Continuously Stirred Reactor Example

Objective:

This exercise will expose the user to the WASP graphical user interface, the steps needed to create an input file and how to examine WASP results. This example will be using a simple continuously stirred reactor. Once the batch reactor is set up, we will run a conservative tracer and then tracer with a first order decay. A continuously stirred reactor is a single WASP model segment that will have a single inflow and outflow into a controlled volume. Everything is considered completely mixed in the CSTR (Figure 1).

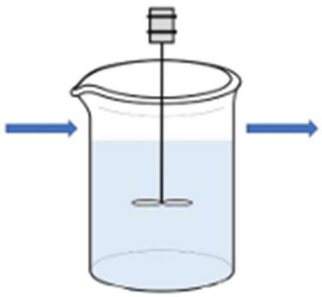


Figure 1 CSTR

Building a WASP Input File:

The following steps will take you through the process of creating a WASP input file for the CSTR. Anywhere you see an icon next to the heading you click on this icon on the interface to enter the form. Users may also use the WASP menus as well.

Load WASP Graphical User Interface:

To load the WASP model, you will need to go to your Systems Start Menu and Select: USEPA WASP8→WASP.

This process may differ depending upon your operating system. The user is encouraged to create a User Shortcut for easier access to WASP. This is not done automatically by the installer because depending upon computer configuration administration privileges would be required. If you create a short cut just click on the WASP Icon.

Create New File:

Click on the 

icon to start the development of WASP Input file. It should be noted clicking the New file icon will cause the interface to re-initialize all data forms potentially losing data.

Save File:

Clicking the Save File icon will save the currently active WASP Input File (*.WIF) to disk. If it is the first time saving the file you will be presented with a standard file dialog box that allows you to select path and define filename. It is very important to make sure that you manage filenames and locations on your computer.

Save the file to the WASP Course installation folder under WASP_Course/Examples/CSTR as: ***CSTR_Example***

Dataset Parameterization:

The dataset parameterization form is where the user selects the model type, time domain and out interval for simulation results (Figure 2). The user must enter information in this form before any of the other input dialogs will become available. Interface needs to know the time domain and the model type so that other forms can be configured appropriately.

Description:

One-line description of your project to help you keep scenarios and model runs organized.

Enter: ***CSTR Example***

Comments:

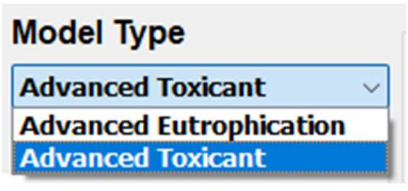
Text dialog box where you can enter comments or task to be done building and/or calibrating the model

Enter: ***WASP Workshop Hands-On Example 1***

Model Type:

This drop-down menu allows you to select the WASP model module you would like to build an input file. The choices are Advanced Eutrophication or Advanced Toxicant Model. The selected model type will cause the graphical user interface to display information specific to that model type.

Using the drop-down menu select: ***Advanced Toxicant***



Start Date/Start Time:

Sets the Gregorian date for the start of the simulation (mm/dd/yyyy). ***01/01/2024***

Sets the start time for the simulation (hh:mm) ***12:00 AM***

End Date/End Time:

Sets the Gregorian date for the end of the simulation (mm/dd/yyyy). ***01/07/2024***

Sets the end time for the simulation (hh:mm) ***12:00 AM***

Model Output Interval:

Defines the output interval for the simulation (days). An example would be if you want output 4 times a day you would enter ***0.25***

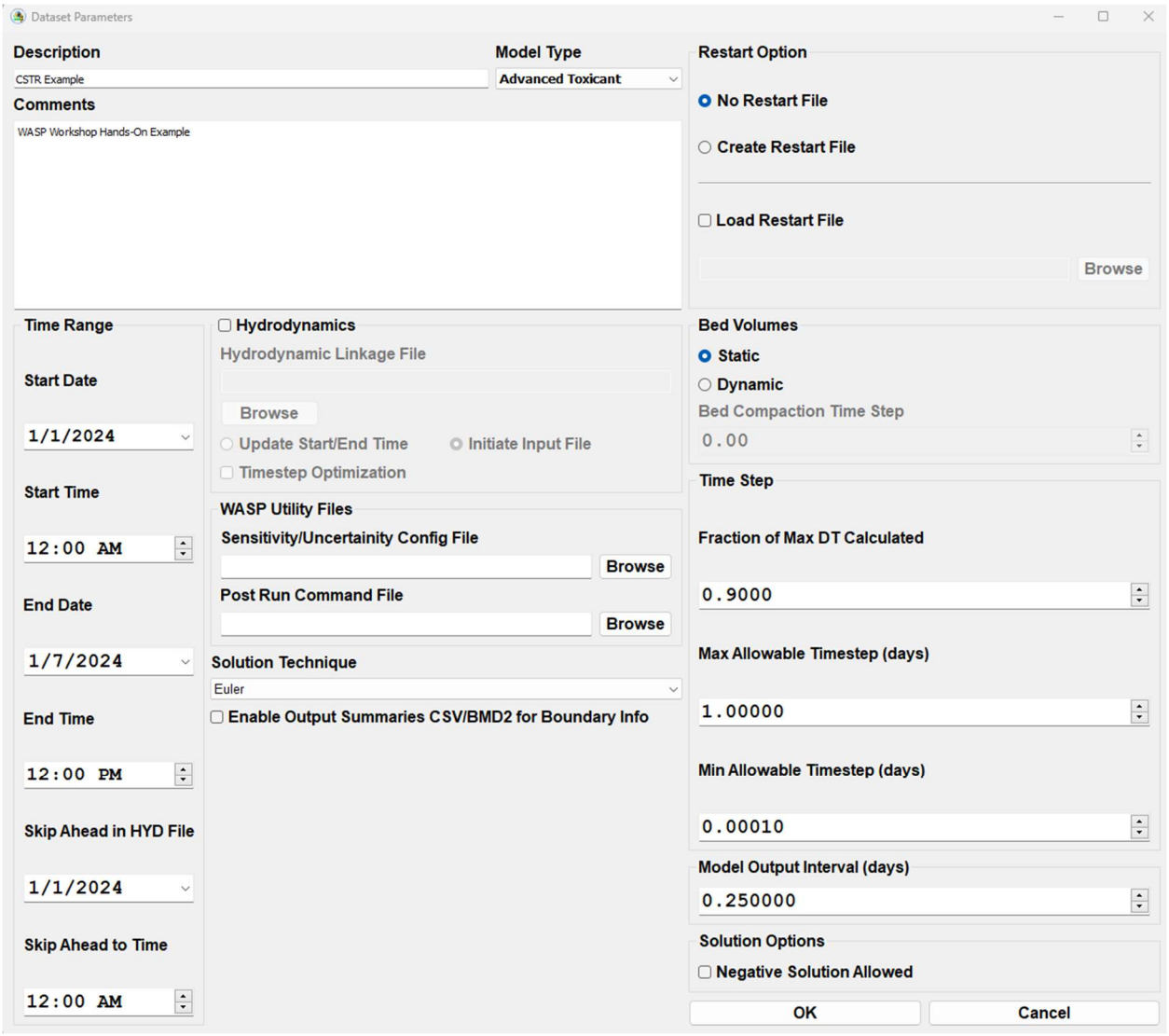


Figure 2 Dataset Parameterization

State Variables:

This is where WASP is very different than other water quality models. WASP does not assume what state variables the user would like to simulate. WASP has been carefully programmed to allow the user to select the level of complexity to perform simulations. Unlike other models where the user must specify information for all state variables whether they are being considered for the model to execute, WASP allows the user to determine which state variables will interact  (Figure 3).

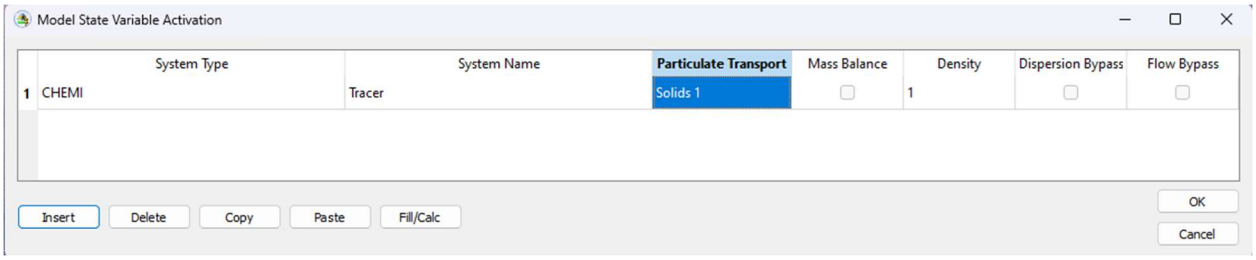


Figure 3 WASP State Variable Options

For our example here, we are using the Advanced Toxicant model to simulate a tracer and eventually a simple decay. We will not be using all the complexities of the Advanced Toxicant model. Click the **Insert Button** once on the bottom of the form. From the drop-down menu select (Figure 4): ***CHEMI***

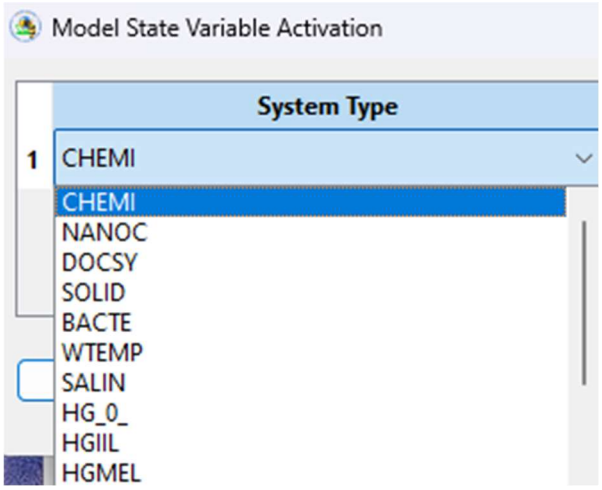


Figure 4 State Variables

Segment Definition:

This data entry form is where you define model segments  . Segments represent computational compartments for your waterbody. In the case of the CSTR we have only

one segment representing our waterbody. Click the **Insert Button** once on the bottom of the form to insert a segment (Figure 5).

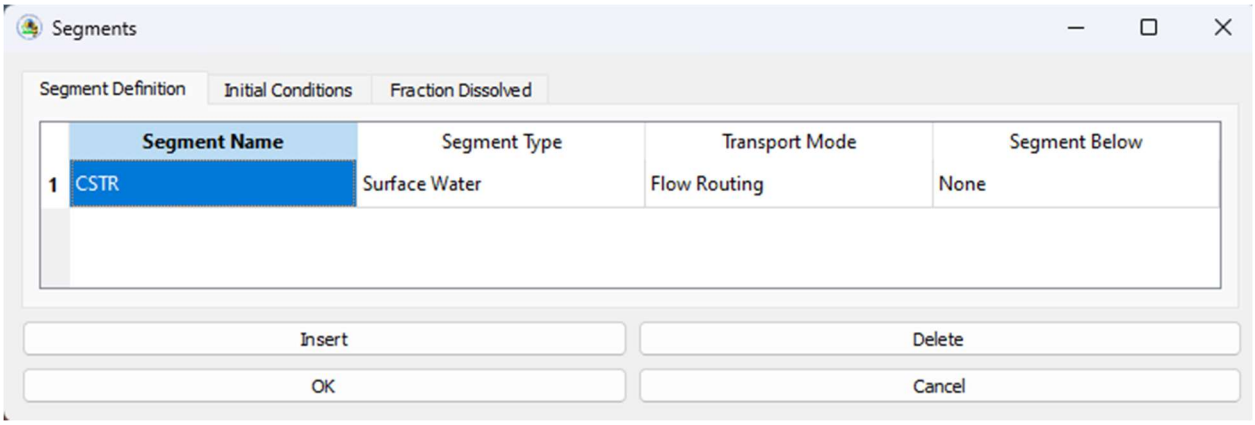


Figure 5 Segment Definition & Transport Mode

Segment Name:

This specifies the name of the segment being defined. This name is carried throughout the graphical user interface as well as the model output file. Please enter ***CSTR***

Segment Type: This specifies the select type.

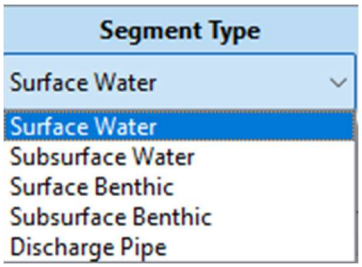


Figure 6 WASP Segment Types

From the drop-down menu select Surface Water

Transport Mode:

This specifies the transport mode that will be used for this segment. From the drop-down menu select ***Flow Routing***

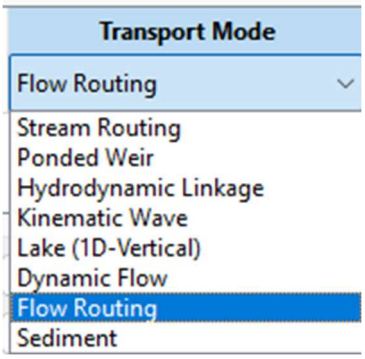


Figure 7 WASP Transport Modes

Segment Below:

If this were a multi-dimensional network, you would use the drop-down menu to select the WASP segment that would be located below the segment currently being defined. In the CSTR example we will leave set to ***None***

Segment Geometry/Flows:

This is a multi-tab screen that allows the user define segment geometry, flow paths and flows . For the CSTR example we will be entering data on the Channel Geometry and Surface Water tabs. For the Channel geometry tab, the available fields that are editable are a function of the selected segment Transport Mode (as defined on Segment Definition Screen). Greyed out columns means that data is not needed for the selected transport mode (Figure 8). For our CSTR example complete the information as described below.

Segment Name:

This field is not editable here, segment name is specified on Segment Definition form.

Volume:

This represents the volume of our CSTR in meters^3. ***1000.00***

Average Depth:

This is the average depth of the CSTR in meters. ***3***

Average Velocity:

This is the average water velocity in the CSTR meters/second ***0.1***

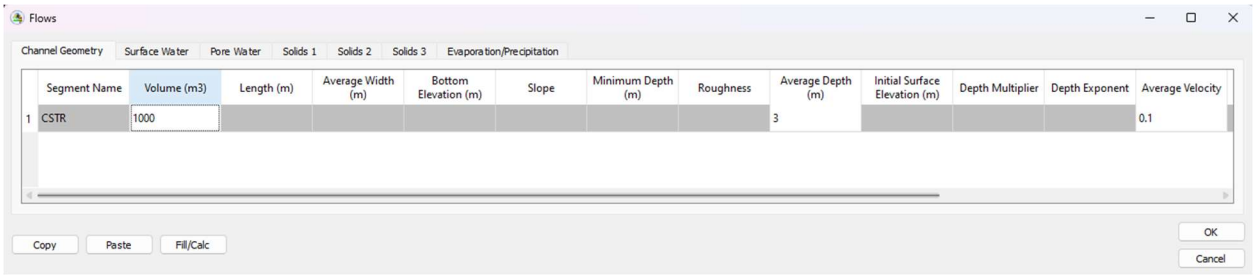


Figure 8 WASP Segment Geometry Information

Surface Water:

This form allows the user to define all the various surface water flow paths for the model network

In the case of this example there will be only one flow path that will be defined. Figure 9 depicts our CSTR example, we will have a single inflow.

Figure 9 CSTR Flow Schematic

The form is broken down into 3 components. The top data entry box allows the user to define multiple flow functions which consists of flow pathways (segment pairs) and time series of flows (Moment Value Pairs) (Figure 10). To activate the input to the flow pathway and flow time series click on the Flow Function in the upper box (arrow designated the active flow function).

At the top of the data entry form the user could set a global scale and conversion factor. The scale and conversion factor will be multiplied by the flow values in the moment/pairs table. An example for the use of the conversion factor is to convert flows from cubic feet per second (entered in the moment/pairs table) to WASP flow units of cubic meters per second. An example of the scale factor would be to see changes if flows were scaled up/down or set to zero.

You will see the Used checkbox throughout the WASP interface. If this box is left unchecked when the model is executed the information in this form will not be passed to the model. Essentially it is the same as deleting the information. This checkbox can be very helpful in diagnosing issues when running WASP.

Plot Window

The plot window displays a graph of the information that the user enters in the moment value pairs. This graph is very useful for determining if information was not entered correctly or pasted in correctly. When dealing with large data sets that contain a lot of time series data you should always be looking at this graph after you complete the data entry procedure.

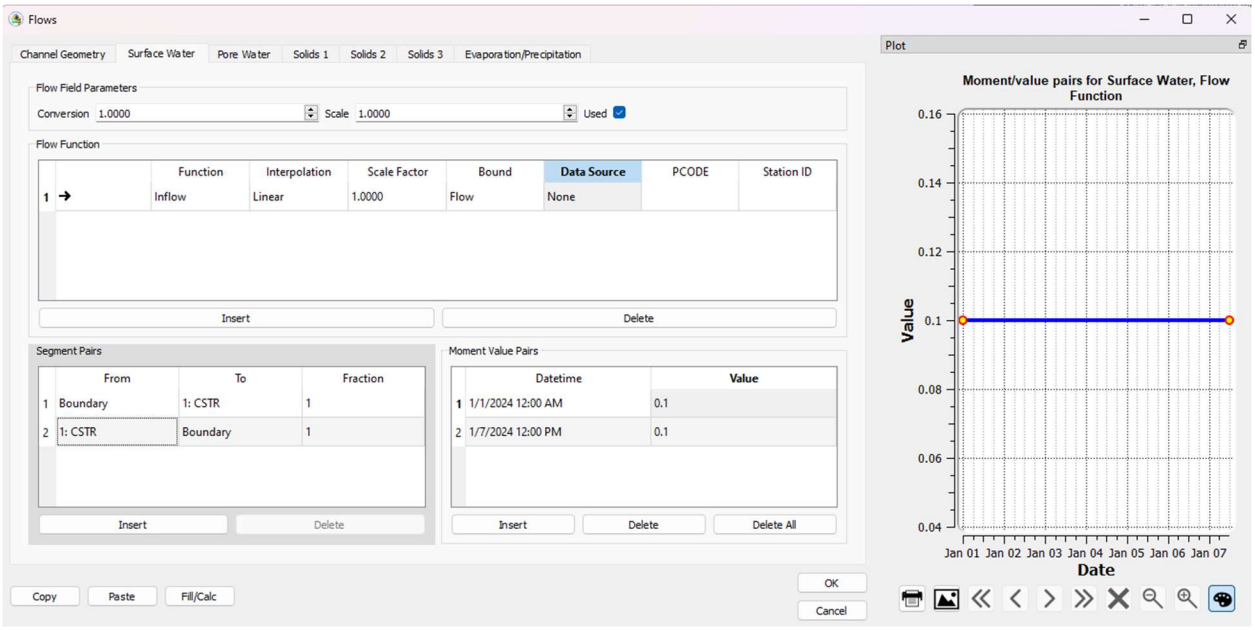


Figure 10 WASP Surface Water Flow Definition

Flow Function Table:

WASP allows you to have as many flow functions as needed to define the waterbody that you are modeling. For each row that you insert a Segment Pairs and Moment Value Pairs table will be created. By selecting the row in the Flow Function table this will cause the display of the Segment Pair for Moment Pair information for that flow path being defined.

Function

The function column allows you to name the flow path being defined. In large scale modeling projects, there can be hundreds of flow paths, naming allows the user to know which flow contribution is being defined. Selecting a row in the Flow Function table will activate the Segment Pairs and Moment Value Pairs table associated with the flow function.

Interpolation:

WASP provides two methods for interpolating the flows that are defined in the Moment Value Pairs table. WASP can utilize moment value pairs at any time interval (day, month,

year, irregular). As WASP simulates through time it uses either a linear interpolation or step function to determine flow to use at the model simulation time. In our example select: ***Linear***

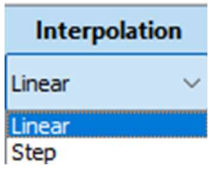


Figure 11 WASP Time Series Interpolation

Scale Factor

The scale factor column works much like the global scale factor described above, but only works on the flow time series associated with the selected flow function. ***1.0***

Boundary Type

WASP supports several boundary types; each has a specified purpose, and the user must understand implications of implementation.

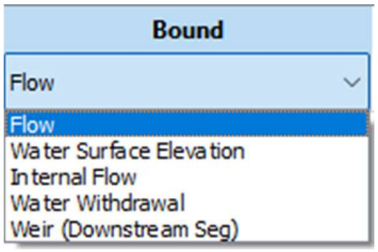


Figure 12 WASP Boundary Types

- Flow – user will describe the flow at the boundary (cubic meters per second). This flow will be propagated downstream and combined with other defined flows as a function of the transport model selected for a given segment. This is the most common boundary type.
- Water Surface Elevation – user will describe changes in water surface elevation over time at the boundary. An example of this would be a tide. The units for water surface elevation are meters.
- Internal Flow – allows the user to specify a flow time series from one model segment to another in the model network.
- Water Withdrawal – allows the user to specify a water withdrawal time series which will remove water and associated constituents from the model network.
- Weir – allows the user to set a downstream weir elevation in which the model transport algorithms will calculate if and how much water will flow over the weir.

Segment Pairs

For each of the flow functions you must provide the flow path through the segments in your model in which the flows are being defined. For this example, we have 2 segment pairs to define. We have a flow coming from outside the model network (which is called a boundary) into our only segment (CSTR) and then a second pair from CSTR to Boundary (Figure 13). The fraction value is typically always 1.0 unless your have diverging flow into different segment. WASP will determine the flow for "From" and "To" segment by multiplying the "Fraction" value time the interpolated flow value from the Moment Value Pair inputs for the flow function (Figure 14).

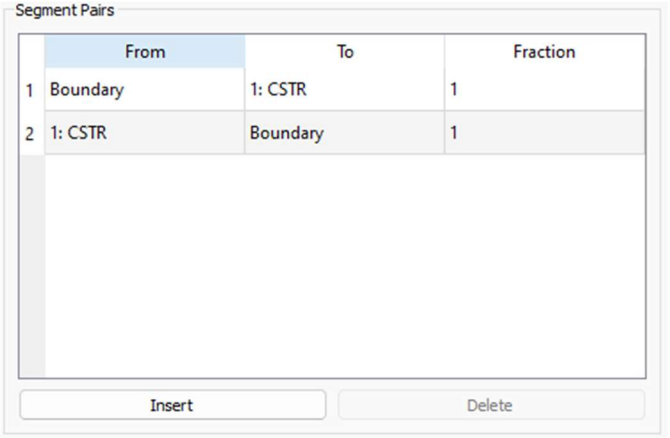


Figure 13 Segment Flow Continuity

Moment Value Pairs/Flow Time Series

This timeseries dialog box is very consistent with all the timeseries data entry forms used in the interface. For any timeseries in WASP you will have to enter at least 2 lines of data. For our CSTR example click the Insert Button to add 2 lines of flow data. The interface automatically adds the start and end time. We are going to set the inflow to a constant 0.1 meter3/second. Under the value column enter ***0.1***.

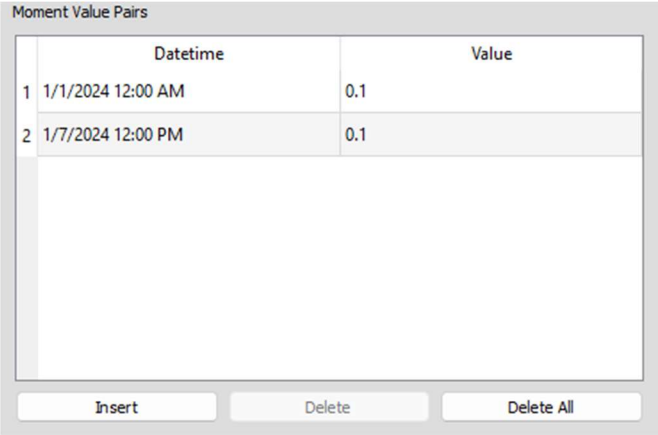


Figure 14 Timeseries of Flows

Boundary Concentrations

The boundary screen allows the user to assign a concentration timeseries for each state variable that is being simulated associated with the inflows from outside the model network (everywhere you have Boundary in Flow Functions). In the case of the CSTR example we only have 1 inflow and 1 State variable (Figure 15). The WASP interface determines which segments have boundaries based upon information provided in the flow pathway definition.

To assign a concentration associated with a boundary for a state variable the upper box (grid) is used. Click on the combination of state variable (column) and boundary segment (row), once highlighted the lower box is used to set concentration. Highlight CHEMI-CSTR and go down to the bottom dialog box and set the value to ***1.0 mg/L.***

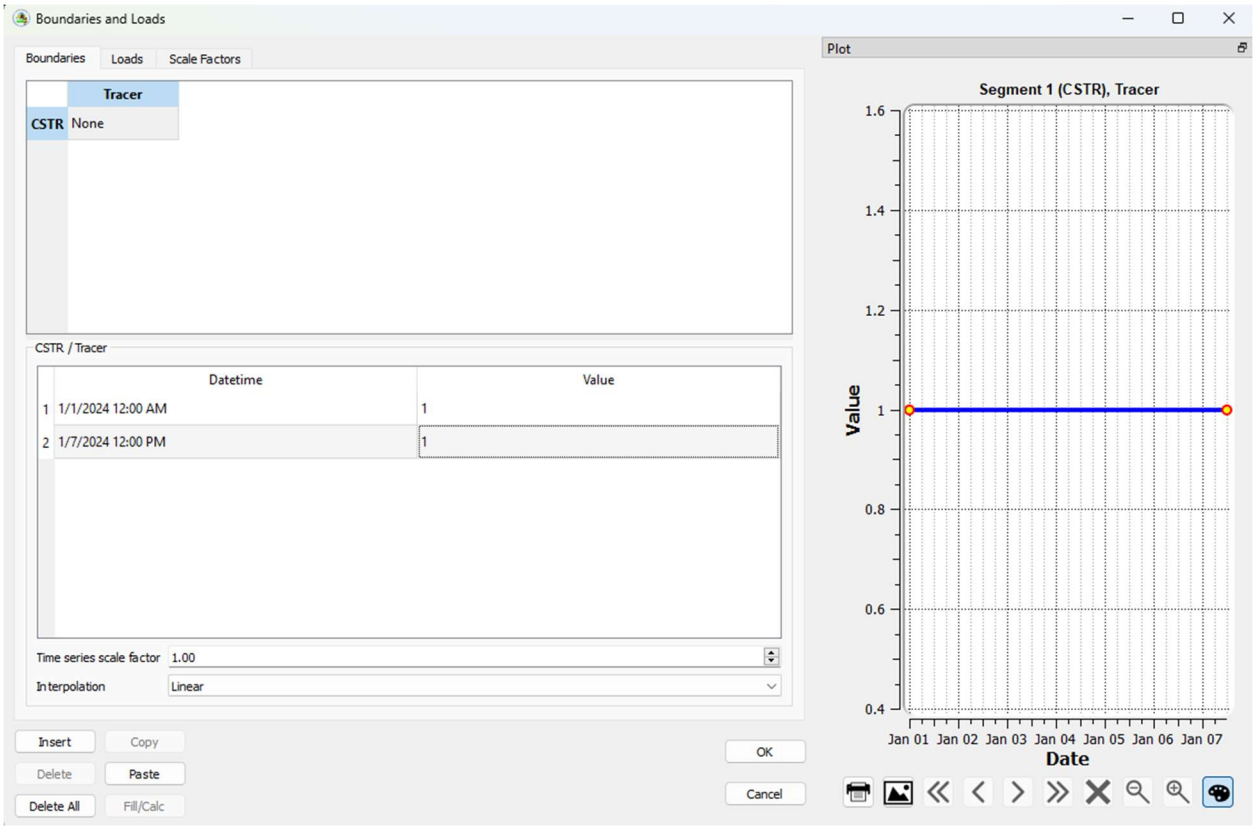


Figure 15 Boundary Concentration Definition

Output Control

The last step in setting up the CSTR input file is select output from the simulation  . Because WASP makes no assumptions on what you are simulating the user must select meaningful output. In our case we are going to select some output that is used to provide information about the transport (Figure 16) and chemical concentration (Figure 17). The selected output will be saved to binary output file for post processing. The file will be called the same as the input file with the exception that file extension will be BMD2 (CSTR_Example.BMD2).

The user can navigate to the various functional output groups by using the drop-down menu option. The case below shows that we are activating output for: Volume and Flow out, this is done by checking the radio box in the output column.

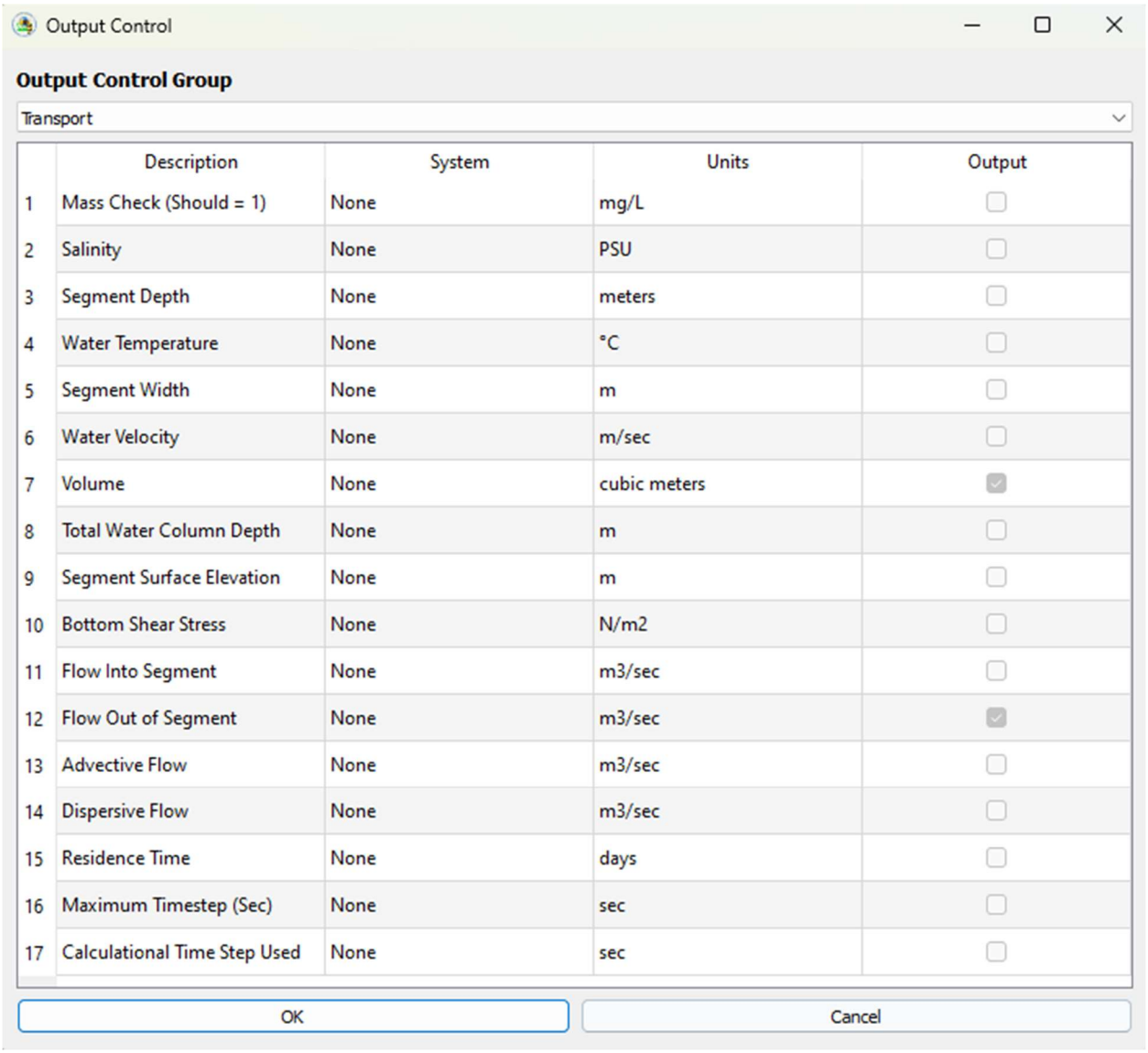


Figure 16 Output Selection Transport

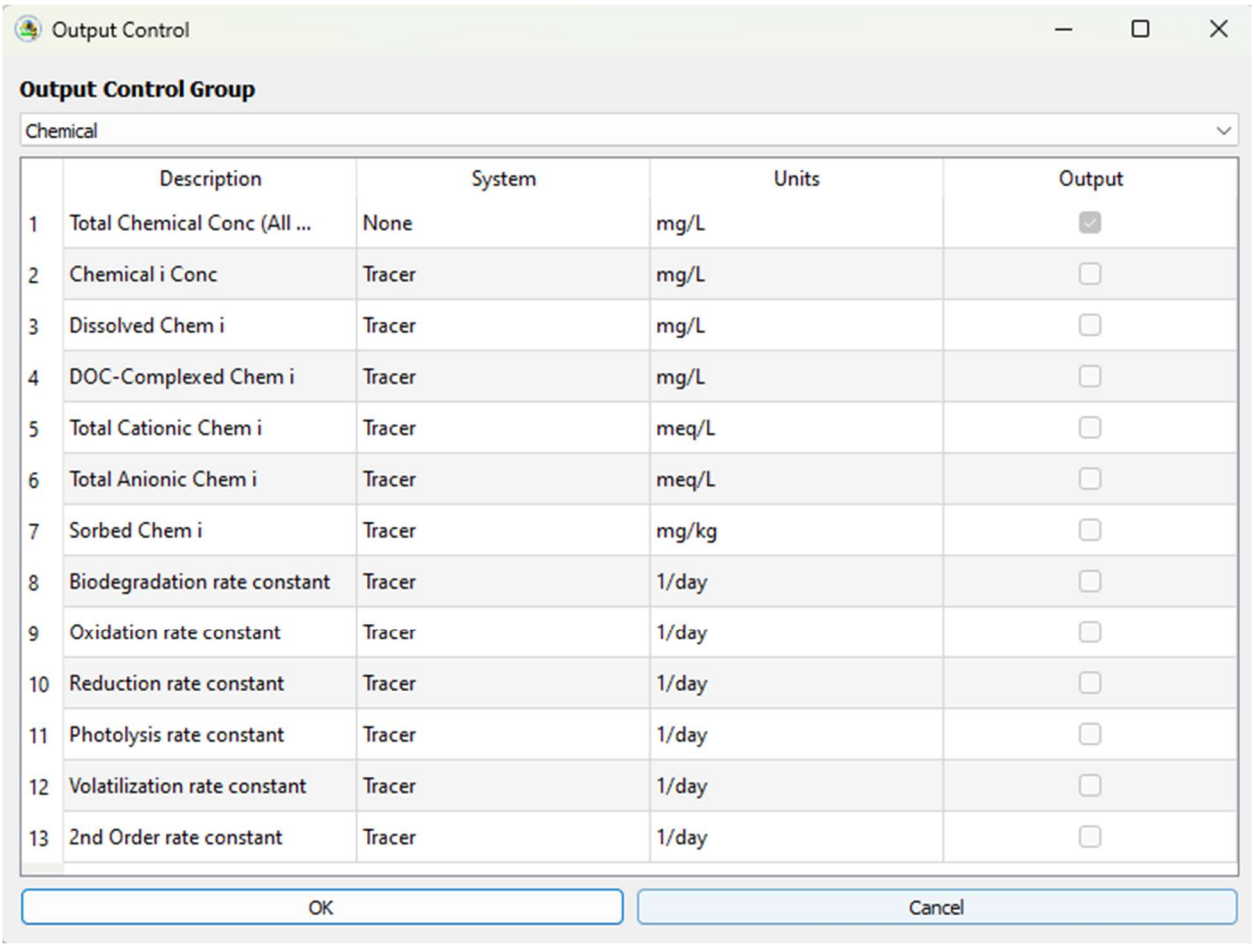


Figure 17 Output Selection Chemical

Executing Model

We are now ready to execute the model. Make sure you SAVE the file before you execute the model. To execute click the icon  . Once the model starts to run you will see Figure 18. The grid on the top shows intermediate model results as the model is simulating. The dialog window below provides informative information as the model is running as well as diagnostic information if the model does not run.

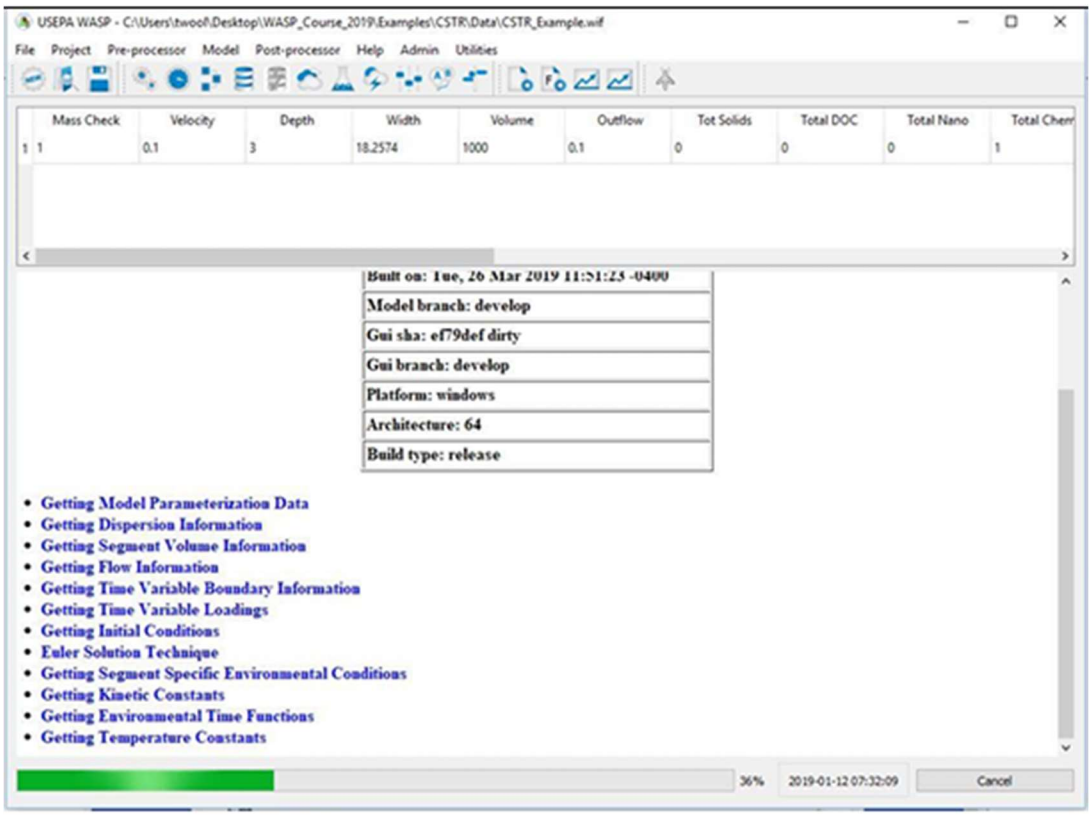


Figure 18 WASP Runtime Screen

Create a Project

To aid in the post processing of model results we are going to create a project which will provide the graphical post processor with appropriate information associated with the CSTR input file. WASP uses a component of the Water Resources Database (WRDB) to create plots of model results. The component is called WRDBGraph which is a separate executable that can be found in the Water Resources Database installation directory. Prior to post processing you should execute WRDB as it sets an environmental variable to tells WASP where WRDBGraph is located.

To create a project, you will have to use the file menu, click on Edit Project it will present Figure 11. Click insert and browse to WASP_Course/Example/CSTR and select CSTR_Example.BMD2. WSAP will use this information when loading the post processor to pass the correct file for processing.

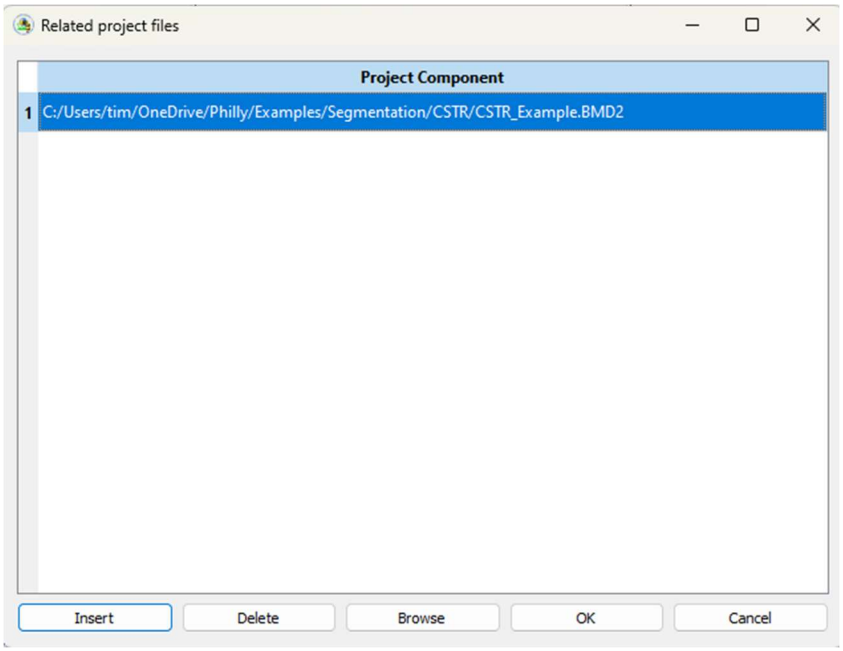


Figure 19 WASP Project File

With project file set you are now ready to load the post processor.

Post Processing

There are 2 icons for loading a post processor  . The first post processor icon (on left) will load BMDUtil which is another utility that is part of the Water Resource Database. We will be using the second icon (on right) will execute WRDBGraph and pass the CSTR_Example.BMD2 file for processing. Figure 20 illustrates the graph configuration screen where the user can select a table or model output file, a table station or model segment and table parameter or WASP output variable. WRDBGraph allows the user to add as many plot lines as needed. User must select a data table, a station and parameter and then click the Add to Left Axis button.

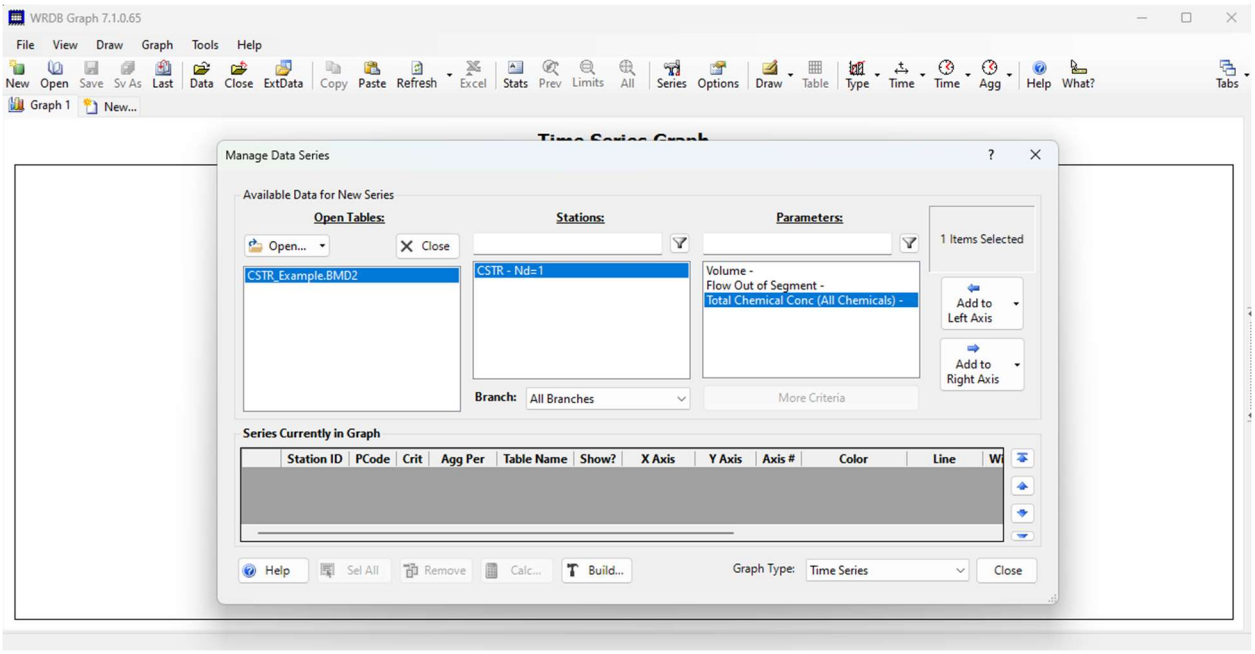


Figure 20 WRDBGraph Graph Parameterization

Figure 21 illustrates a completed plot for the CSTR segment and Total Chemical which was defined in the output control screen.

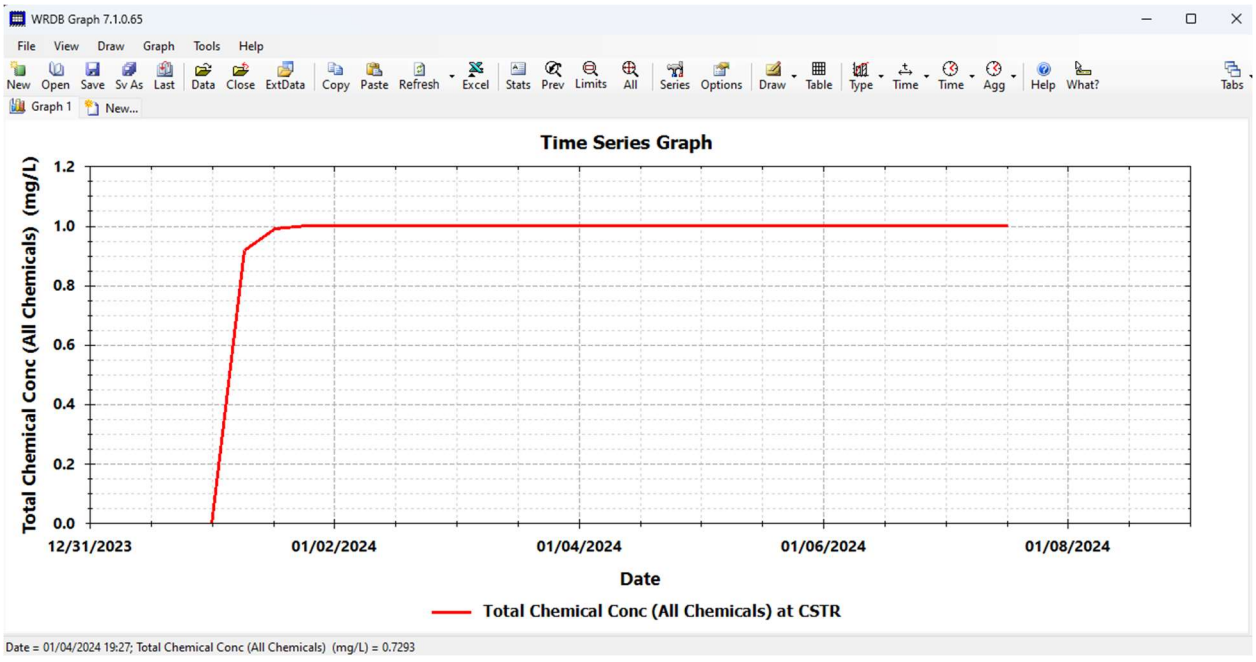


Figure 21 WRDBGraph Plot