# TOXCHEM V4.3

## Modeling the Fate of Toxics in Wastewater Treatment Plants


# USER'S GUIDE

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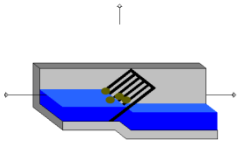
# 1.What's New in Version 4.3

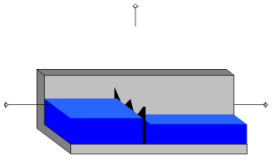
The TOXCHEM V4.3 builds on the features of TOXCHEM V4.2 which was released in 2013. TOXCHEM V4.3 includes a variety of new processes to model the air emissions at the wastewater treatment plant, including a bar screen, V-notch weir, membrane bioreactor, water scrubber, closed surge tank and floating roof storage tank. In addition, the ability to model air emissions from a layer of oil floating on the water surface has been added to preliminary treatment processes, with the inclusion of four procedures for estimating the emission rates. To further improve the ease of use and functionalities of software, selected new features are added to the Graphical User Interface. A brief introduction to new features of TOXCHEM V4.3 is provided below.

## 1.1 NEW UNIT PROCESSES

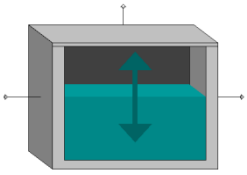
***Bar Screen -*** As wastewater passes through the bars of the bar screen process, resistance to the flow dissipates energy, which can cause turbulence and eddies, thereby resulting in air emissions. The bar screen emission model is developed by converting the head loss in the process to dissipated energy, which is then used to estimate the surface mass transfer coefficient for volatilization.



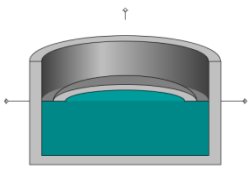
***Weir Process -*** The weir process is provided as a unit for estimating air emission losses of organic compounds as water drops over a V-notch (saw-tooth) weir. The weir model is one of two volatilization mechanisms in primary and secondary clarifiers, surface volatilization being the other mass transfer mechanism. The volatilization models for weirs involving primary- and secondary-treated wastewater as proposed in Pincince (1991) are used.



***Closed Surge Tank -*** The closed surge tank is a vessel in which the volume of wastewater in tank changes over time. The emissions from this tank take place during filling. As the wastewater volume fills the tank during the specified time period, an equivalent volume of headspace air is expelled through an opening in the cover, such as a vent stack or open grate. The model for this unit process assumes that the headspace air inside the tank is at equilibrium with the water phase.

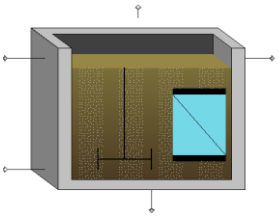


***Floating Roof Tank -*** The emission model for floating roof tank assumes that the main source of air emission from this tank is the exposed clingage of water/oil layer on the periphery of the floating roof tank sidewall. The exposed clingage arises when the floating roof move down due to withdrawal of liquid in the tank. The

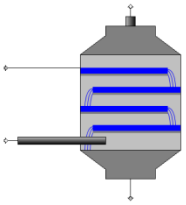


composition of the clingage is assumed to be same as the average composition of the influent tank, Exposed clingage height, clingage thickness and exposure time are used to estimate the amount of emissions.

***Membrane Bioreactor -*** A new air emission model is developed for membrane bioreactor (MBR) considering the effect of the coarse bubble backwash of membranes. The process estimates air emissions from normal aeration and coarse bubble backwash. The total air emissions from the unit process is then calculated based on the on the frequency of the coarse bubble backwash.

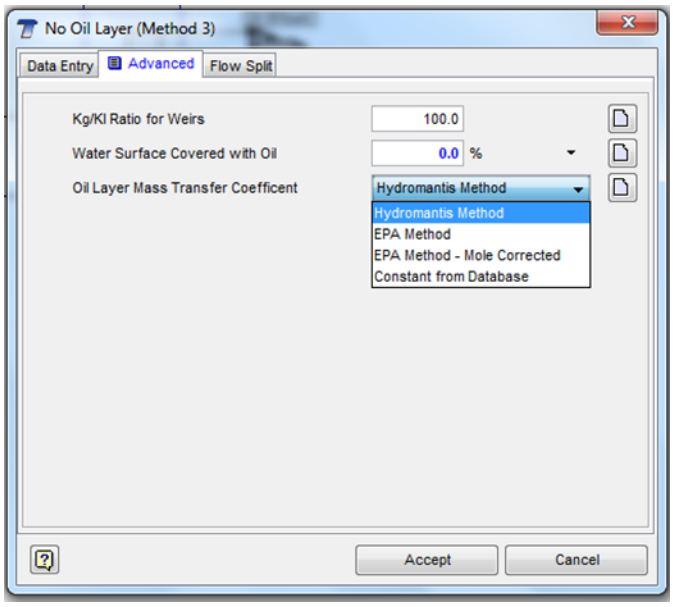


***Water Scrubber -*** The new unit process is added to transfer the contaminant from an air stream to water stream. The emission model for the scrubber uses the same model as the cooling tower model in Toxchem, only with transfer between liquid and gas phases reversed.



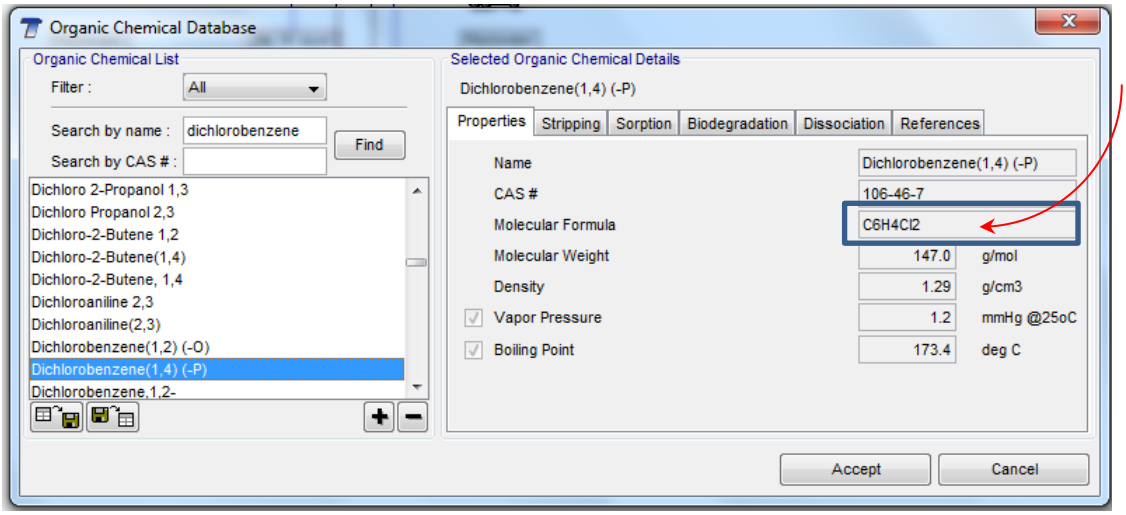
## 1.2 NEW EMISSION MECHANISM FROM FLOATING OIL SURFACES

The issue of modeling of air emissions of organic compounds from a non-aqueous layer floating on a water surface is of growing concern. Originally, Toxchem software was intended to predict the fate of contaminants in wastewater. In certain specific industries, such as petroleum refining, however, it is possible that the surface of the wastewater in collection or treatment process units may be covered by a floating layer of oil, assumed to be of hydrocarbon origin. Users can specify the fraction of the water surface that is covered by the floating oil layer. In Version 4.3, TOXCHEM provides four procedures for estimating emissions of organic contaminants from a floating oil layer. The first approach (default) is based on mass transfer principles similar to volatilization from a water surface. The additional procedures are provided based on 1) an EPA approach as defined the in the document “Air Emission Models for Waste and Wastewater (EPA, 1994), 2) a modified EPA approach considering the mole fraction correction factor for dilute concentration of contaminant in oil and 3) application of direct experimental mass transfer coefficient in the emission calculations.

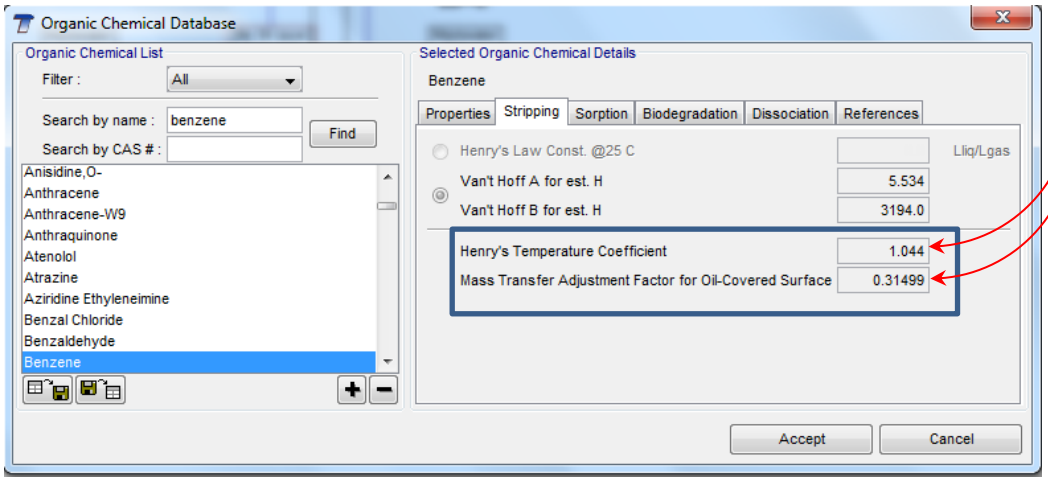



## 1.3 NEW DATABASE PROPERTIES

The organic contaminant database now includes the chemical formula of organic compounds.




For user-defined organic compounds only, a temperature correction coefficient for Henry's law constant can now be specified by a user in place of the default value of 1.044. Also, for user-defined compounds, the mass transfer adjustment factor for estimation of emissions from an oil layer rather than from water is provided in the same tab for "Stripping" properties.



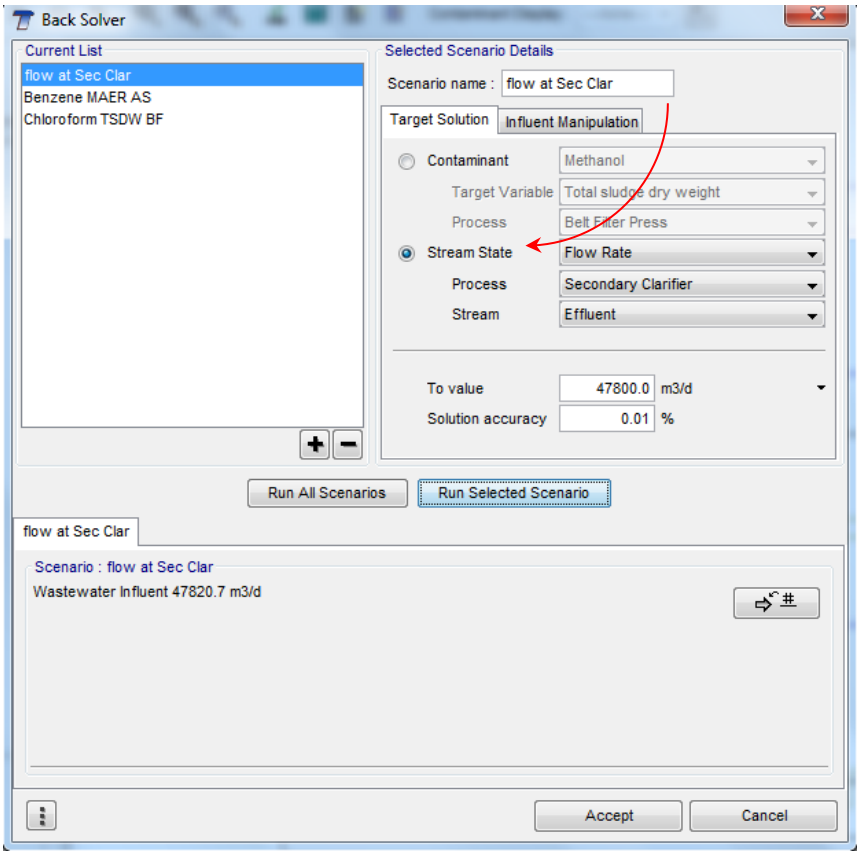

Lastly, the values of dissociation constants for weak acids and bases have been reviewed an updated as needed.

## 1.4 INTERFACE IMPROVEMENTS

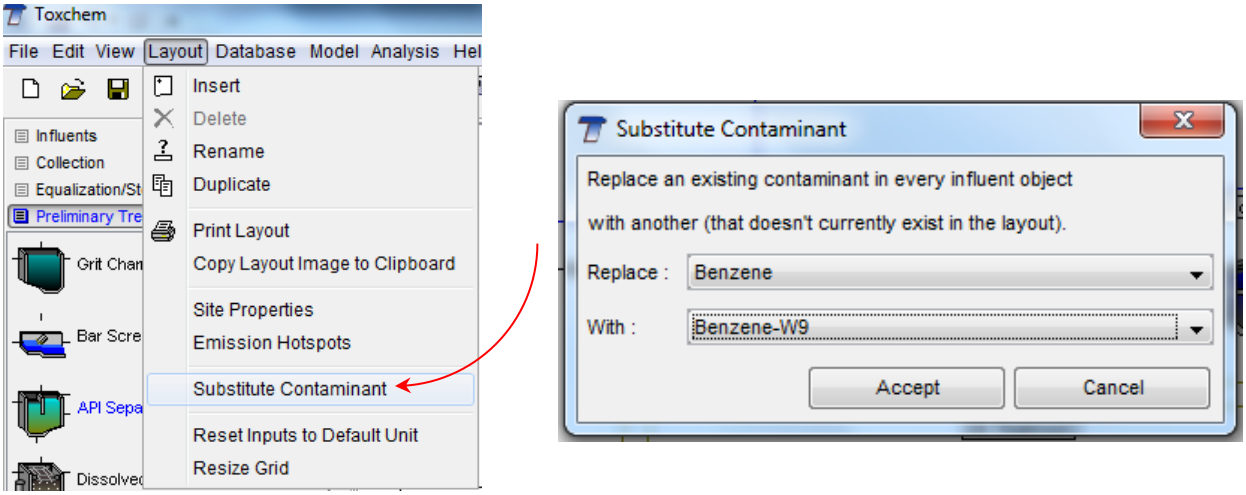
***Quick Adjust Panel -*** The new feature in the Quick Adjust Panel allows the user to include the physical-chemical properties of contaminants for quickly changing the values and running the simulations. The values of the parameters on the quick panel can also be imported from a data file.

***Color-coding of Stream Lines -*** Stream lines representing flows of water effluent, air, sludge and oil are now color-coded to make differentiation of the streams more discernible to users. Stream colors can be preferentially adjusted by a user.

***Extended Functionality of Back-Solver -*** The back-solving function has been extended to allow users to solve back from a state variable such as flow to the influent level. Note that when certain state variables such as suspended solids are specified as a process data entry, setting the target value may result in a process mass balance failure.

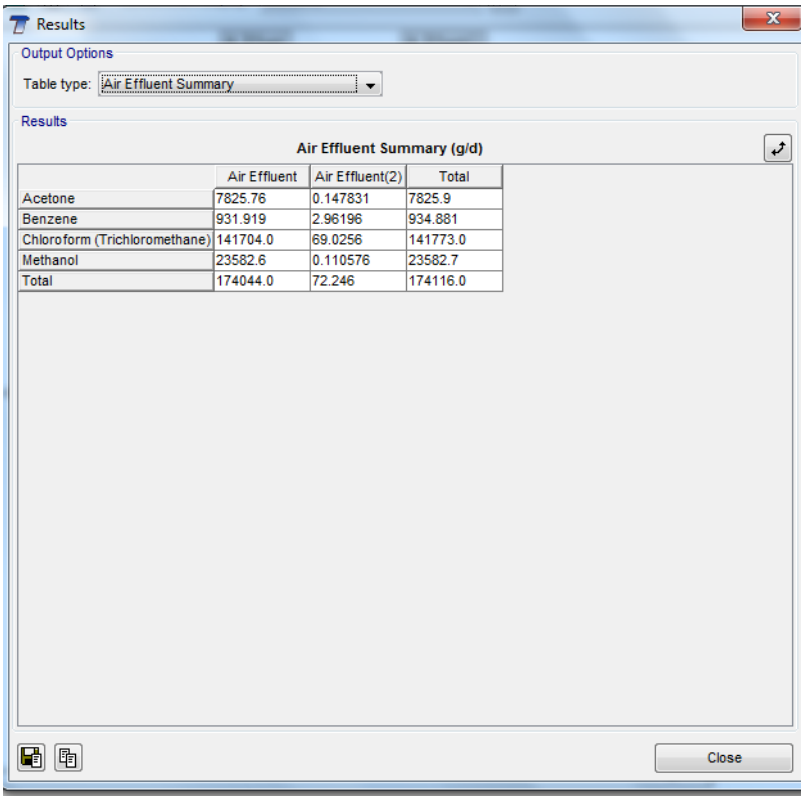



***Contaminant Substitution –*** In larger layouts with many influent process streams, users may find it advantageous to substitute one compound for another during evaluations. For example, a user-defined compound may need to replace the default compound in an assessment. Rather than manually deleting the existing compound and then adding the replacement compound, users may substitute the replacement compound easily.



***Archive Layouts -*** This new feature will bundle any user-defined contaminants that are used in a layout with the layout file so that you can easily send it to a colleague and they can open the layout and be assured that they are using the exact same parameters.

***New Summary Table -*** With this feature, accessed through the “View Summary Results”, users can create and view results without the need to export the data to an Excel file.




| | Air Effluent | Air Effluent(2) | Total |
|---|---|---|---|
| Acetone | 7825.76 | 0.147831 | 7825.9 |
| Benzene | 931.919 | 2.96196 | 934.881 |
| Chloroform (Trichloromethane) | 141704.0 | 69.0256 | 141773.0 |
| Methanol | 23582.6 | 0.110576 | 23582.7 |
| Total | 174044.0 | 72.246 | 174116.0 |

# 2. TOXCHEM INTERFACE BASICS

## 2.1 INTERFACE TERMINOLOGY

A brief introduction of TOXCHEM V4.3 interface is presented in this section to familiarize the user to the organization of various features and functionality available in the simulation system. TOXCHEM starts with a program window as shown in **Figure 2-1**. The program window contains the areas for Menu Bar, Tool Bar, Hot Spot Bar, Process Tool Bar and Layout Drawing. It also contains the two quick output tables summarizing fate of contaminant in each unit process and the system.

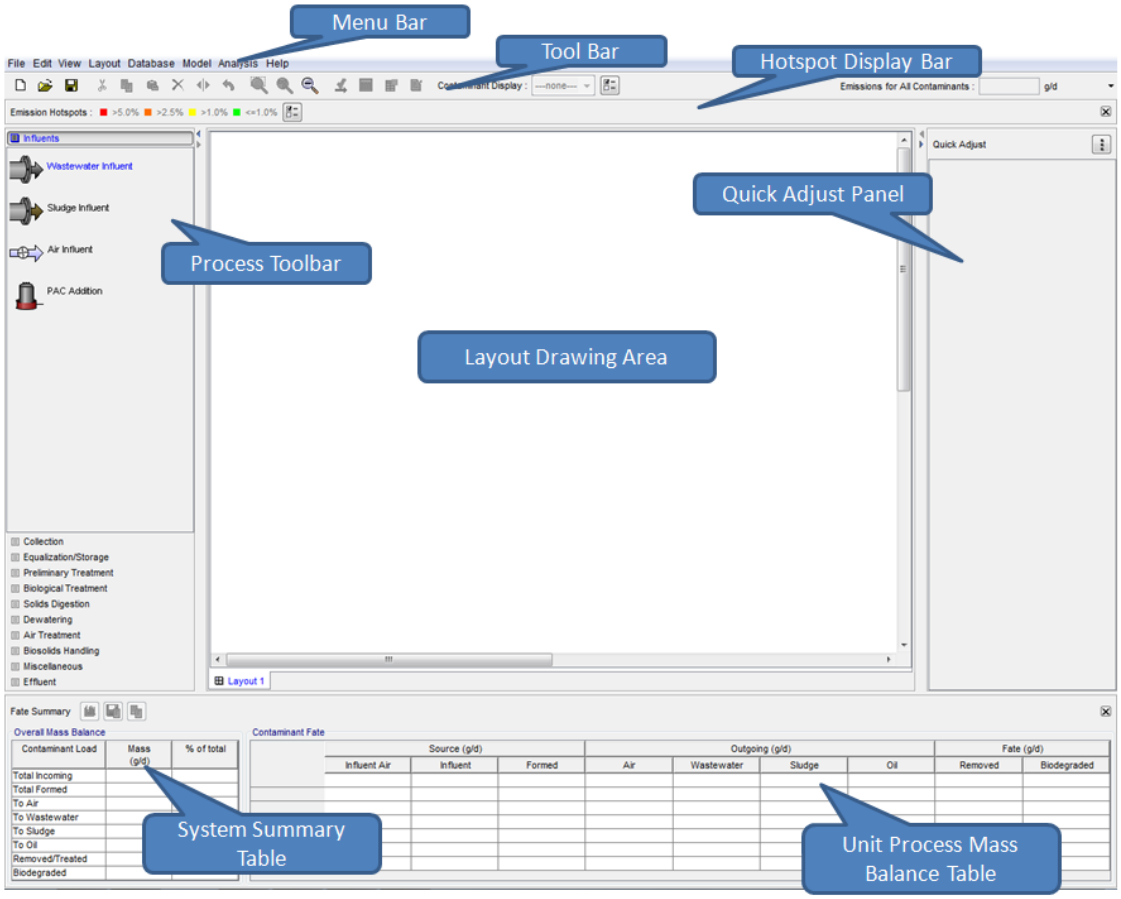



**Figure 2-1 TOXCHEM program window**

## 2.2 INTERFACE COMMANDS/FEATURES

*Menu Bar* - The Menu Bar contains menu items like File, Edit, View, Layout, Databases, Model, Analysis and Help. The various commands available in each menu item are as shown in **Figure 2-2**. The **File** menu contains command for retrieving and saving the TOXCHEM files. The **Edit**

menu provides commands for manipulating the layout on the drawing area. The **View** Menu provides many different options for displaying the layout on the drawing area. The **View** Menu also includes the command for viewing the model Preferences like the system of units, solver accuracy and other user preferences. The **Layout** menu provides command to manage multiple layouts in the same file. It also includes the commands like Site Properties and Emission Hotspots, which are used to set layout specific properties. The **Databases** menu contains commands to access and manipulate the organic contaminant and metal properties database. The **Model** menu includes command for checking, solving and viewing results after a layout is completely defined. The **Analysis** menu provides access to Sensitivity Analysis and Back Solver functions of TOXCHEM. The Help menu may be used to access the User's Guide and Technical Manual.

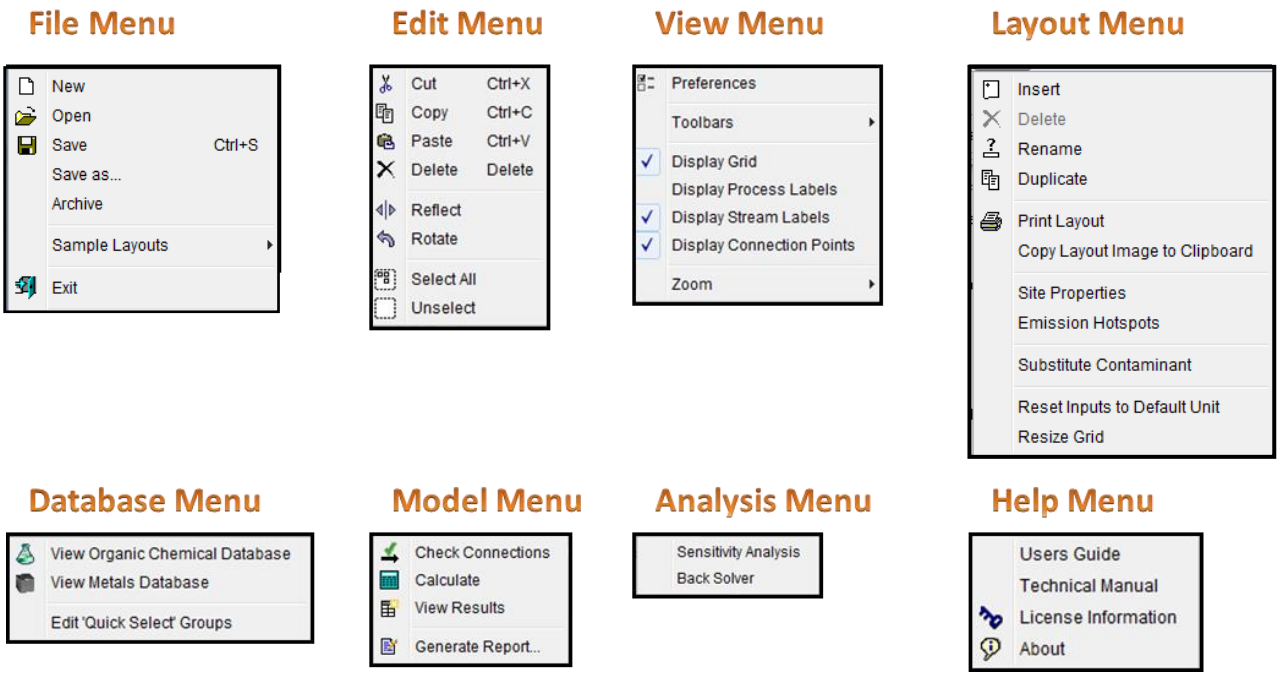



**Figure 2-2 Commands in different Menu items**

*Tool Bar* – The Tool Bar contains buttons for some of most often used commands in TOXCHEM. The menu items and corresponding commands available on the commands on tool bar are as shown in **Figure 2-3.** The Tool Bar also contains a contaminant selection drop down menu which can be used to select a contaminant for which hot spot display and quick outputs needs to be viewed. At the far right end of the Tool Bar, there is a button to access the Contaminant Database.

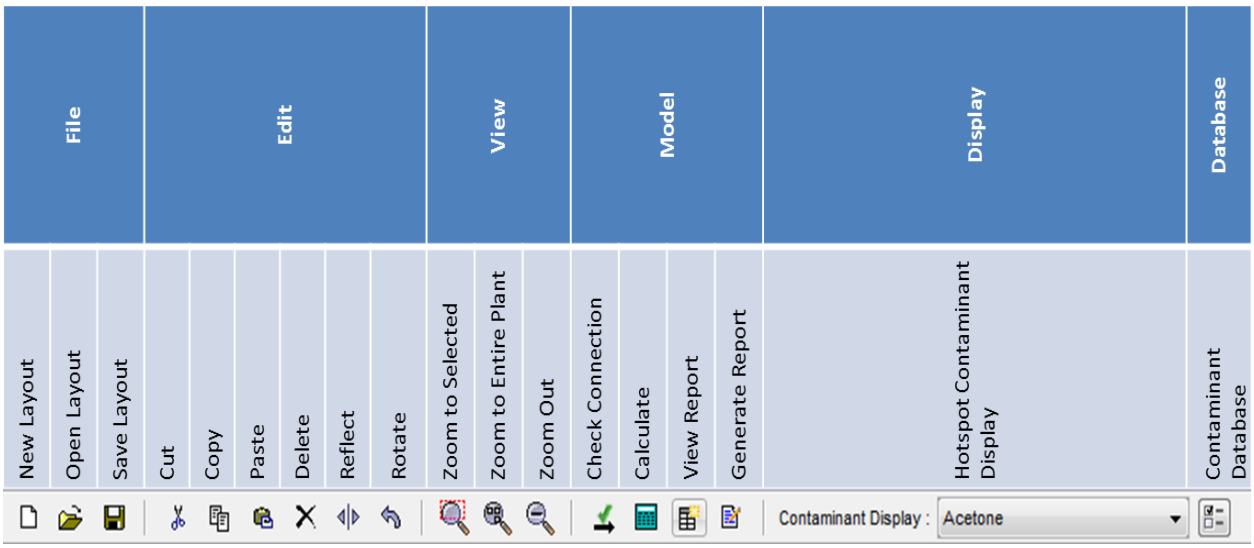



**Figure 2-3 Commands on the tool bar and icon representation**

*Hot Spot Bar* – The Hot Spot Bar provides quick access to view and edit the hot spot display setting. It also shows the current color code used for different emission limits.

*Process Tool Bar* – The Process Tool Bar provides access to all the unit processes available in TOXCHEM for layout building. The process units are compiled in different categories of Influents, Collection, Preliminary Treatment, Biological Treatment, Solid Digestion, Air Treatment, Dewatering, Miscellaneous and Effluents. The unit processes available in any category can be accessed by clicking on the category tab.

*Layout Drawing Area* – The Layout Drawing Area is used for placing the process units and connecting them to make a process flow scheme for analysis. The layout drawing area is specific to the layout name which appears at the bottom-left of the drawing area.

*Unit Process Mass Balance Table* – After the layout is solved, the table is used to show the speciation and mass balance of a selected contaminant for all the unit processes in the layout.

*System Summary Table* – After the layout is solved, the table shows the overall fate of a selected contaminant in the system.

*Quick Adjust Panel* – The quick adjust panel that can be used to place important model parameters which needs to be changed while conducting different simulations. The model parameters placed on the quick panel can also be read from an EXCEL file.

# 3.TUTORIAL

## 3.1 INTRODUCTION

This Tutorial describes various features of TOXCHEM and demonstrates how to conduct a contaminant fate modeling in TOXCHEM. After completing this chapter, user shall be able to understand;

1. How to build a plant layout
2. How to select a contaminant from the ready to use database
3. How to set inputs for process units
4. How to set emission hotspots
5. How to conduct simulation
6. How to view results
7. How to export results
8. How to add user defined contaminants
9. How to conduct sensitivity analysis
10. How to use back-solver

In this tutorial, we will be working with a relatively simple treatment process configuration called the *Tutorial Plant*. The schematic form of the plant is shown in **Figure 3-1**. The liquid process train of the *Tutorial Plant* consists of the following processes:

1. Equalization basin
2. Primary clarifier
3. Aeration basin
4. Secondary clarifier

The solid process train of the plant handles the waste solids and consists of the following processes:

1. Anaerobic digester
2. Belt filter press

In addition to the liquid and solid trains, the plant consists of an air process train which consists of a single unit process of digester gas cleaning process.

The objective of this simulation study is to quantify the pollution loads of selected contaminants in the liquid, solid and air effluents streams from the plant.

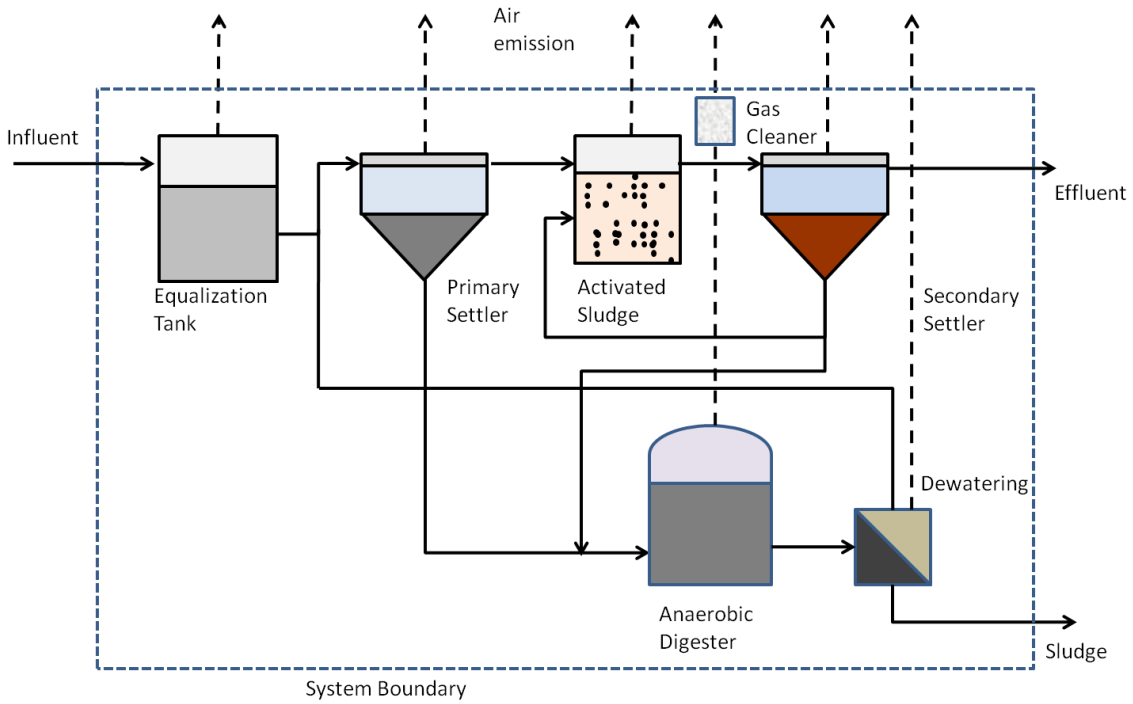



**Figure 3-1 Process Schematic for Tutorial Layout**

## 3.2 CREATING THE PLANT LAYOUT

**Note to Users of TOXCHEM 3 and earlier Versions:** The grid designation system is no longer used since V4. Also the technique for configuring the layout is no longer based on a select and click-in-place action, but a drag-and-drop action.

**Selecting Unit Processes** To prepare the plant layout, select the unit processes from the unit process table available at left side of the drawing board. The unit process table consists of various tabs containing various unit processes. Left clicking on any tab expands the tab and provides the details of unit processes available in that tab. For building the *Tutorial Plant* layout, the process units listed in column 1 of **Table 3-1** will be used. The **Table 3-1** also provides the description of the category under which the process unit is found. To place the unit process on the drawing board, click on the tab under which the process unit is available. Left click on the process unit and drag to the drawing board while keeping the mouse button pressed. Release the mouse button to drop the unit process at the desired location on the drawing board. To remove a unit process from the drawing board, right click the mouse button on the process and click **delete** from the pop-up window. Another way to delete the unit process is by left clicking on the unit process [a red border around the object appears] and then accessing the **delete** command inside edit menu or on Tool Bar. The **delete** key on the keyboard can also be used for deleting the unit process [Note: At present TOXCHEM does not support a “Undo” button]. To move a process unit from one cell to other, left click on the process unit and move the cursor to the new location with the mouse button pressed. Release the mouse button to select the new location. The move operation can be performed for a group of selected process units. When all the process units have

been added to the drawing area, optimize the screen view by clicking on <View/Zoom> and selecting "**to Entire Plant**" [Zoom to Entire Plant command is also available on Tool Bar for quick access]. The drawing board after the unit process placement shall appear as shown in **Figure 3-2** .

**Table 3-1 Process Units Required in Tutorial Layout**

| Unit Process | Category | Comment |
|---|---|---|
| Wastewater Influent | Influents | The influent object are used to specify the wastewater flow rate, contaminants concentration etc. |
| Equalization | Preliminary Treatment | In this exercise the hydraulic mixed tank is used. |
| Primary Clarifier | Preliminary Treatment | - |
| Activated Sludge – Diffused Aeration | Biological Treatment | The diffused aeration unit is selected in this exercise. |
| Secondary Clarifier | Biological Treatment | - |
| Pass Through | Miscellaneous | The Pass Through object allows to visualize the properties of the incoming stream |
| Anaerobic Digester | Solids Digestion | - |
| Belt Filter Press | Dewatering | Belt filter press process unit is used in this exercise. |
| Air Treatment | Air Treatment | - |
| Wastewater Effluent | Effluent | - |
| Air Effluent | Effluent | Used to collect air from all the unit processes except anaerobic digestion |
| Air Effluent | Effluent | Used to collect air from the anaerobic digestion object |
| Sludge Effluent | Effluent | - |

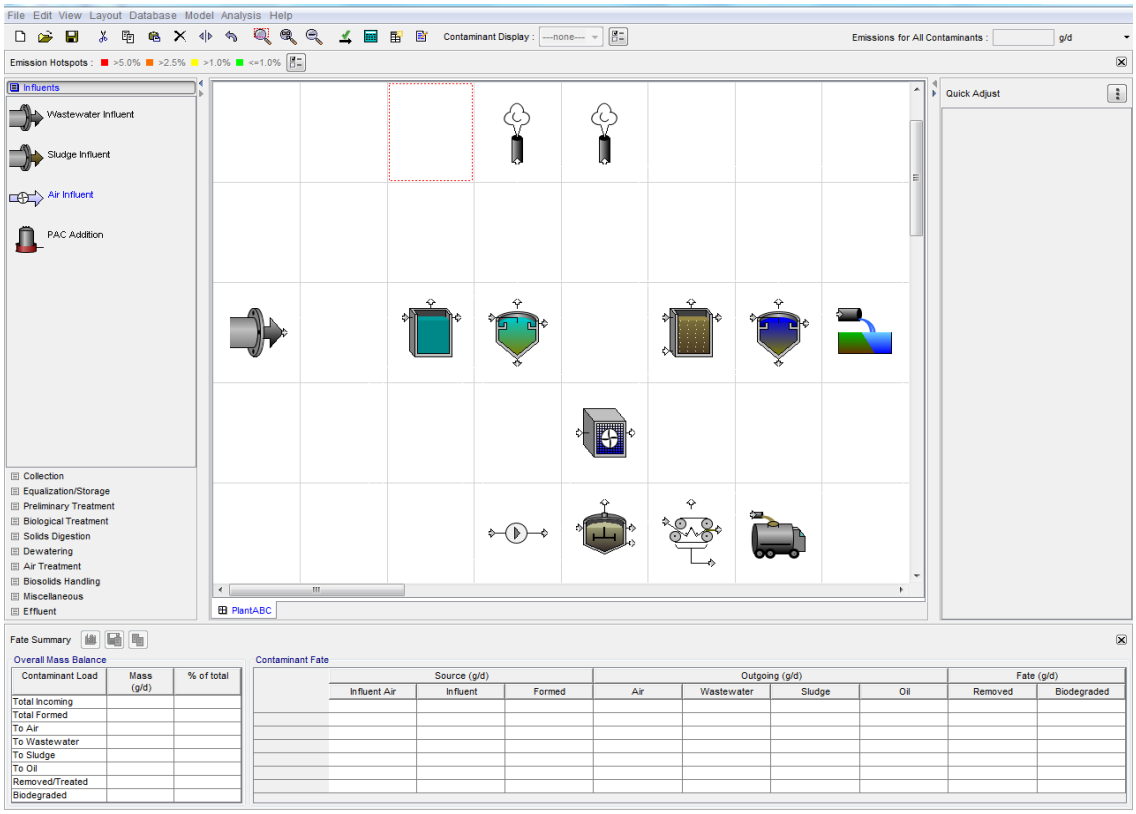



**Figure 3-2 Drawing Board after Placing the Process Units**

**Making Flow Connections** After all the required process units are placed on the drawing board, the flow connections between the unit processes are defined. The process connections required to make the layout are shown in **Table 3-2** which also lists the connection types between the process units.

**Note**: In TOXCHEM, there are four types of connections e.g. wastewater connection, sludge connection, air connection and oil connection available to the user. The nature of the connection points can be checked by right clicking on process unit and then selecting the “Edit Labels” in the popup window. The “Edit Label” window as shown in **Figure 3-3** indicates the nature of the connection. The connection points can also be identified by the fill- colour of arrow which appears when the cursor is placed over the connection point. The wastewater, sludge, air and oil connection points bring up arrow filled with grey, brown, blue and black colour respectively. In TOXCHEM, it is permitted to make a connection between wastewater and sludge lines. However air and oil streams can only be joined to respective colour streams. This means that while the wastewater and sludge connection lines can be interconnected without discretion, the air and oil streams can only be joined to respective connection type.

**Table 3-2 Process Connections for Tutorial Layout**

| From Process | Connection Type | To Process |
|---|---|---|
| Influent | Wastewater | Equalization |
| Equalization | Wastewater | Primary Clarifier |
| Equalization | Air | Air Effluent |
| Primary Clarifier | Wastewater | Diffused Air Activated Sludge |
| Primary Clarifier | Air | Air Effluent |
| Primary Clarifier | Sludge | Anaerobic Digester |
| Diffused Air Activated Sludge | Wastewater | Secondary Clarifier |
| Diffused Air Activated Sludge | Air | Air Effluent |
| Secondary Clarifier | Wastewater | Effluent Discharge |
| Secondary Clarifier | Air | Air Effluent |
| Secondary Clarifier | Sludge | Diffused Air Activated Sludge |
| Secondary Clarifier | Sludge | Flow Through |
| Flow Through | Wastewater | Anaerobic Digester |
| Anaerobic Digester | Wastewater | Equalization |
| Anaerobic Digester | Air | Air Treatment |
| Anaerobic Digester | Sludge | Belt Filter Press |
| Belt Filter Press | Wastewater | Equalization |
| Belt Filter Press | Air | Air Effluent |
| Belt Filter Press | Sludge | Sludge Discharge |
| Air Treatment | Air | Air Effluent 2 |
| Wastewater Effluent | | |
| Air Effluents | | |
| Air Effluents 2 | | |
| Sludge Discharge | | |

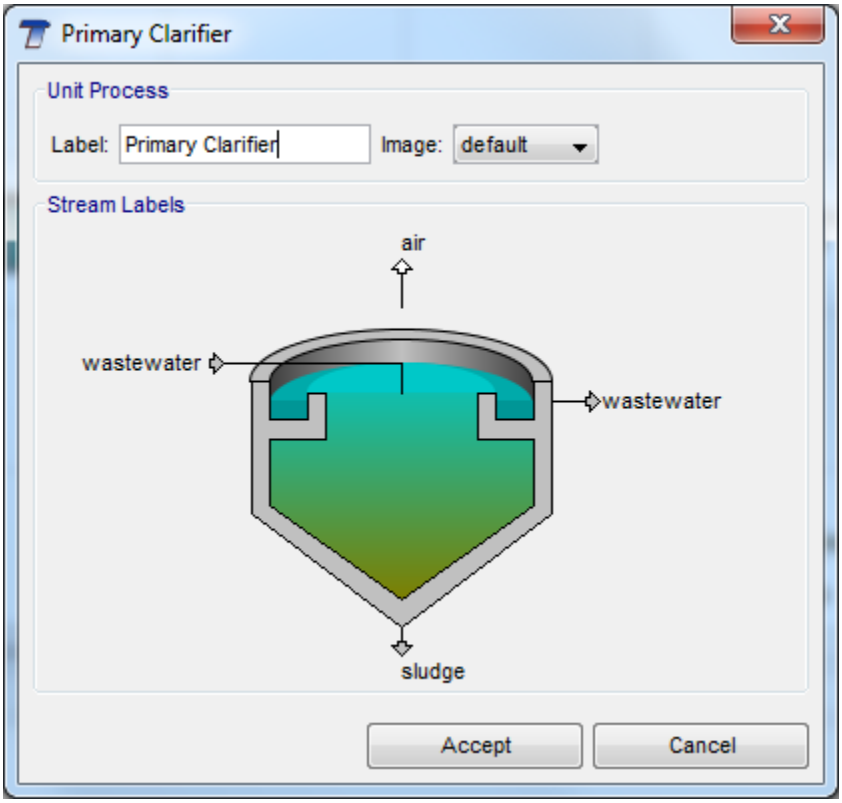



**Figure 3-3 Verification of connection types for primary clarifier**

To collapse the quick adjust panel, click on the right facing triangle available on the divider between the drawing board and the quick adjust panel. The quick adjust panel can be displayed when necessary by clicking on the left pointing triangle. The process tool bar on the left side can also be collapsed/displayed by using the left and right pointing triangles available on the divider between the process tool bar and the drawing board. For this exercise, collapse the quick adjust panel by clicking on the right pointing triangle.

To make a connection between two process units, place the mouse on the outlet arrow connection of the unit process from where the connection starts. Once the cursor is at the right position, a larger right facing arrow will appears. Press the left mouse button to connect to the outlet and drag the mouse cursor to the inlet connection of the unit while keeping the mouse button pressed. When the cursor is at the proper position on the inlet arrow connection, a larger right facing green colour arrow will appear. Release the mouse button to accept the connection. A connection line between the units should appear after the operation. For deleting a connection, right click on the process unit from where the connection to be deleted originates. In the pop-up window, point the cursor on **Delete Connection** and select the connection to be deleted. Another quick way to delete the connection line is to right click on the line and left click on **Delete Connection** in the pop-up window**.**

Follow the connection list in **Table 3-2** and repeat the operation to connect all the unit processes. Both inlet and outlets connection points of process units allows multiple connections as long as they are of same type.

**Note**: TOXCHEM requires that all the outlet connections on all the unit processes are connected to a downstream process unit. Therefore, in a TOXCHEM layout, the wastewater line, sludge line, air line and oil line always terminate at a wastewater effluent, sludge effluent, air effluent and oil effluent process objects [only objects without an output connection] respectively.

When all the connections are complete, verify that all the process connections are valid by left clicking on the green check-mark and arrow button available on the tool bar. Alternatively select the **Check Connection** from the **Model** menu**.** The missing connections in the layout will be displayed in a pop-up information window. Define the missing connections to complete the layout. You can also rearrange the connection lines by dragging then horizontally or vertically. The completed layout will now appear as in **Figure 3-4.**

**Note**: the **Check Connection** feature only identifies the missing connections, it cannot determine if the connections are correct.

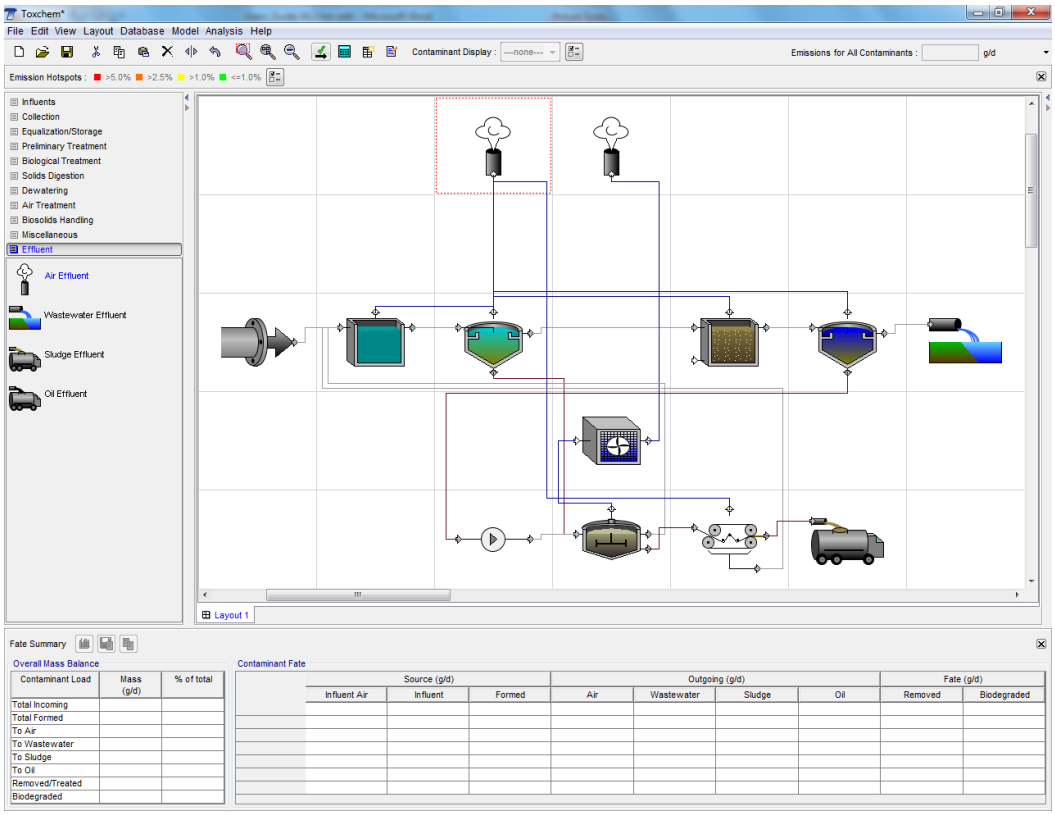



**Figure 3-4 Example Layout with Process Connections**

There are several display options in TOXCHEM which are accessible from the **View** menu. To display/hide the process labels select/unselect the **Display Process Labels** in **View** menu. Similarly, to display/hide the stream labels, select/unselect the **Display Stream Labels** in **View**

menu. The layout with both the process and stream labels selected is shown in **Figure 3-5**. The display of process and stream labels can also be turned On/Off by right clicking in an empty cell on the drawing board and (un)selecting **Display Process Labels** or/and **Display Stream Labels.**

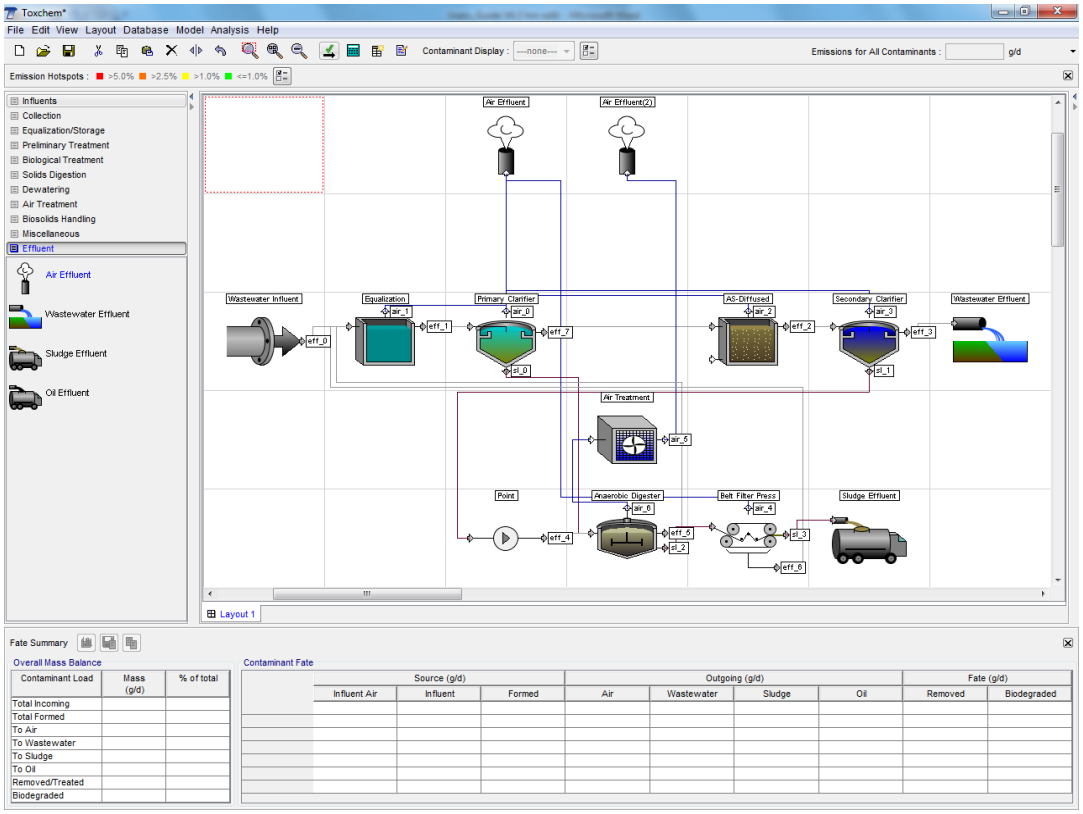



**Figure 3-5 Example Layout with Process and Stream Labels Activated**

TOXCHEM automatically decides the path of the connection lines between two unit processes. At times, the paths of the connection lines may almost appear to overlap, and so are not optimally placed. In such situation, the automatically drawn path of the connection lines can be rearranged by the user. The lines can be moved by left clicking on the line and dragging it in the indicated (horizontal or vertical) direction. It shall be noted that only one segment of the line between two break-points (In automatically drawn lines, the break-points exist at each connection point and at the point of change in direction) can be moved at a time. Additional break-points can be created on a line by left clicking on the line where a break-point is necessary and left clicking on **Create Break Point**. The example layout with the connection lines redrawn is as shown in **Figure 3-6**.

[**Note**: if the unit process is moved, all the connection lines originating from the unit processes will be redrawn by TOXCHEM]

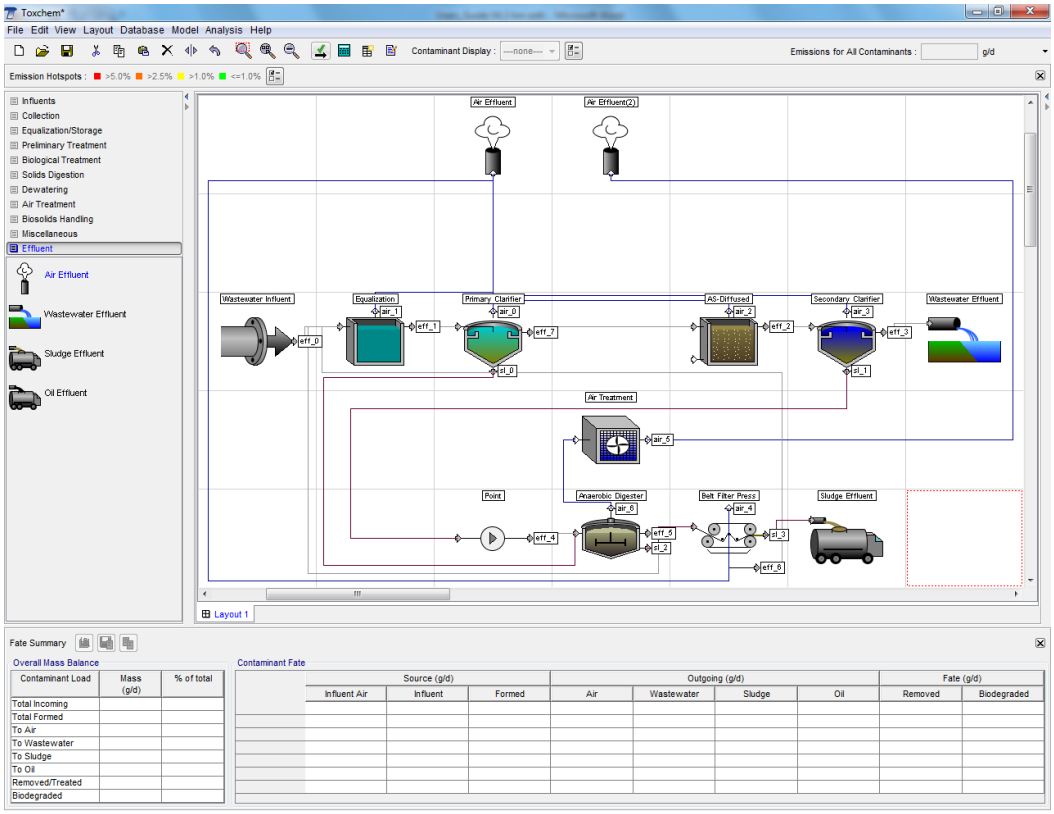



**Figure 3-6 Example Layout with connection lines reorganized**

**Note**: TOXCHEM automatically assigns both the process and stream labels. The process label is assigned when the process object is placed from the process table to the drawing board. A stream label is assigned when the connection point is connected to a downstream object. To change the automatically assigned labels to more user meaningful labels, right click on the process object and select **Edit Labels** in the pop-up window. Enter the new process/stream labels in the process/stream label field of the edit label window. Press **Accept** to confirm the changes.

In this layout, we will change the labels for the secondary clarifier. Right click on the secondary clarifier and select **Edit Labels**. In the Edit Labels window, change the labels as shown in the **Table 3-3**.

To access the second sludge stream of the secondary clarifier, click on the selection box next to the sludge stream and select To-Point and then change the connection label. The Edit Label window after the changes shall be as in **Figure 3-7**.

**Table 3-3 New Stream Labels**

| Stream | New Label |
|---|---|
| From - AS diffused | AS_eff |
| To - Air effluent | Cl_air |
| To - Wastewater effluent | Cl_eff |
| To-AS diffused | RAS |
| To-Point | WAS |

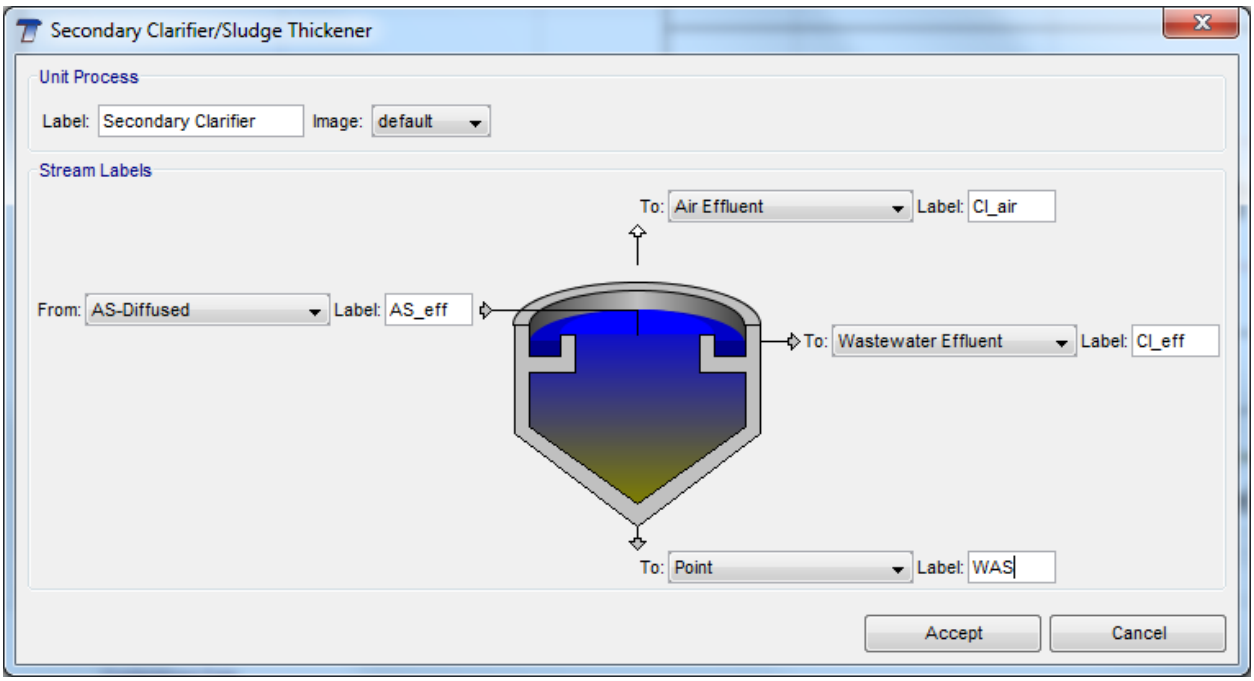



**Figure 3-7 Edit Label Window with New Stream Labels**

## 3.3 DATA ENTRY

**Note**: TOXCHEM organizes data inputs into three categories - Global Data, Layout Specific Data and Unit Process Specific Data. The Global Data form can be accessed by going to **View** Menu and clicking on **Preferences** command. The Global Data controls the display and model settings for all the layouts in the project file. In the Display Settings tab, settings like significant digits in output numbers and Default Unit System (metric, US) are accessible to user. In the Model Settings tab user can set the accuracy of the steady state solver and can choose the biological model for suspended growth processes. The layout specific data is applicable to the layout and can be set for each layout differently. The unit process data is specific for the specific unit process for which the data is provided. In this exercise we will only change the Layout Specific Data and Unit Process Specific Data.

## LAYOUT SPECIFIC DATA

To input the layout specific information, access **Site Properties** in the **Layout** menu. The **Site Properties** window is as shown in **Figure 3-8.** In this exercise, we will leave all the parameters to their default value. Note that the wind speed, which affects surface volatilization is 10 km/h (6.2 mph) and the site elevation and site wide pH value are 100 m (328 ft) and 7.0 respectively.

**Note**: To enter the data in units other than default units, click on the inverted triangle next to the data entry field. Select the required unit in the popup window. TOXCHEM provides a choice to apply SRT based active biomass correction in the biodegradation rate. By default, the correction factor is not applied.

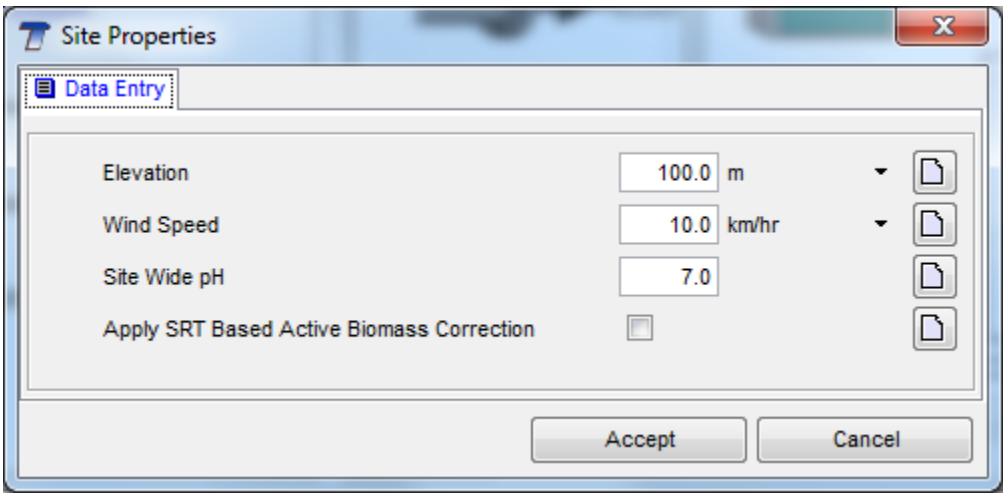



**Figure 3-8 Site Properties input window**

## UNIT PROCESS SPECIFIC DATA

**Note**: Unit process data Entry is now accomplished by right-clicking on the process unit and then clicking on Edit Parameters in pop-up window

***Influent*** - On the **Data Entry** tab of the Influent data input window, set the wastewater flow to 30,000$m^3$/d (7.925 MGD). The temperature and suspended solids concentration of the influent are set to 40$^oC$ (104$^oF$) and 250 mg/L respectively. All the other input parameters are left with their default values. It should be noted that as soon as the default values are changed the display color changes to blue. This change in color helps user keep track of values which are changed in the model. After the changes have been made, the user can view the original default values by pointing the cursor over the field. A tool tip will display the default value. A help button is available at the bottom left of the form to access brief description of the input parameters. The Data Entry form after entering the influent data is shown in **Figure 3-9.**

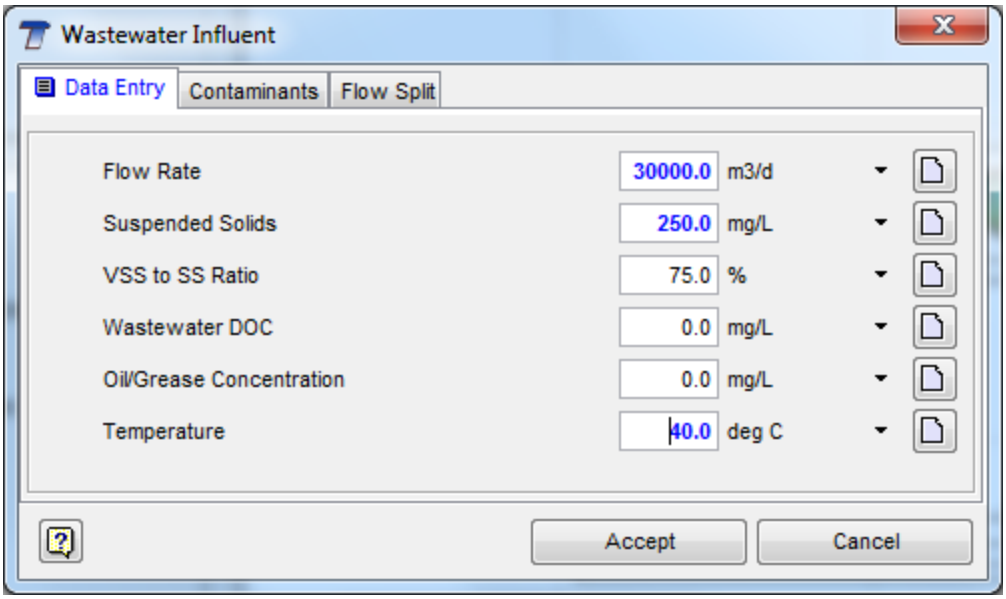



**Figure 3-9 Data Entry tab for the Wastewater Influent**

To select and enter the concentration of contaminants, click on the **Contaminants** tab. The **Table 3-4** shows the contaminants and their concentration which will be included in the fate modeling.

**Table 3-4 Contaminants and Influent Concentrations for Tutorial Layout**

| Compound | Influent Concentration (ug/L) |
|---|---|
| Acetone | 1,000 |
| Benzene | 100 |
| Chloroform (Trichloromethane) | 10,000 |
| Methanol | 50,000 |

Click on the **Add/Remove** button to begin selection of contaminants from the TOXCHEM database. Scroll through the list of contaminants to find the contaminant of interest. To quickly find the contaminant in the list, enter the first letter of the contaminant (or a few letters quickly). Select the contaminant of interest by clicking on it. After selecting the contaminant, click the right-facing arrow button in the center of the window to include the contaminant in the wastewater. The name of the contaminant will appear in the window on the right side of the selection panel. Once all the contaminants have been selected, click on the **Accept** button. Clicking the **Accept** button closes the contaminant selection window and shows data entry window to input the concentration of each selected contaminants. On this screen change the concentrations of the contaminants as shown in **Table 3-4**. The **Contaminants** tab after selecting and entering the contaminant concentration is as shown in **Figure 3-10.** After changing the concentration click the **Accept** button on the window to close the data entry window.

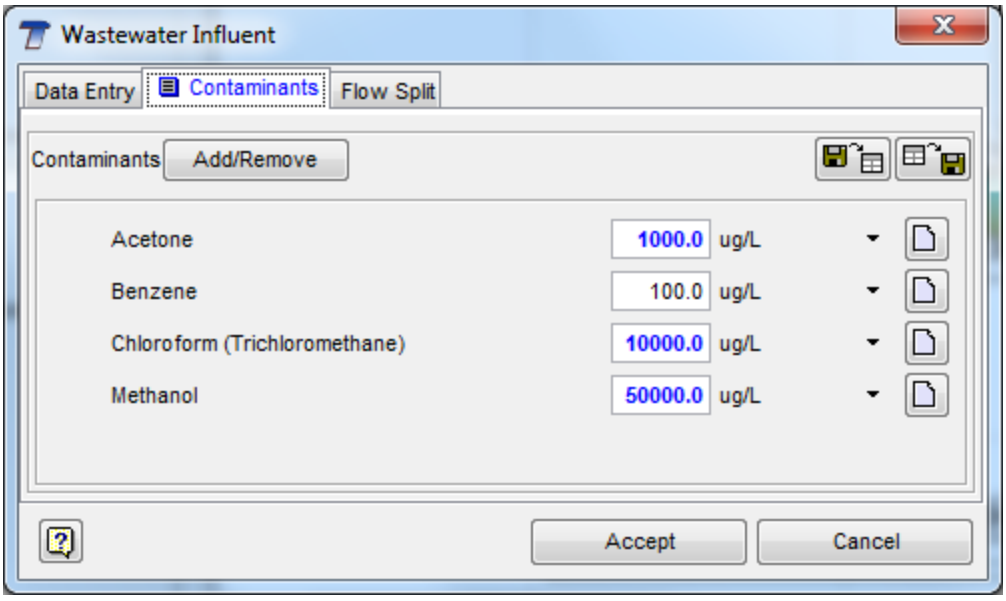



**Figure 3-10 Contaminant tab showing the selected contaminants**

Alternatively, the contaminants and their concentrations can be imported from an EXCEL file by using **Import** button on the window. The procedure to import data from an EXCEL file is described later in Chapter 4- Additional Topics.

***Equalization Basin***-Change the equalization basin depth to 3.5 m and area to 40,000 $m^2$ Use the inverted triangle next to the data entry field to select the correct units (**Figure 3-11**).

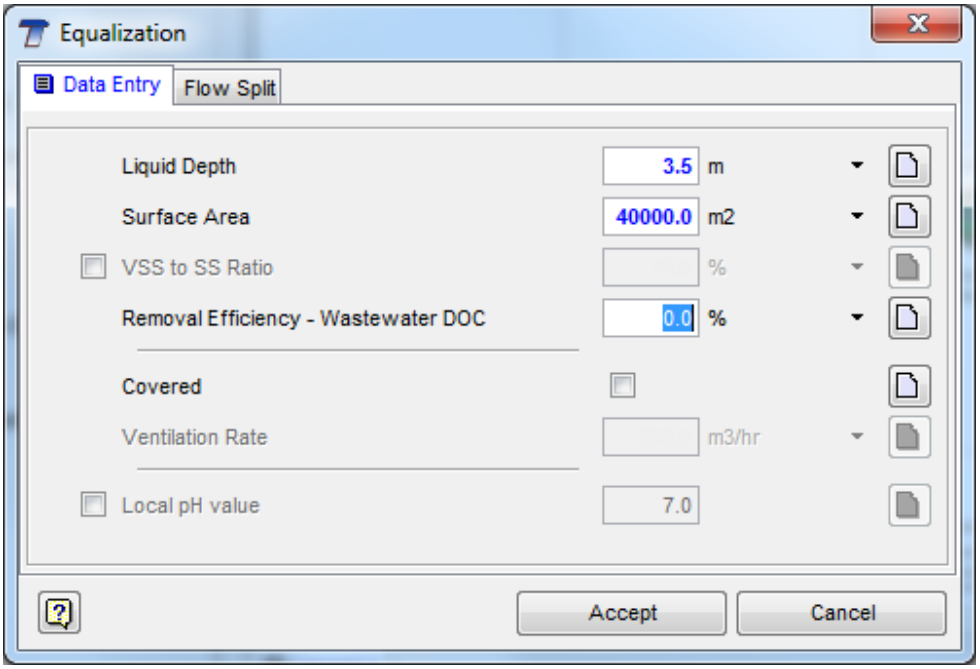



**Figure 3-11 Data Input for equalization basin**

***Secondary Clarifier*** - In the secondary clarifier process, open the data entry form by right clicking on the object and selecting **Edit Parameters**. Once in the data entry window, click on the flow split tab to set the flow split fractions of the sludge stream. Depending on in what sequence the stream connections were made, either RAS or WAS stream fraction may appear with an editable field. In this example, the RAS flow split field is editable. Set a flow fraction of 0.98 and enter to see the recalculated WAS split fraction. Alternatively, if the Waste Activated Sludge (WAS) stream shows up with an editable fraction then set the sludge flow split fraction to 0.02. The Flow Split set up screen for the Secondary Clarifier is shown in **Figure 3-12**. Press enter after typing in the split fraction and make sure that the split fraction of other stream is correctly calculated.

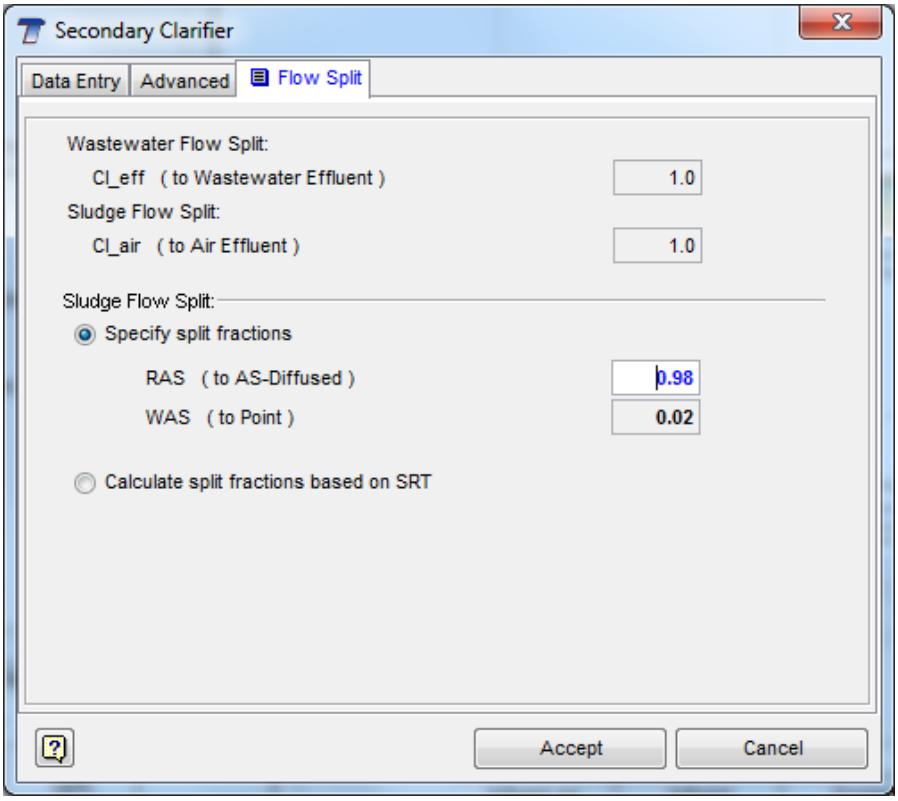



**Figure 3-12 Specifying split fraction of the underflow stream**

**Note**: The split fractions are specified for all but one stream. The split fraction for the unspecified stream is calculated as the difference of one minus the sum of the split fractions of other streams.

For all the other process units, use the default values.

## 3.4 SET EMISSION HOTSPOTS

In TOXCHEM by using the "hotspots" feature, it is possible to visually differentiate the process units which are minor/major source of air emissions in a wastewater treatment facility. When the hotspot feature is activated, the unit processes appear surrounded by different colors, depending on their emission rates. Up to 4 different colors can be used. The classification

ranges can be based on either estimated emission rates (g/d or lb/d), or as a percent of the total input mass.

To set the emission limits for the hotspot, access the **Emission Hotspots** from the **Layout** menu item. For this exercise, the ranges designated will be based on % emission rates. The settings are as shown in **Figure 3-13**. After inputting the values, click the **Accept** button to confirm the settings. The hot spots will be only visible if the hot spot tool bar is activated from **View** – **Toolbars** Menu. It shall be noted that **Emission Hotspots** setting is not applicable to metal, which do not contribute to air emission.

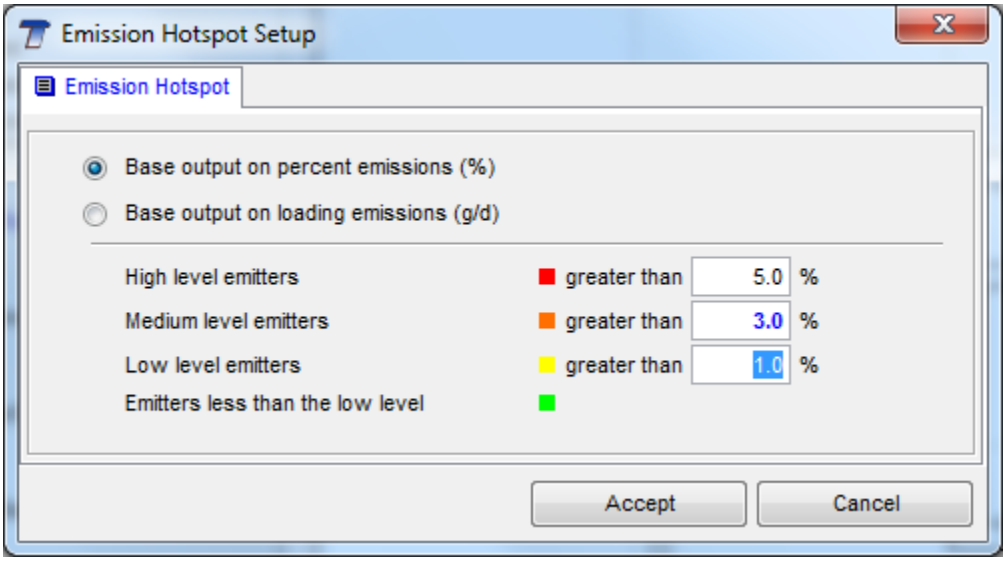



**Figure 3-13 Definition of Hot Spot Emission Categories**

## 3.5 RENAME THE LAYOUT

The name of layout appears at the bottom-left of the drawing area. Right-click on the **Layout1** and select Rename from the drop down menu. Enter **PlantABC** in the layout rename window. Press OK to accept the change.

## 3.6 SAVE THIS PLANT LAYOUT

Save the file as **tutorial.tox** by selecting **Save** from the **File** menu in appropriate directory.

**Note:** Layout files since Version 4 are designated by the file extension <*.tox>. The file name can be different than the name of the layout given in above section.

## 3.7 RUNNING THE SIMULATION

Now that the plant schematic has been prepared and necessary data have been entered, it is time to perform simulation. Click on the **Calculate** button on the toolbar to start the calculation. The solver starts the calculation and solves the model. If no errors are encountered, a pop-up window will appear with the message “Layout successfully solved”. Click the **OK** button to close the popup window. In Version 4.3, a summary of total air emissions of all compounds is displayed in the upper right corner of the layout. After the layout is solved, the unit processes

are presented with different colors around them. If the different colors do not appear, then activate the hotspot display by selecting **Hotspot** toolbar from the **View** – **Toolbars** menu. The hot spot feature provides a quick way to identify the major source of air-emission for a selected compound. To check the emission hot spots for other compounds, select the contaminant from the drop-down box provided in the tool bar for hot spots. The **Figure 3-14** shows the hot-spot coloring for the Chloroform.

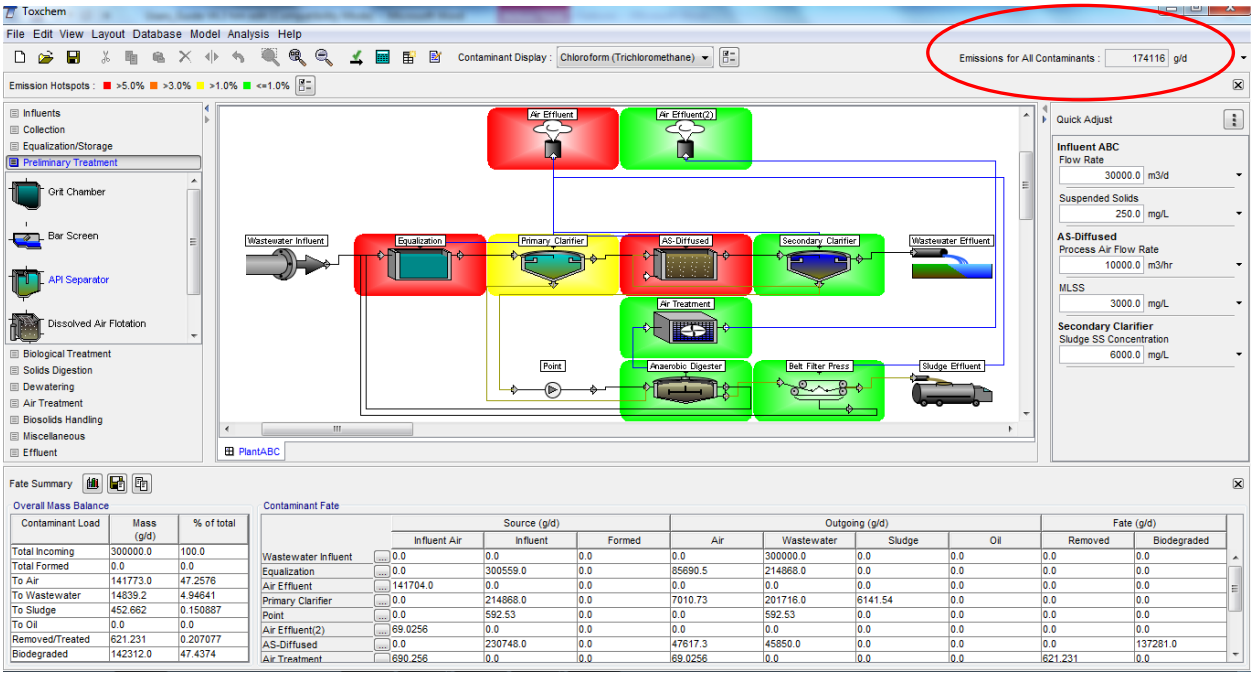



**Figure 3-14 Model Interface with Emission Hotspots Activated**

## 3.8 VIEW AND EXPORT RESULTS

**Note:** TOXCHEM provides many different ways of viewing simulation outputs. In addition, the fate summary table and overall system mass balance tables are displayed on-screen for quick review.

After the layout is successfully solved, the simulation results can be viewed. Right click on the object and select **View Results** to view the outputs for an individual object. To view a detailed summary of the simulation results for complete layout, it is better to use the **View Results** button available on the tool bar.

### VIEW RESULTS FOR UNIT PROCESS

Right click on the activated sludge tank and select **View Results**. In the output window of the process unit (**Figure 3-15**), click on the various tabs for viewing the values of different parameters. The values for different contaminants can be displayed by selecting the chemical from the drop down menu available at the top left corner of output window. The results for every process unit can be viewed similarly.

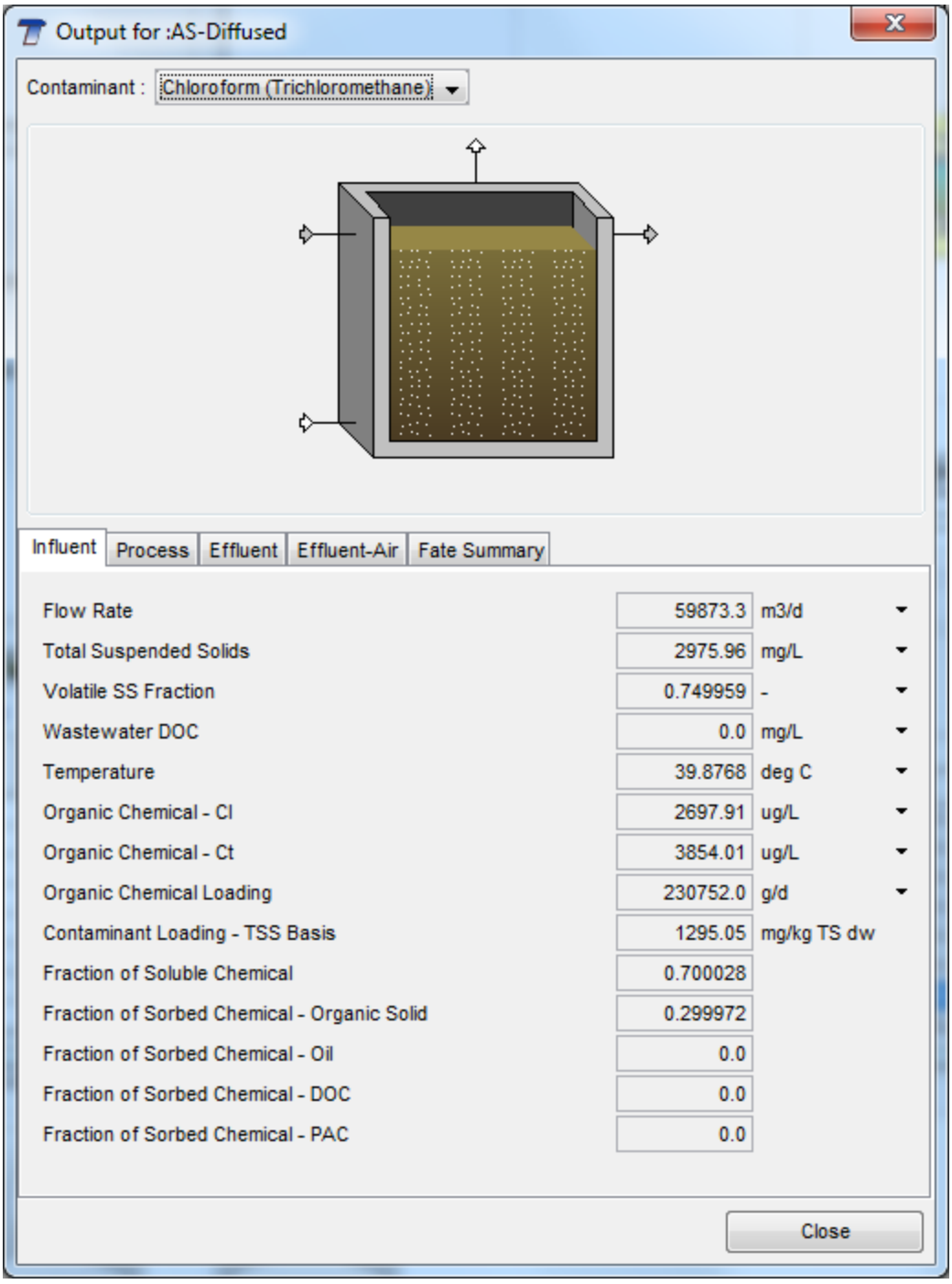



**Figure 3-15 Output window for Activated Sludge-Diffused Air**

Fate summary tab provide the process and overall process emission summary. Open the fate summary tab (**Figure 3-16**) and click on the graph icon at the bottom left of the window for graphical view of the fate summary chart or emission chart.

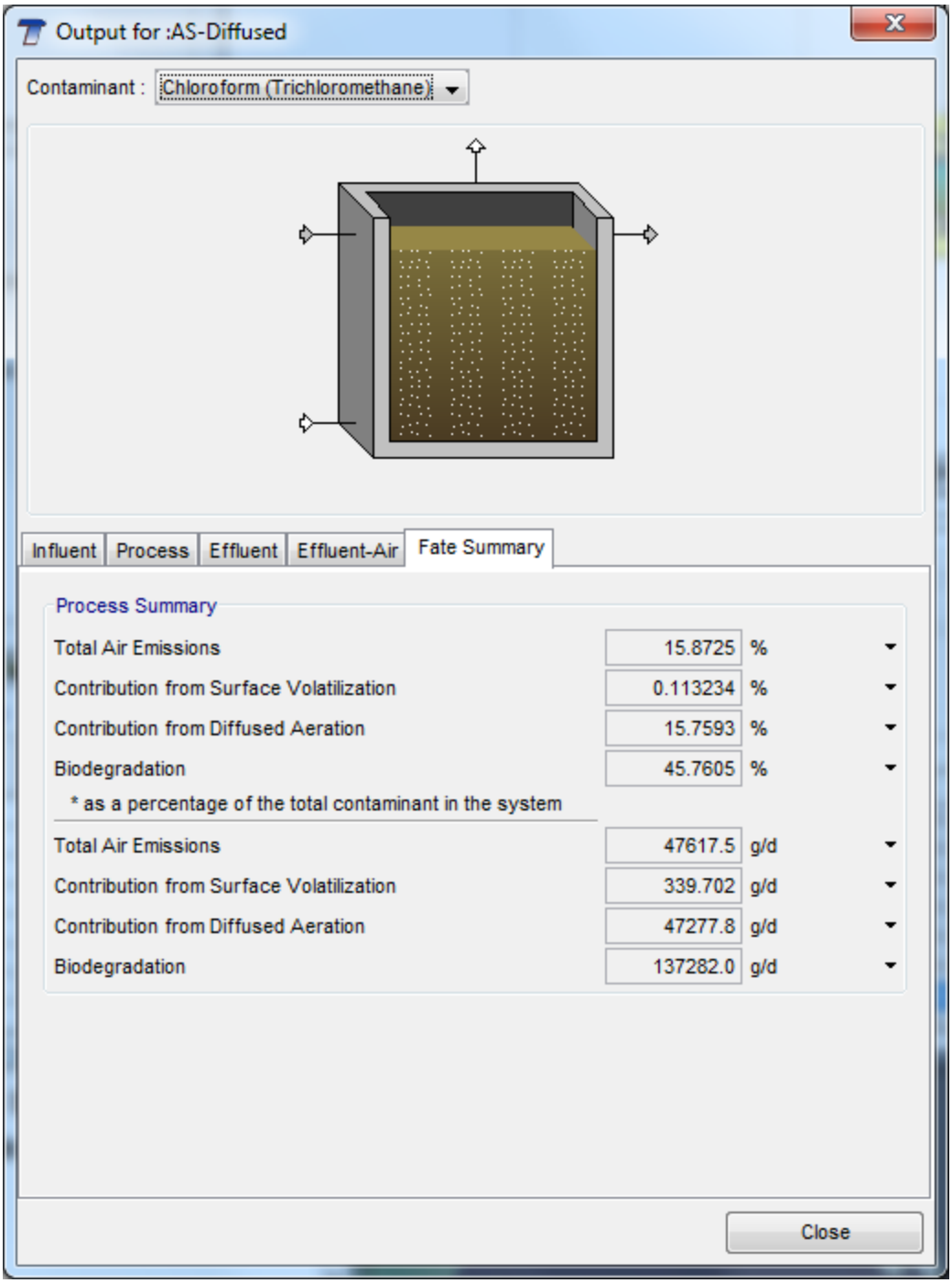



**Figure 3-16 Fate summary tab for Activated Sludge-Diffused Air**

**Note**: depending on the process unit, the output window may consist of different tabs. The parameters on the influent tabs are the values for the combined wastewater and sludge influent lines. For the Effluent-Air stream, all emissions from open tanks are provided as a mass rate only; emissions from covered tanks are provided both as concentration and mass rate.

### CONTAMINANT FATE TABLE

A contaminant fate table is generated as soon as the layout is solved. The contaminant fate table is available for view at the bottom right of the screen (**Figure 3-17**). The table lists all the unit processes in the layout and provides information regarding the total load of incoming contaminant and its fate in the unit process. Left clicking on a unit process in the layout, highlights the corresponding mass balance row in the table and vice-versa. An additional button for viewing results is also provided besides the unit process ID. Clicking on the button, shows the same screen as available from the **View Results** command associated with each unit process.

Contaminant Fate

| | Source (g/d) | | | Outgoing (g/d) | | | | Fate (g/d) | |
|---|---|---|---|---|---|---|---|---|---|
| | Influent Air | Influent | Formed | Air | Wastewater | Sludge | Oil | Removed | Biodegraded |
| Air Effluent | 141703.967 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Primary Clarifier | 0.0 | 214868.542 | 0.0 | 7010.73768 | 201716.262 | 6141.54144 | 0.0 | 0.0 | 0.0 |
| Point | 0.0 | 592.570876 | 0.0 | 0.0 | 592.570876 | 0.0 | 0.0 | 0.0 | 0.0 |
| Air Effluent(2) | 69.0283365 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| AS-Diffused | 0.0 | 230752.235 | 0.0 | 47617.5024 | 45853.1809 | 0.0 | 0.0 | 0.0 | 137281.552 |
| Air Treatment | 690.283365 | 0.0 | 0.0 | 69.0283365 | 0.0 | 0.0 | 0.0 | 621.255029 | 0.0 |
| Anaerobic Digester | 0.0 | 6734.11232 | 0.0 | 690.283365 | 36.7199561 | 975.806029 | 0.0 | 0.0 | 5031.30297 |
| Secondary Clarifier | 0.0 | 45853.1809 | 0.0 | 1384.42271 | 14840.2144 | 29628.5438 | 0.0 | 0.0 | 0.0 |

**Figure 3-17 Contaminant fate table**

### OVERALL MASS BALANCE TABLE

On the left side of unit process contaminant fate table, an overall mass balance table is provided. The table shows the total incoming contaminant load and its fate in the system. The mass balance table for chloroform is as shown in **Figure 3-18**. It can be seen that, 47.3% of the incoming Chloroform is expected to go in the air stream, while 47.4% is expected to biodegrade.

Overall Mass Balance

| Contaminant Load | Mass (g/d) | % of total |
|---|---|---|
| Total Incoming | 300000.0 | 100.0 |
| Total Formed | 0.0 | 0.0 |
| To Air | 141772.996 | 47.2576652 |
| To Wastewater | 14840.2144 | 4.94673813 |
| To Sludge | 452.679886 | 0.150893295 |
| To Oil | 0.0 | 0.0 |
| Removed/Treated | 621.255029 | 0.20708501 |
| Biodegraded | 142312.855 | 47.4376183 |

**Figure 3-18 Overall mass balance table for Chloroform**

Just above the overall mass balance table, three command buttons are provided for visualizing the outputs in the graphical format, exporting the data to EXCEL and copying the Tables to

clipboard. Click on the **Show Graph** button to visualize the fate summary data in a graphical format. The Fate Summary tab contains a chart (**Figure 3-19**) providing a visual depiction of the various fate mechanisms of the contaminant for the whole layout. On the other hand the Emissions Summary tab contains a chart shows the mass emission rate from each process unit in the facility.

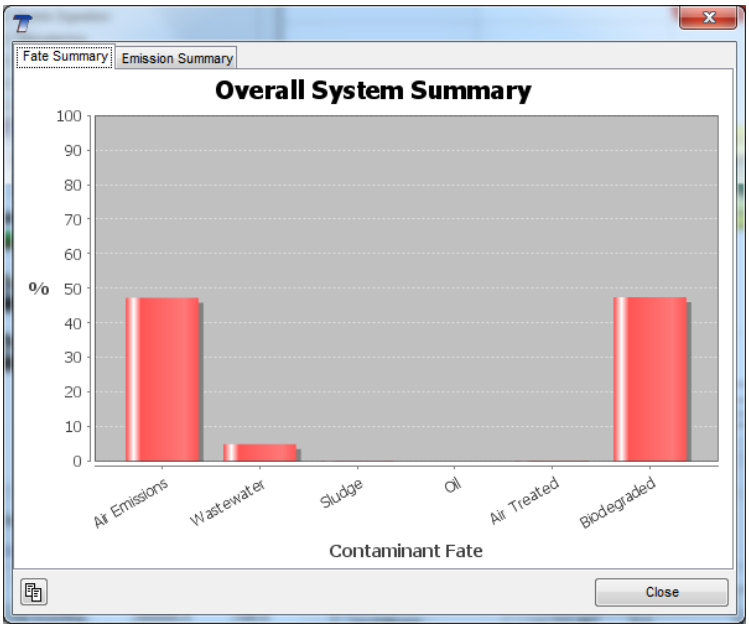



**Figure 3-19 Emission Summary chart**

### VIEW RESULTS FOR COMPLETE LAYOUT

To view the results for the layout in other formats, select the **View Results** in the **Model** menu. Alternatively, click on the **View Results** button available on tool bar. Activation of **View Results** opens a Results window with 4 output options. The output from each option is described below.

1. Air Emissions – Air emissions are tabulated for each contaminant from each process or vice versa.
2. Contaminant Fate – Group by contaminant – The fate of selected contaminant for all unit processes in the layout is summarized.
3. Contaminant Fate – Group by unit process – The fate of all contaminant at a selected unit process is summarized.
4. System States – Group by contaminant – For a given contaminant, the states are tabulated for each stream in the layout.

The first option of Air Emissions provides the summery of air emissions that can be used for preparing emission reports (**Figure 3-20**). The column and rows in the air emission table can be switched by using the row –column invert button provided on the top right of the table.

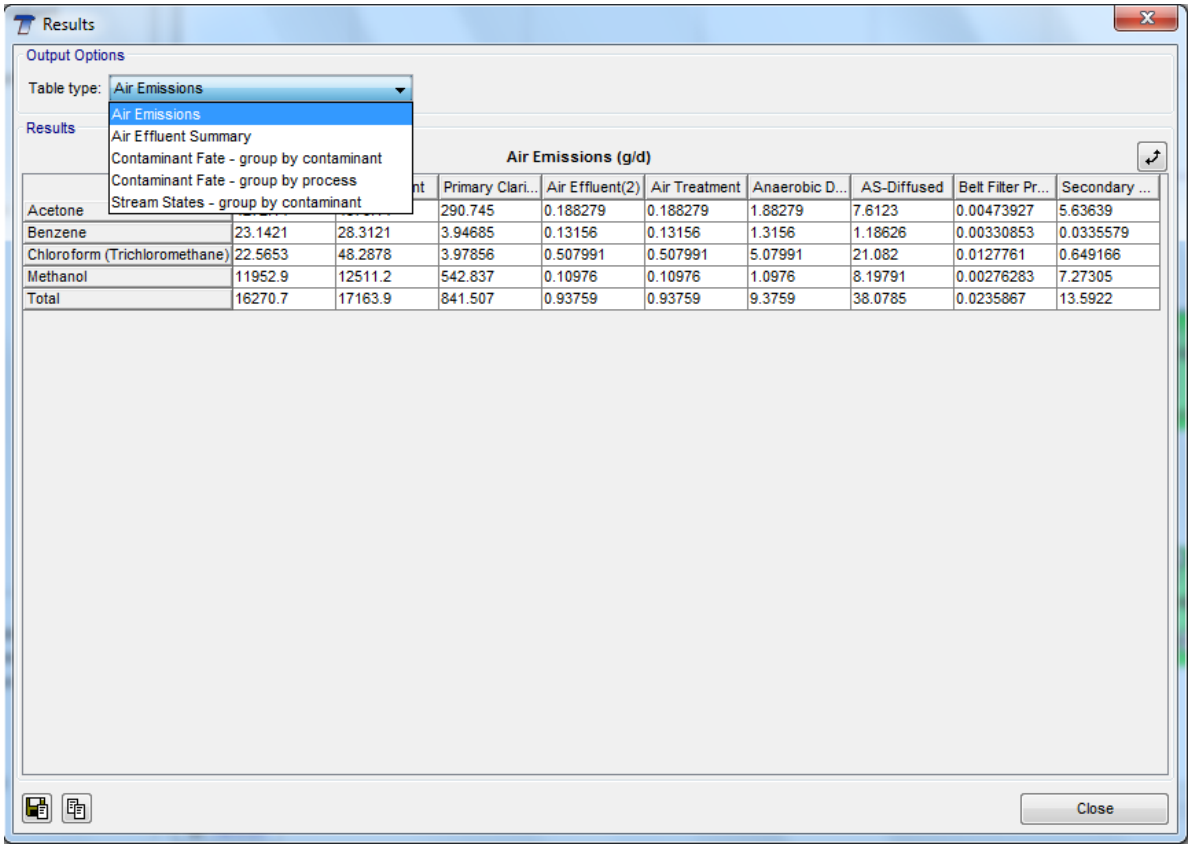



**Figure 3-20 Output Options Window for different Table Types**

Custom reports can be generated by using the Stream States – group by contaminant option. The user can click the Edit Properties button on the top right side of the table to select the Process Streams (effluent, sludge, air) and the state variables of interest associated with the process streams. In the stream and state selection window, all the streams and state variables are selected by default. Click on the **None** button for both the Process Stream choices and State Variable choices. Now, under the Process Stream choices, click to select the following:

Wastewater Influent
Air Effluent
Secondary Clarifier
Air Effluent (2)
Sludge Effluent

The individual influent and effluent streams for any unit process can be accessed by clicking on the + mark on the left of the process unit. Click on the + sign next to the Secondary Clarifier process to see all the influent and effluent streams. Depending on the requirement, the stream outputs can be included or excluded by selecting/deselecting the stream. For the Secondary Clarifier, de-select the stream with labels AS_eff, RAS (return activated sludge), Cl_air (air emission from clarifier) and WAS (waste activated sludge). Only Cl_eff remains selected, which is the treatment plant effluent.

Now expand Air Effluent process to see all the incoming streams. As all of the incoming air streams contribute to the total plant air emissions, let all the streams be selected. Note that Cl_air is the secondary clarifier air emission, which was de-selected in the clarifier unit process.

Now the state variables to be included in the report need to be selected. From the checklist, select Flow Rate, Total Suspended Solids, Organic Chemical Mass, Organic Chemical $C_l$, Organic Chemical $C_t$ and Temperature. The $C_l$ and $C_t$ represent the liquid phase and total (liquid and solid phase) concentrations of the organic chemical. The selections for the streams and states are shown in **Figure 3-21**. Click on the **Accept** button to see the output screen as shown in **Figure 3-22**.

The data shown in the screen is for Chloroform. To view the data for other compounds, simply click on the contaminant dropdown list above the table and select the compound of interest for the fate summary.

The tabulated data can be exported to EXCEL or clipboard by using the Export Data and Copy Table to Clip Board button provided at the top left side of the table.

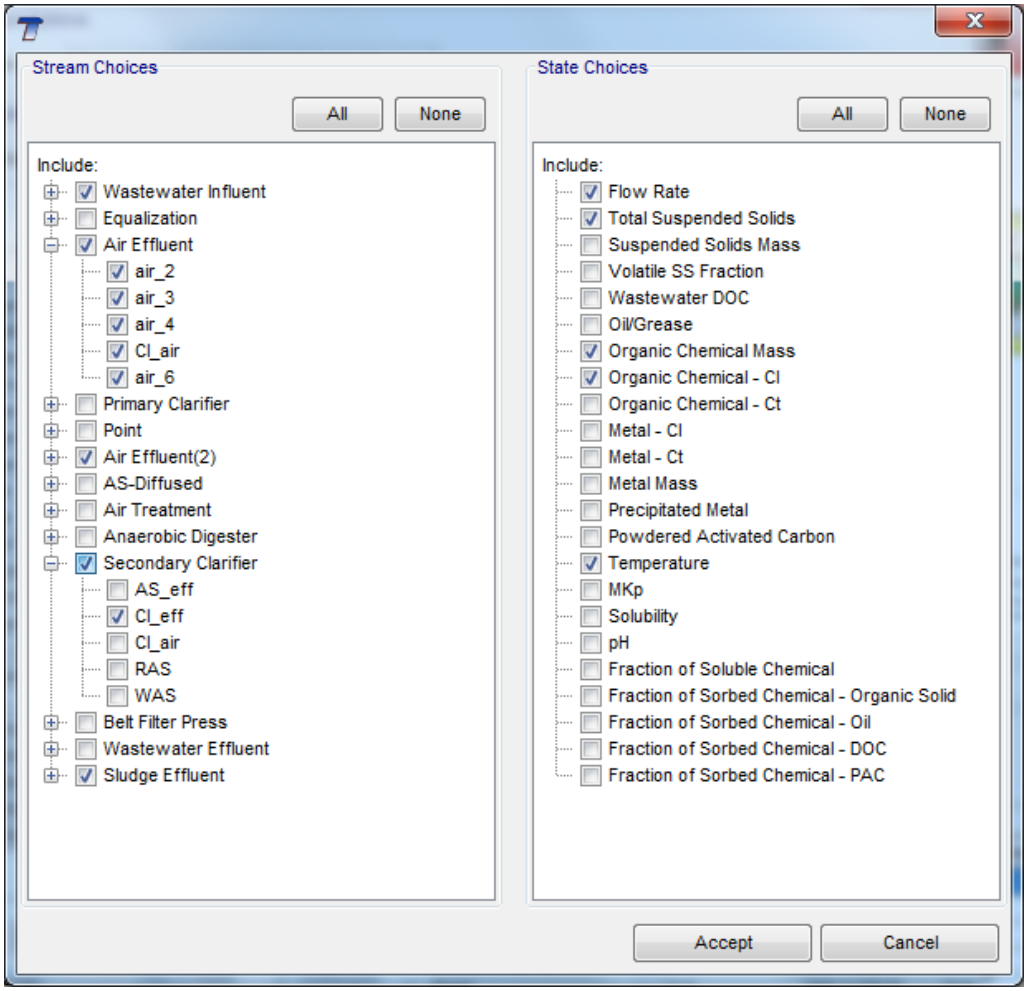
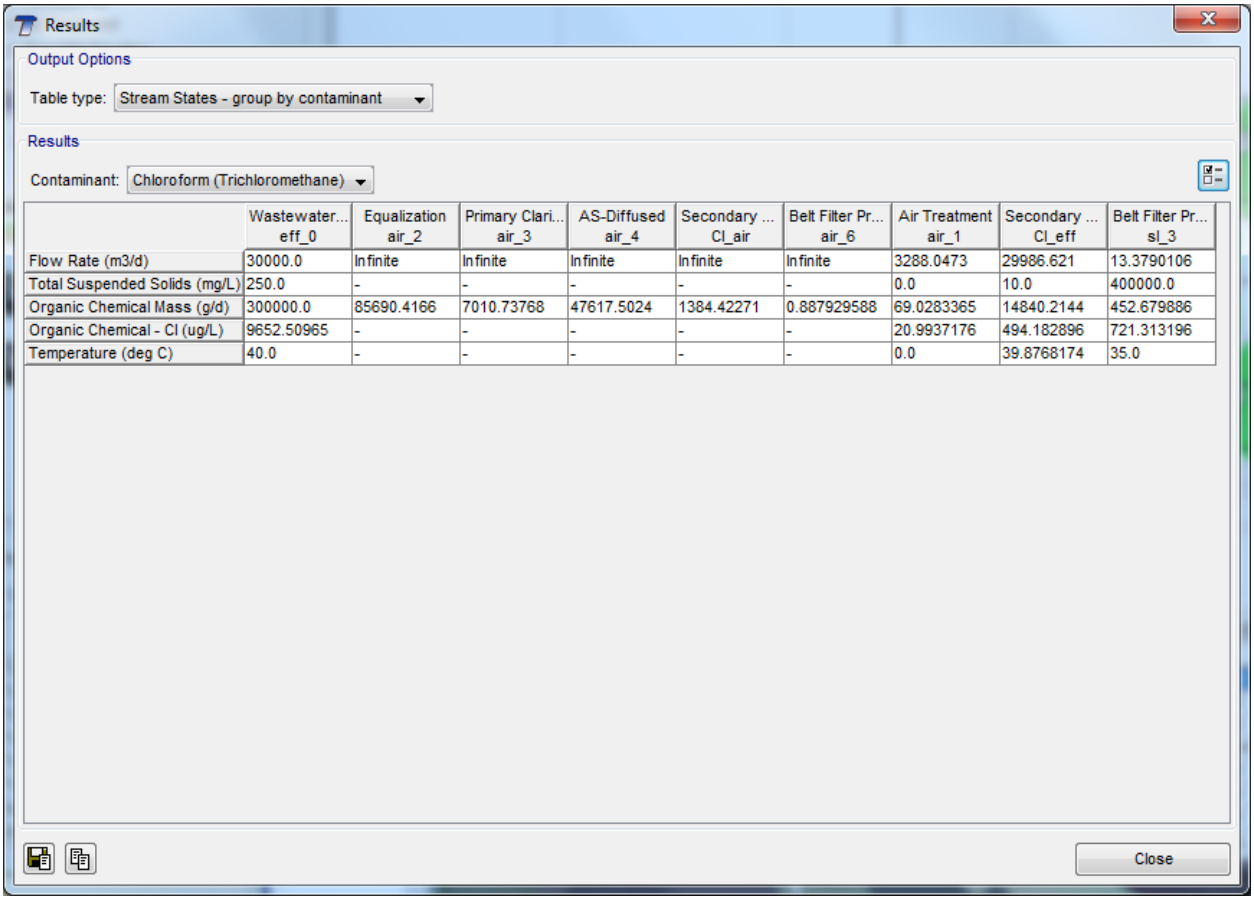



**Figure 3-21 Selection of Process Streams and State Variables for Report**




| | Wastewater... eff_0 | Equalization air_2 | Primary Clari... air_3 | AS-Diffused air_4 | Secondary ... Cl_air | Belt Filter Pr... air_6 | Air Treatment air_1 | Secondary ... Cl_eff | Belt Filter Pr... sl_3 |
|---|---|---|---|---|---|---|---|---|---|
| Flow Rate (m3/d) | 30000.0 | Infinite | Infinite | Infinite | Infinite | Infinite | 3288.0473 | 29986.621 | 13.3790106 |
| Total Suspended Solids (mg/L) | 250.0 | - | - | - | - | - | 0.0 | 10.0 | 400000.0 |
| Organic Chemical Mass (g/d) | 300000.0 | 85690.4166 | 7010.73768 | 47617.5024 | 1384.42271 | 0.887929588 | 69.0283365 | 14840.2144 | 452.679886 |
| Organic Chemical - Cl (ug/L) | 9652.50965 | - | - | - | - | - | 20.9937176 | 494.182896 | 721.313196 |
| Temperature (deg C) | 40.0 | - | - | - | - | - | 0.0 | 39.8768174 | 35.0 |

**Figure 3-22 Output Report for the Selected Streams and State Variables**

## 3.9 GENERATE REPORT

In addition to the above features for viewing and exporting data, TOXCHEM allows user to generate an elaborate report containing information for all the process units and flow streams. To generate a report, select **Generate Report** from the **Model** menu. In the Report Setup window (Figure **3-23**), keep the default settings in the Options and File Format items. Press **Accept** to start the process of report generation. If required, change the name of the file and/or directory where the file should be saved. If *view report on completion* selection box was checked in the Report Setup window then the report will be displayed in the Excel file format which was selected on the Report Setup window.

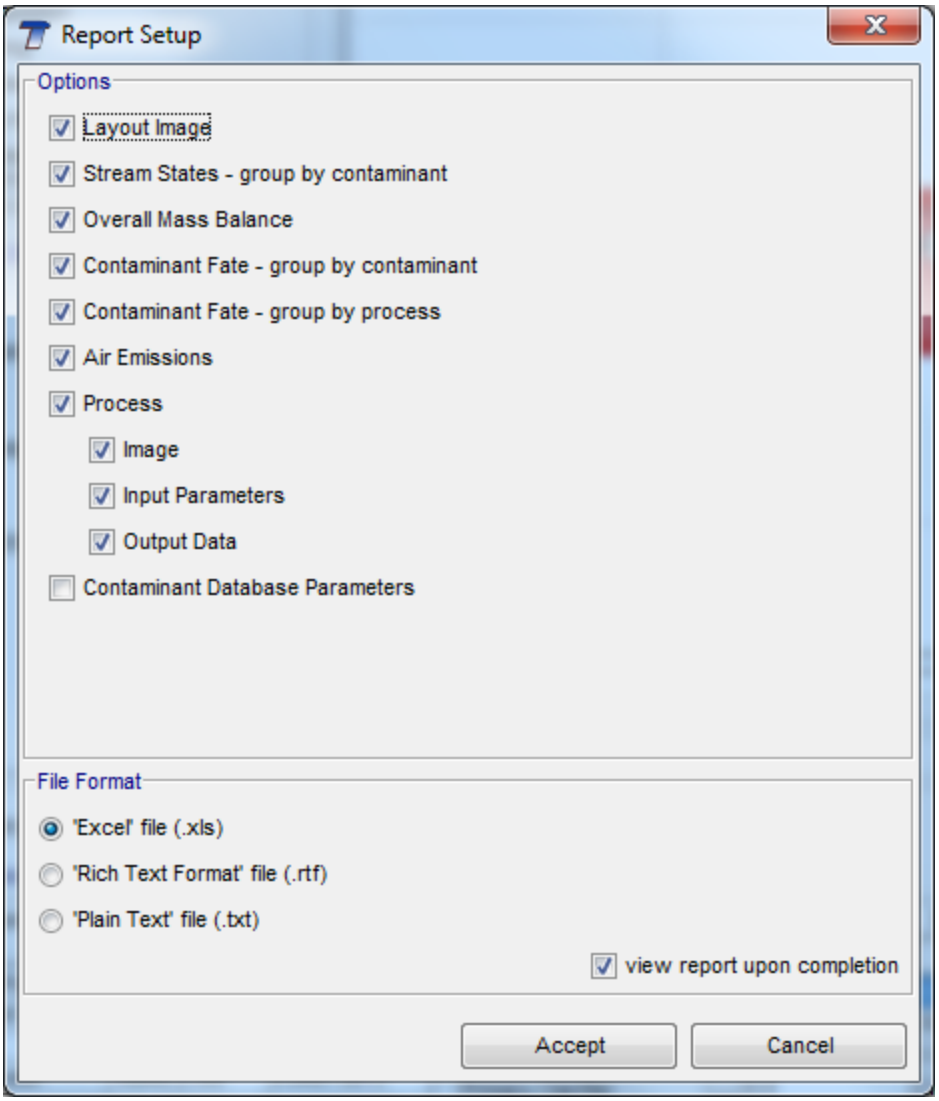



**Figure 3-23 Report Setup Window**

## 3.10 ADDING PARAMETERS ON THE QUICK ADJUST TOOLBAR

Display the quick adjust panel by clicking on the left pointed arrow on the divider between the drawing board and the quick adjust toolbar. In this exercise we will place the following parameters (**Table 3-5**) for different unit processes on the quick adjust panel.

**Table 3-5 Parameters to be Placed on Quick Adjust Toolbar**

| Object | Parameter |
|---|---|
| Influent | Flow Rate |
| Influent | Suspended Solids concentration |
| AS- Diffused Air | Air Flow Rate |
| AS- Diffused Air | MLSS concentration |
| Secondary Clarifier | Sludge SS concentration |

To place a parameter on the quick adjust toolbar, open the Data Entry form by right clicking on the object and selecting Edit Parameters. Right click on the parameter that needs to be placed on the quick adjust toolbar and click on the "Pin to Quick Adjust Toolbar" (**Figure 3-24**). Repeat the steps for each parameter to be placed on the quick adjust toolbar.

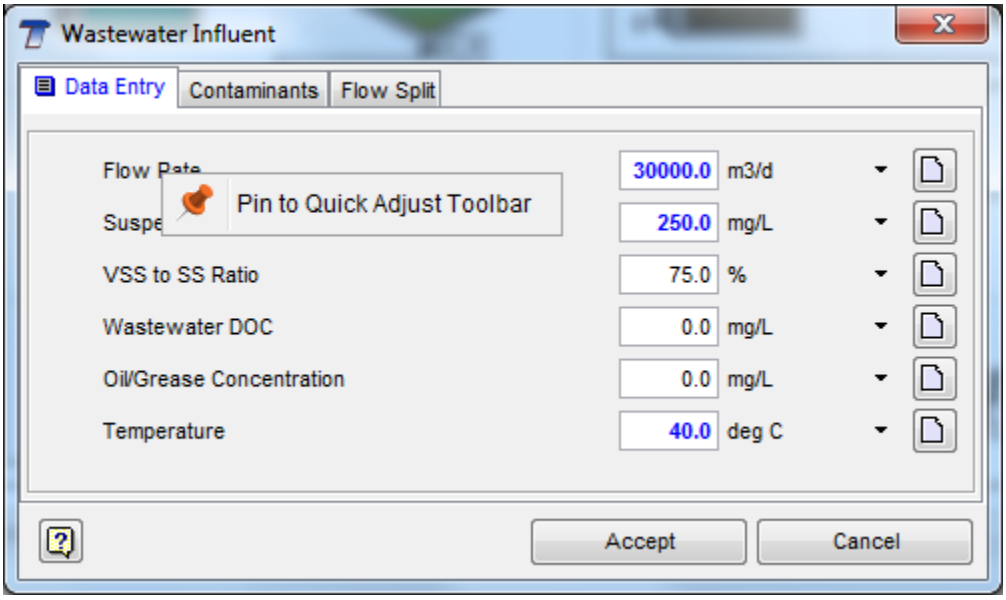



**Figure 3-24 Data Entry Form for Selecting Parameters for Quick Adjust**

After completion of the above procedure the Quick Adjust Toolbar on the right hand side look like **Figure 3-25**.

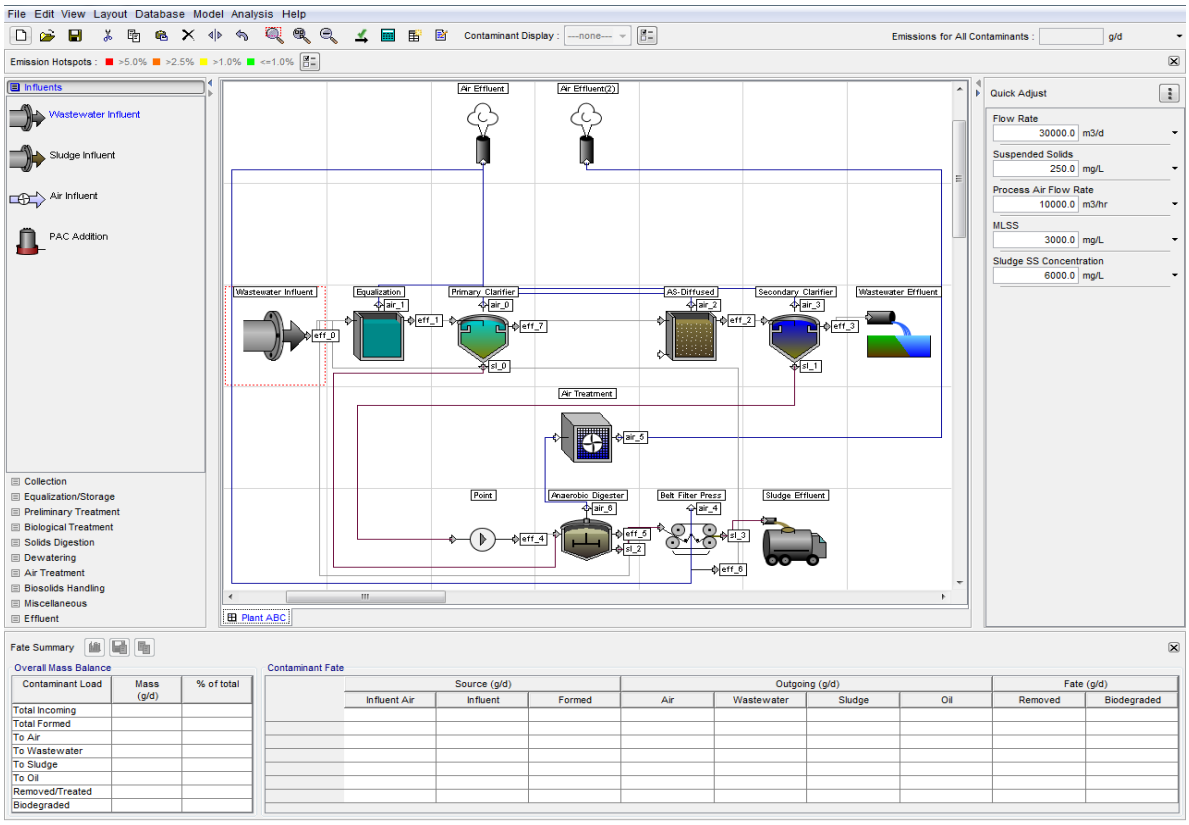



**Figure 3-25 Quick Adjust Panel with Selected Parameters**

To differentiate between various parameters, it is a good idea to label these using the “Add a Label” command from the Options button available at the top –right of the quick adjust panel. Select the parameter above which a label needs to be placed e.g. Flow Rate and click on the Options button and Select “Add a Label”. In the New Label, add Influent ABC and press OK. The label Influent ABC will appear above the Flow Rate Parameter. Similarly add AS-Diffused and Secondary Clarifier Labels to distinguish the parameters belonging to different unit processes. After adding the labels, the completed model shall appear as shown in **Figure 3-26**. If while adding the label, the label appears at wrong place, it is possible to click and move it around. To remove a label, right click on the label and select Remove Label.

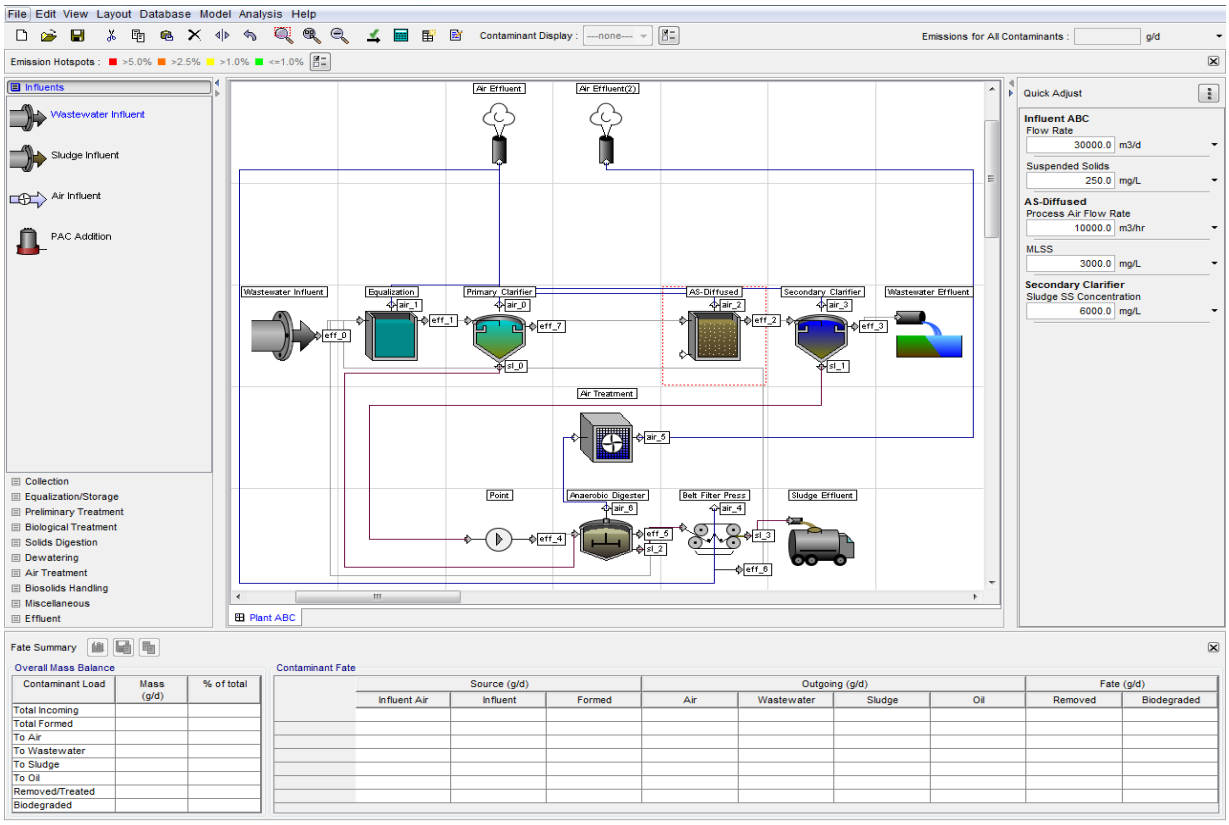



**Figure 3-26 Quick Adjust Toolbar with Labels**

New in V4.3 is the ability to vary the values of compound physical and chemical properties of user-defined chemicals. For example, the impact of varying a first order biodegradation rate coefficient can be tested by pinning the parameter to the toolbar. First create a user-defined compound representing triclosan, an anti-bacterial agent. Find and select the user-defined compound in the database. Click on the "biodegradation" tab, then right click on the aerobic biodegradation rate (Kb) at 20 $^{o}$C for liquid processes. Click on the "Pin to Quick Adjust Toolbar" box to send the rate coefficient to the toolbar. Once it appears on the Quick Adjust toolbar, create a label for the property indicating it is the biodegradation rate coefficient for the user-defined compound triclosan. The Quick Adjust toolbar now looks like the figure below.

.

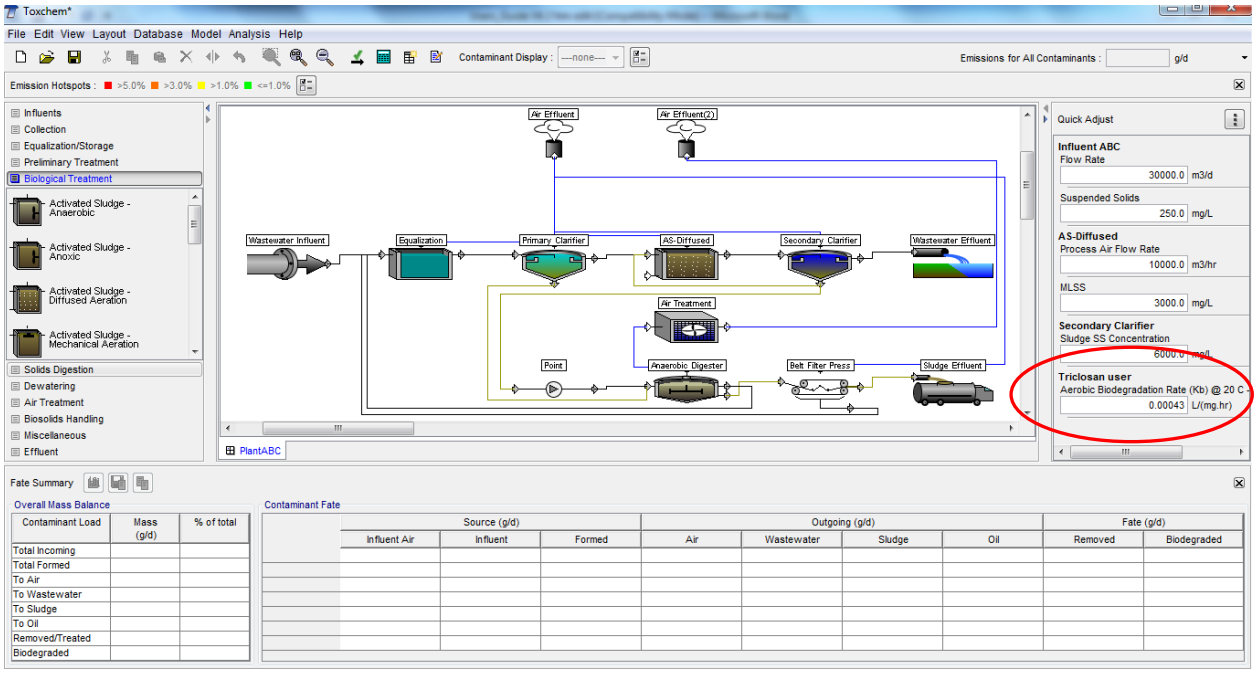



**Figure 3-27 Quick Adjust Panel with Selected Parameters**

Once the important parameters are placed on the Quick Adjust Toolbar, it is possible to easily change the parameters values for different simulations. In this exercise change, the Influent flow rate from 30,000 $m^3$/d to 50,000 $m^3$/d and run the model to see the changes in the air emission. Change the value back to 30,000 $m^3$/d before continuing with the following exercise.

## 3.11 ADDING USER-DEFINED COMPOUNDS

Although the compound database in TOXCHEM is extensive (~800), the compound of user interest may not be available in the database. Compounds can be added to the TOXCHEM database and used in modeling. Adding new compound is often useful if user wants to compare the fate of compound with different values of a chemical property (or more than one property). Compounds with user defined properties can be saved as compoundname-1, compoundname-2, and so on, in the database. The user defined compounds then can be included in the influent wastewater as compounds for evaluation. Afterwards, any compound which is no longer of interest can be deleted from the database.

### ADDING A NEW COMPOUND

**Note**: The chemical property set associated with each organic compound has an updated look since V4. A set of tabs are used to group similar properties. A few additional properties such as weak acid/base dissociation coefficients are added in the database.

In the present example, we are going to add a new compound called "test1" in the organic chemical database. From the tutorial plant configuration established above select the **Organic**

**Chemicals Database** from the **Database** menu. The first compound in the Organic Chemical Database list is 1-2 Dimethylnapthalene, as shown in **Figure 3-28**.

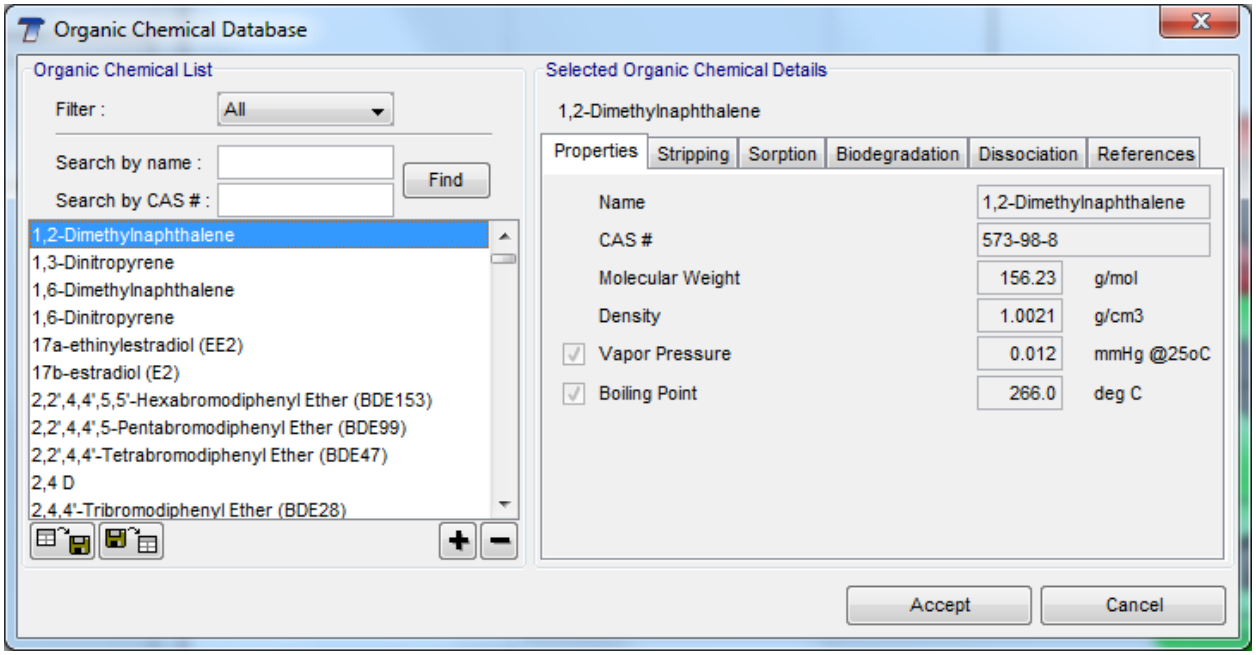



**Figure 3-28 Organic Chemicals Property Set**

To add a new contaminant in the list, click on the Create New Contaminant (+ sign) button available at the bottom right of the contaminant list window. Clicking on the + button create a copy of the compound which was selected initially. As soon as new compound is created, all the property fields become editable. To change the name of the compound click on the Name field and change the name to *test1.* This will change the name of the compound and shift its location in the list according to the alphabetical order. Change the properties of the *test1* according to the values provided in **Table 3-6**. After entering all the information, set the contaminant Filter to User-Defined to see the *test1* in the contaminant list (**Figure 3-29**). Once the user compound is added, press enter to close the window. Do not forget to press **Accept** to save the compound in the database. It is better to create a copy of the contaminant which has similar property to the new compound. To search a compound of interest, use the Search by Name or Search by CAS# search options.

**Table 3-6 Property values for input to User Compound "Test1"**

| Parameter | Value | Tab |
|---|---|---|
| CAS No. | 108-21-4 | Properties |
| Molecular Weight | 102.13 | Properties |
| Density | 0.87 | Properties |
| Vapor Pressure | Unchecked | Properties |
| Boiling Point | Unchecked | Properties |
| Henry's Law Coefficient at 25$^{o}$C | 0.01517 | Stripping |
| Van't Hoff A for estimating H | Unchecked | Stripping |
| Van't Hoff B for estimating H | Unchecked | Stripping |
| Log Octanol/Water Partition ($K_{ow}$) | 1.36 | Sorption |
| Sorption Suspended Growth, $K_p$ | 0.085 | Sorption |
| Sorption Fixed Growth, $K_p$ | Unchecked | Sorption |
| Sorption- Wastewater DOC ($K_{doc}$) | Unchecked | Sorption |
| Isotherm for Carbon ($K_c$) | Unchecked | Sorption |
| Isotherm for Carbon (1/n) | Unchecked | Sorption |
| Sludge Process - Anaerobic Biodegradation Rate | Unchecked | Biodegradation |
| Sludge Process – Aerobic Biodegradation Rate | 0.0037 | Biodegradation |
| Liquid Process - Aerobic Biodegradation Rate $K_b$ | 0.0037 | Biodegradation |
| Liquid Process - Aerobic $K_s$ | Unchecked | Biodegradation |
| Liquid Process – Anoxic Reduction Factor | 0.8 | Biodegradation |
| Liquid Process – Anaerobic Reduction Factor | 0.1 | Biodegradation |
| Classification | Acid | Dissociation |
| First Acid Dissociation Coefficient | 6.8 | Dissociation |
| Second Acid Dissociation Coefficient | Unchecked | Dissociation |

**Note:** To add multiple compounds, press + after one compound is entered and repeat the steps described above. There is no need to press **Accept** after entering each compound. However, once all the compounds are entered, it is necessary to press **Accept** to confirm the changes. A user defined contaminant can be deleted by selecting the compound from the contaminant list and pressing Delete Contaminant (- sign) button next to Create New Contaminant (+ sign) button. To incorporate the new contaminant in the layout calculation, follow the same procedure as described in data entry for influent object.

Any user-defined compound will be added alphabetically to the database list and its name appears in blue color. Compounds with numbers (e.g. 1,4 dichlorobenzene) appear before alphabetical characters that start compounds. A user-defined compound is identified by a blue font compared to the black font of the pre-defined compounds. To quickly view the list of user-defined compounds, use the "Filter" dropdown selection and click on **User-defined**. It may be a good idea to create new contaminants with a specific prefix (e.g. User_ etc.) for easy identification.

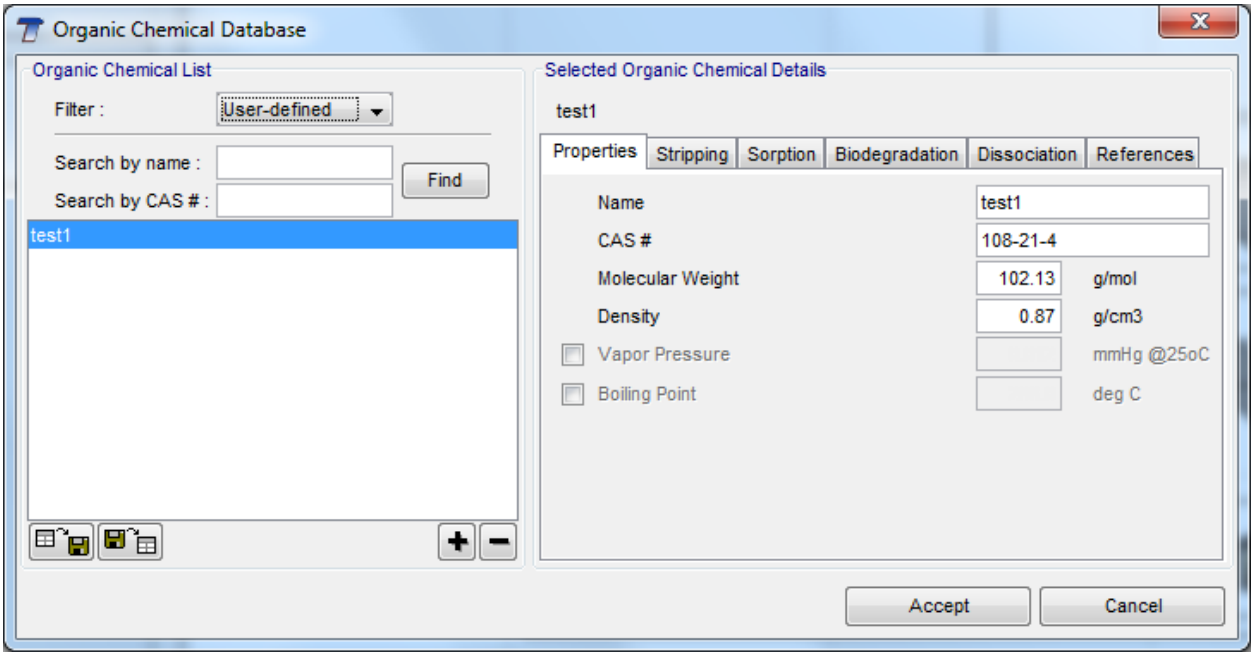



**Figure 3-29 User Defined Contaminant**

## 3.12 SENSITIVITY ANALYSIS

The sensitivity analysis feature is a useful tool in TOXCHEM. It allows the user to see the effect of various design and operating conditions on the fate of the contaminants in the wastewater treatment plant. In essence, the sensitivity analysis adjusts the magnitude of the parameter of interest while holding all other test conditions constant. This enables the user to assess which factors are the most important in governing air emission rates or effluent concentrations.

To illustrate the use of the sensitivity analysis, the effect of a change in the aeration rate in the diffused activated sludge process on the fate of chloroform will be evaluated.

### SETTING THE SENSITIVITY ANALYSIS

Once a treatment plant layout is properly configured, it is possible to run the sensitivity analysis. To setup a sensitivity analysis, select **Sensitivity Analysis** from the **Analysis** menu. On the Sensitivity Setup window (**Figure 3-30**) set the Chloroform, AS-diffused and Air flow rate in the Contaminant, Process and Parameter selection fields respectively. Leave the View effect field at its default value.

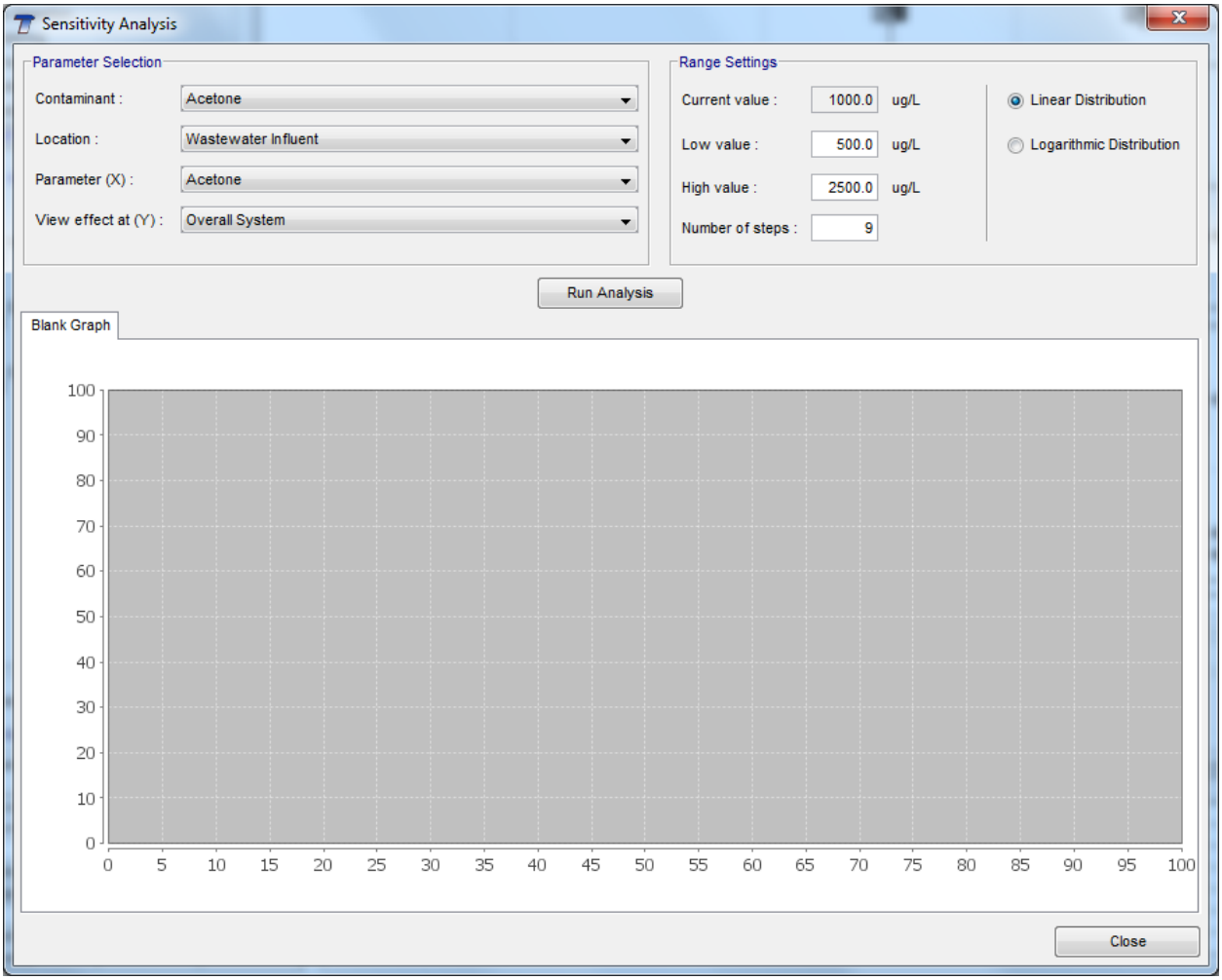



**Figure 3-30 Sensitivity Analysis window**

## SETTING THE SENSITIVITY RANGE

The range over which the sensitivity analysis is to be assessed must be specified. To do this, first note the current value specified in the process unit is10,000 $m^3$/h. Suppose that the analysis is to examine the effect on chloroform fate over a range of 5,000 to 50,000 $m^3$/h of air flow rate. Set the low value for the range at 5000 $m^3$/h and the high value for the range at 50,000$m^3$/h. Set the number of steps at 10 to obtain a sufficient number of points for assessment.

## RUNNING THE SENSITIVITY ANALYSIS

Click the **Run Analysis** button to initiate the sensitivity analysis. When it is finished, the results of the analysis are reported under different tabs of Percentage-graph, Mass Loading-graph, Percentage - table and Mass Loading- table. By default, the sensitivity analysis results are shown on the Percentage-graph tab (**Figure 3-31**). The graph on Percentage-graph tab indicates that the increase in aeration rate increases the fraction of chloroform that is stripped/volatilized, while decreasing the fraction biodegraded. On the left side of the graph, the

yellow color Up and Down arrows may be used to change the scale of the graph. Use the yellow color rectangle to reset the scale. The graph legend may be turned On/Off by using the Graph Legend button below the yellow arrow pointing down. To copy the graph to the clip board, use the Copy Image to Clipboard button available below the Graph Legend button. Try clicking on other tabs of Mass Loading-graph, Percentage-table and Mass Loading- table to familiarize with the sensitivity analysis outputs.

In some cases, the range of the sensitivity analysis variable may span over several orders of magnitude. In such situation, it may be better to plot the data on a logarithmic scale rather than on a linear scale. In the Range Settings header box, user can easily switch between the options of Linear Distribution/Logarithmic Distribution. Note that the data curves in the charts remain essentially unchanged after the selection is changed from Logarithmic to Linear Distribution, however, on the X-axis there are more data points at lower air flow rates than that in the linear distribution.

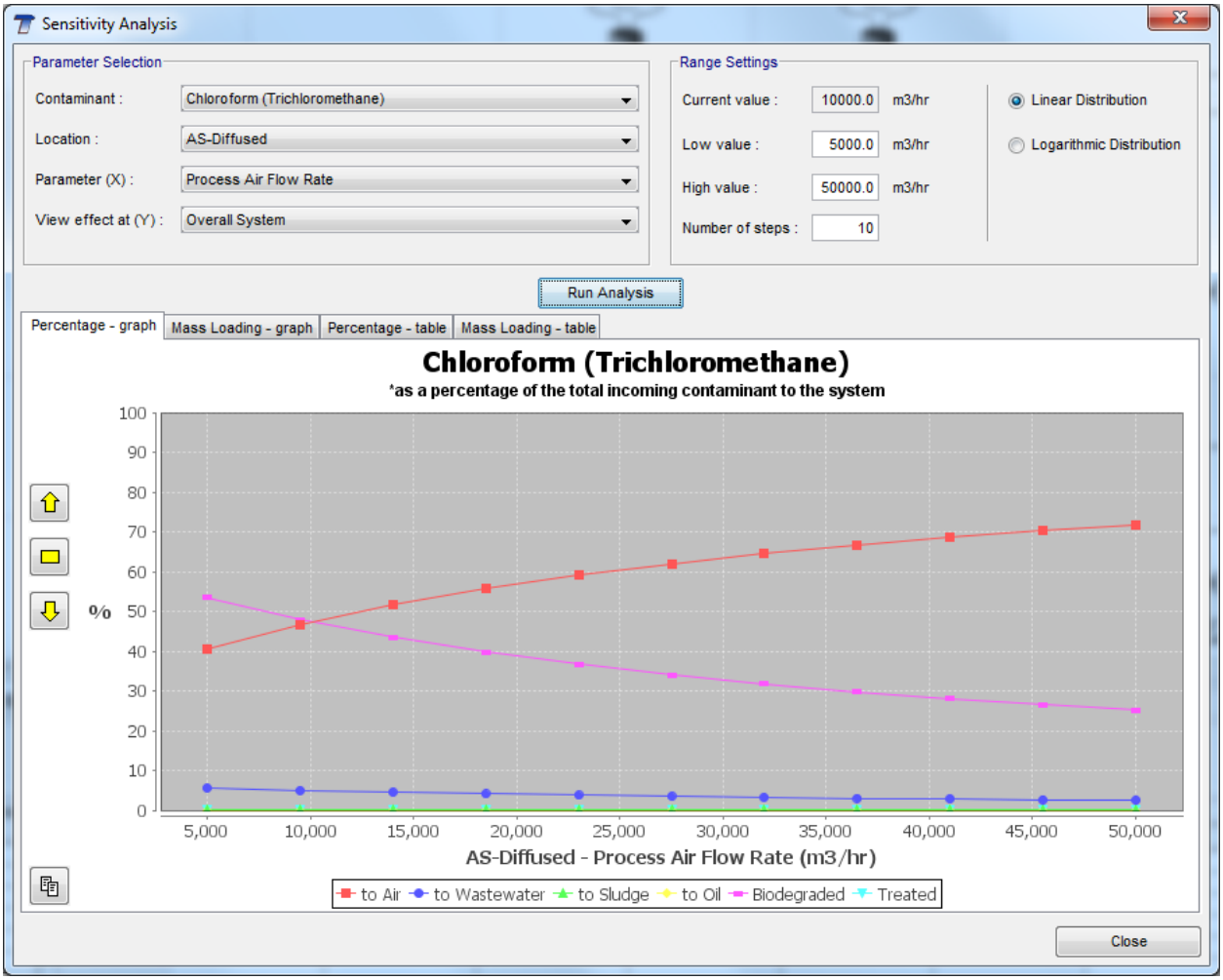



**Figure 3-31 Sensitivity Analysis Output Chart**

## 3.13 USE OF BACK-SOLVER FEATURE

The back-solver feature of TOXCHEM enables user to determine, for example, the required concentration of a contaminant in influent to meet certain specified emission criteria in a downstream process unit for a selected contaminant. There are a number of possible ways that back-solving may be applied. For example, to stay within total emission limits, the air loading from an activated sludge tank is not to exceed a certain mass rate. The back-solver can work from the specified maximum air loading of the contaminant to arrive at the maximum concentration arriving at the treatment plant. As another example, one may wish to check the concentration in an air stream to ensure that the compound does not exceed the lower explosive limit (LEL). By back-solving from the gas concentration in an enclosed headspace to the influent concentration, it is possible to determine the maximum allowable concentration arriving at the plant to avoid exceeding the LEL in the headspace location. Another application may relate to the quality of residual solids disposed of off-site. Suppose the concentration of a contaminant is not to exceed a certain value in the residual sludge disposed of off-site. We can determine what the maximum concentration in the influent will be to avoid reaching the ceiling value.

The TOXCHEM back-solver can be setup with respect to following output variables:

Soluble aqueous concentration

Total aqueous concentration

Gas concentration

Mass air emission rate

Solid sludge concentration

Total sludge concentration

Total sludge dry weight.

### Configuring the Back-Solver Window

**Note**: The layout of the back-solver window has been substantially altered from previous versions to provide a simpler interface for set-up.

The back-solver set up window can be accessed by selecting **Back-Solver** from the **Analysis** menu. In the back-solver setup window, the setup options are organized under two tabs i.e. “Target Solution” and “Influent Manipulation”. For this example, three scenarios as listed in **Table 3-7** will be tested. On the Target Solution tab, enter the values from **Table 3-7**. Move through the Table one contaminant at a time. Click on the “+” button to add the next scenario after all the inputs for the first contaminant are complete. Repeat the process for the third contaminant. When the three scenarios have been entered, the dialog box should appear as in **Figure 3-32**.

**Table 3-7 Inputs for Tutorial Back-Solver Scenarios**

| Scenario Name | Contaminant | Solution Type | Process Location | Solve to Value |
|---|---|---|---|---|
| Methanol Ct SC | Methanol | Total aqueous concentration | Secondary Clarifier | 0.02 mg/L |
| Benzene MAER AS | Benzene | Mass Air Emission Rate | AS-diffused | 1.0 g/d |
| Chloroform TSDW BF | Chloroform | Total Sludge Dry Wt. | Belt Filter Press | 0.5 mg/kg TS |

Notes: leave the solution accuracy at 0.01%.

On the Influent Manipulation tab, leave the influent maximum concentration and influent manipulation to its default value for all the scenarios.

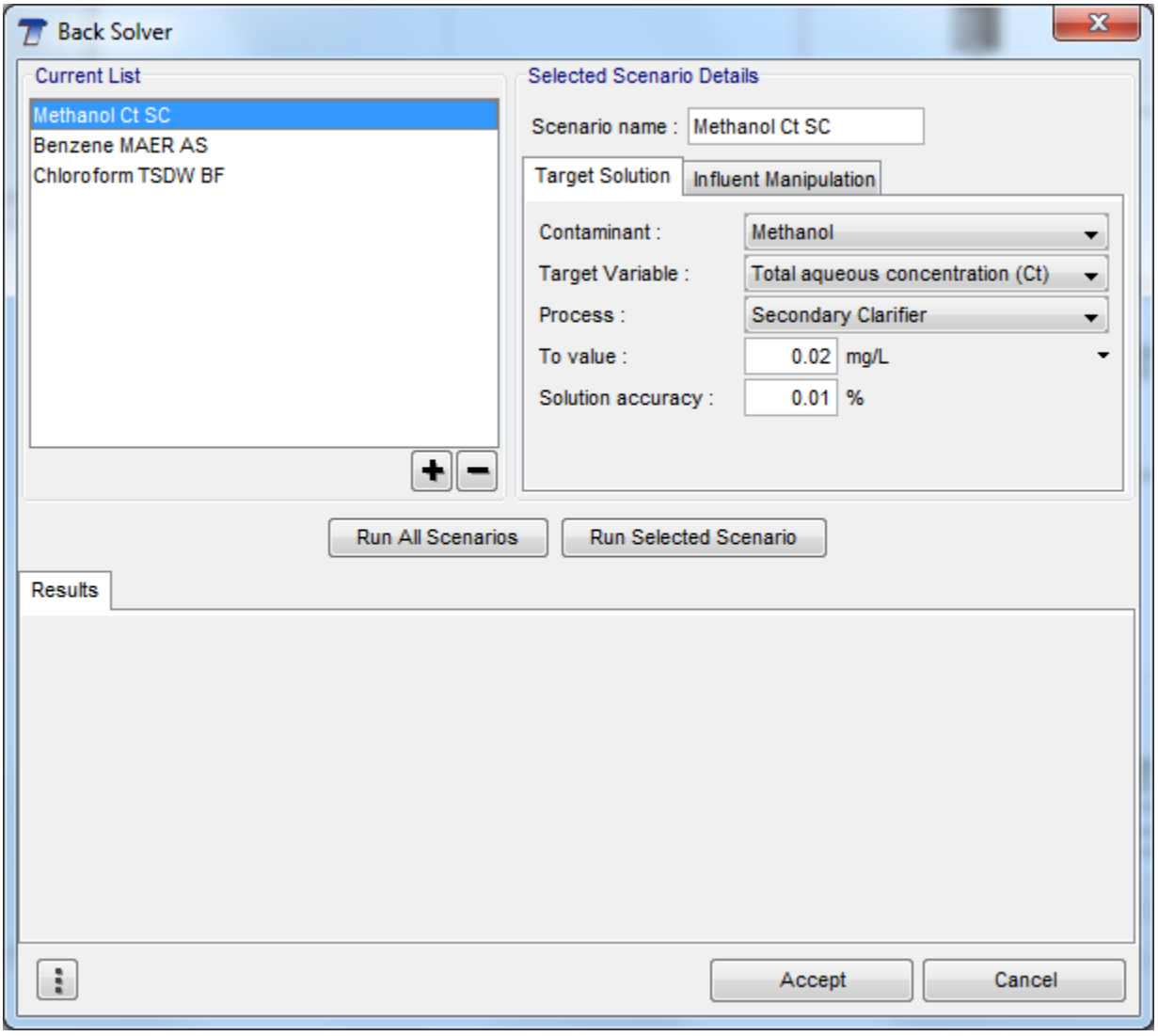



**Figure 3-32 Completed Back-Solver Scenarios**

## RUNNING SCENARIOS

The configured scenarios can be solved by pressing **Run All Scenario** button or **Run Selected Scenario** button. For example, click on the chloroform scenario and then click on the **Run Selected Scenario** button. The back-solver iterates to the solution and outputs the results of simulation in the Results tab. In this exercise, press the **Run All Scenario** button to run all the scenario one after other. The **Back-Solver** results are presented in individual scenario named tabs. The typical output from back-solver scenario analysis is as shown in **Figure 3-33**.

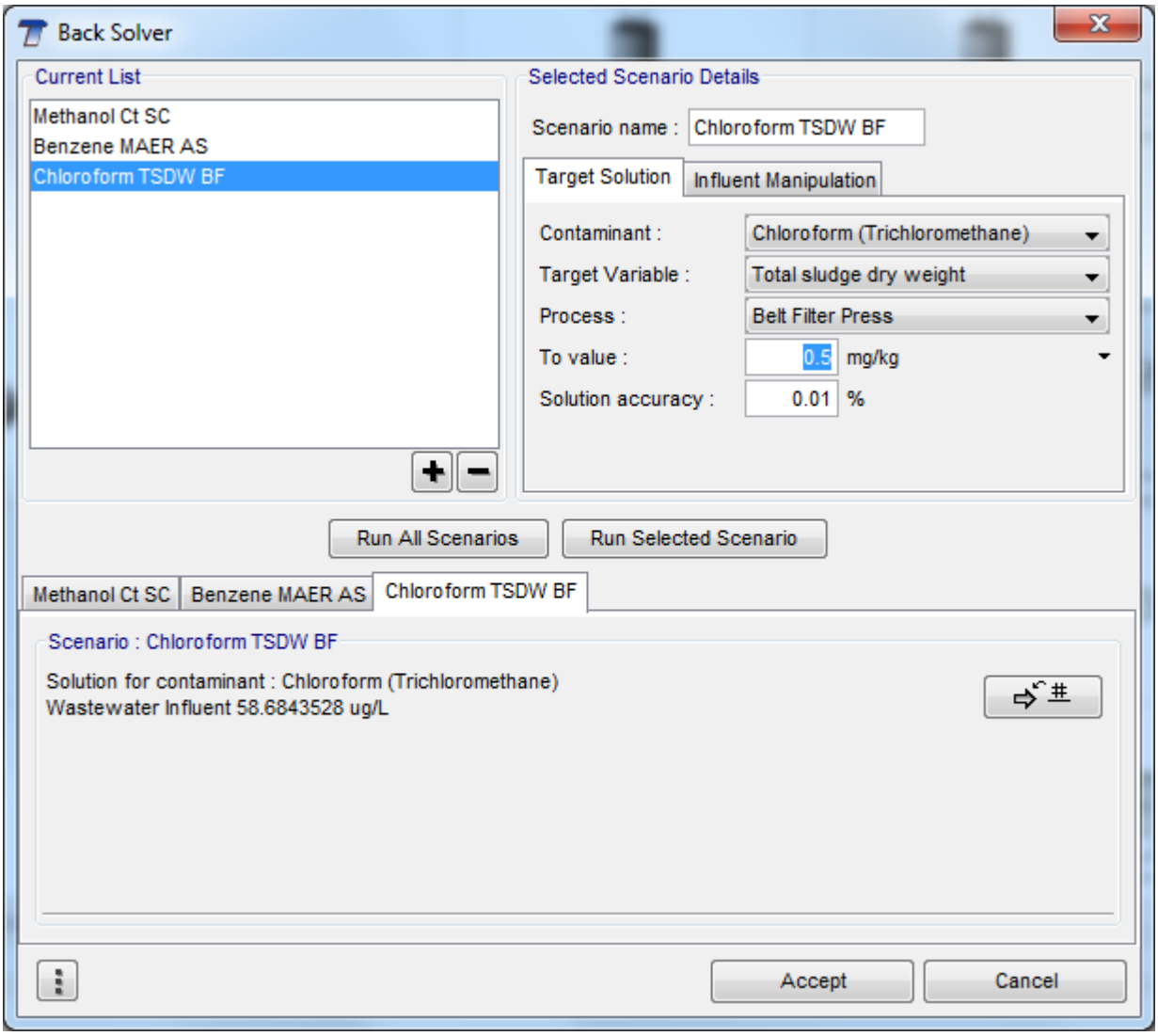



**Figure 3-33 Results for Back-Solving of Chloroform Scenario**

The back solver estimated influent concentration can be directly transferred to the influent wastewater data input by clicking on the button to the right of the solution (a right-pointing arrow and # sign). A pop up confirmation message appear. Click on the transfer button to transfer the estimated value for all the three contaminants from respective tab. Close the Back Solver

window and go to influent unit process and check that the estimated concentration values are correctly updated. Run the simulation again with the new values and verify that the outputs at the respective unit process are as expected with the new influent concentrations.

The options button at the bottom left of the window presents other options of exporting/ importing back solver scenario settings to/from EXCEL file. Also the option of transferring back solver estimated values for different scenarios to the influent object is available for easy transfer of estimated values.

Consider now the ability added in V4.3 to solve for the required influent flow rate that would result In a sludge flow rate of 480 $m^3$/d from the primary clarifier. After accessing the back-solver, for the Target Solution, click on the Stream State button, and select “Flow Rate” from the list of state variables, Primary Clarifier as the Process and Effluent-Sludge as the stream type. Setr the target flow of primary sludge to 480 $m^3$/d. Call the scenario name “Sludge flow at Prim Clar”. The scenario result provides an influent wastewater flow rate as indicate in the **Figure 3-34** below.

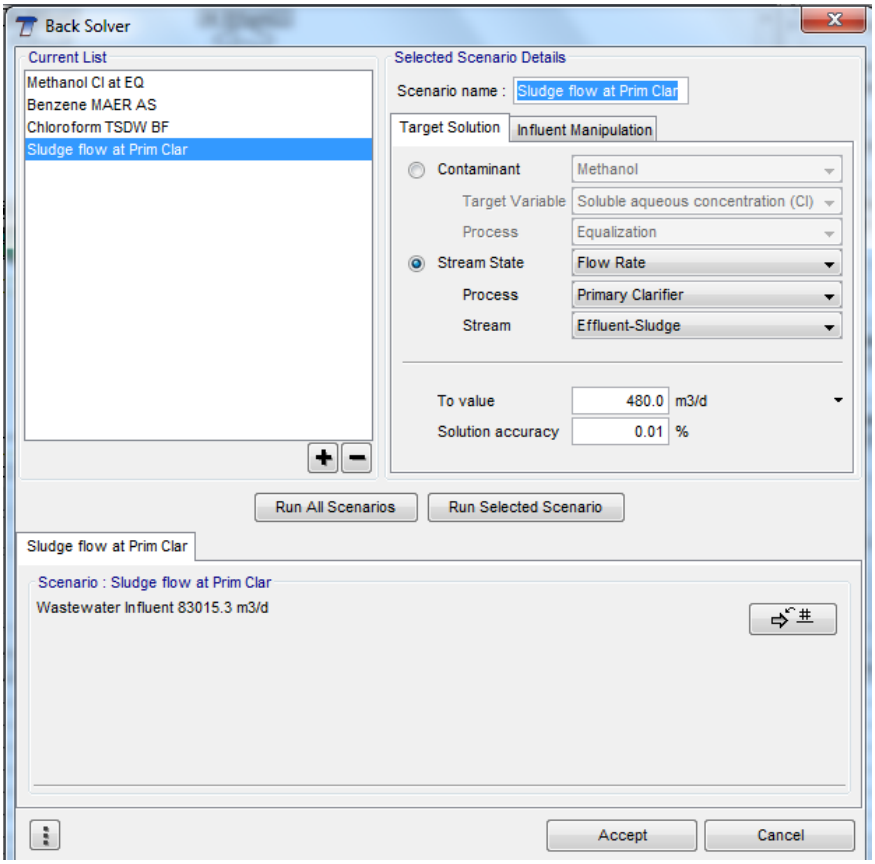



**Figure 3-34 Back-solver results for flow rate**

# 4.ADDITIONAL TOPICS

In this chapter a few additional topics are discussed to help the user understand TOXCHEM V4.3 functionalities.

## 4.1 IMPORTING V3 LAYOUTS

### LAYOUTS WITH COMPOUNDS IN STANDARD DATABASE

For importing the layouts in which only the contaminants from the standard V3 database are modeled, use the **File – Open** command to open the V3 layouts with .wtp extension. If the layout contains unit process of DAF, newly defined oil connection will have to be connected to an oil effluent before the layout could be simulated.

### LAYOUTS WITH USER DEFINED COMPOUNDS

If the layout contains a user defined contaminant in it, then it is first necessary to import the user defined compound database in the V4 database before importing the layout. The V3 user defined contaminant database file shall be available in the TOXCHEM V3 install directory. The user chemical and metal database files are named USCHEM3.DB and USMETAL3.DB respectively. To import these V3 user database files in V4 and later, following step may be used for importing organic chemical compound data.

1) Select **View Organic Chemical Database** from the **Databases** menu item
2) Click on the **Import Database from File** command button available on the bottom left of the organic compound display panel.
3) Select the database file

If the name of the user defined contaminant does not conflict with the compound name already existing in the database, the compounds will be imported into the database. Set the filter to User-Compounds to see the list of imported compounds. If a conflict is found then a pop-up window will show up (**Figure 4-2**), presenting several choices for overwriting, skipping or appending a descriptor to the name of the conflicting compounds.

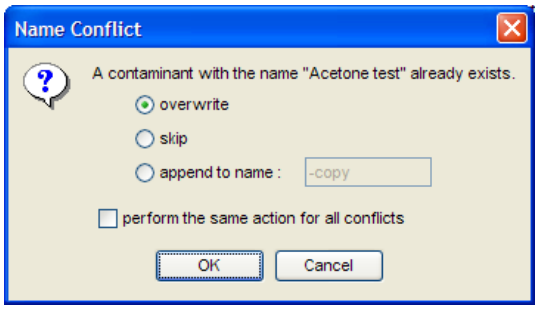



**Figure 4-1Choices when importing user compound which pre-exist in database**

Same steps can be followed for importing the metal compounds, except that in step #1, select **View Metals Database** instead of **View Organic Chemical Database** from the **Database** menu**.**

After importing the user defined database, import the layout by following the steps listed in previous section.

**Caution**: Due to the differences in the grid structure of V3 and V4 (or later versions), it is sometimes possible that all of the unit processes defined in V3 are not imported in V4. In such situation, user may have to modify V3 layout to make it compatible for V4 import. If you encounter this issue, please contact Hydromantis for more details regarding how to modify your V3 layout.

## 4.2 HOW TO CREATE USER DEFINED GROUP OF CONTAMINANTS

The user can create a user defined group of contaminants, which are regularly used in analysis. By using a user defined group of contaminant, the user can avoid the step of individually selecting the contaminant each time. Following steps may be used to create a user defined group of contaminants.

1) Select **Edit 'Quick Select' Groups** from the **Database** menu item
2) In the Quick Select Contaminant Groups window as shown in **Figure 4-2**, click on the + button next to select group and enter the name of the group in the pop up window.
3) Find the contaminant name from the organic chemicals or metals and press the transfer arrow to transfer the contaminant to the Current chemicals window.
4) For example, if you enter "Test" as the group name containing Benzene, Ammonia and Dichlorobenzene 1,2, the Quick Select Contaminant Groups window should look as shown in **Figure 4-3** after the first three steps.
5) Press **Accept** to create the group.
6) You can easily add the group of contaminants in an influent object by pressing on the **Quick Select** button (**Figure 4-4**) and selecting the contaminant group of choice.

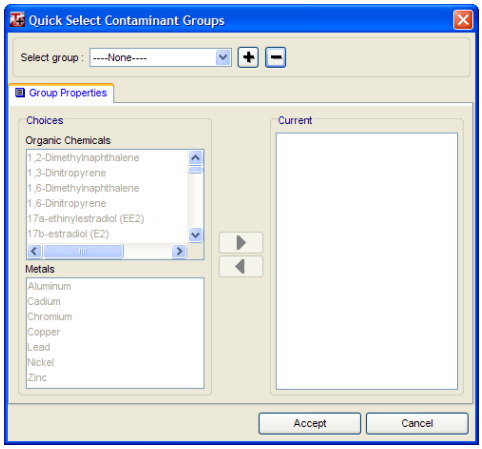



**Figure 4-2 Quick Select Contaminant Groups window for creating/editing contaminant groups**

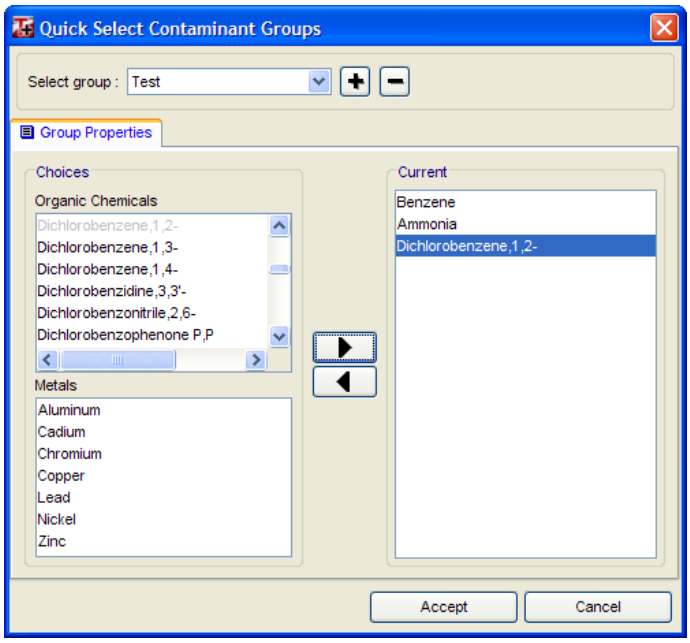



**Figure 4-3 Window showing the user defined contaminant group "Test"**

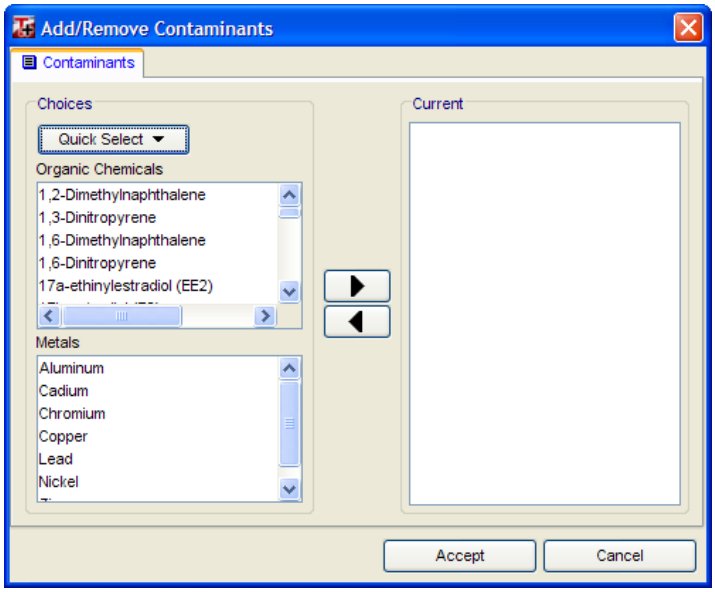



**Figure 4-4 Using Quick Select to add the contaminant group to an influent object**

## 4.3 HOW TO SET SRT BASED WASTAGE IN SECONDARY CLARIFIER

TOXCHEM V4 (and later) allows users to automatically estimate the Waste Activated Sludge (WAS) flow rates based on the Sludge Retention Time (SRT) specified in the biological tanks. This SRT based WAS flow waste algorithm is in addition to the method of specifying the sludge flow rate split fractions. The SRT based WAS flow rate estimation method is available only when there are two streams originating from the underflow of the secondary clarifier. To setup the SRT based WAS flow rate estimation, following steps may be used.

1) After the process layout is completed with all the stream connections, right click on the secondary clarifier object and select **Edit Parameters** item. Access the **Flow Split** tab. The Secondary Clarifier with the Flow split tab shall appear as shown in **Figure 4-5**.
2) In the **Flow Split** tab select the Calculate split fractions. This shall change the Flow Split window to as shown in **Figure 4-6**.
3) SRT based WAS flow rate estimation require a) specification of the biological tanks, the biological mass of which will be used in WAS flow rate estimation and b) the correct specification of the WAS flow line.
4) The biological tanks which are included in the wastage flow calculation can be selected from the list of tanks that appears by clicking on Edit button (**Figure 4-7**). Select the tanks whose sludge mass needs to be considered in the SRT based WAS estimation. In this example, select the AS-diffused tank.
5) Next we need to specify the WAS stream correctly. If the indicated WAS stream is not correct, the WAS and Recycle flow lines can be switched. In this example, the Sl_0 shall

be Recycle while Sl_1 shall be the WAS line. Pressing on the  should change the order.

6) After the setup, the final window shall look like **Figure 4-8.**
7) Press **Accept** to commit the changes.

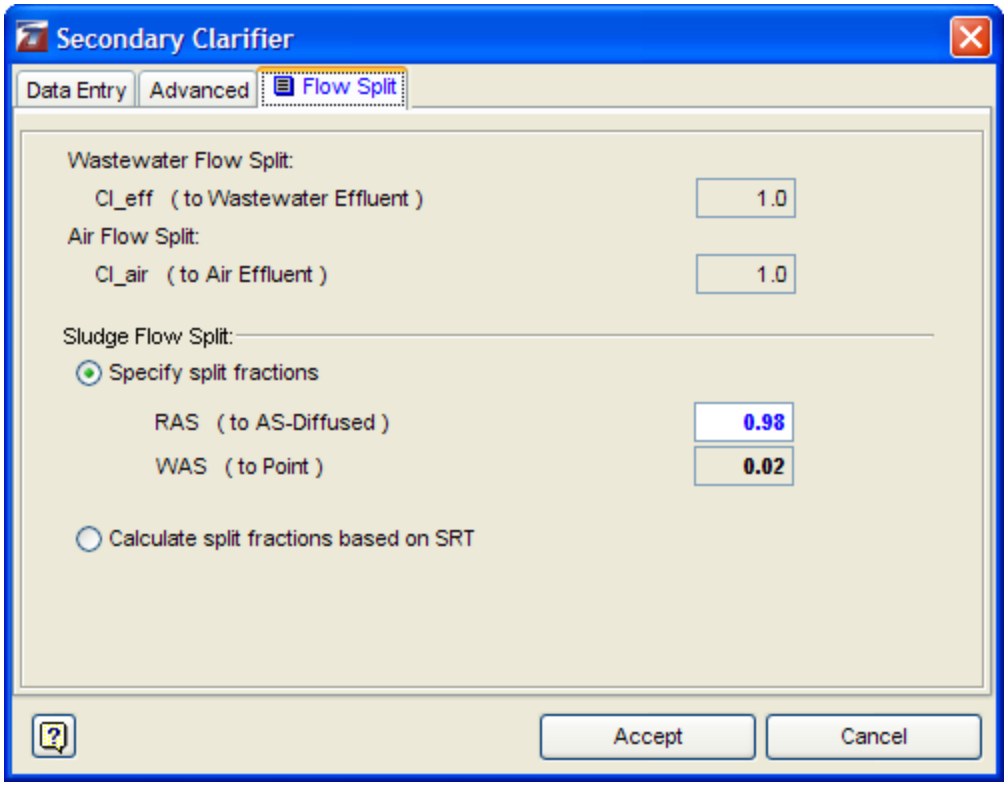



**Figure 4-5 Flow Split tab of secondary clarifier process unit**

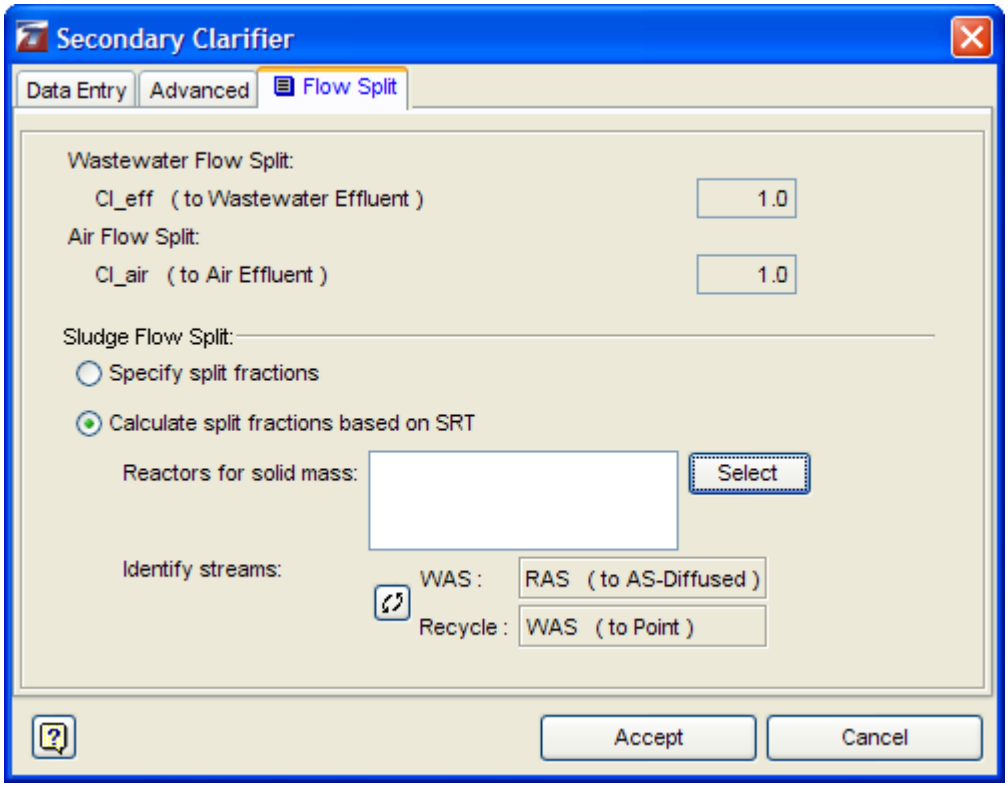



**Figure 4-6 The Flow Split tab after selecting the Calculate Split fraction method**

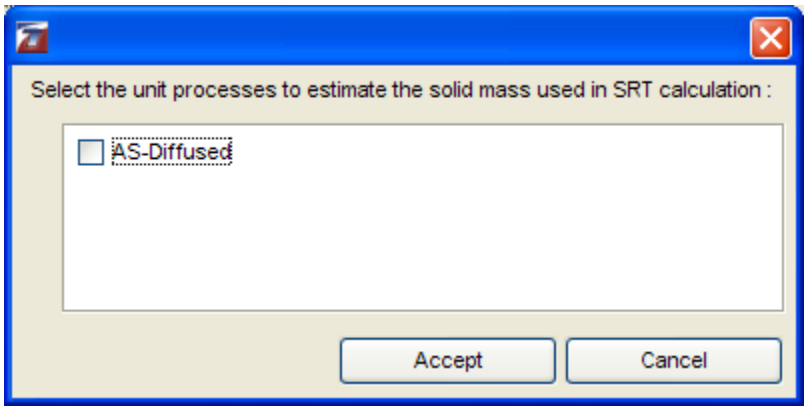



**Figure 4-7 List of tanks that can be used in WAS split calculation (layout specific)**

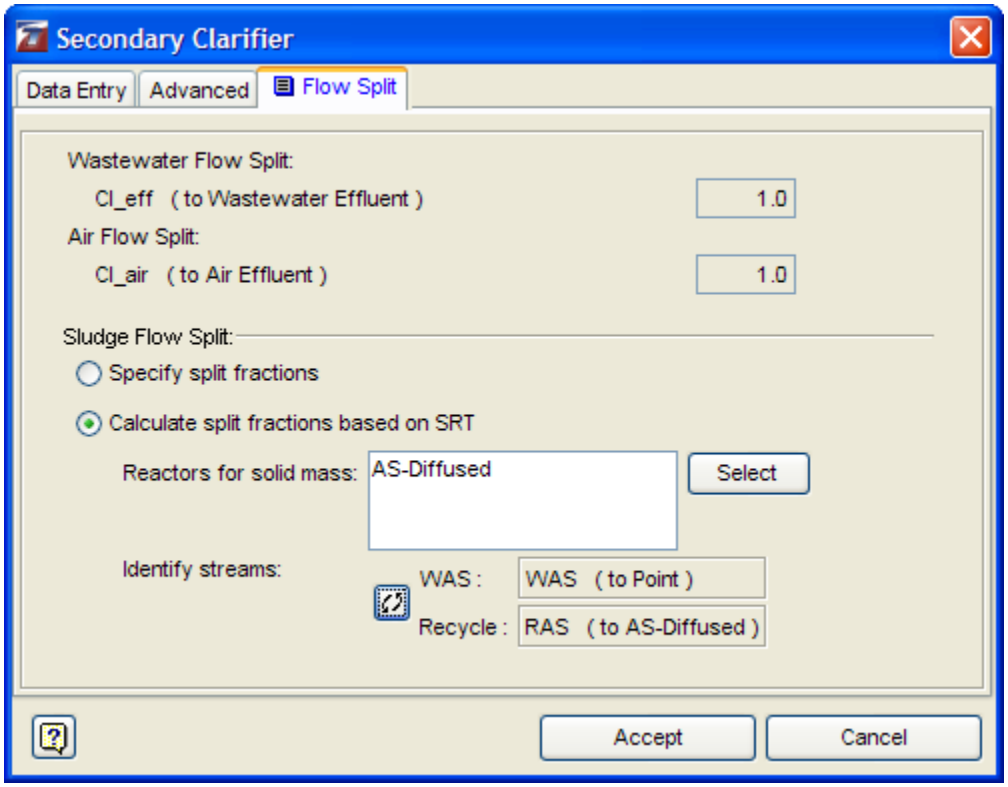



**Figure 4-8 Flow Split Tab after correct specification for SRT based WAS flow rate estimation**

## 4.4 HOW TO CREATE MULTIPLE LAYOUTS IN SAME FILE

TOXCHEM V4 (and later) allows user to work with different process layouts in one file. This is useful to the user, if it is required to compare two or more different process layouts with few changes. The new layouts can be added in the file by using the following steps.

1) From the **Layout** menu choose **Insert** to add a blank layout to the file. To create a duplicate of a layout, use the **Duplicate** item inside **Layout** Menu.
2) The layout name can be changed by accessing the **Rename** item from the **Layout** menu.

In **Figure 4-9**, the Layout1(2) is created by using the Duplicate command on Layout1. The commands associated with Layout menu may also be accessed by right clicking on the Layout Name shown at the bottom left of the drawing area.

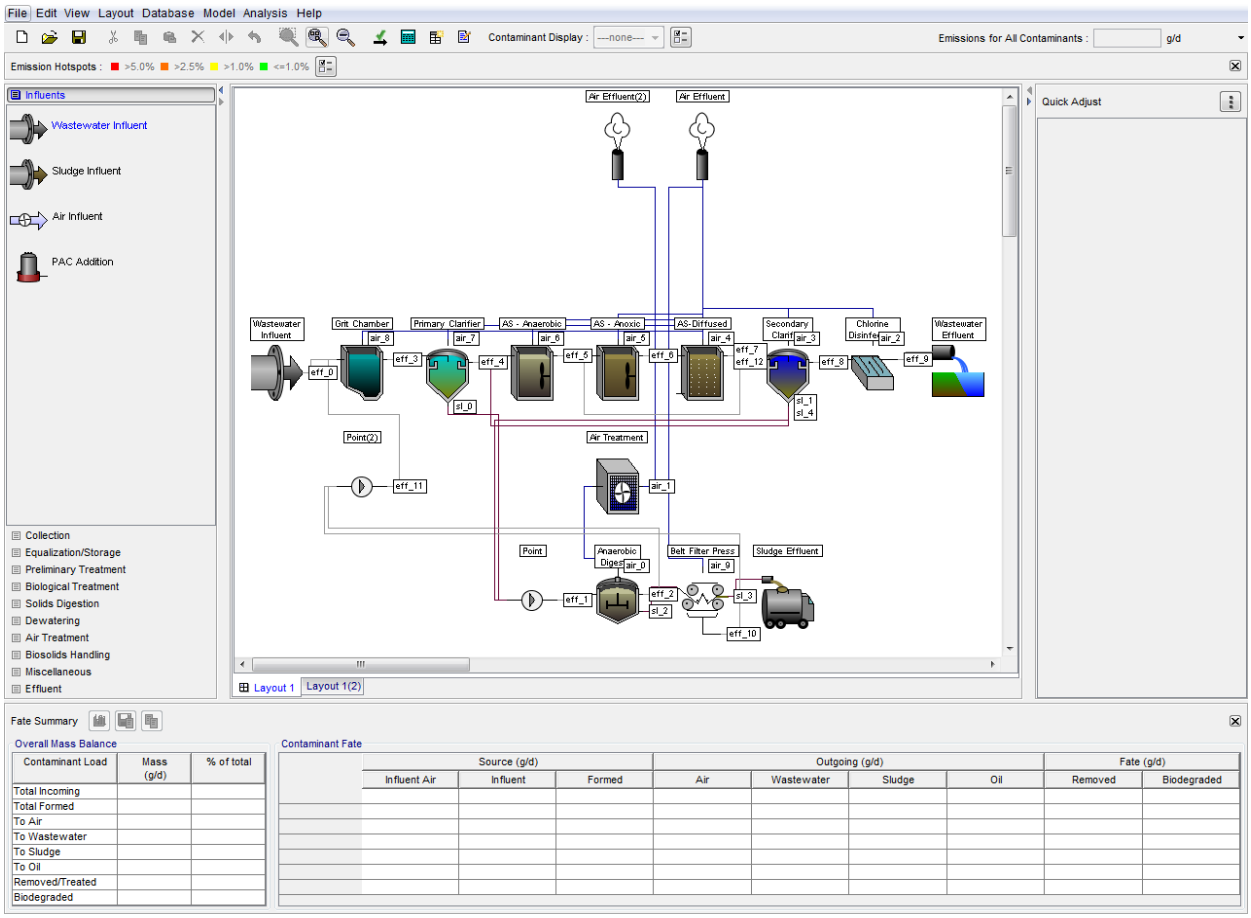



**Figure 4-9 Screen showing multiple layouts in same file**

## 4.5 HOW TO CHANGE THE PH GLOBALLY AND LOCALLY

TOXCHEM V4 and later allows the user to model the volatilization of compounds considering pH dependent dissociation. The pH value in each unit process of the layout can be either changed globally or locally. For example if the pH value in all the unit processes is same then it is easier to change the global pH value. By default the global pH value is set to 7.0. To change the global pH value, following steps may be used.

1) In **Layout** menu, click on the **Site Properties**.
2) Set the value in the **Site Wide pH**

It shall be noted here, that the set values are specific to the layout which is active at the time of setting.

The pH for an individual unit process may be changed in the Data Entry window of the process unit (right click on object and select **Edit Parameters** to open the Data Entry window). Click on the selection box next to **Local pH Value** to activate the data entry field. Enter the local pH (**Figure 4-10** ) and press **Accept** to confirm the change.

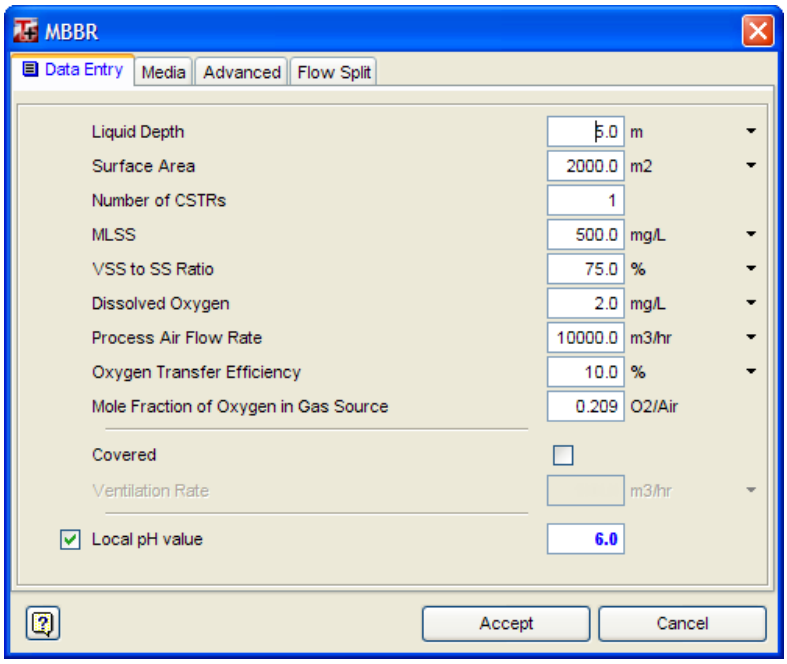



**Figure 4-10 Changing local pH value**

## 4.6 HOW TO ZOOM IN-ZOOM OUT

The user can use the **View → Zoom** command to Zoom In – Zoom out the layout. Three Zoom buttons are also provided on the tool bar. The **Zoom Selected Area** button on the tool bar may be used to zoom in the selected grid. The **Zoom Plant** button may be used to zoom to the region occupied by the layout. An additional **Zoom Out** command button is also provided on the tool bar. This button may be used to increase the number of rows and columns in the drawing board view.

## 4.7 HOW TO TURN ON/OFF THE PROCESS TABLE, FATE SUMMARY AND HOT SPOTS TOOL BARS

The default user interface of TOXCHEM V4 shows the panels for Process Table, Fate Summary Tables and Hot Spots Setup (**Figure 4-11**). The panel views can be turned ON/OFF by using the **View → Toolbars** command. Select or unselect the **Unit Process**, **Hotspot** or **Fate Summary** to open or close these panels. **Figure 4-12** shows the interface when all the panels are closed.

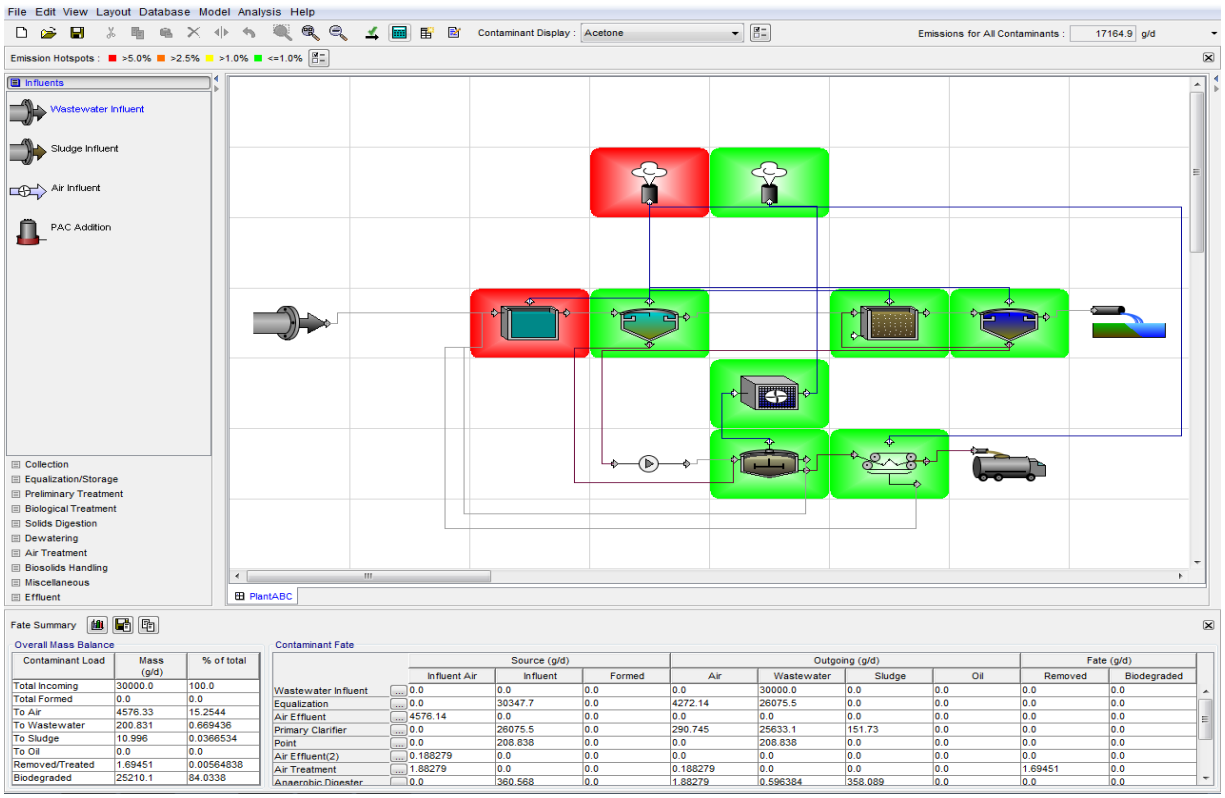



**Figure 4-11 Default interface view with Process Table, Fate Summary and Hot Spot panel views turned ON**

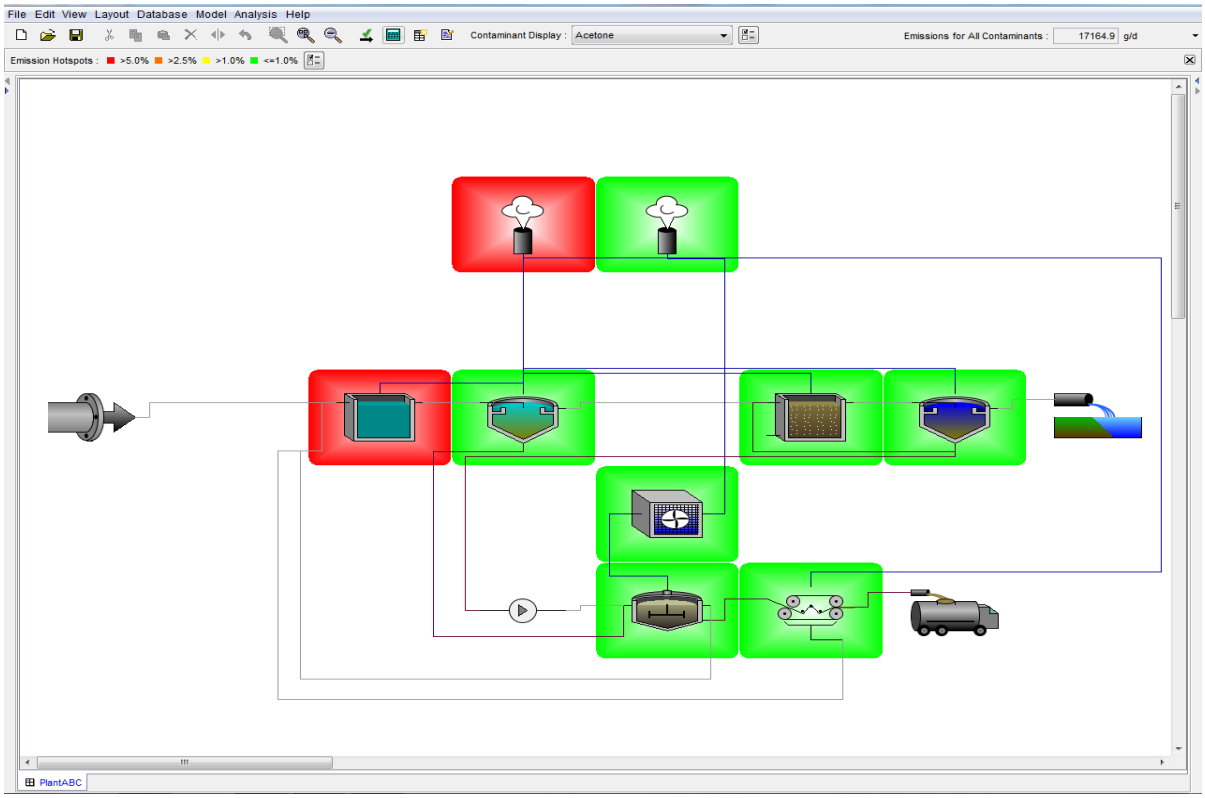



**Figure 4-12 Interface view with all the panel views turned OFF**

## 4.8 HOW TO REARRANGE THE FLOW LINES

The flow lines can be rearranged for better representation and better tracing of the connection points. Rearranging the flow lines can improve the appearance of the plant layouts. In addition to moving the flow lines in horizontal and vertical directions, it is possible to add break points to create additional line segments. Following step demonstrate the procedure.

1. Place the cursor on the line which you want to move. The mouse cursor will change into an arrow and the selected connection line will automatically turn into red color (**Figure 4-13**). Press the Left mouse button and move the line in indicated direction.

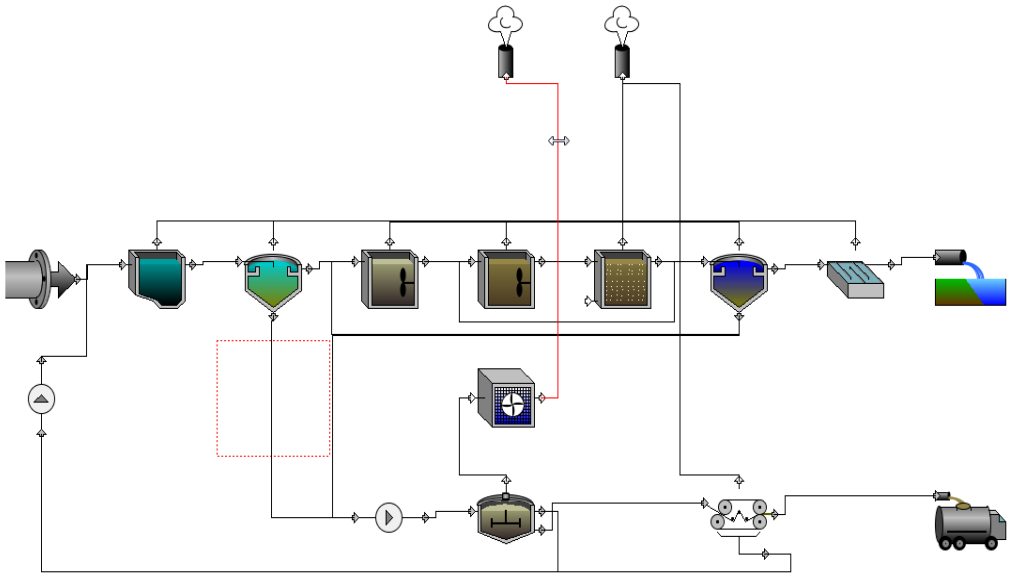
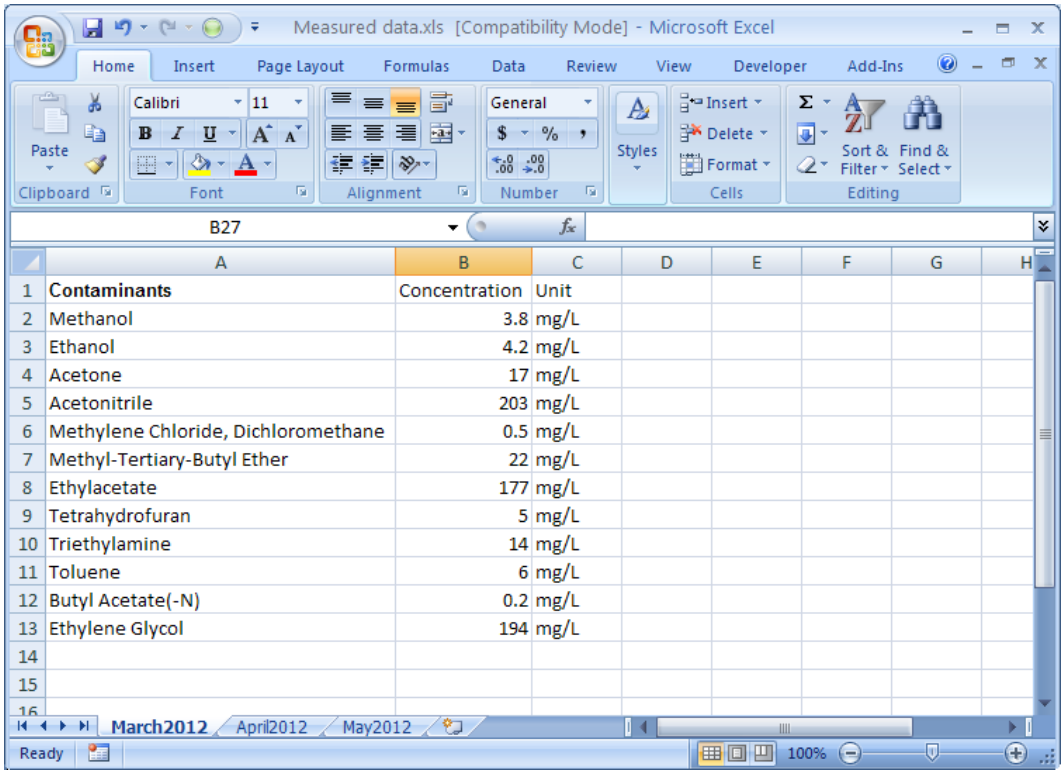


**Figure 4-13 Highlight the connection line for rearranging**

2. For creating a break-point, right click the line at the point where the break point is desired. From the pop-up menu, click on break point.

## 4.9 HOW TO READ CONTAMINANT CONCENTRATION FROM EXCEL FILE

This feature allows user to import concentration of contaminants in the influent object from an EXCEL file. This is useful when concentrations of a large group of contaminants are recorded in EXCEL sheet and is required for analysis. This feature saves time in data entry and eliminates chances of erroneous input. Following procedure may be used to import contaminant concentration data. In the following example, we will be importing the contaminant and their concentration shown in the March2012 worksheet of the EXCEL workbook (**Figure 4-14**). [Note: the contaminants names in the EXCEL sheet should correspond to the exact name in the database. If a contaminant does not exist in the database, it will not be imported from the worksheet. Also use only the A, B, C columns for contaminant name, concentration and unit respectively. The concentration unit shall be the one that is recognized in TOXCHEM (g/m3, mg/L, ug/L, g/L or ppm) ].




| | A | B | C |
|---|---|---|---|
| 1 | **Contaminants** | Concentration | Unit |
| 2 | Methanol | 3.8 | mg/L |
| 3 | Ethanol | 4.2 | mg/L |
| 4 | Acetone | 17 | mg/L |
| 5 | Acetonitrile | 203 | mg/L |
| 6 | Methylene Chloride, Dichloromethane | 0.5 | mg/L |
| 7 | Methyl-Tertiary-Butyl Ether | 22 | mg/L |
| 8 | Ethylacetate | 177 | mg/L |
| 9 | Tetrahydrofuran | 5 | mg/L |
| 10 | Triethylamine | 14 | mg/L |
| 11 | Toluene | 6 | mg/L |
| 12 | Butyl Acetate(-N) | 0.2 | mg/L |
| 13 | Ethylene Glycol | 194 | mg/L |
| 14 | | | |
| 15 | | | |

**Figure 4-14 EXCEL data file**

Click on the Contaminants tab in the Influent object Edit Parameters menu (**Figure 4-15**).

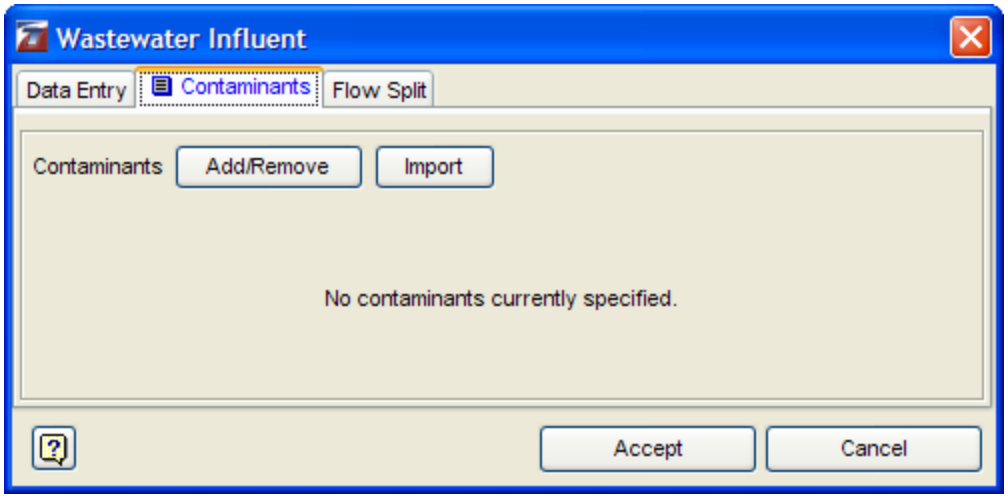



**Figure 4-15 Import button in wastewater influent**

1. Click on Import button to import the contaminant concentrations from the EXCEL worksheet. Select the location where the EXCEL data file is stored, select the file and open it.
2. A Worksheet Selection window (**Figure 4-16**) pops up to confirm which sheet to import data from. In this example March 2012 is selected. Press Accept.
3. An error window (**Figure 4-17** ) will appear and report any rows are that are not imported due to contaminant name or unit mismatch. In this example the first row contains the header in the worksheet and this is ignored. Close the error window.

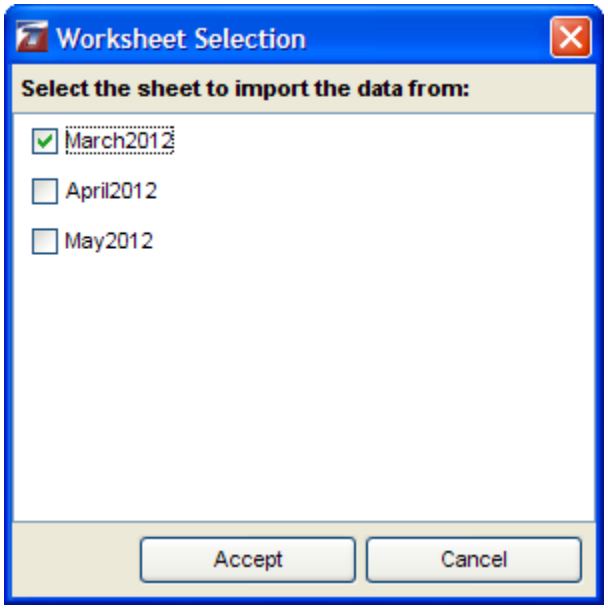



**Figure 4-16 Sheet Selection for data import**

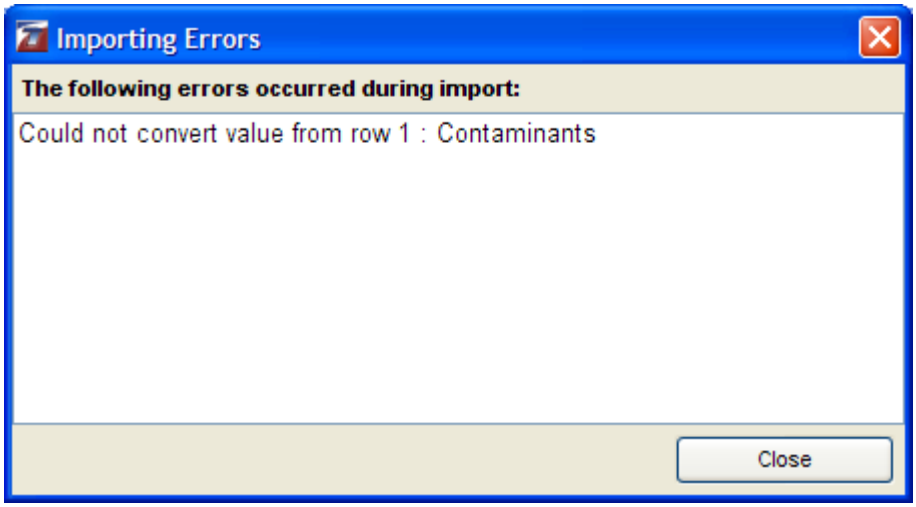



**Figure 4-17 Error reporting window**

The contaminants and their concentration can be seen the contaminant window (**Figure 4-18**). Accept to close the window.

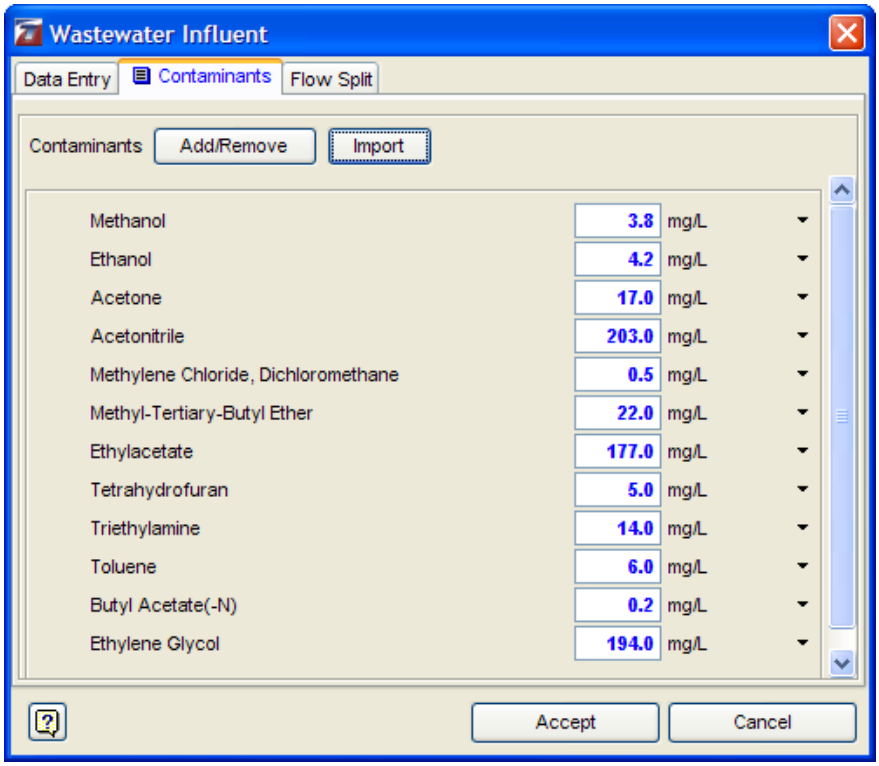



**Figure 4-18 Imported contaminant and concentrations (March2012)**

Now, if we use the import feature one more time and import the data from the April2012 sheet, the concentrations changes as in **Figure 4-19**.

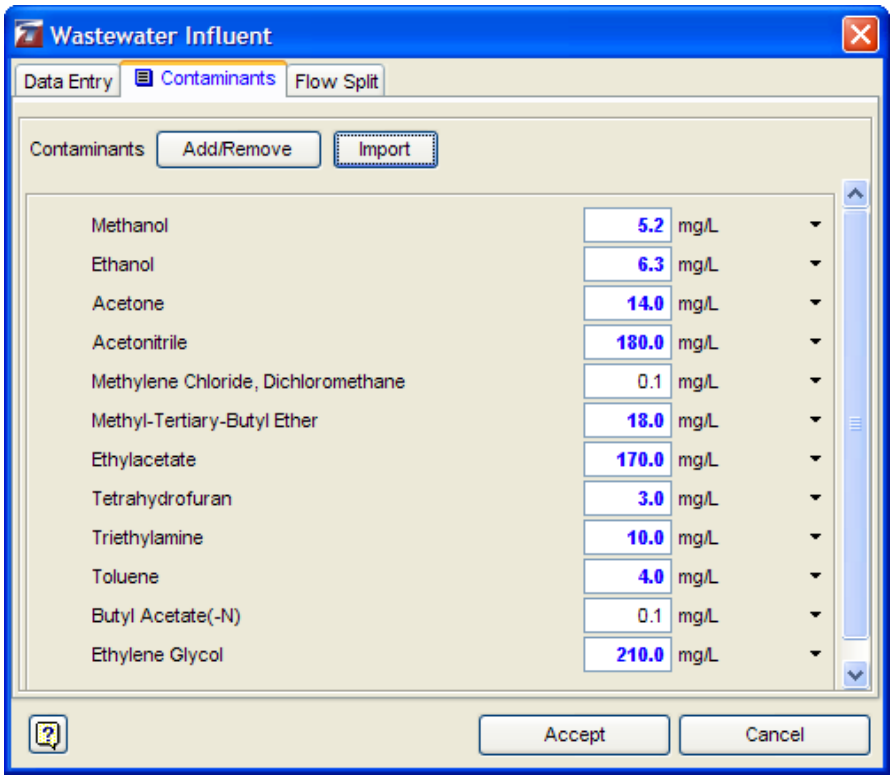



**Figure 4-19 Imported contaminant and concentrations (April2012)**

## 4.10 HOW TO VIEW STREAM PROPERTY QUICKLY

To view the properties of a stream, right click on the stream and select “View Stream States”. The pop-up window will show the calculated values of the stream properties as in Figure 4-20.

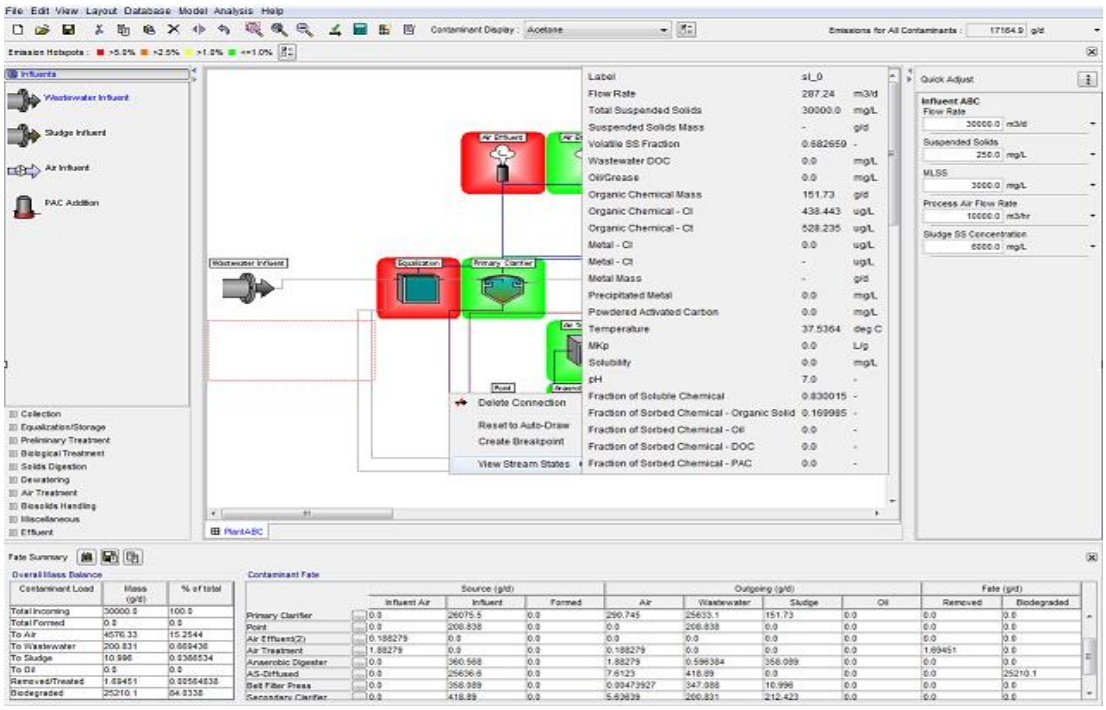
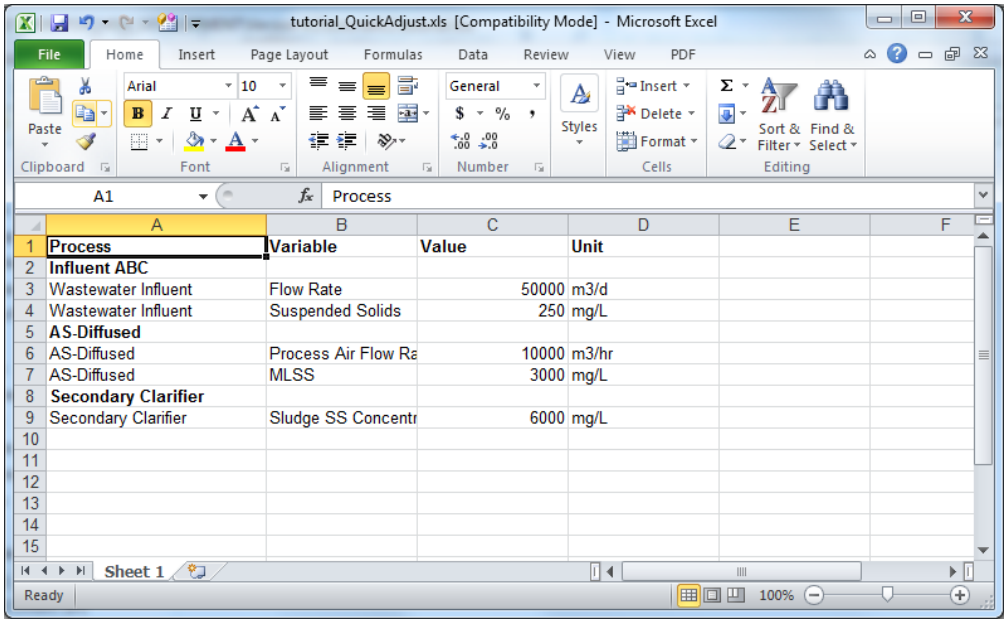


**Figure 4-20 Viewing Stream Properties**

## 4.11 HOW TO IMPORT FILE DATA FOR VARIABLES ON QUICK ADJUST TOOLBAR

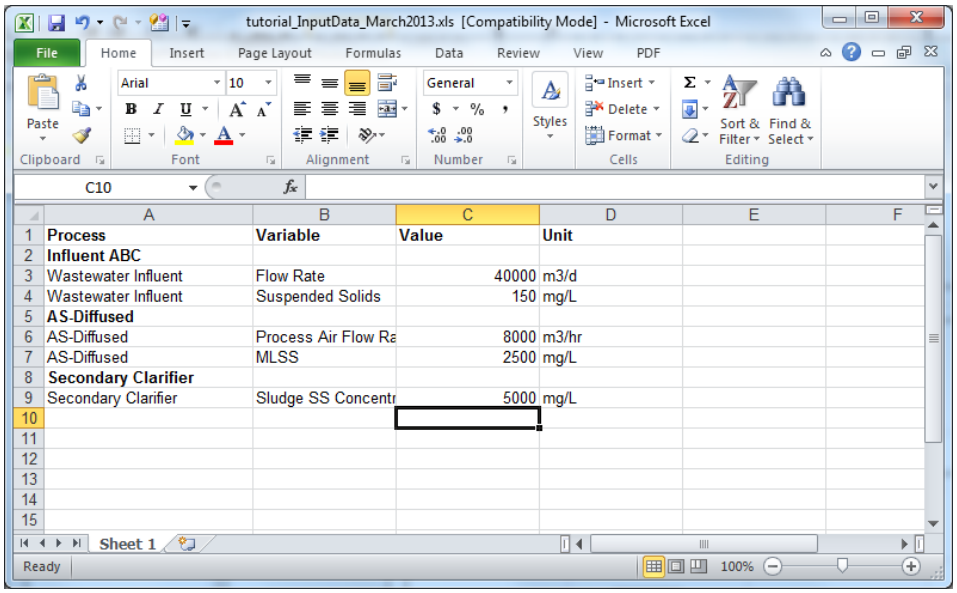
Toxchem allows user to export and import data of model variables from an EXCEL file. For the export and import of variable data to wok, the selected variables shall be available on the Quick Adjust Toolbar. A data import file with correct format can be created by first exporting data from the Quick Adjust Toolbar to an EXCEL file. In the Tutorial example, an export EXCEL file can be created by clicking on the Options button on Quick Adjust Toolbar and selecting “Export Values to File”. Save the file with appropriate name. The data format in the saved file will appear as shown in Figure 4-21.




| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| 1 | **Process** | **Variable** | **Value** | **Unit** | | |
| 2 | **Influent ABC** | | | | | |
| 3 | Wastewater Influent | Flow Rate | 50000 | m3/d | | |
| 4 | Wastewater Influent | Suspended Solids | 250 | mg/L | | |
| 5 | **AS-Diffused** | | | | | |
| 6 | AS-Diffused | Process Air Flow Ra | 10000 | m3/hr | | |
| 7 | AS-Diffused | MLSS | 3000 | mg/L | | |
| 8 | **Secondary Clarifier** | | | | | |
| 9 | Secondary Clarifier | Sludge SS Concentr | 6000 | mg/L | | |

**Figure 4-21 Excel File Created Using Data Export Feature**

For a situation where monthly emission reports needs to be prepared, a user can create data input files for each month by changing the observed operational values. For example, a data file for March 2013 can be created by changing the values and saving the file as tutorial_InputData_March2013.xls as shown in Figure 4-22.




| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| 1 | **Process** | **Variable** | **Value** | **Unit** | | |
| 2 | **Influent ABC** | | | | | |
| 3 | Wastewater Influent | Flow Rate | 40000 | m3/d | | |
| 4 | Wastewater Influent | Suspended Solids | 150 | mg/L | | |
| 5 | **AS-Diffused** | | | | | |
| 6 | AS-Diffused | Process Air Flow Ra | 8000 | m3/hr | | |
| 7 | AS-Diffused | MLSS | 2500 | mg/L | | |
| 8 | **Secondary Clarifier** | | | | | |
| 9 | Secondary Clarifier | Sludge SS Concentr | 5000 | mg/L | | |

**Figure 4-22 Data Input File for March 2013**

Once the input data file is created, the file data can be imported to the variables on the Quick Adjust Toolbar. The data can be imported by accessing the “Import Values From File” command from the Options button on the Quick Adjust Toolbar. Select the correct input file from where data needs to be imported (tutorial_InputData_March2013.xls). After the import, the data values on the Quick Adjust Toolbar shall appear as shown in Figure 4-23.

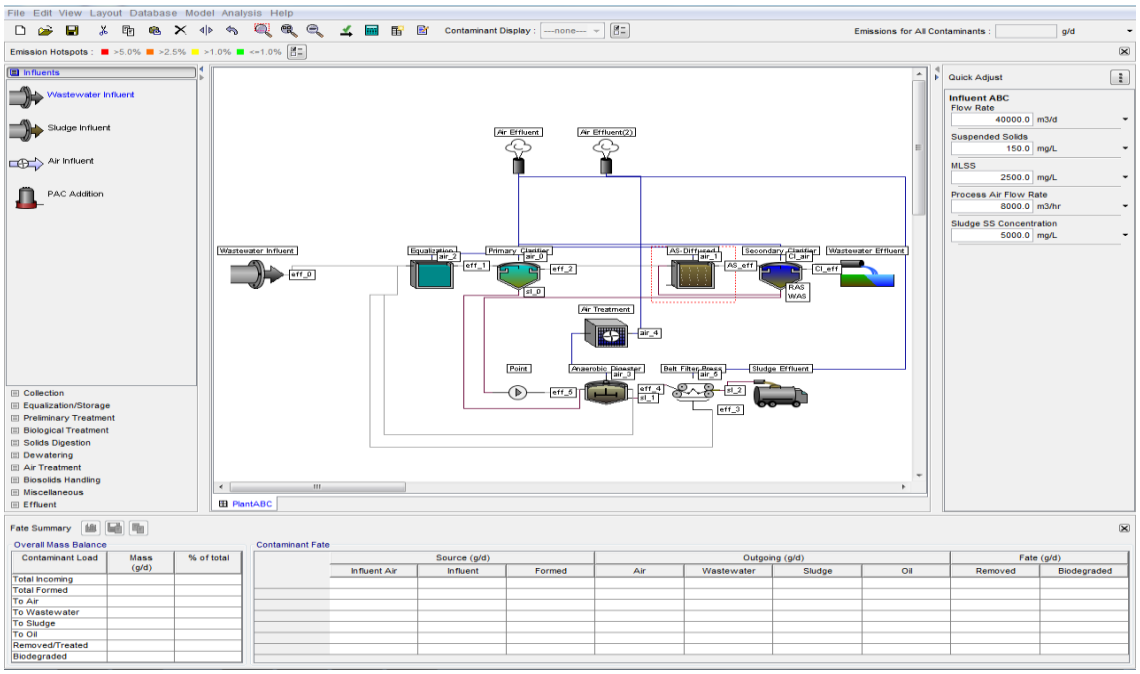



**Figure 4-23 Variable Values On Quick Adjust Toolbar After Data Import**

# 5. APPENDIX-A

## 5.1 Version 4

Some of the parameter values which were hard coded in V3 simulation system are now provided in the advanced parameter setting tab. Based on experience over the years, some of these hard coded values were updated with new defaults in TOXCHEM V4 (and later). The changes in the parameter default values are as shown in **Table 5-1**. These new default values are carried forward in TOXCHEM V4.3.

## 5.2 Version 4.1

Corrections to EPA air emission database compounds: Please refer to Technical Memorandum No. 2012-001. These updates were made in TOXCHEM V4.2.

Corrections were made in the oxygen density estimation procedures. Please refer to Technical Memorandum No. 2012-002.

## 5.3 Version 4.3

The technical literature for values of Henry's law coefficients for ammonia and hydrogen sulfide was reviewed extensively. Based on the data reviewed, new values of Henry's law coefficients of 0.000661 $L_{liq}/L_{gas}$ for ammonia and 0.4035 $L_{liq}/L_{gas}$ for hydrogen sulfide were adopted and carried forward in V4.3. The detailed documentation regarding the selection of the values for these two compounds is provided in Technical Memorandum No. 2014-001.

## Table 5-1 Changes in default parameter values

| Unit Process/Parameter | Unit | V3 Default | V4 (and later) Default | Explanation |
|---|---|---|---|---|
| Drop Structure - Closed | | | | |
| Kg/Kl Ratio for Drop | | 3 | 100 | Same as Weir |
| Drop Structure - Open | | | | |
| Kg/Kl Ratio for Drop | | 3 | 100 | Same as Weir |
| Grit Chamber | | | | |
| Kg/Kl Ratio for Diffused System | | 40 | 3 | Air bubble coming in contact with Liquid |
| Equalization - Mixed/Aerated | | | | |
| Kg/Kl Ratio for Diffused System | | 40 | 3 | Air bubble coming in contact with Liquid |
| Dissolved Air Flotation | | | | |
| Oxygen Transfer Efficiency | % | 50 | 25 | OTE reduced based on experience |
| Kg/Kl Ratio for Diffused System | | 40 | 3 | Air bubble coming in contact with Liquid |
| Activated Sludge - Diffused Aeration | | | | |
| Kg/Kl Ratio for Diffused System | | 40 | 3 | Air bubble coming in contact with Liquid |
| Activated Sludge - Diffused/Mechanical Aeration | | | | |
| Kg/Kl Ratio for Diffused System | | 40 | 3 | Air bubble coming in contact with Liquid |
| Trickling Filter | | | | |
| Kg/Kl Ratio | | 4 | 40 | Same as mechanical aeration in which liquid droplets come in contact with air |
| Biofilm Thickness | mm | 0.1 | 1 | Based on experience from modeling fixed film processes |
| Stagnant Liquid Layer Thickness | mm | 0.1 | 0.05 | Based on experience from modeling fixed film processes |
| Rotating Biological Contactor | | | | |
| Kg/Kl Ratio | | 4 | 40 | Same as mechanical aeration in which liquid droplets come in contact with air |
| Biofilm Thickness | mm | 0.1 | 1 | Based on experience from modeling fixed film processes |
| Stagnant Liquid Layer Thickness | mm | 0.1 | 0.05 | Based on experience from modeling fixed film processes |
| Channel | | | | |
| Oxygen Transfer Efficiency | % | 2 | 6 | |
| Cooling Tower | | | | |
| Kg/Kl Ratio | | 700 | 40 | Same as mechanical aeration in which liquid droplets come in contact with air |
| Volatilization Mass Transfer Coefficient | m/d | 0.8 | 0.2 | Same value as in the trickling filter |
| Aerobic Digester | | | | |
| Kg/Kl Ratio for Diffused System | | 40 | 3 | Air bubble coming in contact with Liquid |