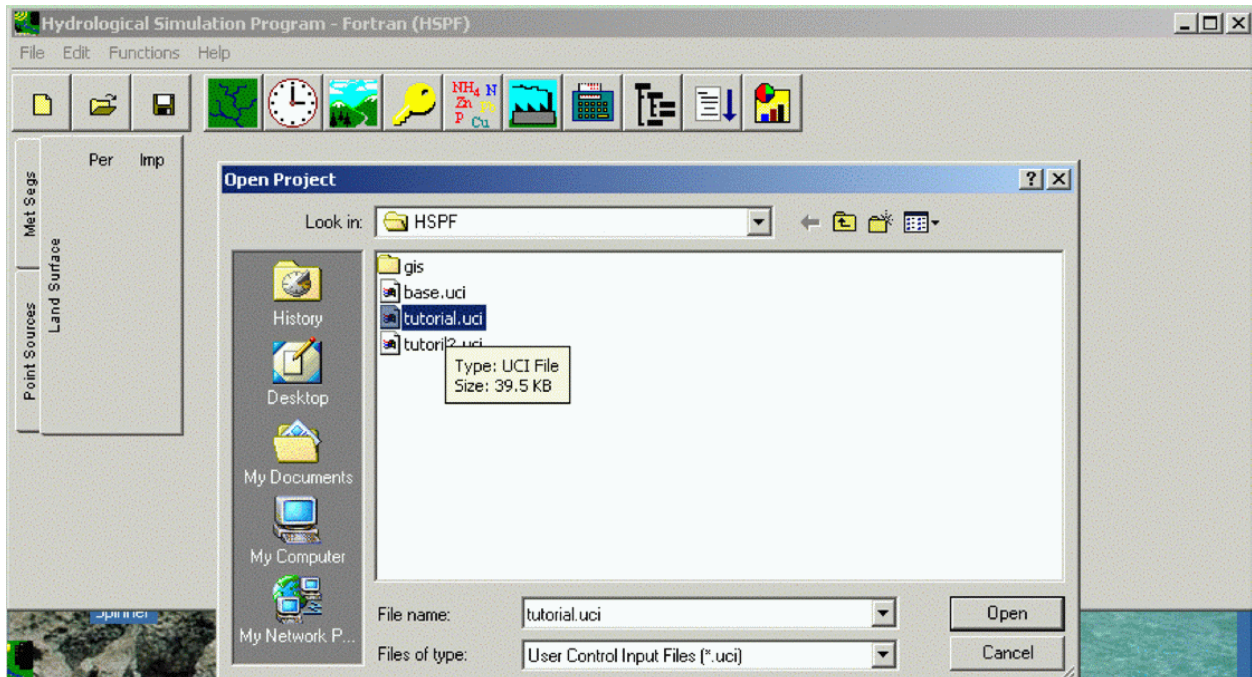
Start by selecting the tutorial watershed file. Select the “BASINS\data\tutorial\HSPF\tutorial.wsd” file as shown above. Next, select the Met WDM file. Select the “BASINS\data\met_data\tutorial.wdm” file. Finally, specify the project WDM file. This file is used to store model output and does not have to be a previously existing file.

Once the met WDM file has been specified, the “Initial Met Station” list will be populated with the identifier corresponding to met stations available for use in the new HSPF project. One item from this list should be selected in order to have some met data included in the HSPF simulation. Select the first met station on the list (Johnstown) as shown above.

In the Model Surface Segmentation radio buttons, the Grouped option creates a single model segment for all collective subbasins, and the Individual creates a single model segment for each subbasin. For this tutorial leave the selection set to Grouped. Then click the OK button to call the algorithms that build the new UCI file. The new UCI file will be written to the “BASINS\data\tutorial\HSPF” directory.

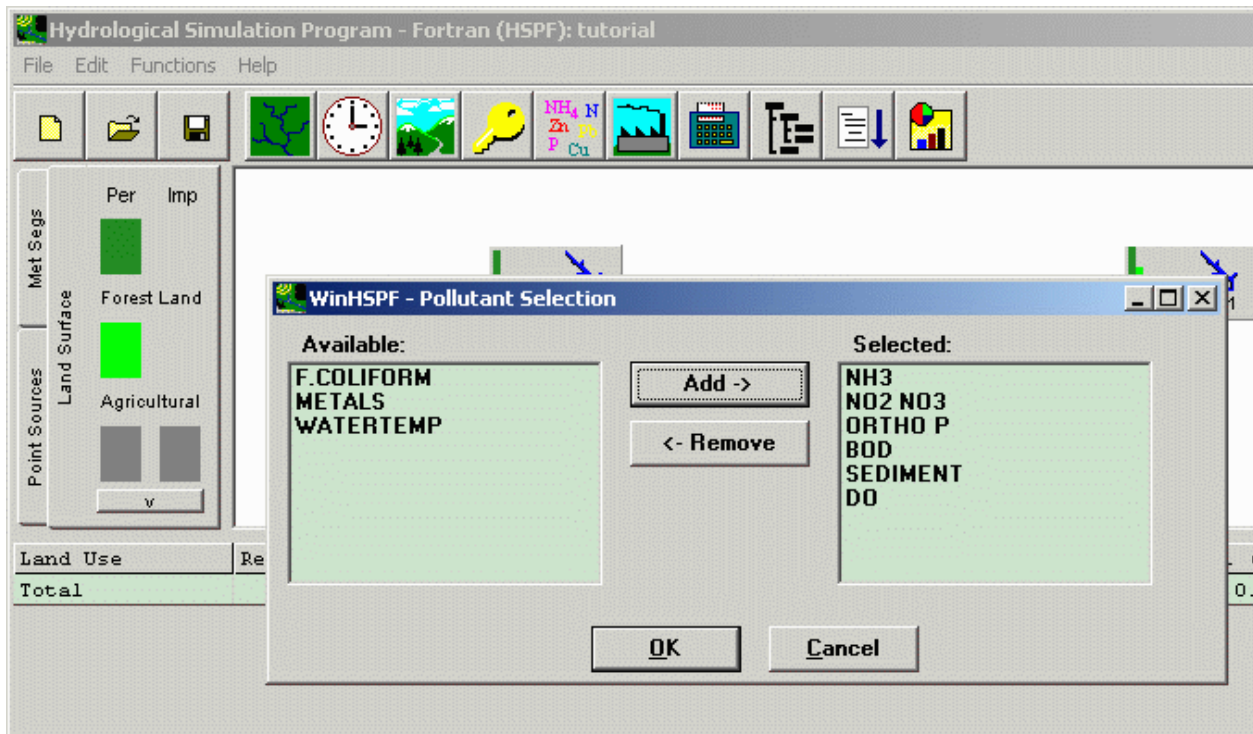
For more information on using the “Create” screen within WinHSPF, see Lesson 1 in the Tutorial within the WinHSPF manual (found in the BASINS\docs directory).

After you have left the “Create” screen, the UCI file will have been created and opened. In the future, you may open this UCI by clicking on “File,” then “Open.,” and then selecting the file.



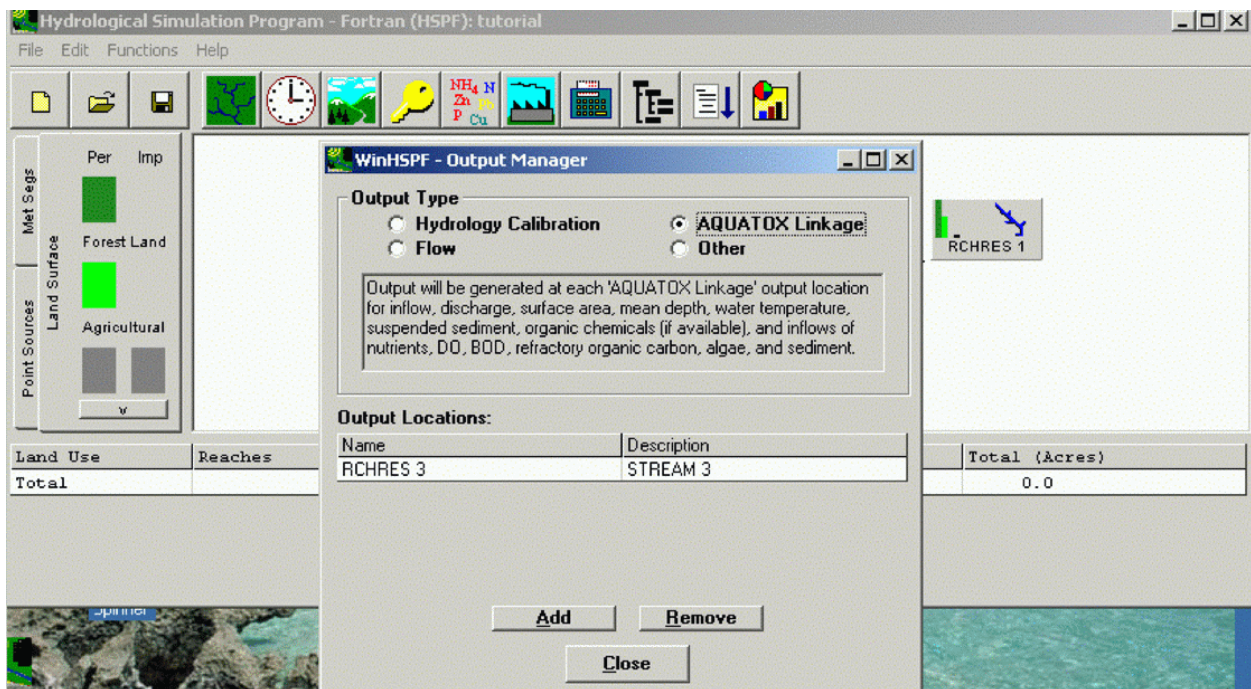
2.2 Selection of Pollutants

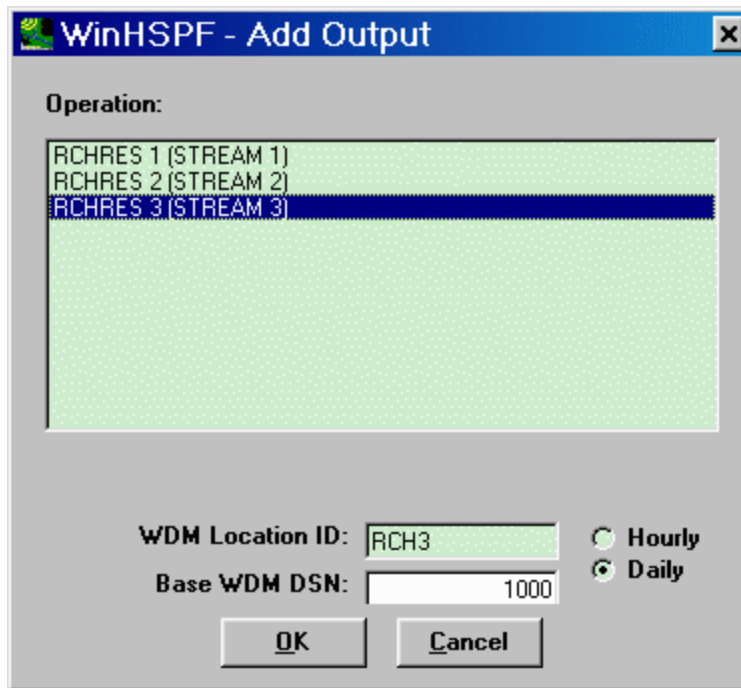
In order to pass water quality data to AQUATOX, a user must include several water quality categories within their HSPF simulation. Click on the Pollutant Selection button. Add NH₃, NO₂ and NO₃, Ortho P, BOD, DO, and Sediment. Click “OK” when finished.



2.3 AQUATOX Linkage

Specify AQUATOX output by clicking on the Output Manager button, choosing the “AQUATOX Linkage” radio button, and clicking on “Add.” Choose one or more reaches in the next dialog, click “OK,” and “Close.” (Note: If “AQUATOX linkage” is not visible in the Output Manager window, then the AQUATOX extension has not been installed. Obtain a copy of the AQUATOX extension and install it. To do this, the file “b3mo_aquatox.avx” must be obtained and installed into the BASINS\etc\Extensions\Models\ directory)

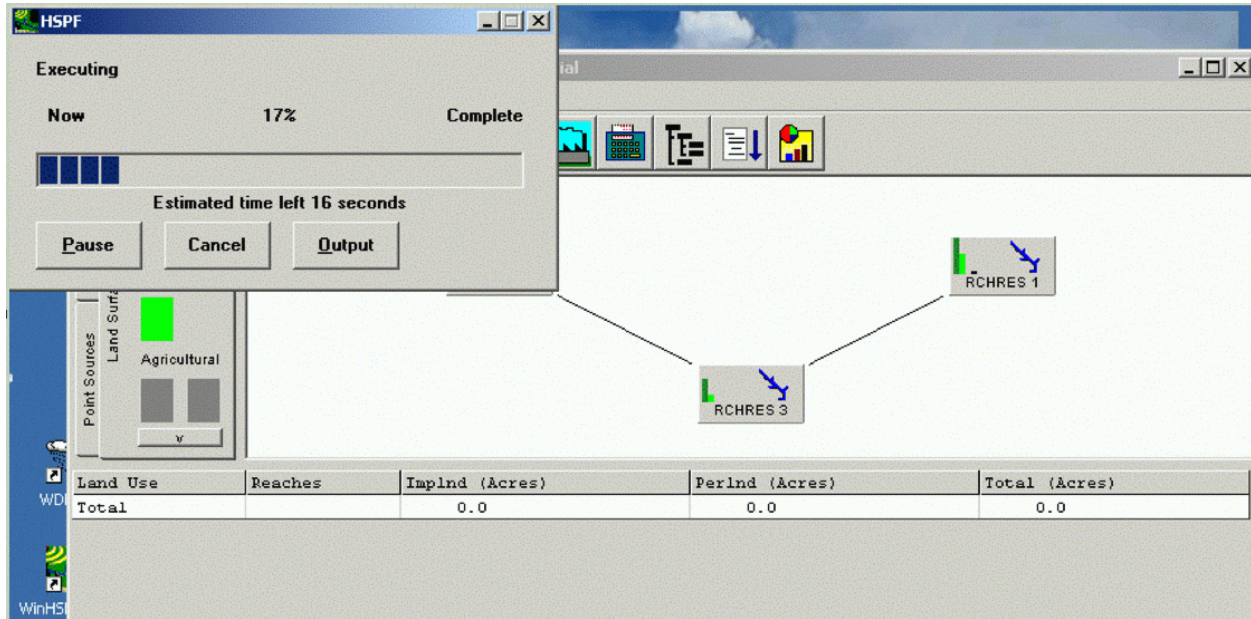




The above dialog box appears when you have chosen to add an AQUATOX output location. If using WinHSPF “build 2.3 revision 1” or higher, when adding AQUATOX output, there will be options to output time-series on an hourly or a daily basis. AQUATOX release 2.1 allows only daily time-series to be imported so this feature is not relevant to Release 2.1. If hourly data are chosen, AQUATOX Release 2.1 will aggregate the hourly data into daily values. Future versions of AQUATOX will allow the input of hourly time-steps so this feature is provided for forward compatibility.

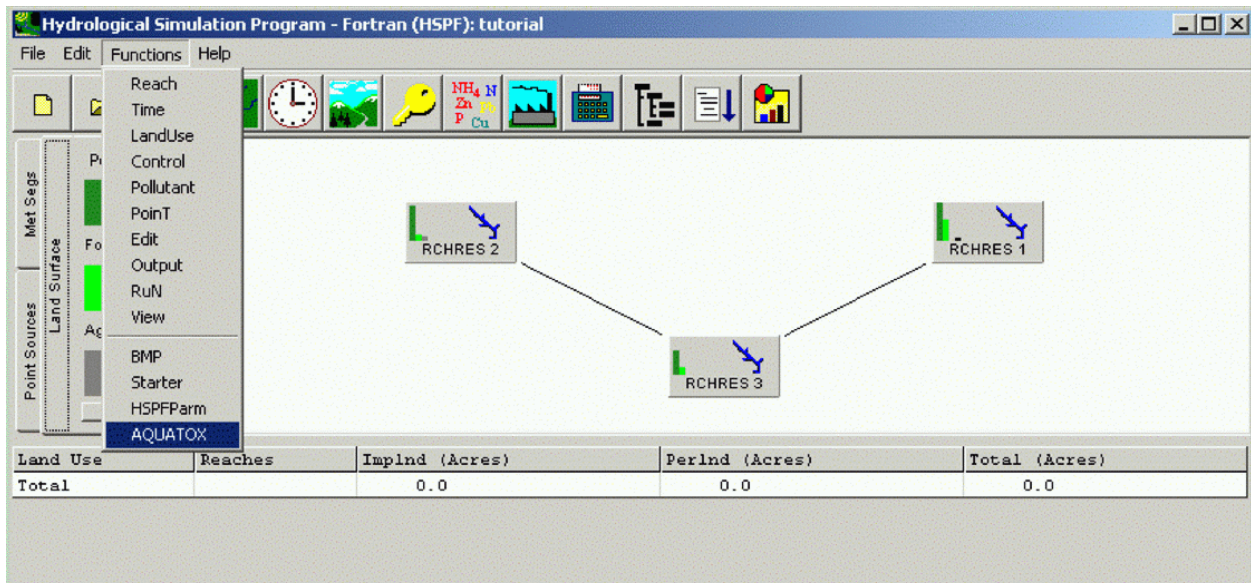
2.4 Obtain HSPF Watershed Simulation

Click on the Run HSPF button to obtain a simulation of the watershed.

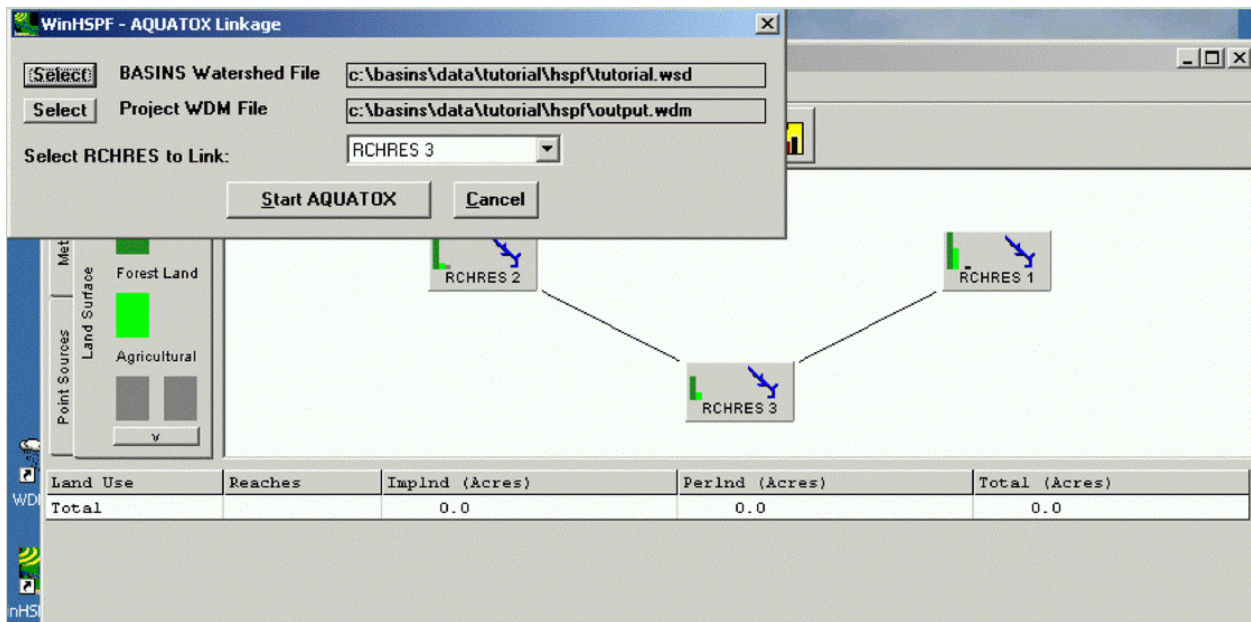


2.5 Running AQUATOX from WinHSPF

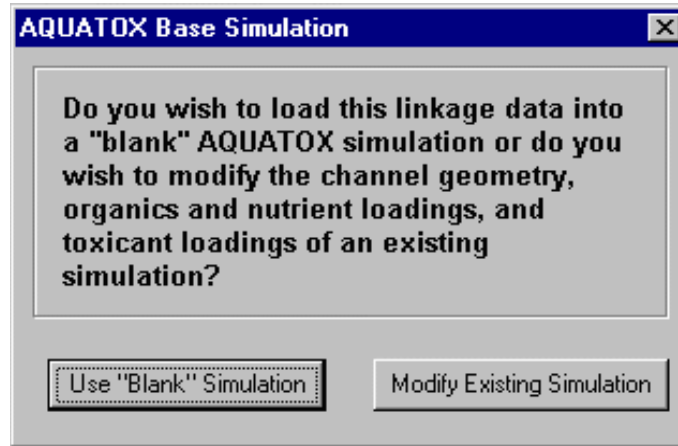
From the Functions menu choose AQUATOX.



In the WinHSPF-AQUATOX Linkage dialog window, select the reach to link (only one at a time). Also, check to make sure the BASINS Watershed File is specified. If you are running the tutorial and WinHSPF does not find the default, use “tutorial.wsd” from \basins\data\tutorial\hspf\. Otherwise, choose the Watershed File that is relevant to the HSPF simulation you are running. If no watershed file is specified, AQUATOX will not be able to locate the BASINS GIS files that are relevant to this particular HSPF simulation. In this case, Channel Length, Channel Slope, Channel Depth, and Maximum Depth data will not be read from the GIS data.



To initiate AQUATOX, click the “Start AQUATOX” button. (If AQUATOX was installed after BASINS, you may need to locate the “AQUATOX.EXE” program file in the “PROGRAM” directory of your AQUATOX installation.) After AQUATOX has started, you will be asked if you wish to create a new simulation or modify an existing AQUATOX simulation. To continue stepping through this tutorial, you should choose a “blank” simulation.

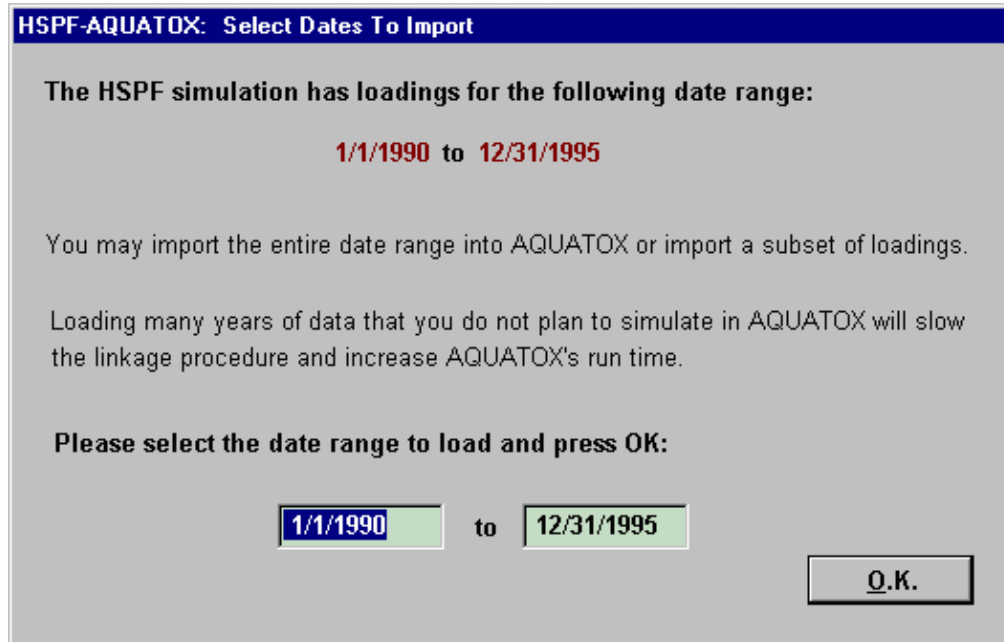


If you choose to use a “blank” simulation, the only parameters within the AQUATOX simulation will be taken from the BASINS linkage. If you choose to modify an existing AQUATOX simulation, data from BASINS will be used to overwrite variables and time-series from the original simulation. *Note:* if you choose to modify an existing AQUATOX simulation, AQUATOX will rename the file-name of the simulation so that the original simulation remains intact. You will be able to see exactly which variables in the original simulation were overwritten by examining the linkage log file as discussed below.

Choosing “modify existing simulation” is often useful because the HSPF-AQUATOX linkage does not pass any information about plants or animals in the system. Therefore a user can take an existing AQUATOX simulation with extensive information about plants and animals and see how it will respond to the flow, nutrient, and toxicant regime found in the BASINS simulation.

Additionally, a user can perform experiments and see how a particular set of plants and animals will respond to a different set of flow and nutrient parameters from different reaches within BASINS or different calibrations of the same BASINS river reach.

Next, you will be asked for which dates you wish to import loadings from the HSPF simulation.



If the HSPF simulation is fairly long in duration, you may wish to reduce the amount of loadings you bring into AQUATOX. The more years of loadings that you import into AQUATOX, the longer the linkage process will take, the larger the AQUATOX simulation will be on disk, and the slower the AQUATOX simulation will run.

HSPF-AQUATOX Linkage: Phosphate Loadings

HSPF includes several forms of phosphorus as listed below. AQUATOX can accept all of these forms or a subset of these depending on how the check-boxes are set below:

Phosphate Forms to Link

include dissolved orthophosphate

include adsorbed orthophosphate

include organic phosphate

The phosphorus state variable is designated "Total Soluble P." Phosphorus that is not bioavailable (i.e. immobilized phosphorus/ acid soluble phosphorus) may be specified using the FracAvail parameter:

Bioavailable Fraction

AQUATOX can model inflow phosphate as Total Soluble P. Alternatively, inflow can be modeled as Total P by accounting for phosphorus contributed by detrital and phytoplankton loads and back-calculating the amount available as freely dissolved nutrients.

Inflow is Total Soluble P

Inflow Represents Total P

O.K.

If using WinHSPF “build 2.3 revision 1” or higher, you will next see the above dialog box asking for the characterization of phosphate as modeled in HSPF. Total Phosphate in HSPF includes dissolved orthophosphate, adsorbed orthophosphate, and organic phosphate. These compartments need to be transformed into bioavailable phosphate within AQUATOX. To do this, you can choose which of the HSPF forms of phosphate to link, choose a bioavailable fraction, and also select whether the phosphate being linked best represents Total Soluble P or Total P. If you don’t have any particular information about the bioavailability of the phosphate you are modeling in HSPF, a reasonable assumption is to pass all phosphate forms and use the Total P linkage as shown above. Choosing a bioavailable fraction of 1.0, as shown above, indicates that all phosphate being passed is bioavailable (perhaps through P-solubilizing bacterial action).

When using earlier versions of WinHSPF, dissolved orthophosphate is the only form of phosphate that is automatically passed into AQUATOX.

Next you will need to characterize the organic matter loadings that are being read into AQUATOX from HSPF. AQUATOX models organic matter in the water column as four compartments by splitting organic matter into refractory and labile fractions and dissolved and particulate fractions.

AQUATOX has a single parameter that characterizes the percentage of inflow loadings that are labile versus refractory. This parameter remains constant throughout the course of an AQUATOX simulation. From HSPF, AQUATOX can obtain two different daily loadings (BOD and refractory organic carbon) with different refractory to labile splits. BOD is assumed to be mostly labile in nature, while refractory organic carbon is refractory by definition. If a user has additional information about the refractory and labile split of BOD modeled within HSPF, the next dialog screen allows this information to be incorporated into the linkage. To get the best representation of organic matter coming into the system, the linkage software sums these two loadings. Then, using a weighted average, AQUATOX determines the most representative percentage of labile vs. refractory for this total mass of incoming organic matter. In this manner, the total labile and refractory loadings will be averaged out over the course of the entire AQUATOX simulation.

Organic matter loadings must also be broken down into particulate and dissolved fractions for use in AQUATOX. This percentage may also be entered in the dialog screen shown below. The default value of 10% particulate is a generally accepted percentage, but this can vary depending on site-specific conditions.

BASINS-AQUATOX Linkage: Please Characterize Organic Carbon Loadings

AQUATOX will import BOD from the HSPF simulation. This must be characterized as Labile or Refractory organic matter. It is generally assumed that BOD is predominantly Labile in nature.

AQUATOX will assume that 10% of the BOD is Refractory (90% Labile) unless a different number using is specified using this screen.

% of BOD that is Refractory

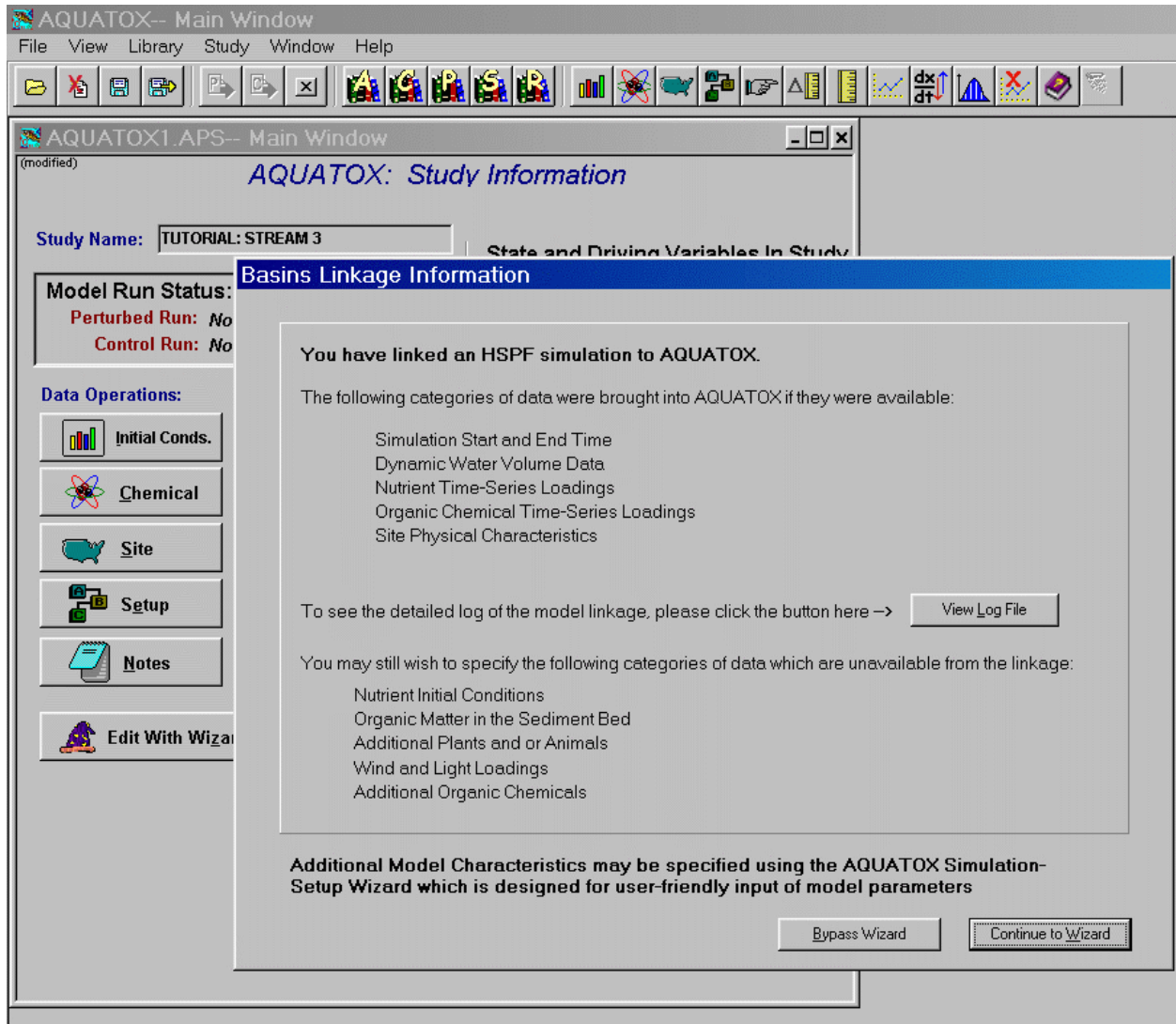
Additionally, AQUATOX must characterize incoming loads of organic matter (BOD and Refractory Organic Carbon) as Dissolved or Particulate in nature.

AQUATOX will assume that the organic loadings are 10% particulate unless a different number is specified with this screen:

% of Organic Loadings that are Particulate

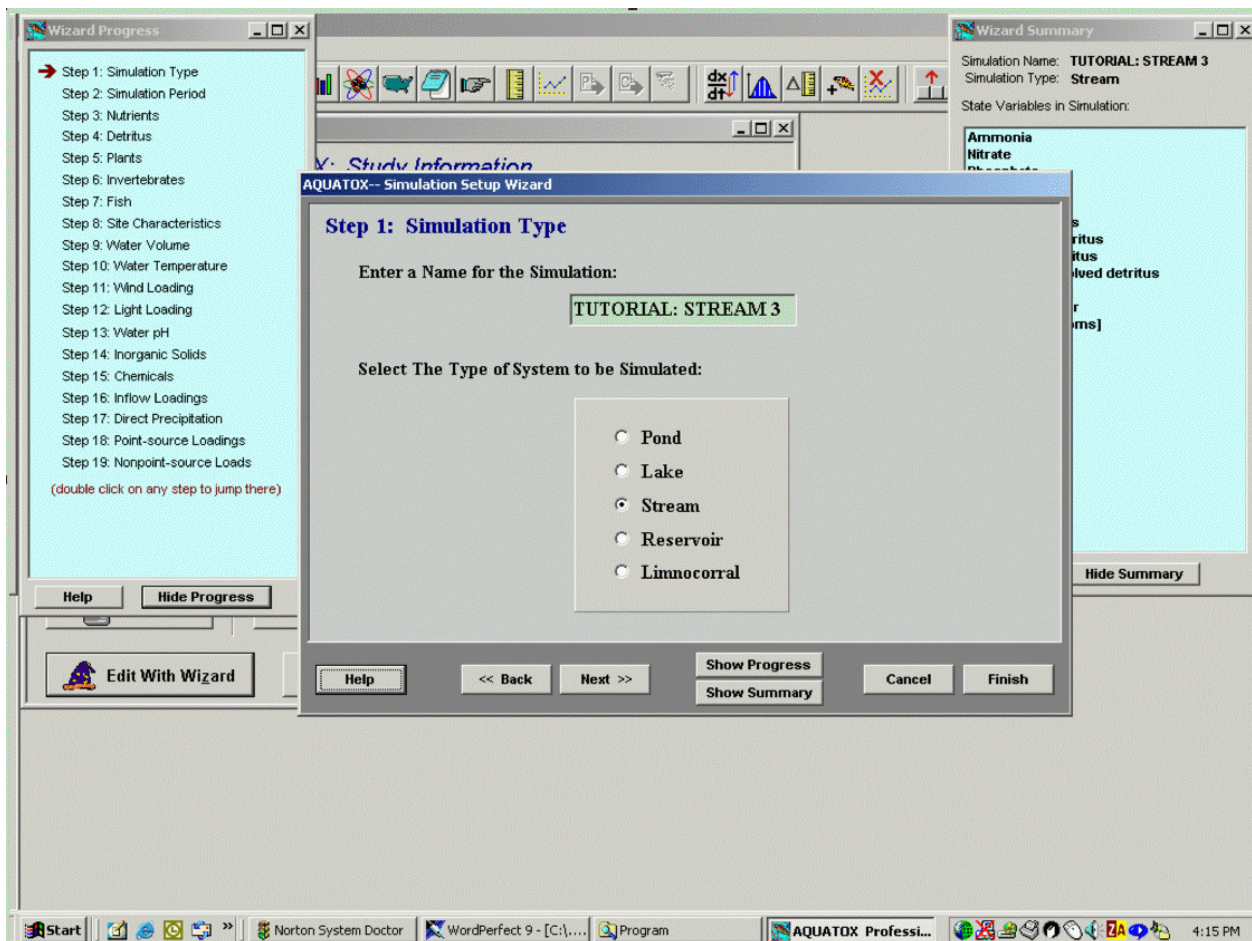
2.6 Linked Simulation

At this point, the linkage procedure should complete itself and the below screen will be displayed. You may wish to click on “View Log File” to see what actions were taken; the log file name and location is also copied into the set of notes associated with the AQUATOX study. These notes can be displayed by clicking on the “Notes” button from that main study screen (*Note: the Notes button is not available when the linkage windows or the Wizard is open*).



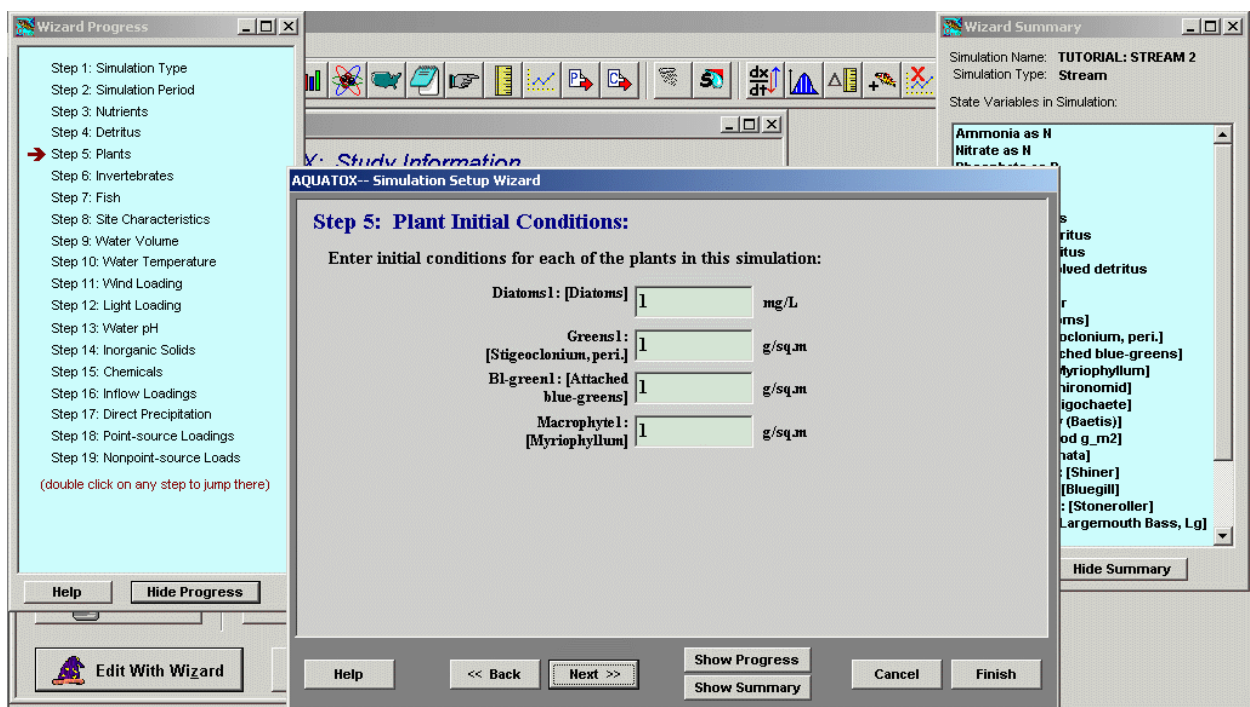
2.7 Specification of Additional State Variables and Loadings

Especially if linking to a blank simulation, the user is advised to click the “Continue to Wizard” button to facilitate specification of state variables and loadings that are not available from the linkage. There are 19 steps with context-sensitive help. Unless discussed below, the default values are appropriate for the initial simulation. This section will discuss how a user can set up the basic ecosystem variables after linking to a blank simulation. You may also reference the AQUATOX Users Manual (EPA-823-R-04-001) for more information on using the AQUATOX wizard.

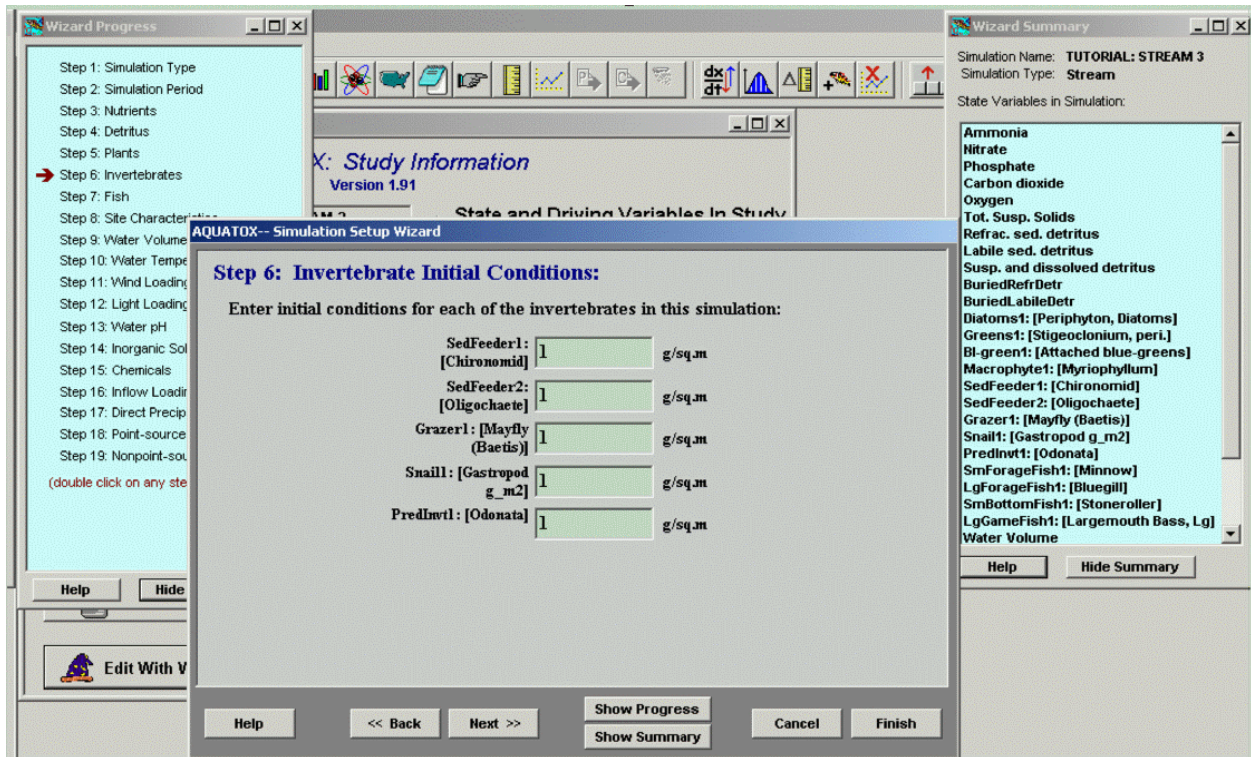


Note: While the AQUATOX linkage reads BOD data from HSPF, it converts these data into organic matter and then adds the data to the time-series of refractory organic carbon data for a complete set of organic carbon loadings. Therefore, the user should maintain a selection of “organic matter” in Wizard Step 4.

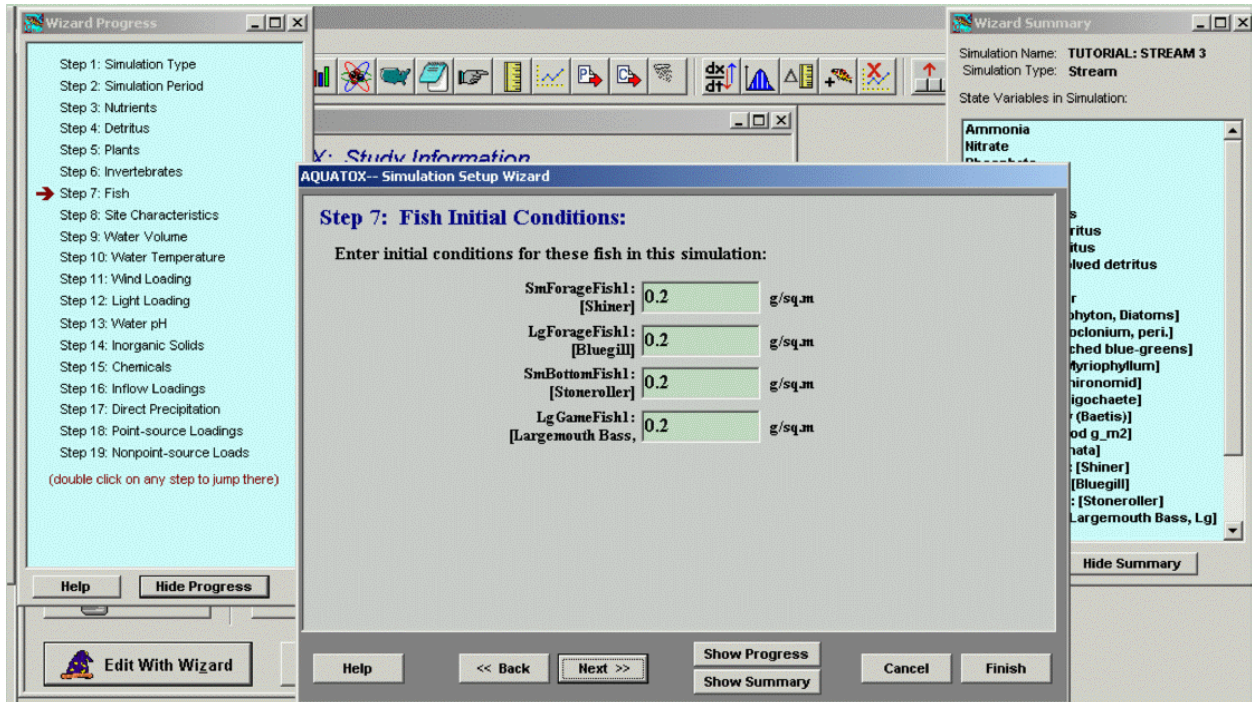
For a typical stream you should add Diatoms, periphytic Diatoms, Greens, and Blue-greens, and Macrophytes. Set their initial conditions to 1 g/m² in a subsequent screen (unless of course you have site specific data). You should run the model for several years to “spin up” the model and avoid transient conditions from the initial guesses; you can then take the end conditions and substitute them for the original initial conditions in subsequent simulations.



Several invertebrates should be chosen, and their initial conditions also set to 1, as shown.



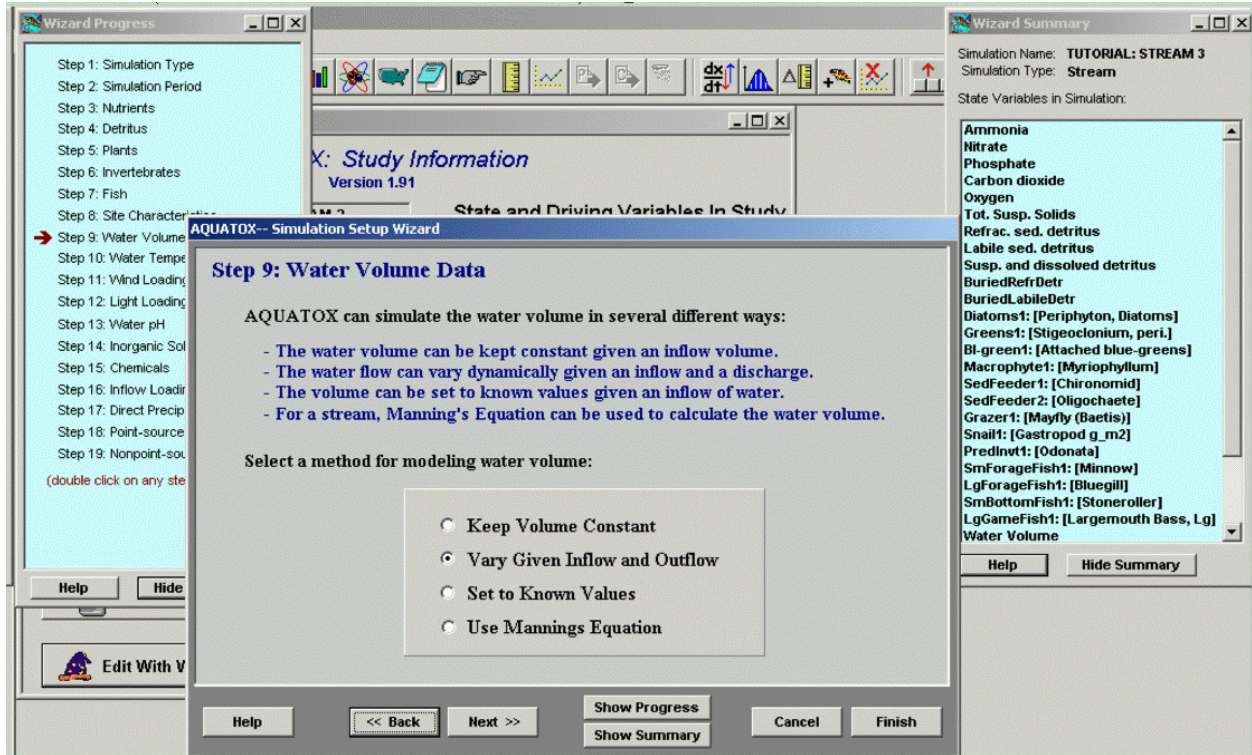
Likewise, several fish would usually be chosen. Initial conditions of 0.2 g/m² are suggested.



In the wizard step 8, site characteristics that have been imported from HSPF will be displayed. Note that the stream bottom is assumed to be 100% run. If the site has significant riffle and pool features, change these parameters accordingly.

Next, water volume data will be loaded from HSPF so that the water volume in the AQUATOX reach is identical to the HSPF water volume over the course of the simulation. To make this possible, the inflow water loaded into AQUATOX has been adjusted for the evaporation and precipitation predicted by HSPF.

To use the HSPF water volume data, the “Vary Given Inflow and Outflow” option should remain checked as shown below. For more information about the other water volume modeling choices on this screen, you can select the “Help” button from this wizard step.

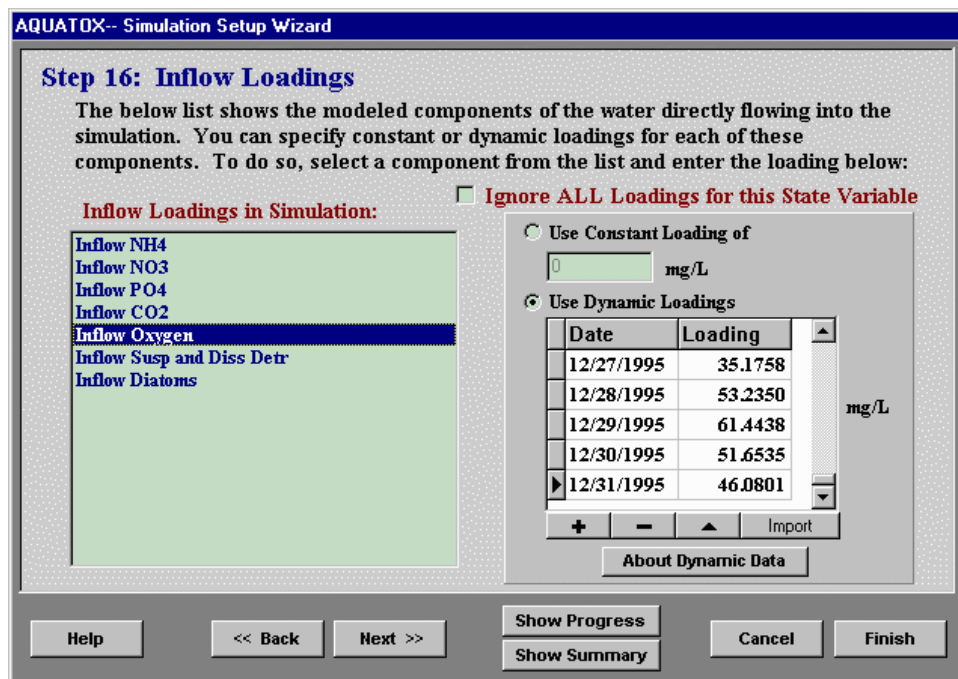


Because a time-series of water temperature is generally imported from the HSPF linkage, the user should select the option "Use time-varying temperature" in Wizard Step 10.

Stream simulations are generally not sensitive to wind, so use the default with a mean value of 3 m/s.

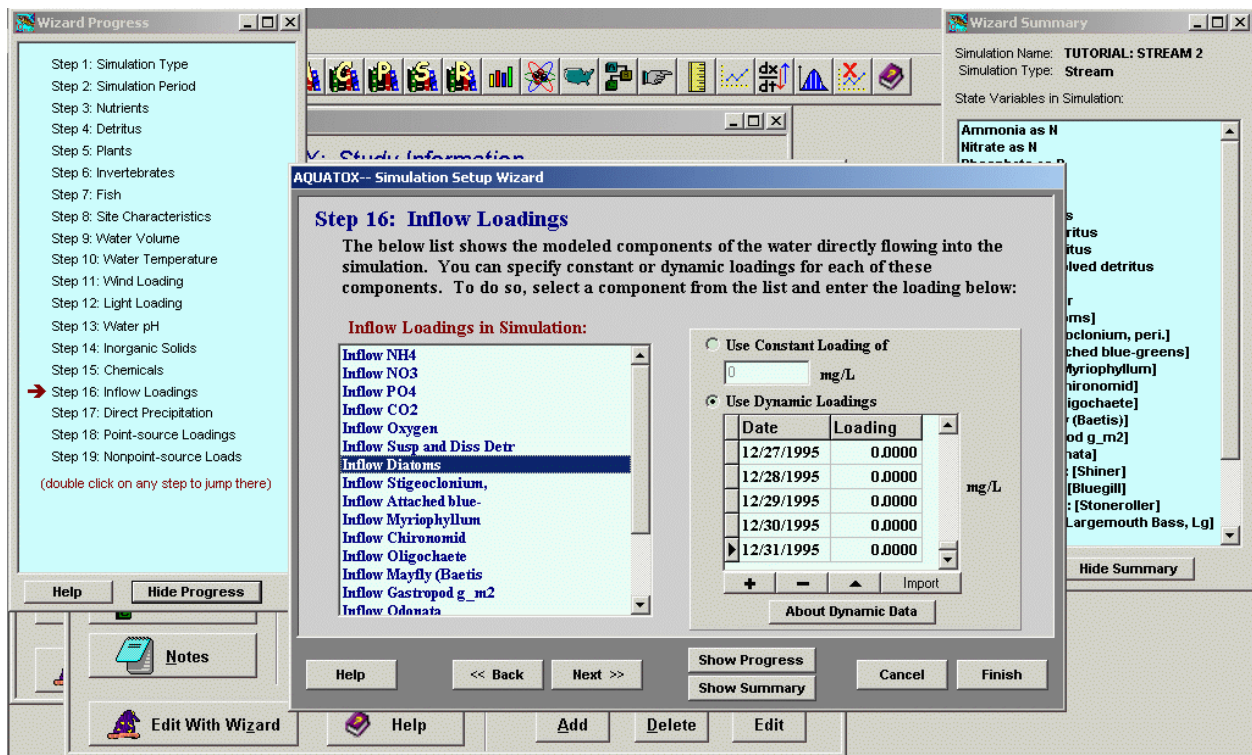
Wizard step 14 displays inorganic solids loadings within the AQUATOX simulation. Currently TSS concentrations are linked from HSPF as the summation of modeled sand, silt, and clay. TSS concentrations can affect light extinction within a simulation, affecting algal growth. A user can also choose to model sand, silt, and clay as state variables within AQUATOX, but not directly through the linkage at this time. (As light extinction is currently the only feedback between inorganic sediments and modeled biota, HSPF simulated TSS concentrations provide a sufficient source of data. In the future, if more complex feedbacks between sand silt and clay and the biotic components within AQUATOX are developed, linkage to categorized sand, silt, and clay data from HSPF will be appropriate.)

Oxygen loadings have been converted from kg\hr as predicted by HSPF into mg\L of inflow water for integration into the AQUATOX interface. Because of this translation, the oxygen concentration predicted within the AQUATOX reach will be essentially identical to the oxygen concentration predicted by HSPF. Because of the translation from kg\hr to mg\L of inflow water, in some cases the inflow loading value may appear to be too high within AQUATOX. However, when these loadings are brought into the system, and matched with the volume of inflow water in that time-step, the oxygen concentration within the AQUATOX reach will match the oxygen concentration predicted by HSPF at that time.



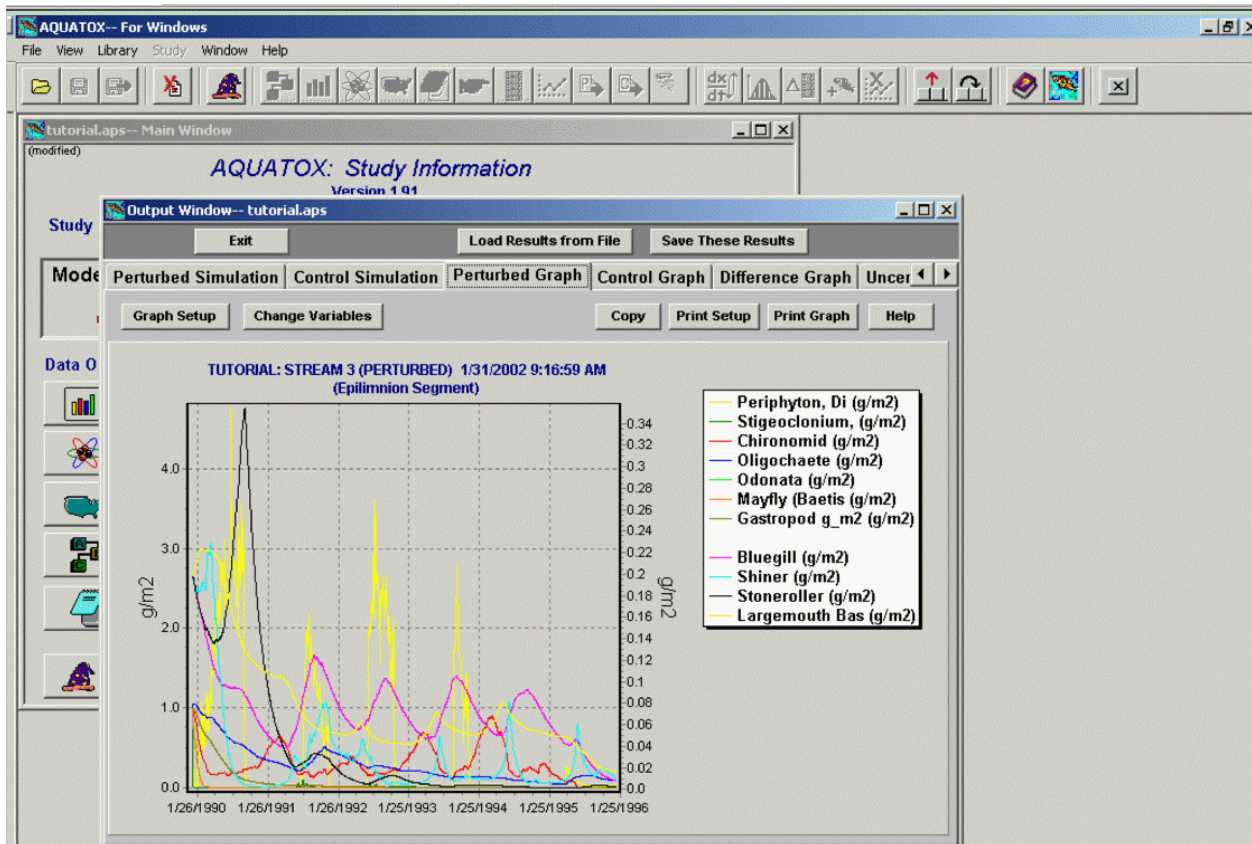
Inflow loadings serve two purposes: they can be realistic time-series predicted by HSPF, or they can be “seed” values to account for colonization and recruitment. The recommendation is to use loadings of 0.00001 for plants, fish, and invertebrates other than insects. A value of 0.0001 is suggested for insects to account for drift and eggs from free-flying adults.

There are usually many modeled components of the water that directly flow into each AQUATOX simulation. This wizard step is provided so that you may check and edit inflow loadings for each of these inflow components. You can scroll through the list to see which of these items have already had dynamic data loaded into them from the HSPF to AQUATOX linkage. As mentioned above, for several of the new animals you added to the simulation within the wizard, a “seed” loading may also be appropriate.



2.8 Run AQUATOX and Plot Results

Run the model for several years and plot the results to see what changes may need to be made. The “Change Variables” button allows you to select which AQUATOX variables are currently plotted and whether to plot variables on one or two axes. For further information on the AQUATOX output capabilities, please see the Users’ Manual (referenced below).



(Note: Plotted results above are given as an example only. Your results will vary depending on the specific data libraries utilized, the stream reach modeled and the initial conditions chosen)

A site-specific parameter that often needs to be adjusted is mortality for the fish. As mentioned previously, it may be desirable to take the end biomass values and use them as initial conditions to avoid a transient response in the first year or two due to inappropriate values. In this example, all fish started with initial conditions that are too high, and the shiners and stonerollers attained even higher levels before crashing. (Reasons for the decline can be determined by saving and plotting the rates.) The decline of all state variables toward the end of the simulation is the result of declining water levels.

For more information on how to use AQUATOX see:

AQUATOX (Release 2)--Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems. Volume 1: User's Manual, January 2004, 823-R-04-001.

It is available on-line at: <http://www.epa.gov/waterscience/models/aquatox/>

3 BASINS GIS TO AQUATOX LINKAGE

3.1 Introduction

A user may link data from the BASINS GIS data layer directly to AQUATOX through the ArcView interface. This can be helpful for gathering information about a site even when there is no related HSPF or SWAT simulation. The categories of data that are relevant to AQUATOX within the BASINS GIS layers are listed below:

- Reach Name
- Channel Length
- Mean Depth of Reach
- Channel Slope
- Channel Depth

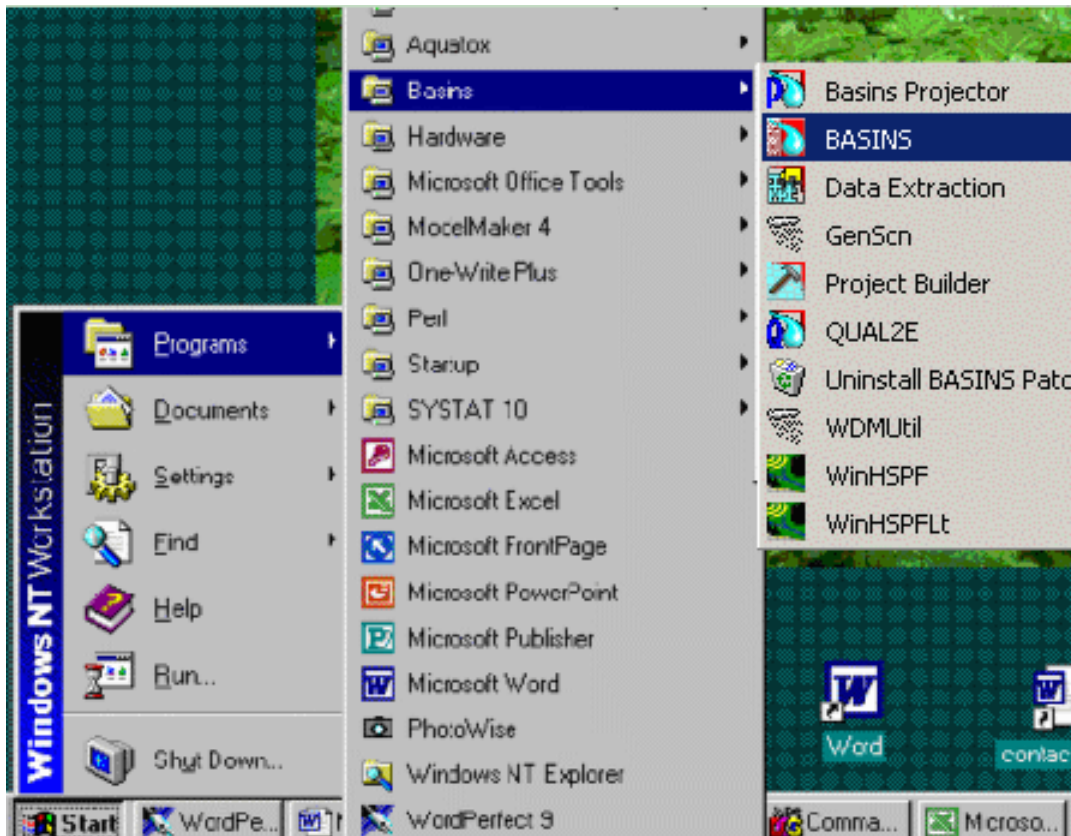
The steps that are required to link BASINS GIS data to AQUATOX are as follows

- Verify that the AQUATOX and delineation extensions are active.
- Manually or automatically delineate the watershed sub-basins.
- Select the stream segment to be modeled within AQUATOX.
- Execute AQUATOX from the BASINS interface.
- Setup and Run the AQUATOX simulation.

3.2 Performing the BASINS to AQUATOX Linkage

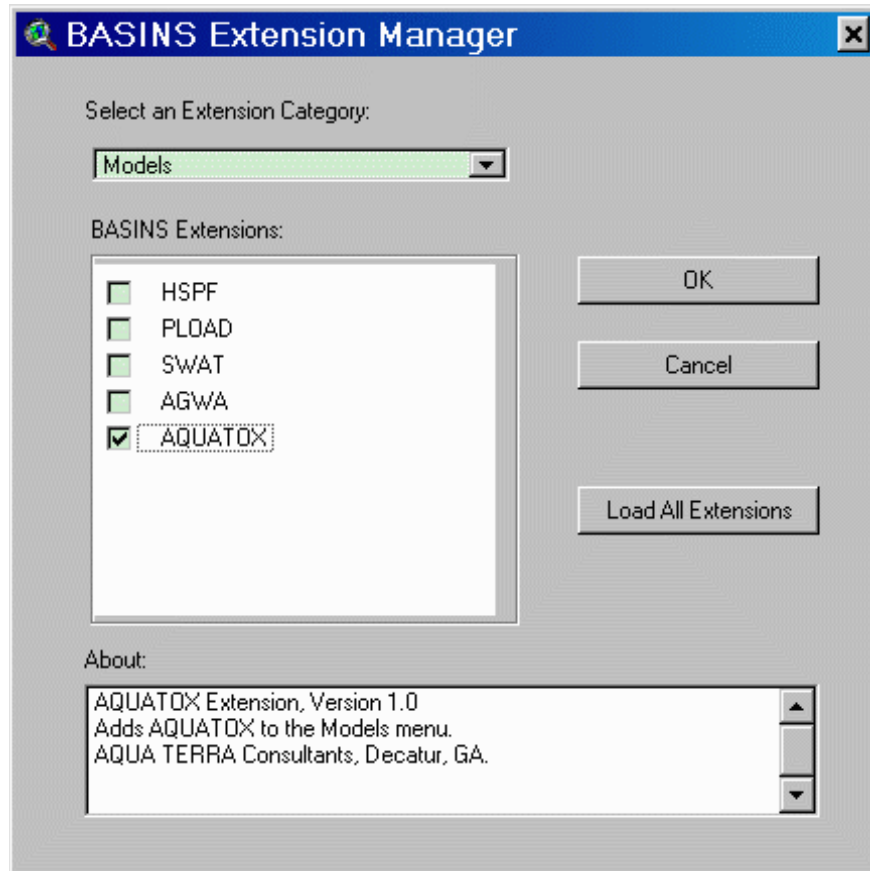
Performing this linkage is very similar to linking a stream reach from the BASINS GIS data layer to HSPF, except that it starts from the BASINS interface rather than the WinHSFP interface. The following steps are required:

Open a BASINS project by selecting BASINS from the “Programs” menu as shown.



Open “TUTORIAL.APR” or whichever BASINS project file you wish to work with.

Next, verify that the AQUATOX extension is active in your BASINS project by typing Ctrl+B from the BASINS View and selecting the Models item from the Extension Categories drop-down list. The AQUATOX entry in the BASINS Extensions list should be visible and selected.



If AQUATOX is not visible in the BASINS Extensions list when the Models item has been selected, then the AQUATOX extension has not been installed. Obtain a copy of the AQUATOX extension and install it. (*To do this, the file “b3mo_aquatox.avx” must be obtained and installed into the BASINS\etc\Extensions\Models\ directory*)

If AQUATOX is not selected (checked), click on it to select it.

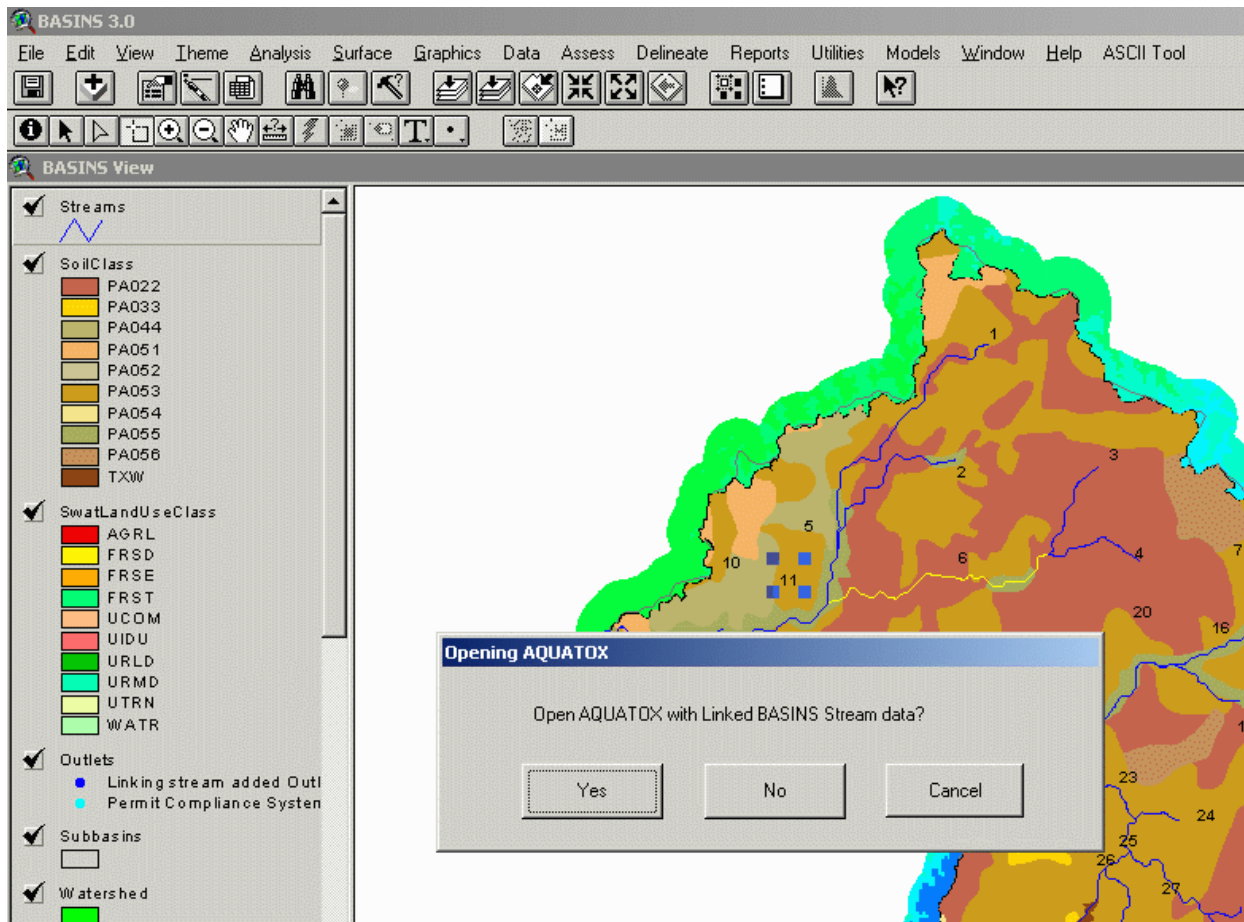
Also, to use the AQUATOX extension to create an AQUATOX simulation, you must first run the manual or automatic delineation extensions to create the watershed, sub-basins, streams, and outlets themes. See section 8 of the BASINS User Manual for details on watershed delineation. This step requires that the automatic or manual watershed delineation tools are selected in the “Delineate” extension category within the BASINS Extension Manager. (*Note: automatic delineation requires the ArcView Spatial Analyst software package.*)

When delineating the watershed sub-basins, a user should keep in mind that the primary stream in each sub-basin will become the AQUATOX reach simulated. On an ecological basis, fast-flowing upstream river segments may be significantly different than downstream slow-flowing

backwaters. Therefore, a user should try to keep the size of the reaches small enough so that dramatically different ecosystems are not simulated within a single AQUATOX reach.

After the watershed has been delineated, the user must select the stream segment that is to become an AQUATOX stream simulation. Select the “streams” theme and use the “select feature” tool to make the relevant stream reach turn yellow. Then, select AQUATOX from the “Models” menu at the top of the screen.

As shown below, you will next be asked whether you wish to “Open AQUATOX with Linked BASINS Stream data.” (*Note: Screen capture based on TUTORIAL.APR*)

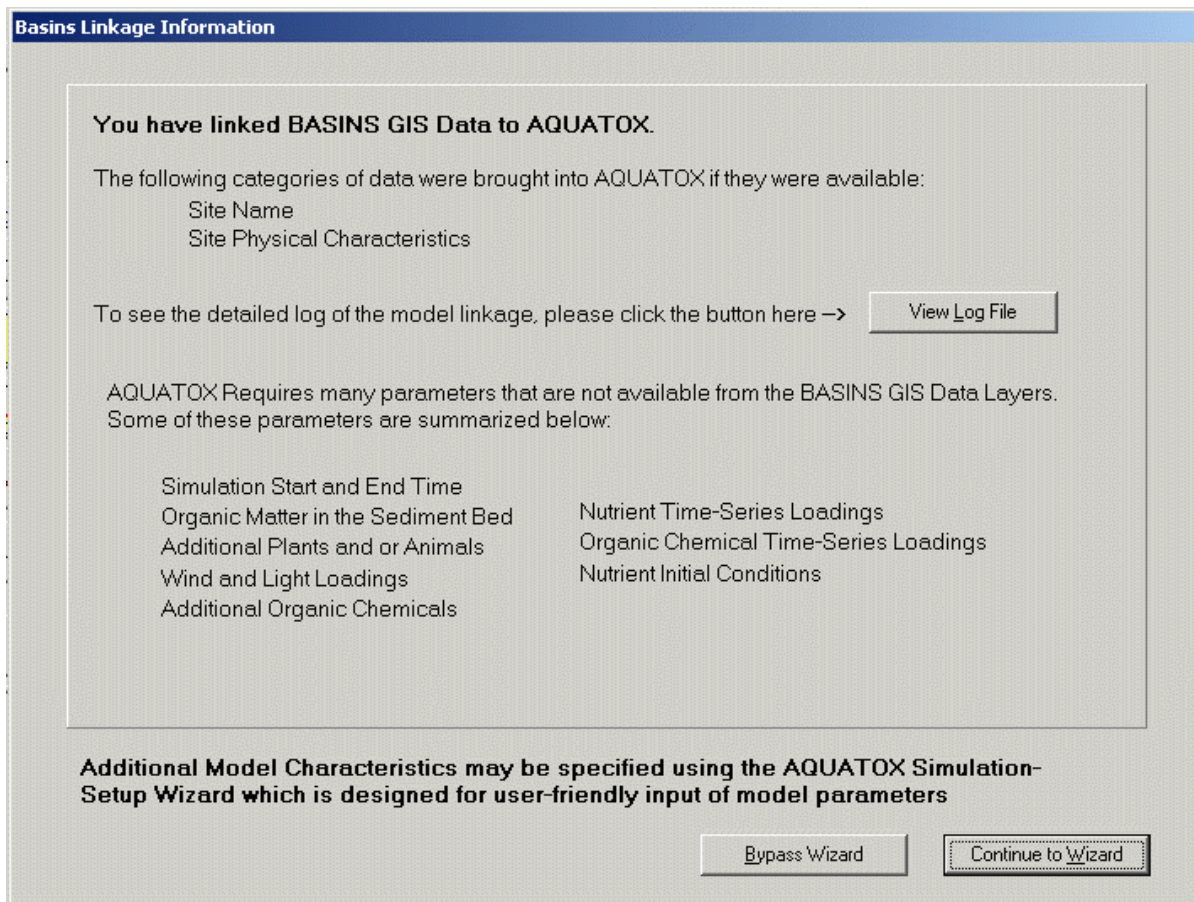


Selecting “Yes from this dialog” will open AQUATOX with linked data. Selecting “No” will open AQUATOX but with no linked data.

3.3 Using AQUATOX after a BASINS to AQUATOX Linkage

As was the case for the HSPF linkage, a user may choose to link to a blank AQUATOX simulation or overwrite relevant parameters and loadings in an existing AQUATOX simulation. See Section 2.5 for more information about this choice.

Next, the AQUATOX Linkage Information screen becomes visible. This screen shows the types of information that have been linked to AQUATOX and the additional parameters that are required to fully specify an AQUATOX simulation.



All parameters that are loaded from the GIS data layers are logged in a text file. The user may view and print the log file from this screen by selecting the “View Log File” button. (If a user wishes to refer to the log file at a later time, the location of this log file is written into the “Notes” dialog, available through the main screen of the AQUATOX interface.)

An expert AQUATOX user may choose to bypass the user-friendly AQUATOX simulation setup wizard. Beginning users are encouraged to continue to the wizard to finish specifying the required parameters.

4 SWAT TO AQUATOX LINKAGE

4.1 Introduction:

AQUATOX has the capability to read input and output data from SWAT (Soil and Water Assessment Tool) version 2000. AQUATOX will read data about channel geometry, nutrient and pesticide loadings, simulation period, water flow, and organic and inorganic sediment loadings.

To perform this linkage, the following steps must take place.

- The user must complete the specification and calibration of a SWAT 2000 simulation using the BASINS 3.0 interface. (*This requires the ArcView Spatial Analyst software package.*)
- The user must start AQUATOX and select the SWAT output file that contains the relevant data.
- The SWAT sub-basin the user wishes to gather data from will then be selected.
- AQUATOX will read all relevant data from the SWAT input and output files.
- Finally, the user is required to fill in AQUATOX parameters that are not available through the SWAT linkage.

When the process is complete an AQUATOX simulation that corresponds to the main channel within a SWAT sub-basin will have been created. This SWAT to AQUATOX linkage process is described in more detail below.

4.2 Running a SWAT Simulation

This section will outline some relevant points about running SWAT if a user intends to link the SWAT simulation to the AQUATOX model. Complete documentation as to how to run the SWAT 2000 model can be found in the **B2SWAT.chm** file located in the BASINS\DOCS directory following the installation of BASINS 3.0.

The steps required to run a SWAT model are roughly outlined below:

- Automatically delineate the watershed.
- Define land use and soil themes for the SWAT model
- Define the HRUs (hydrologic response units) distribution for the SWAT model
- “Edit Input” within the SWAT view
- Write all input data files within the SWAT view (under the “Input” menu)
- Run the SWAT model

At each step of the above process, a user should bear in mind that the main reach within a single SWAT sub-basin will later correspond to a single AQUATOX reach. This may affect a user's choices within the automatic delineation or input choices for the SWAT model. Smaller sub-basins are generally most appropriate for an AQUATOX simulation so that the ecosystem does not change dramatically within a single sub-basin.

When a user has completed all the steps required above, and has chosen to "Run SWAT," the following dialog box appears:

Set Up and Run SWAT model simulation

Period of simulation:

Starting date: January 1 1993
Ending date: December 31 1995

Rainfall/Runoff/Routing: Daily rain /CN / Daily

Rainfall distribution:
 Skewed normal
 Mixed exponential

Potential ET method:
 Priestley-Taylor method
 Penman-Monteith method
 Hargreaves method
 Read in

Crack flow:
 Not active
 Active

Channel water routing method:
 Variable Storage
 Muskingum

Channel degradation:
 Not Active
 Active

Stream Water Quality Processes:
 Not Active
 Active

Lake Water Quality Processes:
 Not Active
 Active

Printout frequency:
 Daily
 Monthly
 Yearly

Routing Pesticide: Weed-B-Gon

Watershed parameters:
 Basin Input File: Bsn
 General Water Quality Input File: Wwq

Buttons: Help, Exit, Setup SWAT Run, Chek Input Ranges, Run SWAT

As can be seen from the lower left portion of this screen, the SWAT model can produce output in "daily," "monthly," or "yearly" time steps. To link the model to AQUATOX, daily or monthly time-steps must be chosen. Annual time-steps do not provide the data resolution required by AQUATOX.

A user also can select the SWAT simulation period at the top of this screen. If the SWAT model has many sub-basins and is being run for many years, choosing monthly time-steps is probably the best choice as output file sizes become unwieldy otherwise.

When run with monthly time steps, SWAT sums mass loadings over the course of each month and averages concentrations over the course of each month. In the case of summed mass loadings, AQUATOX divides the total loading by the days in the month to get an average daily loading. Then, in order to prevent interpolation between data-points, AQUATOX loads these values as data points at the beginning and the end of each month. This creates some “stair-stepping” of input data into AQUATOX, but presents the best accounting for mass and concentration data as provided by SWAT.

While the SWAT model can track several pesticides over land within a simulation, it only tracks the movement of a single pesticide through the main channel. This means only a single pesticide may be passed from SWAT to AQUATOX at a given time. The choice of which pesticide to move into the main channel can be seen under the “Routing Pesticide” header within the screen shown above. If the user wishes to track a specific pesticide from SWAT within AQUATOX, it must be selected within this dialog box.

Because AQUATOX only models organic chemicals, the linkage assumes that any pesticide data passed to AQUATOX is in the form of an organic chemical. The user will later be asked to specify the organic chemical being modeled from a list of available chemicals, or will be required to input chemical-specific data about the organic chemical utilized.

Finally, a user may select to have “Stream Water Quality Processes” be “active” or “not-active” within a SWAT simulation. Within SWAT, nutrient transformations in the stream are controlled by the in-stream water quality component of the model. Even if active nutrient transformations within the stream are not utilized, SWAT still calculates the movement of nutrients through the system due to inflow loadings, and loadings from point and non-point sources. More information about SWAT’s modeling of nutrients within a stream may be found in Chapter 25 of the SWAT user’s manual (swat2000.PDF, located in the BASINS\DOCS\SWAT directory).

Nutrients that can be modeled within SWAT include Ammonia, Nitrate, Phosphate, Oxygen, and Biochemical Oxygen Demand. As AQUATOX also models each of these nutrient compartments, these variables can be linked directly into AQUATOX from SWAT. Total suspended solids (TSS) may also be linked from SWAT to AQUATOX.

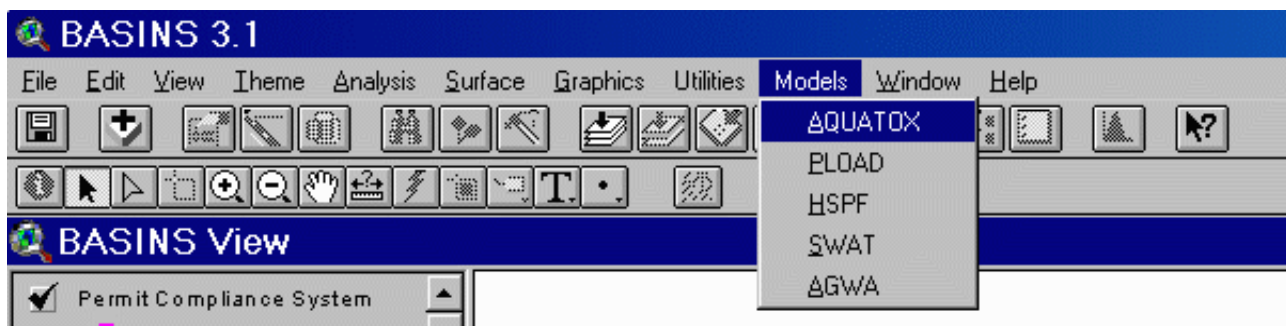
In-stream water-quality processes modeled by SWAT within the sub-basin that is linked to AQUATOX will not affect the AQUATOX simulation. AQUATOX only reads the inflow loadings of nutrients within a particular SWAT reach and calculates in-stream water-quality processes within its own derivatives. However, in-stream water-quality processes that occur

upstream of the AQUATOX reach will affect the loadings of nutrients into AQUATOX, so the user may still wish to utilize this option within SWAT.

Important Note: By using a text file editor and editing the SWAT Input Control Code file (*.COD file) a user may select to limit the number of variables that are output in a SWAT reach file (*.RCH file). As the SWAT-AQUATOX linkage requires most of the variables from a SWAT reach file to be present, the linkage will not work properly when the RCH files are limited in this manner.

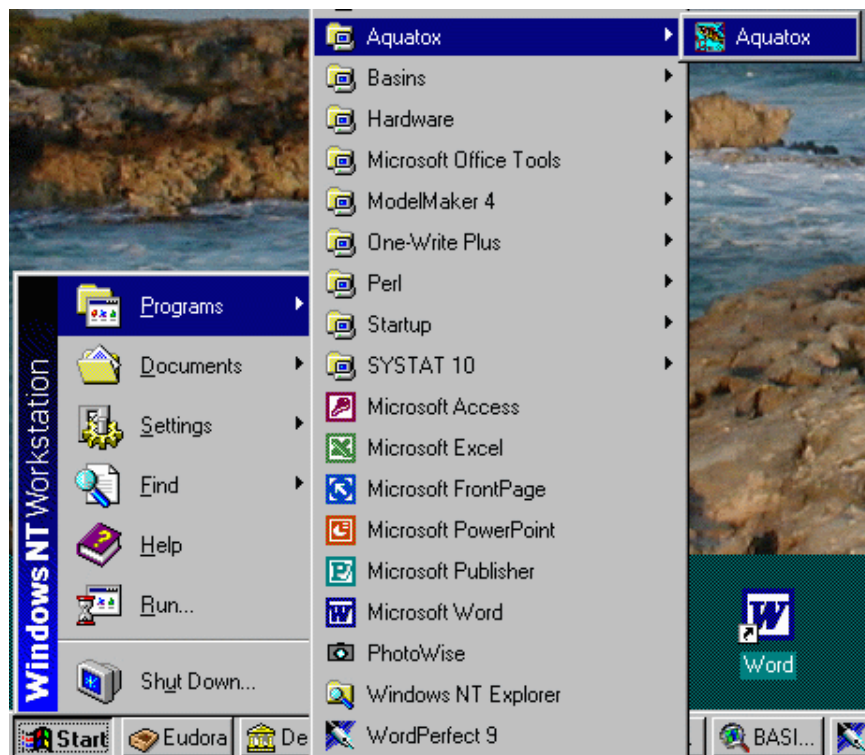
4.3 Loading SWAT data into AQUATOX

To load SWAT data into AQUATOX, a user must first start AQUATOX. This can be done in two ways. The user can run AQUATOX directly from the BASINS 3.0 menu by selecting “AQUATOX” from the “Models” menu within the BASINS view:



The user will then be asked whether she\he wishes to “Open AQUATOX with Linked BASINS Stream data.” Selecting “No” indicates to the BASINS interface that the user is not trying to link GIS data to AQUATOX. AQUATOX will then be started with no attached data.

If a user has already run the SWAT model and does not need to have BASINS open, the user can run AQUATOX directly from the “Start” menu.



Once AQUATOX has started, a user can load SWAT data into AQUATOX by clicking on the “Import Data from SWAT” button in the toolbar.

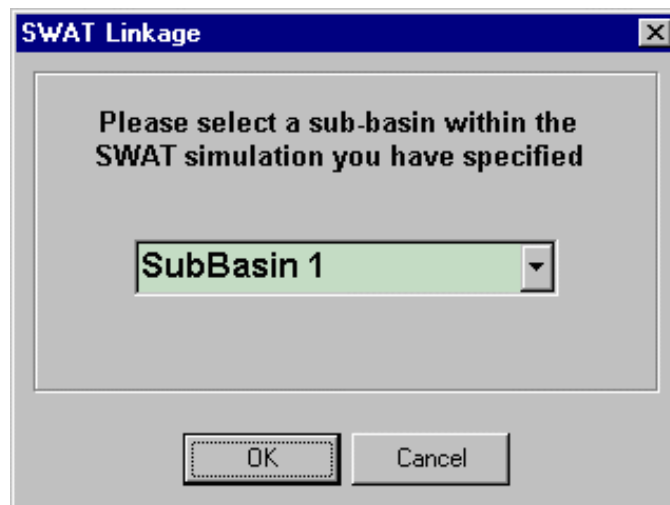


Alternatively, a user may select the “Import Data from SWAT” option from the “File” menu at the upper left of the screen.

Next, a dialog box appears asking the user to select the completed SWAT simulation from which to import data. The user must select the “Control Input/Output File” (File.CIO) that is associated with the SWAT simulation that is to be linked. This file will be found in the “txtinout” directory under the directory named after your SWAT project. The full directory structure will look as follows:

```
"BASINS\MODELOUT\SWAT\{your_project_name}\TXTINOUT\FILE.CIO"
```

The user will then see the following dialog box:



All sub-basins that are included in the SWAT simulation will be shown within the pull-down interface. The user should select the relevant sub-basin to be linked to AQUATOX. The resulting AQUATOX water body will correspond to the main channel within this sub-basin.

4.4 The Linkage Process

As with all BASINS-AQUATOX linkages, a user may choose to link SWAT parameters to a “blank” AQUATOX simulation or overwrite relevant parameters and loadings in an existing AQUATOX simulation. See Section 2.5 for more information about this choice.

AQUATOX models organic matter in four compartments:

- Labile Dissolved Organic Matter
- Labile Particulate Organic Matter
- Refractory Dissolved Organic Matter
- Refractory Particulate Organic Matter

Within SWAT, BOD data is not broken down into these compartments. For this reason, a user must specify the percentage of BOD that is Refractory and the percentage of BOD that is Particulate organic matter. Default values are provided within the AQUATOX dialog box as shown, and these values should be used if the user has no additional information about the BOD loading.

BASINS-AQUATOX Linkage: Please Characterize Organic Carbon Loadings

AQUATOX will import BOD from the SWAT simulation. This must be characterized as Labile or Refractory organic matter. It is generally assumed that BOD is predominantly Labile in nature.

AQUATOX will assume that 10% of the BOD is Refractory (90% Labile) unless a different number using is specified using this screen.

% of BOD that is Refractory

10

Additionally, AQUATOX must characterize incoming loads of BOD as Dissolved or Particulate in nature.

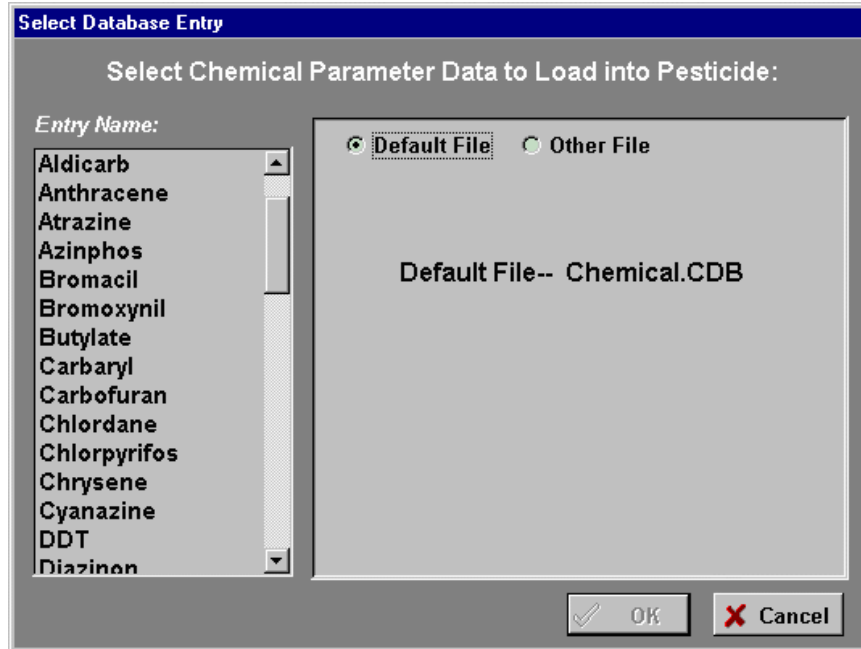
AQUATOX will assume that the organic loadings are 10% particulate unless a different number is specified with this screen:

% of Organic Loadings that are Particulate

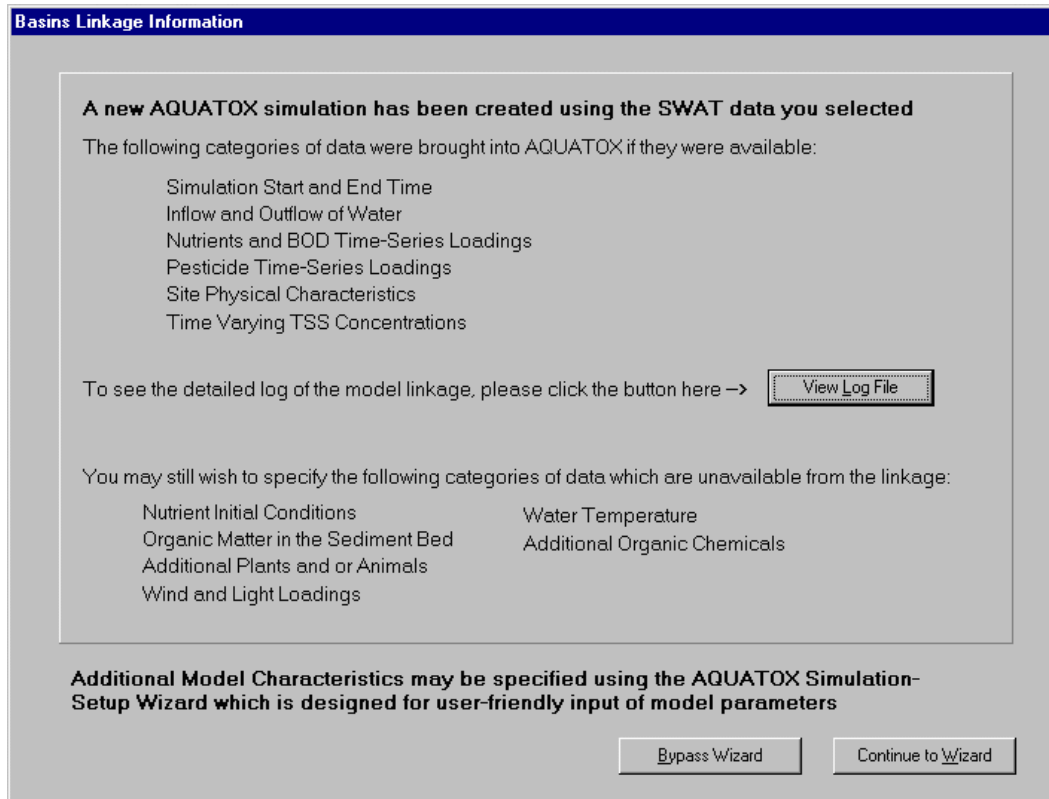
10

O.K.

The user will then be prompted as to whether a pesticide is tracked within the SWAT reach. If the user selects “yes,” the loadings of the “Routing Pesticide” specified above will be linked into the AQUATOX simulation. To model an organic toxicant within AQUATOX, parameters are required about the chemical properties and toxicity of the substance. After selecting to model the routing pesticide, the user will be prompted to load these chemical parameters from a database of organic toxicants. Alternatively, the user can press “cancel” and enter these chemical parameters later, within the AQUATOX “chemical underlying data” interface.



From the SWAT linkage, AQUATOX will load data about channel geometry, nutrient and pesticide loadings, simulation period, water flow, and organic and inorganic sediment loadings. In each case when a parameter value or time-series is loaded, AQUATOX writes the source and result of the linkage into the log file. The log file can be viewed by pressing the “View Log File” button from the screen shown below.



From this screen, the user may continue to the AQUATOX Wizard to complete setting up the new AQUATOX simulation or may bypass this step and work with AQUATOX through the main AQUATOX interface.

The data required to finish specifying a SWAT simulation are almost identical to those required after an HSPF to AQUATOX linkage. The only difference is that water temperature is available from an HSPF simulation but must be specified after a SWAT to AQUATOX linkage. For more information about finishing the specification of the AQUATOX simulation, please see sections 2.7 and 2.8 (“Specification of Additional State Variables and Loadings” and “Run AQUATOX and Plot Results”) in the “WINHSPF to AQUATOX Linkage” chapter .


5 AQUATOX TO GENSCN LINKAGE

5.1 Introduction

After an AQUATOX simulation has been run, a user may view output data using AQUATOX's output screens, a user may export the data to several database and spreadsheet formats, or the user may choose to send the output data to GenScn, the post-processor within BASINS. GenScn offers several statistical functions that are not available through the AQUATOX output screen such as comparison of predicted and observed time-series and duration analysis.

5.2 Linking to GenScn

There are three ways to link to GenScn from within AQUATOX.

1. Select "Export to GenScn" from the "File" menu.
2. Click the Export to GenScn button in the toolbar as shown here: .
3. Click the "Export All Results to GenScn" button on the Export Results Dialog.

All three of these options are enabled when AQUATOX has run a simulation and has results in memory. These options are not enabled if GenScn has not been installed on a user's computer.

When AQUATOX exports data to GenScn, a set of two files are written to the AQUATOX "OUTPUT" directory. (*This is the "OUTPUT" sub-directory within the directory in which AQUATOX was installed*). A file with an "RDB" extension is written that contains all of the AQUATOX time-series results (control and perturbed), and a file with an "STA" extension is written that tells GenScn the format and location of the RDB file.

5.3 Using GenScn

The AQUATOX linkage produces a set of GenScn data within a single "Location" (the AQUATOX river reach). There are up to two "Scenarios" produced, "Control" and "Perturbed," depending on which types of AQUATOX runs have been executed. (The "OBSERVED" scenario that appears within GenScn is empty and should be ignored.) Finally, each AQUATOX output variable is available under the GenScn "constituent" menu.

To produce a graph, a user can select the location, scenario, and constituent to graph and then press the plus button at the top of the "Time Series" list. The constituent will appear as a new item on the "Time Series" list. With this item selected, the user can then click on the "Generate Graphs" button at the bottom of the screen and a graph generation dialog is created.

For more information about how to use GenScn see GenScn.pdf located in the BASINS\DOCS\GENSCN directory.