

# WatPro

Water Treatment Simulator for Predicting Water Quality



## USER'S GUIDE

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Hydromantis Environmental Software Solutions, Inc. (HESS, Inc.)

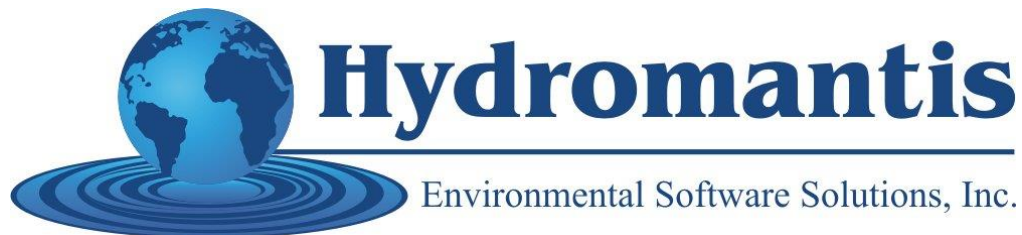
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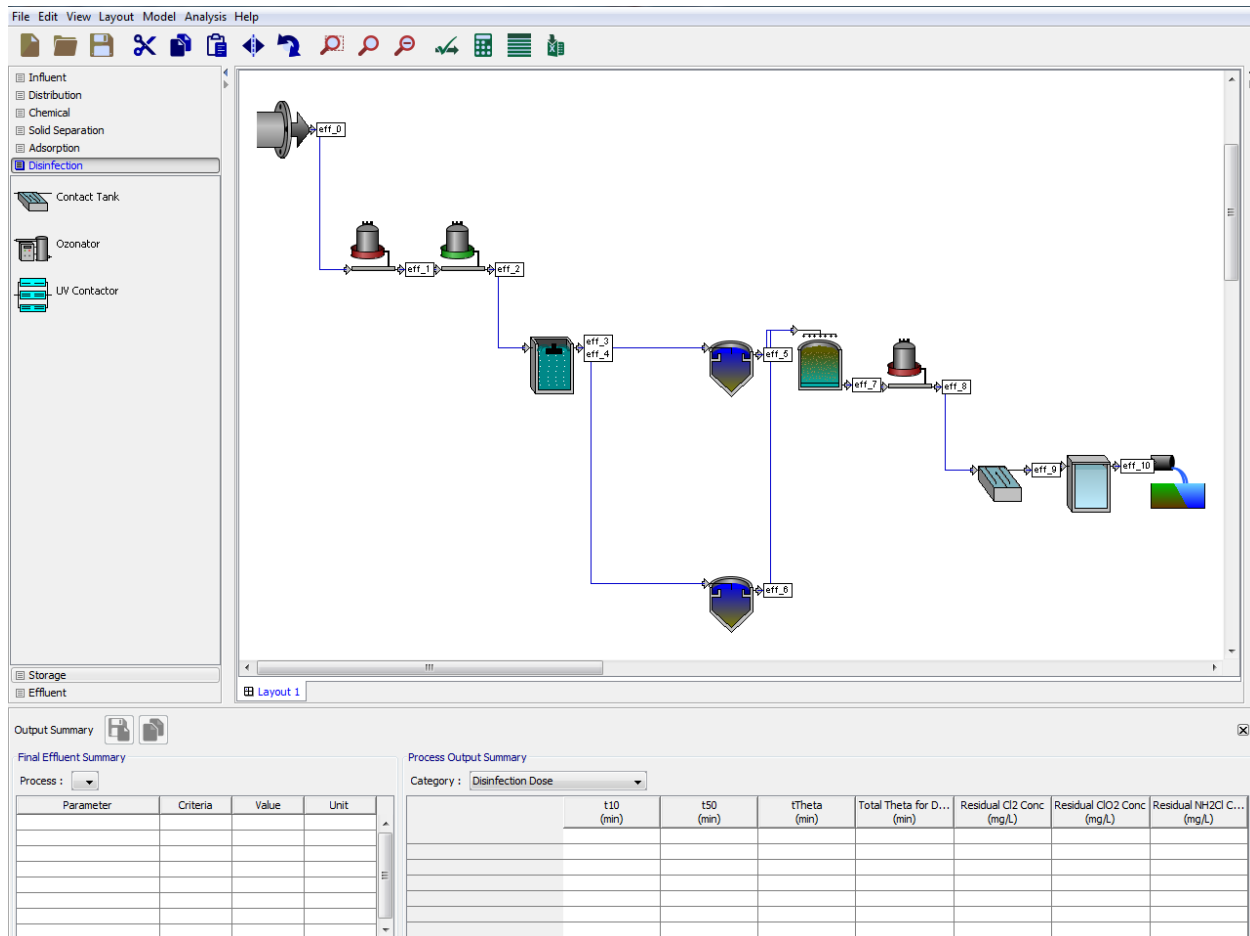
# 1 Introduction

## 1.1 Overview of WatPro

WatPro software provides a quick and easy way to evaluate the performance of drinking water treatment processes from a microbial and chemical standpoint. The software models (at steady-state) disinfection by-product (DBP) formation, inactivation of Giardia and viruses, organic matter removal, disinfectant decay and pH. The treatment train to be modeled is represented as a schematic diagram.

## 2 Design of a Water Treatment Facility

The water treatment facility schematic is the center of the WatPro model. An example water treatment schematic is displayed, as illustrated by the figure below.



### 2.1 Example Water Treatment Plant

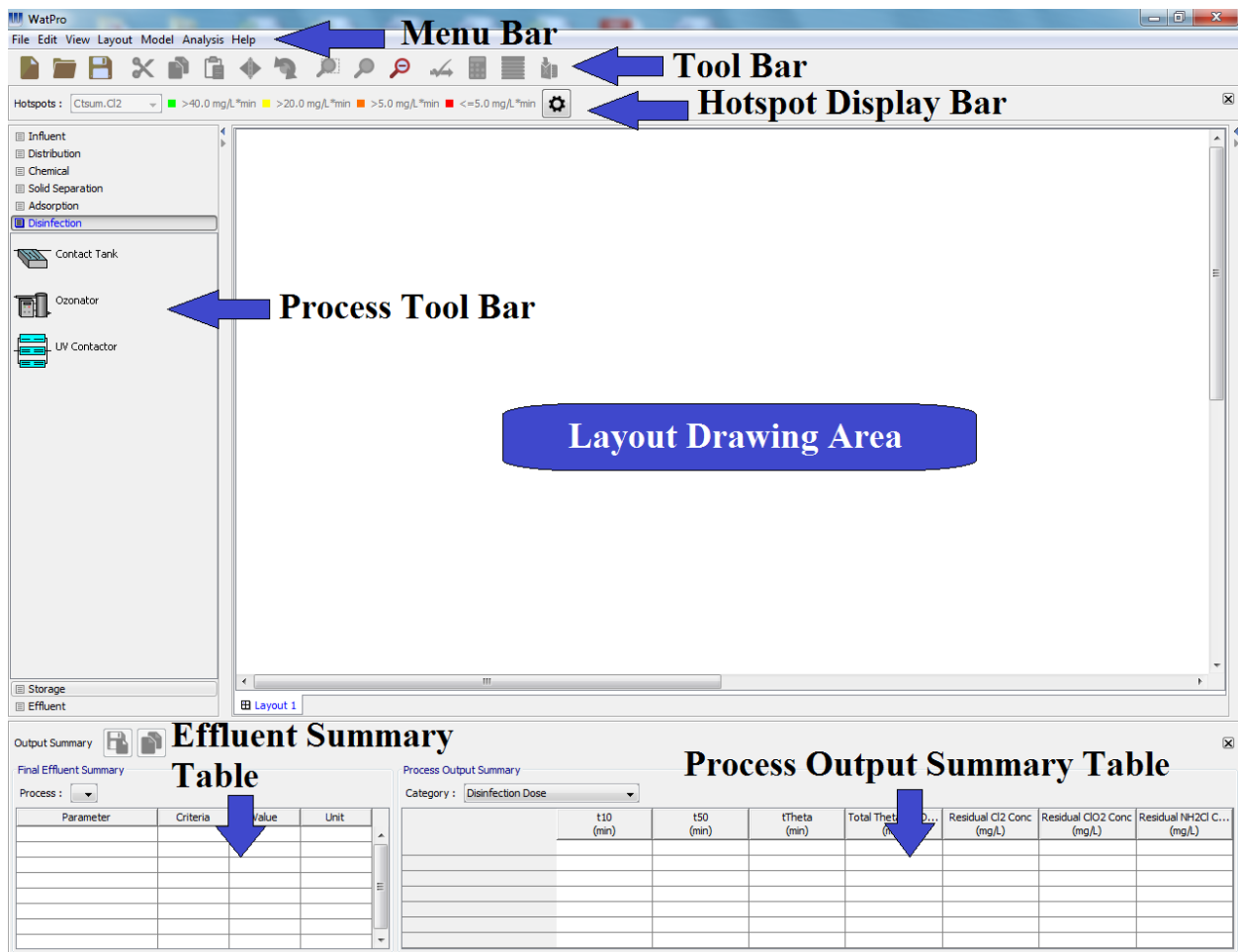
The example plant consists of the following processes:

- Raw water influent
- Pre-Disinfection (chlorine) and chemical input (alum)
- Rapid mix/flocculator
- Settling basin
- Filters
- Post-Chlorination and contactor

- Chemical input (ferrous chloride)
- Clear Well
- Effluent

## 2.2 Toolbars and Menus

A brief introduction of WatPro interface is presented in this section to familiarize the user to the organization of various features and functionality available in the simulation system. WatPro starts with a program window as shown below. 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 effluent quality and process outputs in the system.



**Menu Bar** - The Menu Bar contains menu items like File, Edit, View, Layout, Model, Analysis and Help. The various commands available in each menu item are as shown in the figure below.

The **File** menu contains command for retrieving and saving the WatPro 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.

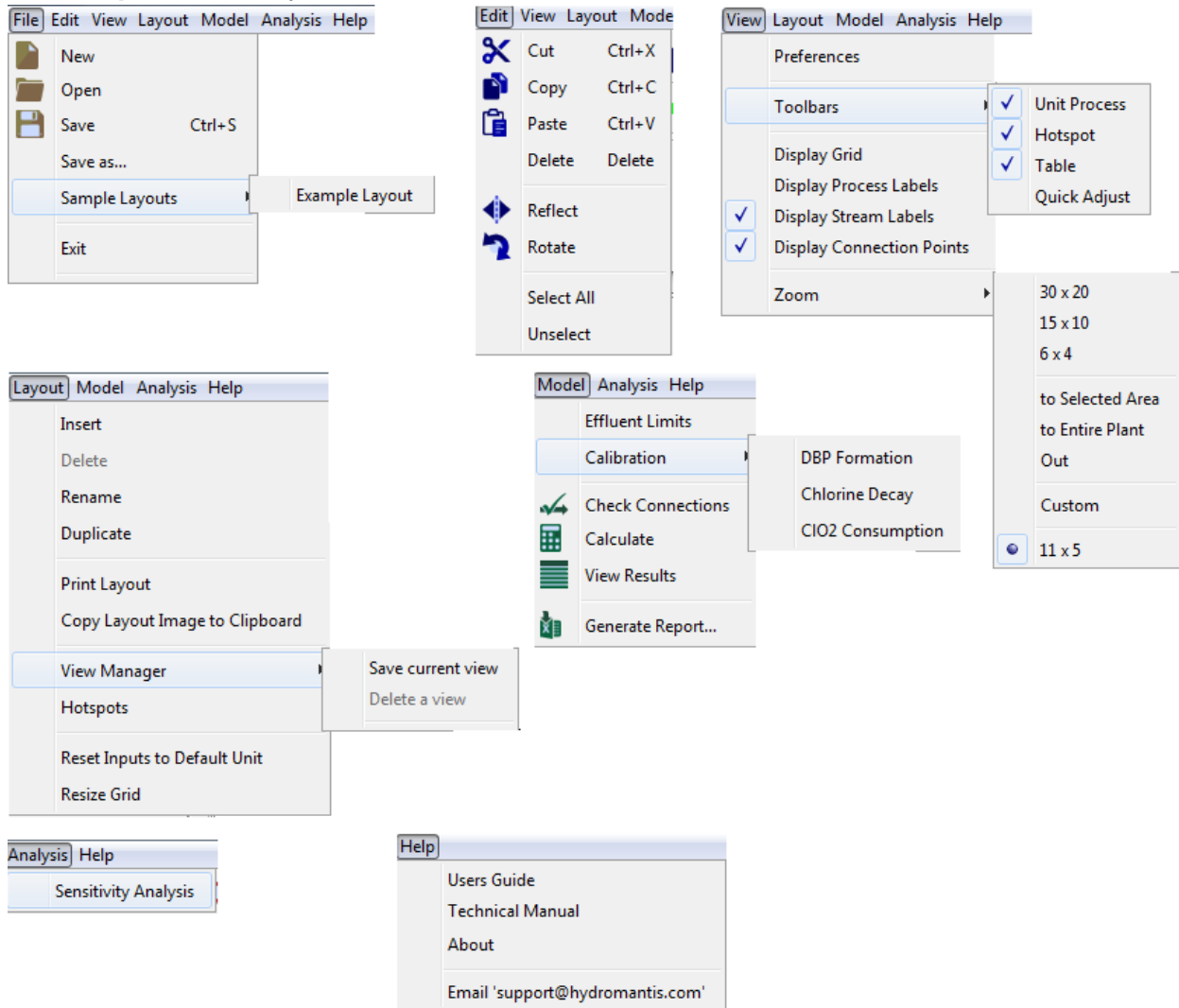
The **Layout** menu provides command to manage multiple layouts in the same file. It also includes the commands like Site Properties and Hotspots, which are used to set layout specific properties.

The **Model** menu includes command for checking, solving and viewing results after a layout is completely defined. The Model mode has options to verify that process connections are complete, to define the format of an output report, to run the model, to customize the model with site-specific calibrated parameters, and to identify disinfection byproduct hotspots.

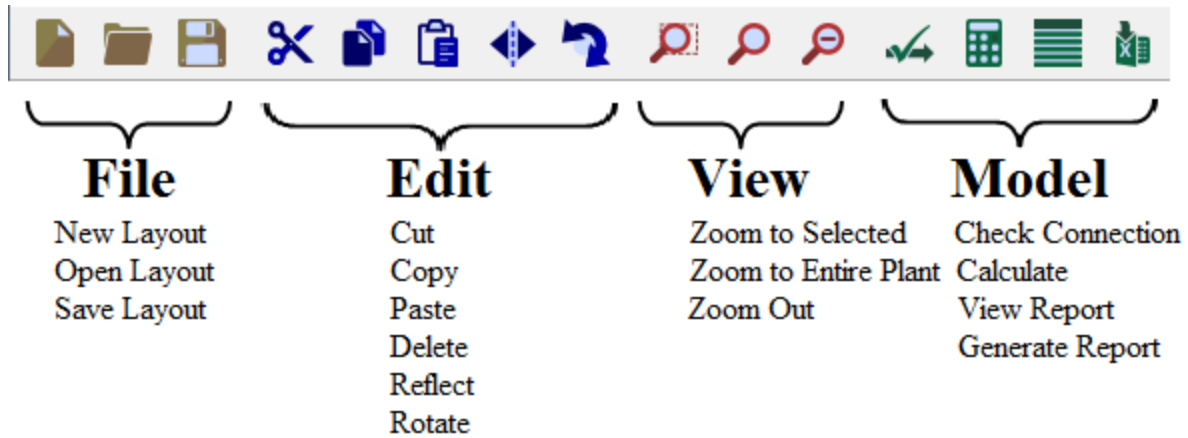
The **Analysis** menu provides access to Sensitivity Analysis that enables users to investigate the effects of a modeling parameter on DBP formation, microbial disinfection efficiency, or on other water quality parameters.



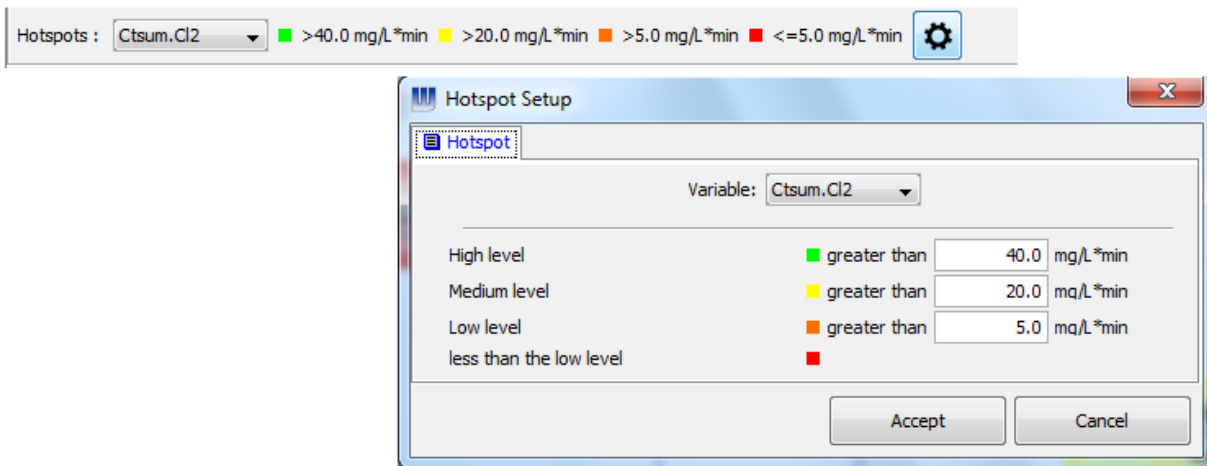
The **Help** menu may be used to access the User's Guide and Technical Manual.



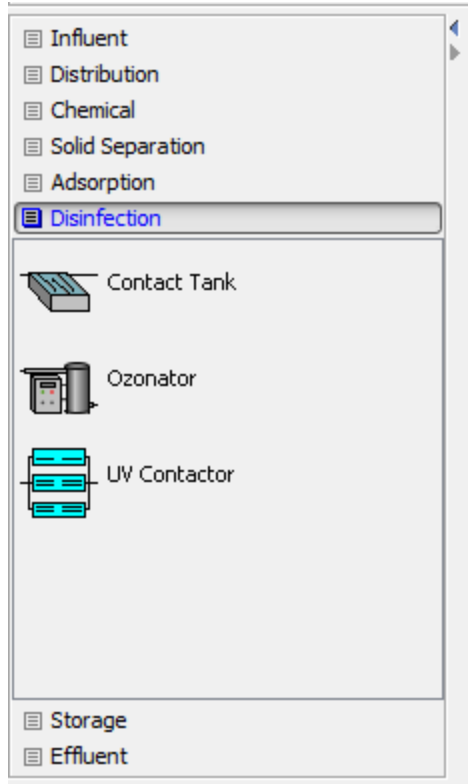
*Tool Bar* – The Tool Bar contains buttons for some of most often used commands in WatPro. The menu items and corresponding commands available on the commands on tool bar are as shown below.



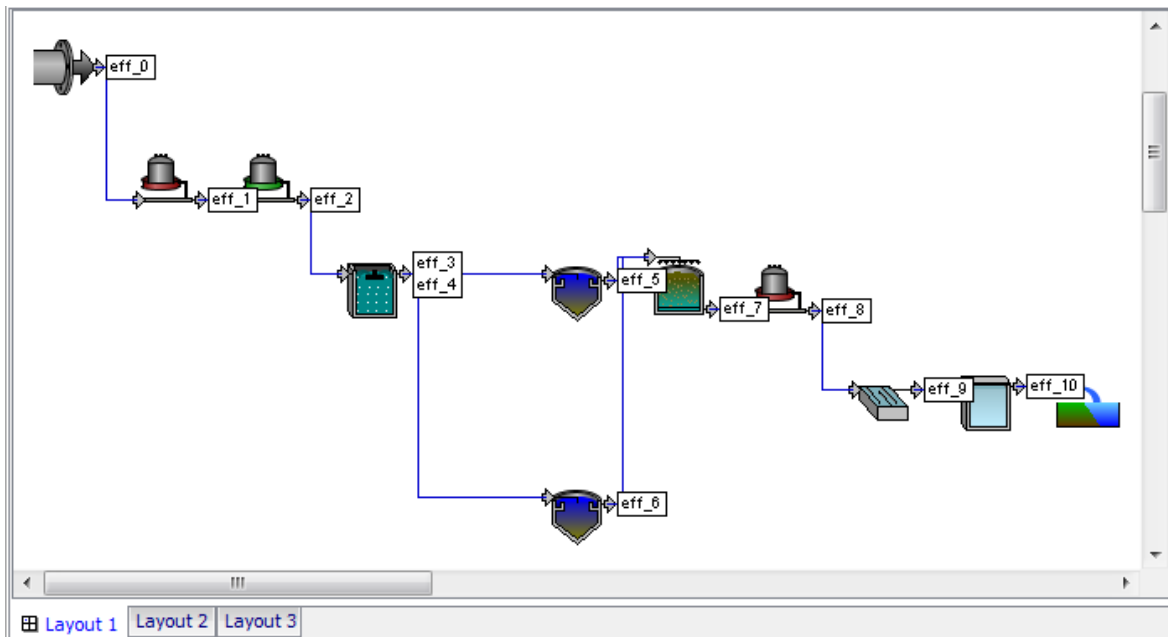
*Hot Spot Bar* – The Hot Spot Bar provides quick access to view and edit the hot spot display setting. It also shows the current color code used for different parameter limits.



*Process Tool Bar* – The Process Tool Bar provides access to all the unit processes available in WatPro for layout building. The process units are compiled in different categories of Influent, Distribution, Chemical, Solid Separation, Adsorption, Disinfection, Storage 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.



*Final Effluent Summary Table* – After the layout is solved, the table is used to show the final effluent quality and compliance for the layout.

Process Output Summary Table – After the layout is solved, the table shows the outputs of all the process units in the system.

The screenshot shows two summary tables. The 'Final Effluent Summary' table lists parameters like Disinfectants, DBPs, and Chlorite with their respective criteria, values, and units. The 'Process Output Summary' table shows the 'Disinfection Dose' category with columns for t10, t50, tTheta, Total, and Residuals across various process units like Influent, Flocculator, and Filtration.

Parameter	Criteria	Value	Unit
<b>Disinfectants</b>			
Effluent Chlorine	4.0	1.0399	mg/L
Effluent Chlorine Dioxide	0.8	0.0	mg/L
Effluent Chloromines	1.0	0.0	mg/L
<b>DBPs</b>			
THMs	100.0	86.0314	ug/L
HAA5s	100.0	116.315	ug/L
Chlorite	1.0	0.0	mg/L

	t10 (min)	t50 (min)	tTheta (min)	Total ... (min)	Residu... (mg/L)	Residu... (mg/L)	Resid... (mg/L)
Influent	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Disinfectant Addition	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Chemical Addition	0.0	0.0	0.0	0.0	2.0	0.0	0.0
Flocculator	5.76	40.32	57.6	40.32	0.394336	0.0	0.0
Settling Basin	11.52	80.64	115.2	120.96	0.316137	0.0	0.0
Settling Basin(2)	11.52	80.64	115.2	120.96	0.316137	0.0	0.0
Filtration	43.2	77.76	86.4	198.72	0.268027	0.0	0.0

## 2.3 Quick Overview of Building a Layout

To construct a water treatment facility begin with a blank drawing area by clicking on the menu item **File→New**.

### 2.3.1 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. Clicking on any tab expands the tab and provides the details of unit processes available in that tab.

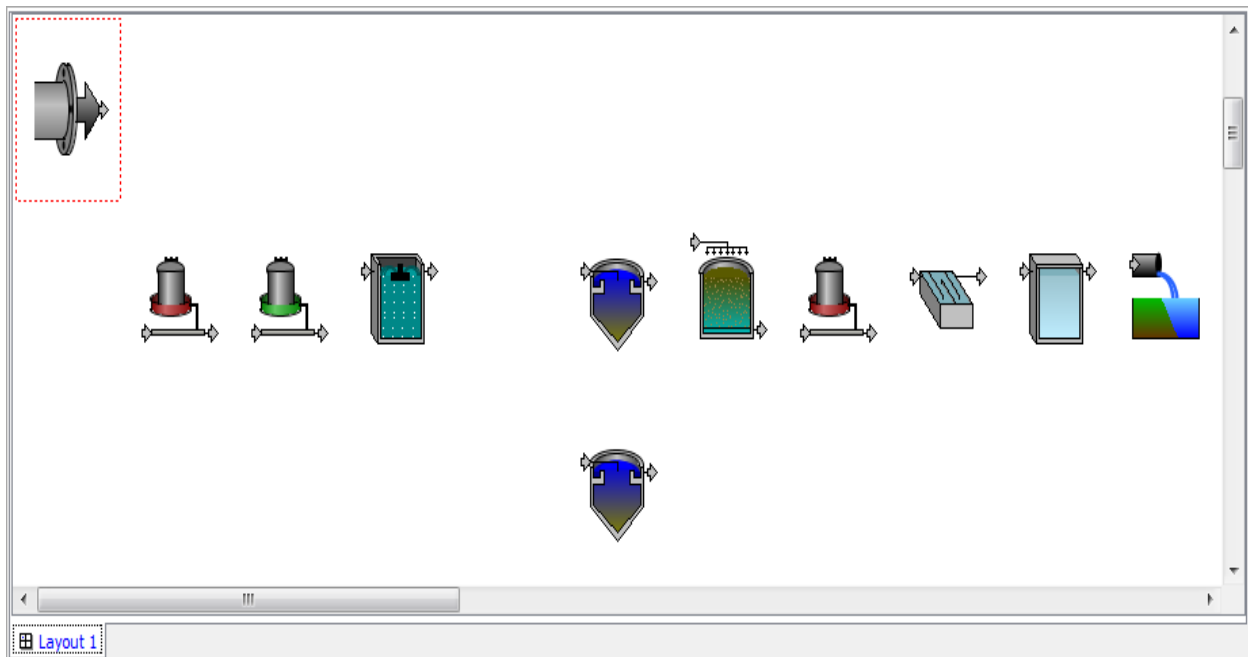
To place the unit process on the drawing board, click on the tab under which the process unit is available then drag-n-drop the process onto the desired location on the drawing board.

To remove a unit process from the drawing board, right-click the mouse button on the process and select 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.

To move a process unit from one cell to other, simply drag-n-drop the process to a new location. The move operation can also 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” (Note: the “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 the figure below.



Continue to click on the process icons and drop them on the drawing area until the process schematic is complete.

### 2.3.2 Making Flow Connections

After all the required process units are placed on the drawing board, the flow connections between the unit processes are defined.

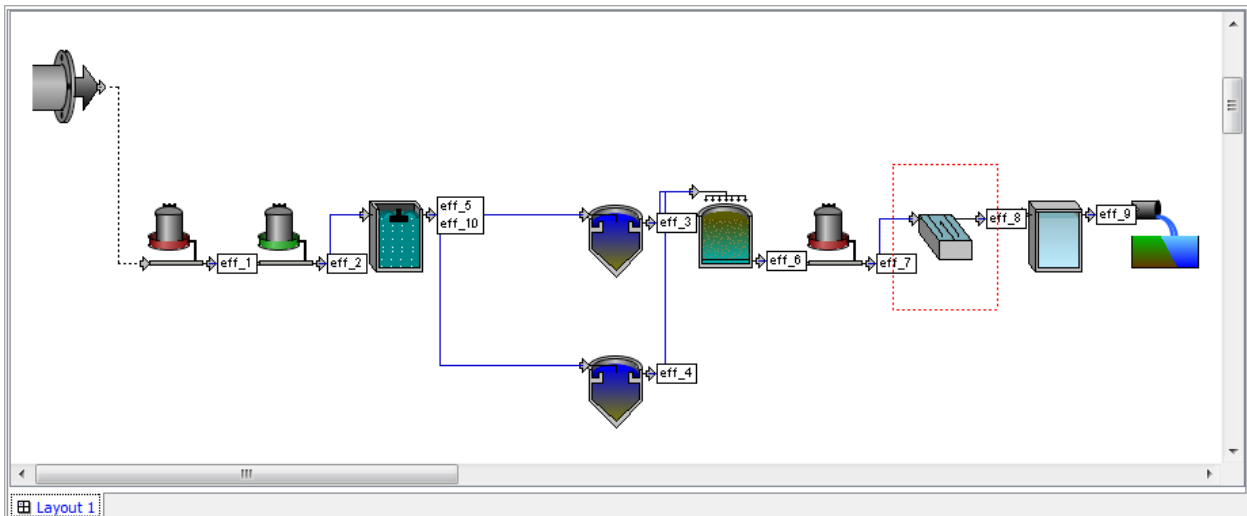
To make a connection between two process units, place the mouse on the outlet arrow connection of the unit process from where the connection starts. Once the cursor is at the right position, the cursor will change to a grey arrow.



Click-and-drag the arrow from that outlet to the desired inlet on another process. When the cursor is at the proper position on the inlet arrow connection, the cursor will change to green to indicate that it is an acceptable connection.

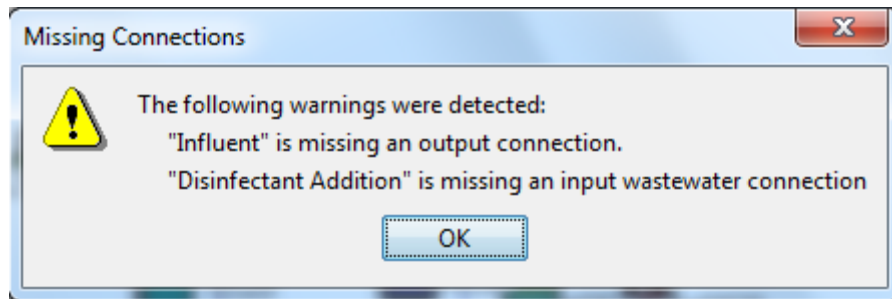


Release the mouse button and a connection line between the units will appear. If a connection has been made incorrectly or needs to be modified, the existing connection may be deleted by right-clicking on the connection between the processes and selecting “Delete Connection”.



After all the process connections have been completed, select the menu command "Model/Check Connections". If a process connection is missing, the model will indicate the location of the process that needs the connection.

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



There are several display options in WatPro 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 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**.

**Note:** Watpro 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 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.

### 2.3.3 Data Entry

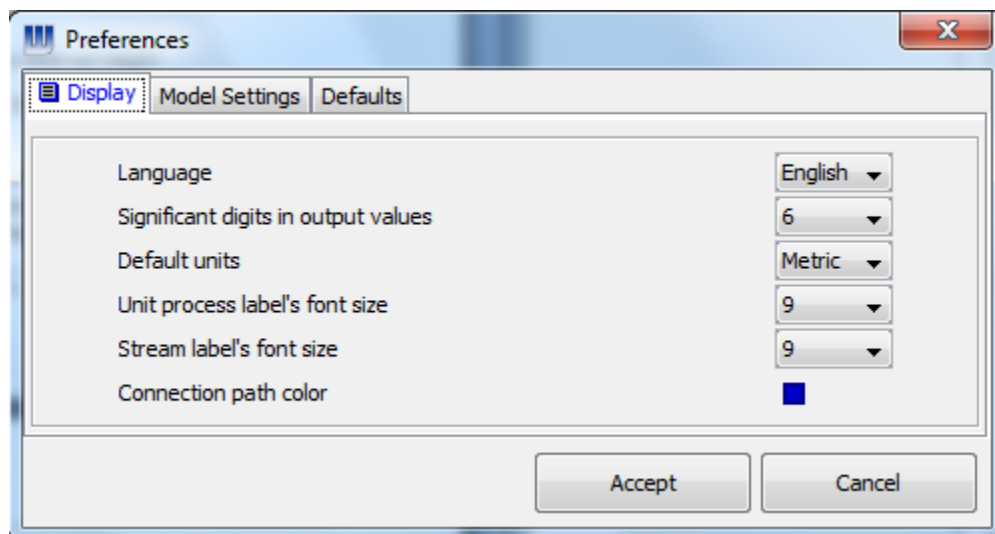
Once the schematic has been verified, entering of the process data can begin.

**Note:** WatPro organizes data inputs into three categories - Global Data, Layout Specific Data and Unit Process Specific Data.

#### 2.3.3.1 Global 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.





### 2.3.3.2 Layout Specific Data

The layout specific data is applicable to the layout and can be set for each layout differently.

These data values are the Hotspot settings under the **Layout** menu and the **Effluent Limits**, and **Calibration** options under the **Model** menu.

The effluent limits dialog box is used to enter concentration limits needed to be met in the effluent.

Parameter	Value	Unit
Max Effluent Chlorine Concentration	4.0	mg/L
Max Effluent Chlorine Dioxide Concentration	0.8	mg/L
Max Effluent Chloramine Concentration	1.0	mg/L
Max Effluent TTHMs	100.0	ug/L
Max Effluent HAA5s	100.0	ug/L
Max Effluent Chlorite	1.0	mg/L
<input type="checkbox"/> Total Giardia Reduction Required		log(10)
<input type="checkbox"/> Total Virus Reduction Required		log(10)
<input type="checkbox"/> Total Crypto Reduction Required		log(10)
Max Effluent Turbidity	0.5	NTU

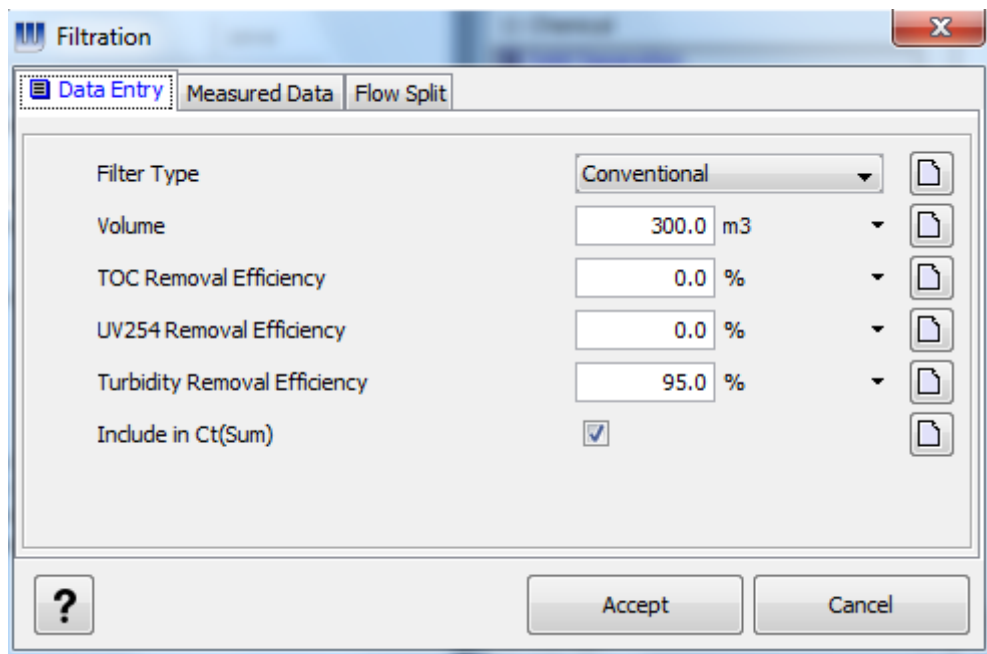
If the facility final treated water exceeds the maximum allowable concentrations for disinfection by-products (total THMs, HAA<sub>5</sub>, chlorite, chlorate), disinfectant residuals, (chlorine, chloramine, chlorine dioxide) or turbidity, the water is considered to be out of compliance. The Final Effluent Summary table discussed previously will reveal the non-compliant parameters.

WatPro determines a plant's requirements for *Giardia* and virus inactivation based on the influent water *Giardia* cyst concentration as specified by the EPA's Surface Water Treatment Rule. These requirements can be superseded by checking the box.

### 2.3.3.3 Unit Process Data

In order to specify unit process data, right-click on each process on the drawing area, select *Edit Parameters*, and complete the data entry dialog boxes. 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.

**Note:** To enter the data in units other than default units, click on the unit label and select the required unit in the popup window.



The screenshot shows a dialog box titled "Filtration" with a close button (X) in the top right corner. The dialog has three tabs: "Data Entry" (selected), "Measured Data", and "Flow Split". The "Data Entry" tab contains the following fields:

Parameter	Value	Unit	Action
Filter Type	Conventional		Dropdown
Volume	300.0	m3	Dropdown
TOC Removal Efficiency	0.0	%	Dropdown
UV254 Removal Efficiency	0.0	%	Dropdown
Turbidity Removal Efficiency	95.0	%	Dropdown
Include in Ct(Sum)	<input checked="" type="checkbox"/>		Checkbox

At the bottom of the dialog, there is a help button (question mark) on the left, and "Accept" and "Cancel" buttons on the right.

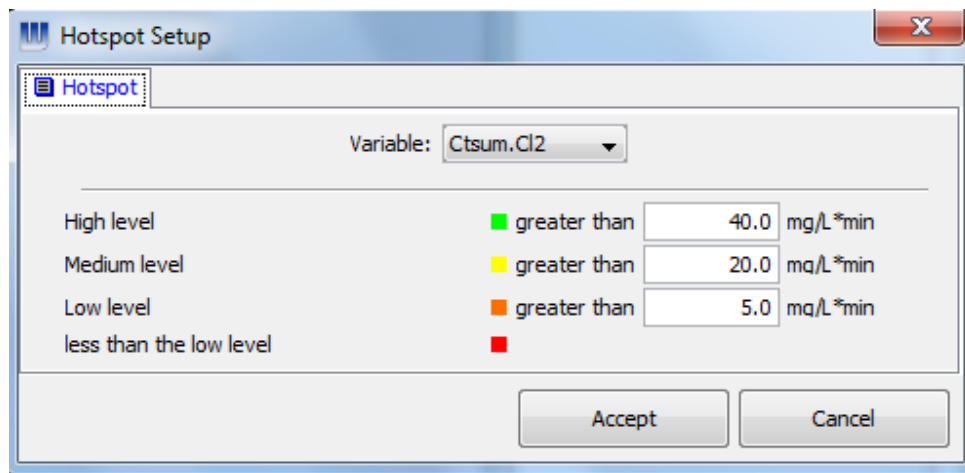
**Note:** The "Help" button shown in the lower-left corner will give a more in-depth description of what each of the input parameters mean.

### 2.3.4 Set Hotspots

By using the “hotspots” feature, it is possible to visually differentiate the process units which are minor/major source of the selected variable in the facility. When the hotspot feature is activated, the unit processes appear surrounded by different colors, depending on their concentration.

To set the levels for the hotspot, access the **Hotspots** from the **Layout** menu item. After changing 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.



### 2.3.5 Rename the Layout

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

# 3 Simulation and Outputs

## 3.1 Running the Simulation

Click on the **Calculate** button on the toolbar to start the calculation.



After the layout is solved and if the hotspots are enabled, 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 hotspot feature provides a quick way to identify the major source of the selected parameter.

The screenshot shows the WatPro software interface. At the top, there is a menu bar (File, Edit, View, Layout, Model, Analysis, Help) and a toolbar with various icons. Below the toolbar, there is a 'Hotspots' section with a dropdown menu set to 'Ctsum.Cl2' and four color-coded indicators: green (>40.0 mg/L\*min), yellow (>20.0 mg/L\*min), orange (>5.0 mg/L\*min), and red (<=5.0 mg/L\*min). The main workspace displays a process flow diagram with units represented by icons and labeled with effluent points (eff\_0 to eff\_10). The units are color-coded according to the hotspot legend. On the left, there is a 'Process' tree with categories like Influent, Distribution, Chemical, Solid Separation, Adsorption, Disinfection, Storage, Clear Well, and Fixed/Variable Volume Tank. At the bottom, there are two summary tables.

**Final Effluent Summary**

Parameter	Criteria	Value	Unit
<b>Disinfectants</b>			
Effluent Chlorine	4.0	1.0399	mg/L
Effluent Chlorine Dioxide	0.8	0.0	mg/L
Effluent Chloramines	1.0	0.0	mg/L
<b>DBPs</b>			
TTHMs	100.0	86.0314	ug/L
HAA5s	100.0	116.315	ug/L
Chlorite	1.0	0.0	mg/L

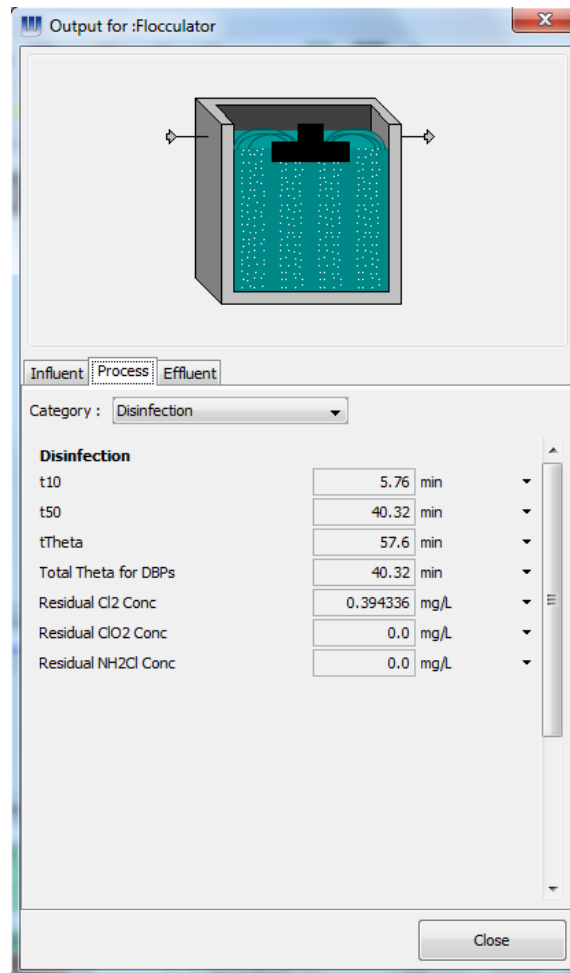
**Process Output Summary**

Category	t10 (min)	t50 (min)	tTheta (min)	Total ... (min)	Residu... (mg/L)	Residu... (mg/L)	Resid... (mg/L)
Influent	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Disinfectant Addition	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Chemical Addition	0.0	0.0	0.0	0.0	2.0	0.0	0.0
Flocculator	5.76	40.32	57.6	40.32	0.394336	0.0	0.0
Settling Basin	11.52	80.64	115.2	120.96	0.316137	0.0	0.0
Settling Basin(2)	11.52	80.64	115.2	120.96	0.316137	0.0	0.0
Filtration	43.2	77.76	86.4	198.72	0.268027	0.0	0.0

## 3.2 View Results

After the layout is successfully solved, the simulation results can be viewed in several different ways.

- (1) Right-click on the process and select **View Results** to view the outputs for that individual process.



- (2) To view a detailed summary of the simulation results for the complete layout, it is better to use the **View Results** button available on the tool bar.



Results

	Influent eff_0	Disinfectant... eff_1	Chemical A... eff_2	Flocculator eff_3	Flocculator eff_4	Settling Basin eff_5
Flow Rate (m3/d)	5000.0	5000.0	5000.0	2500.0	2500.0	2500.0
pH (-)	7.5	7.5	7.5	7.03503	7.03503	7.03503
TOC (mg/L)	3.0	3.0	3.0	2.26281	2.26281	2.26281
UV254 (1/cm)	0.8	0.8	0.8	0.313375	0.313375	0.313375
Temperature (deg C)	20.0	20.0	20.0	20.0	20.0	20.0
Ammonia (mg/L)	0.05	0.05	0.05	0.0	0.0	0.0
Alkalinity (mg/L)	100.0	100.0	100.0	87.9615	87.9615	87.9615
Hardness (mg/L)	100.0	100.0	100.0	100.0	100.0	100.0
Turbidity (NTU)	0.5	0.5	0.5	0.5	0.5	0.25
Ca(aq) (mg/L)	80.0	80.0	80.0	80.0	80.0	80.0
Mg(aq) (mg/L)	20.0	20.0	20.0	20.0	20.0	20.0
Carbonates(aq) (mg/L)	214.914	214.914	214.914	214.914	214.914	214.914
CaCO3(p) (mg/L)	0.0	0.0	0.0	0.0	0.0	0.0
MgOH(p) (mg/L)	0.0	0.0	0.0	0.0	0.0	0.0
Other Anion (Ca') (moles/L)	0.0020018	0.00203001	0.00223191	0.00223726	0.00223726	0.00223726
Other Cation (Cb') (moles/L)	0.00199827	0.00199827	0.00199827	0.00199827	0.00199827	0.00199827
TTHM (ug/L)	0.0	0.0	0.0	39.0175	39.0175	47.3995
CHCl3 (ug/L)	0.0	0.0	0.0	32.1192	32.1192	38.3212
CHBrCl2 (ug/L)	0.0	0.0	0.0	5.09138	5.09138	6.80943
CHBr2Cl (ug/L)	0.0	0.0	0.0	0.724498	0.724498	1.03984
CHBr3 (ug/L)	0.0	0.0	0.0	1.08248	1.08248	1.22898
Chlorite (mg/L)	0.0	0.0	0.0	0.0	0.0	0.0
Chlorate (mg/L)	0.0	0.0	0.0	0.0	0.0	0.0
HAA5 (ug/L)	0.0	0.0	0.0	63.1493	63.1493	70.9455
MCAA (ug/L)	0.0	0.0	0.0	0.570924	0.570924	0.751165

- (3) The **Final Effluent Summary** table and **Process Output Summary** table displays simulation results for the final effluent and every process unit. This data can be exported to Excel or the system clipboard by using the Export Data and Copy Table to Clip Board buttons provided at the top left side of the table.

Output Summary

Final Effluent Summary

Process : **Water**

Parameter	Criteria	Value	Unit
<b>Disinfectants</b>			
Effluent Chlorine	4.0	1.0399	mg/L
Effluent Chlorine Dioxide	0.8	0.0	mg/L
Effluent Chloramines	1.0	0.0	mg/L
<b>DBPs</b>			
TTHMs	100.0	86.0314	ug/L
HAA5s	100.0	116.315	ug/L
Chlorite	1.0	0.0	mg/L

Process Output Summary

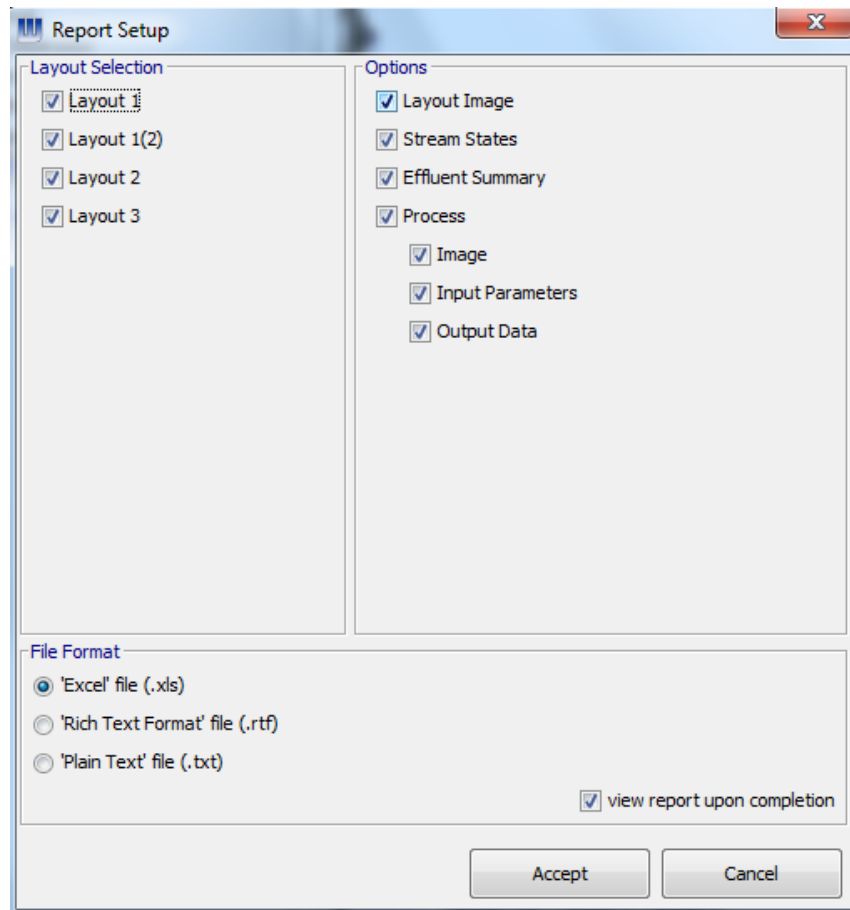
Category : **Disinfection Dose**

	t10 (min)	t50 (min)	tTheta (min)	Total ... (min)	Residu... (mg/L)	Residu... (mg/L)	Residu... (mg/L)
Influent	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Disinfectant Addition	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Chemical Addition	0.0	0.0	0.0	0.0	2.0	0.0	0.0
Flocculator	5.76	40.32	57.6	40.32	0.394336	0.0	0.0
Settling Basin	11.52	80.64	115.2	120.96	0.316137	0.0	0.0
Settling Basin(2)	11.52	80.64	115.2	120.96	0.316137	0.0	0.0
Filtration	43.2	77.76	86.4	198.72	0.268027	0.0	0.0

### 3.3 Generate Report

In addition to the above features for viewing and exporting data, WatPro 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 and select the desired settings.



## 4 Model Calibration

In WatPro, a number of modeled parameters may be calibrated to specific site data. The parameters which may be calibrated include:

- \* DBPs formed (total THMs, HAAs, chlorite, chlorate)
- \* chlorine consumed (initial demand, decay, filter demand)
- \* chlorine dioxide consumed (initial demand, consumption)

Before calibrating the equations in WatPro, it is recommended that the user become familiar with the mathematical models associated with the parameters being calibrated (Please refer to the Technical Reference document for details).

### 4.1 Disinfection By-Product Formation

#### 4.1.1 TTHM Formation Calibration

The total trihalomethanes (TTHM) formation calibration dialog is accessed under the Model/Calibration/DBP Formation menu.

DBP Formation Calibration

TTHM Chlorite Chlorate

$$\text{TTHM} = K1 \cdot (\text{TOC} \cdot \text{UV}_{254})^{K2} \cdot (\text{BR}+1)^{K3} \cdot (\text{pH}-2.6)^{K4} \cdot T^{K5} \cdot \text{Cl}_{\text{dose}}^{K6} \cdot (t^{K7} - t_p^{K7})$$

K1	0.00309	K5	1.06
K2	0.44	K6	0.409
K3	0.0358	K7	0.265
K4	0.715		

Accept Cancel

**K1 ..... K7:** Variables assigned to calibrate the general TTHM equation.



**TOC:** total organic carbon concentration in water

**UV<sub>254</sub>:** absorbance of UV light at wavelength 254 nm by 1 cm of water (cm<sup>-1</sup>)

**BR:** bromide concentration in water (mg/L)

**CIDose:** assigned chlorine dose for unit process

**T:** temperature (deg C)

**t:** time (t<sub>50</sub>) at the end of the unit process being considered (hr)

**tp:** time (previous) (t<sub>50</sub>) at the beginning of the unit process being considered (hr)

Calibration of the WatPro Total THM (TTHM) model improves the predictive accuracy of the model relative to the un-calibrated Amy model (Amy et al., 1987), particularly as the temperature of the water source declines below approximately 15 °C (60°F).

Calibration of the TTHM model may be accomplished using either spreadsheet packages or a statistical software package. The calibration is performed using a routine that minimizes the sum of the squared differences between the measured TTHM concentrations and those predicted by the calibrated model.

The default parameters in the Amy model (see Mathematical Models Chapter) are as follows:

Parameter	Default Value	Parameter	Default Value
K1	0.00309	K5	1.06
K2	0.440	K6	0.409
K3	0.0358	K7	0.265
K4	0.715		

In the calibrated model, these parameters are adjusted by the procedures indicated above to make the formation model match more closely the observed measured TTHM concentrations.

The model calculates the TTHM concentrations formed in each batch reactor. Thus, if several calibration points are used through the process train, the cumulative predicted TTHM concentrations must be used in the exercise. The increment of time between calibration points is used in the model. When a new chlorine addition point is encountered, the time value used in the calibration of the model is reset to zero at the point of injection, and the reaction time begins to increase again thereafter. The Amy model uses chlorine reaction time in units of hours.

The Amy model predicts TTHM formation in units of  $\mu\text{mole/L}$ . The average molecular weight (AMW) expression from the Mathematical Models Chapter is used to convert the concentrations from units of  $\mu\text{mole/L}$  to  $\mu\text{g/L}$ .

#### 4.1.2 Chlorite Formation Calibration

The chlorite formation calibration dialog is accessed under the Model/Calibration/DBP Formation menu.

DBP Formation Calibration

TTHM | Chlorite | Chlorate

$$\begin{aligned} \log(\text{Chlorite}) = & K1 + K2 \cdot \log(\text{pH}) + K3 \cdot \log(T) + K4 \cdot \log(\text{ClO}_2+1) + K5 \cdot \log(\text{RT}+1) + K6 \cdot \log(\text{TOC} \cdot \text{UV}_{254}) \\ & + K7 \cdot \log(T) \cdot \log(\text{ClO}_2+1) + K8 \cdot \log(\text{ClO}_2+1) \cdot \log(\text{RT}+1) + K9 \cdot (\log(\text{pH}) \cdot \log(\text{ClO}_2+1)) \\ & + K10 \cdot \log(\text{TOC} \cdot \text{UV}_{254}) \cdot \log(\text{ClO}_2+1) + K11 \cdot \log(\text{TOC} \cdot \text{UV}_{254}) \cdot \log(\text{RT}+1) \end{aligned}$$

K1	-0.346	K7	0.293
K2	-0.07	K8	0.393
K3	-0.0253	K9	1.27
K4	-0.597	K10	0.67
K5	-0.136	K11	-0.161
K6	-0.0038		

Accept Cancel

**K1 ..... K11:** Variables assigned to calibrate the general chlorite equation

**T:** Temperature (deg C)

**ClO<sub>2</sub>:** Chlorine dioxide dose concentration, mg/L

**RT:** Reaction time (hours)

WatPro uses a multi-parameter non-linear polynomial expression to estimate chlorite formation in each reactor. Terms for two-parameter interactions are included in the equation, which was developed by Korn (1998). In this equation used in WatPro, TOC has been used in place of the non-purgeable organic carbon (NPOC) parameter specified by Korn (1998). Calibration of the chlorite formation model is possible to try to improve the predictive accuracy of the model relative to the un-calibrated expression.

The default values of the empirical parameters used in the equation developed by Korn (1998) are as follows:

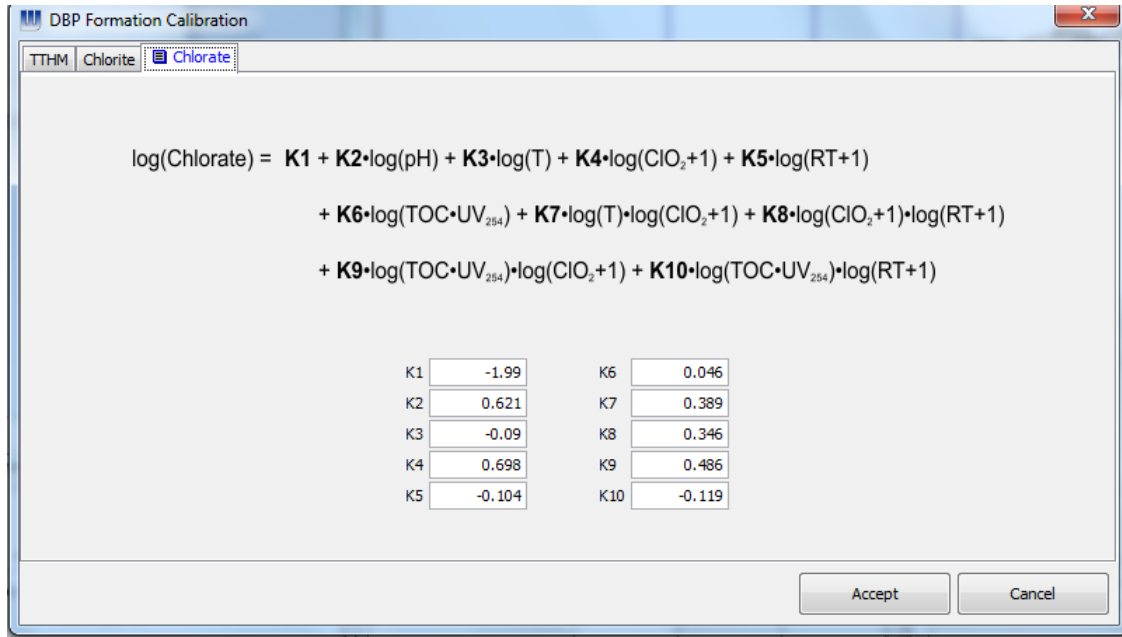
Parameter	Default Value	Parameter	Default Value
K1	-0.346	K7	0.293
K2	-0.07	K8	0.393
K3	-0.0253	K9	1.27
K4	-0.597	K10	0.67
K5	-0.136	K11	-0.161
K6	-0.0038		

Calibration of the model may be accomplished using either spreadsheet packages or a statistical software package. The calibration is performed using a routine that minimizes the sum of the square differences between the measured chlorite concentrations, and those predicted by the calibrated model.

The model calculates the log chlorite concentration (in mg/L) formed in each batch reactor. Thus, if several calibration points are used through the process train, the cumulative chlorite concentration must be used in the exercise. The increment of time between the calibration points is used in the model. When a new chlorine dioxide addition point is encountered, the time value used in the calibration of the model is reset to 0 at the point of injection, and the reaction time begins to increase again thereafter. At each new chlorine dioxide addition point, an initial demand of  $\text{ClO}_2$  is only asserted if the residual concentration at that point is zero.

#### 4.1.3 Chlorate Formation Calibration

The chlorate formation calibration dialog is accessed under the Model/Calibration/DBP Formation menu.



WatPro uses a multi-parameter non-linear polynomial expression to estimate chlorate formation in each reactor. Terms for two-parameter interactions are included in the equation, which was developed by Korn (1998). In this equation used in WatPro, TOC has been used in place of the non-purgeable organic carbon (NPOC) parameter specified by Korn (1998). Calibration of the chlorate formation model is possible to try to improve the predictive accuracy of the model relative to the un-calibrated expression.

The default values of the empirical parameters used in the equation developed by Korn (1998) are as follows:

Parameter	Default Value	Parameter	Default Value
K1	-1.99	K6	0.046
K2	0.621	K7	0.389
K3	-0.09	K8	0.346
K4	0.698	K9	0.486
K5	-0.104	K10	-0.119

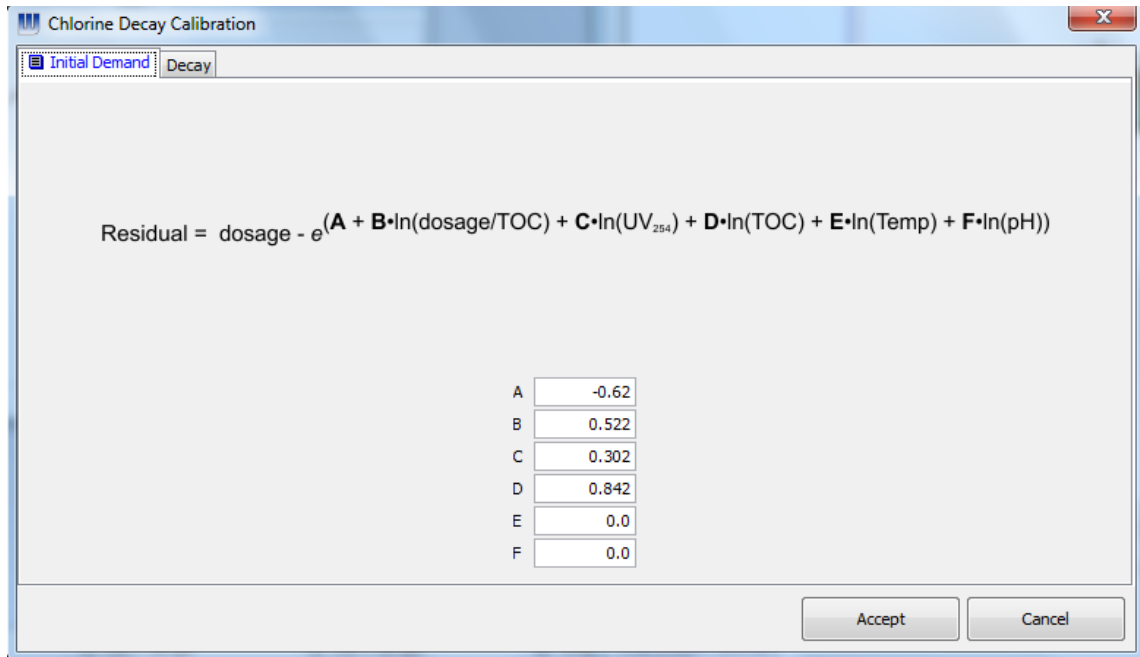
Calibration of the model may be accomplished using spreadsheet packages or a statistical software package. The calibration is performed using a routine that minimizes the sum of the square differences between the measured chlorate concentrations, and those predicted by the calibrated model.

The model calculates the log chlorate concentration (in mg/L) formed in each batch reactor. Thus, if several calibration points are used through the process train, the cumulative chlorate concentration must be used in the exercise. The increment of time between the calibration points is used in the model. When a new chlorine dioxide addition point is encountered, the time value used in the calibration of the model is reset to 0 at the point of injection, and the reaction time begins to increase again thereafter. At each new chlorine dioxide addition point, an initial demand of ClO<sub>2</sub> is only asserted if the residual concentration at that point is zero.

## 4.2 Chlorine Decay

### 4.2.1 Chlorine Initial Demand

The initial chlorine demand calibration dialog is accessed under the Model/Calibration/Chlorine Decay” menu.



The default values of the empirical parameters used in the initial chlorine demand equation are as follows:

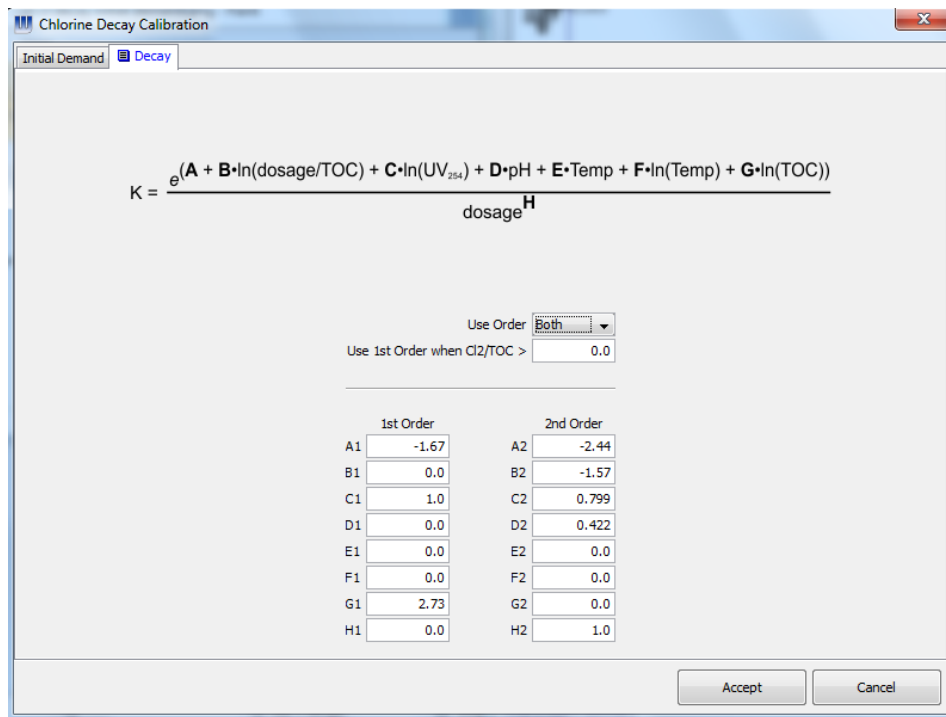
Parameter	Default Value	Parameter	Default Value
A	-0.62	D	0.842
B	0.522	E	0
C	0.302	F	0

The form of the calibratable initial chlorine demand equation is similar to the default equation used by WatPro (see Mathematical models chapter). The additional terms of temperature (Temp) and pH have been included to provide more flexibility. It should be noted that when calibrating the initial demand equation, the demand due to the presence of ammonia is considered separately. As a result, the chlorine dosage should reflect the concentration after ammonia demand has been satisfied.

Calibration of the initial demand model may be accomplished using either experimental data or, if sufficient data are available (e.g. short sample intervals), using field data. Spreadsheet software or a statistical package can be used for calibration purposes.

### 4.2.2 Chlorine Decay Calibration

The chlorine decay calibration dialog is accessed under the Model/Calibration/Chlorine Decay menu.



The default values of the empirical parameters used in the initial chlorine demand equation are as follows:

Parameter	Default Value		Parameter	Default Value	
	1 <sup>st</sup> order	2 <sup>nd</sup> order		1 <sup>st</sup> order	2 <sup>nd</sup> order
A	-1.67	-2.44	E	0	0
B	0	-1.57	F	0	0

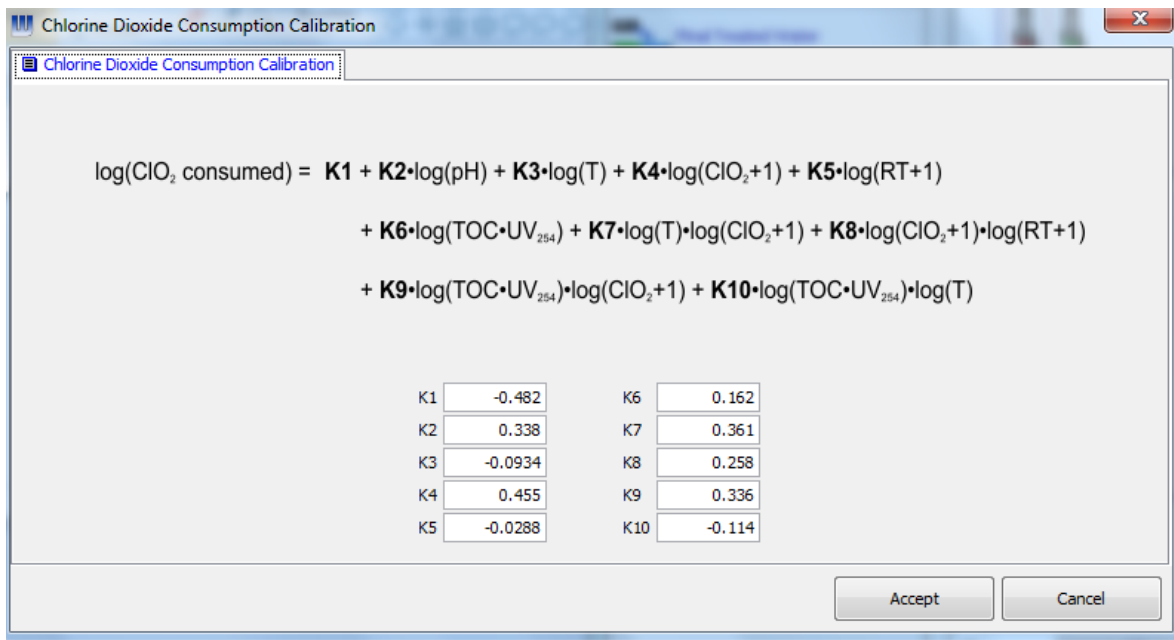
C	1	0.799	G	2.73	0
D	0	0.422	H	0	1

The form of the decay equation is similar to the default model used by WatPro (see Mathematical Models Chapter). The additional terms to account for temperature (Temp) have been included to provide more calibration flexibility. The value of G allows the user to maintain the same form of the first and second order equations as presented in the Mathematical Models Chapter. For example, if G were set to 0 then the form of the equation would be similar to the first order decay equation presented in the Mathematical Models Chapter. The order option (set at “Both” in the above figure) and the chlorine dosage to TOC ratio boxes are used to indicate if the decay equation to be used should be first or second order or if a combination of both should be used. If both are to be used, then the chlorine dosage to TOC ratio is used to determine at point the decay is first order and what point it is second order.

Calibration of chlorine decay may be accomplished using either experimental data or using field data. Spreadsheet software or a statistical package can be used for calibration purposes.

### 4.3 Chlorine Dioxide Consumption

The chlorine dioxide consumption calibration dialog is accessed under the Model/Calibration/CLO2 Consumption menu.



The form of the calibratable chlorine dioxide consumption equation is similar to the default equation used by WatPro (see Mathematical Models chapter).

WatPro uses a multi-parameter non-linear polynomial expression to estimate chlorine dioxide consumption in each reactor. Terms for two-parameter interactions are included in the

equation, which was developed by Korn (1998). In this equation used in WatPro, TOC has been used in place of the non-purgeable organic carbon (NPOC) parameter specified by Korn (1998). Calibration of the chlorine dioxide consumption model is possible using either experimental data or field data to try to improve the predictive accuracy of the model relative to the un-calibrated expression. A recent spreadsheet software package (such as MS Excel) or a statistical package can be used for calibration purposes. The default values of the empirical parameters used in the equation developed by Korn (1998) are as follows:

Parameter	Default Value	Parameter	Default Value
K1	-0.482	K6	0.162
K2	0.338	K7	0.361
K3	-0.0934	K8	0.258
K4	0.455	K9	0.336
K5	-0.0288	K10	-0.114



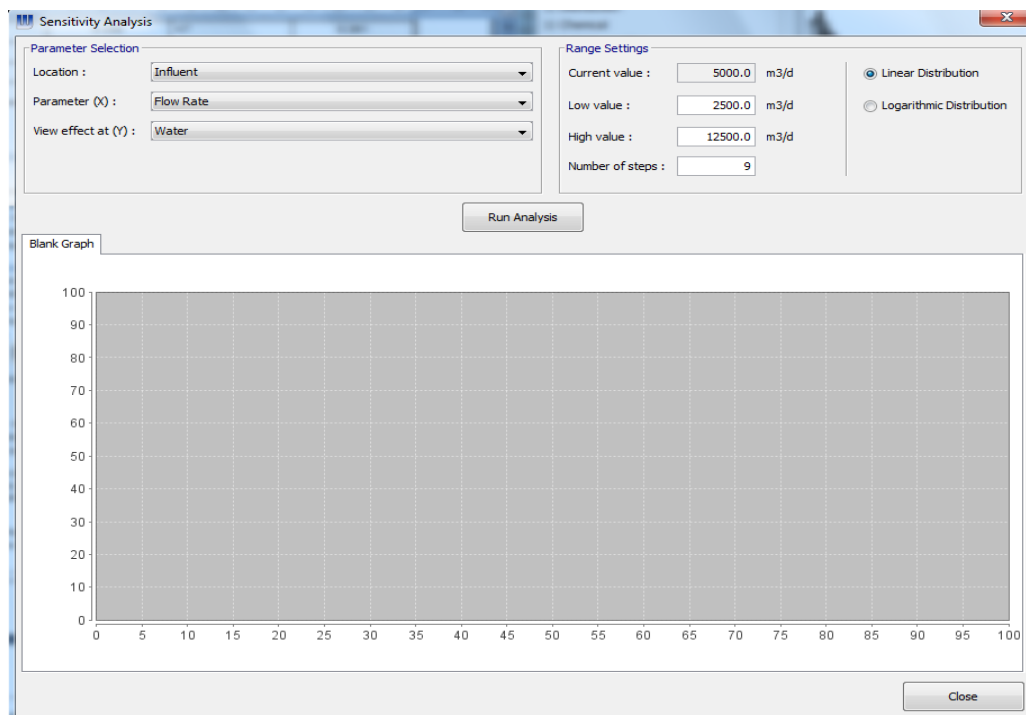
# 5 Sensitivity Analysis

The sensitivity analysis feature allows the user to see the effect of various design and operating conditions 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 effluent concentrations.

## 5.1 Setup of 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, set the process location, independent parameter (X), and dependent parameter (Y).

An example sensitivity analysis dialog box is presented below.



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. Then set the low value and the high value for the range the effect is to be examined. Set the number of steps to obtain a sufficient number of points for assessment.

### **Sensitivity Analysis Options**

**View Effect At (Y):** If the treatment plant has more than one process stream as the treated plant effluent, the selection is made here. If there is only one treated water stream, it is selected by default.

**Location:** The unit process which contains the parameter to be varied is selected using a scroll down menu.

**Parameter (X):** The parameter to be varied (independent variable, X) is selected using a scroll down menu.

**Current Value:** This indicates the current value of the independent parameter entered in the unit process, and cannot be varied.

**Low Value:** User input for the lowest value to be used for the independent variable (X)

**High Value:** User input for the highest value to be used for the independent variable (X).

**Number of Steps:** This indicates the number parameter values that will be used (between the low and high X values) for testing the sensitivity analysis.

### **Scale Option**

The range of the sensitivity analysis may vary over a small range or over several orders of magnitude. Depending on the portion of the sensitivity analysis curve of greatest interest, a user may choose to have the intermediate points of the range estimated on a linear basis or on a log basis.

**Linear Distribution:** The range, as determined by setting the low and high factors, is divided by the number of steps -1 (for the initial step with 0 increment). . Each step is incremented by the quantity:

$$\Delta X = (X_{\max} - X_{\min}) / (\#steps - 1)$$

and

$$X_{n+1} = X_n + \Delta X$$

**Log Distribution:** The range is established as the difference of the log values of the minimum and maximum, and the increment becomes the difference of the log values of the minimum and maximum, divided by the number of steps -1 (for the initial step with 0 increment). . Each step is incremented by the quantity:

$$\Delta X = [\log(X_{\max} - \log(X_{\min}))]/(\#steps - 1)$$

and

$$X_n = 10^{(1 + (n - 1) * \Delta X)}$$

## 5.2 Output of Sensitivity Analysis

Once the sensitivity analysis parameters have been set, the analysis can be run by clicking the Run button. The sensitivity analysis will be performed over the specified number of steps and displayed as a graph and table of values. When it is finished, the results of the analysis are reported under different tabs.

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. To copy the graph to the clip board, use the Copy Image to Clipboard button available below the Graph Legend button.

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.



## 6 Additional Topics

### 6.1 How to Create Multiple Layouts in the Same File

WatPro allows users 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 either:

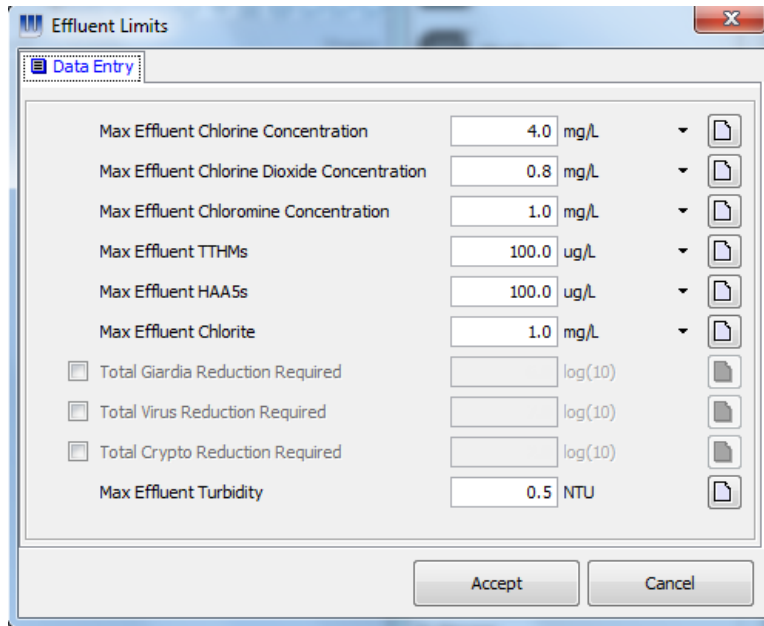
- (1) From the **Layout** menu choose **Insert** to add a blank layout to the file. Alternatively to create a duplicate of the current layout, use the **Duplicate** option.
- (2) Right-click on the layout name tab (at the bottom-left of the drawing board) and select the **Insert** option.

### 6.2 How to Zoom In/Out

The user can use the **View→Zoom** command to zoom in and out of 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.

### 6.3 How to Set Effluent Limits

After any simulation run, WatPro compares treated effluent quality to maximum allowable concentrations (MACs) specified by the user for certain parameters, including disinfection by-products (THMs, HAA<sub>5</sub>, and chlorite), and disinfectant residual concentrations (chlorine and chlorine dioxide). These parameters can be set in the Effluent Limits dialog box accessible from the **Model→Effluent Limits** menu.

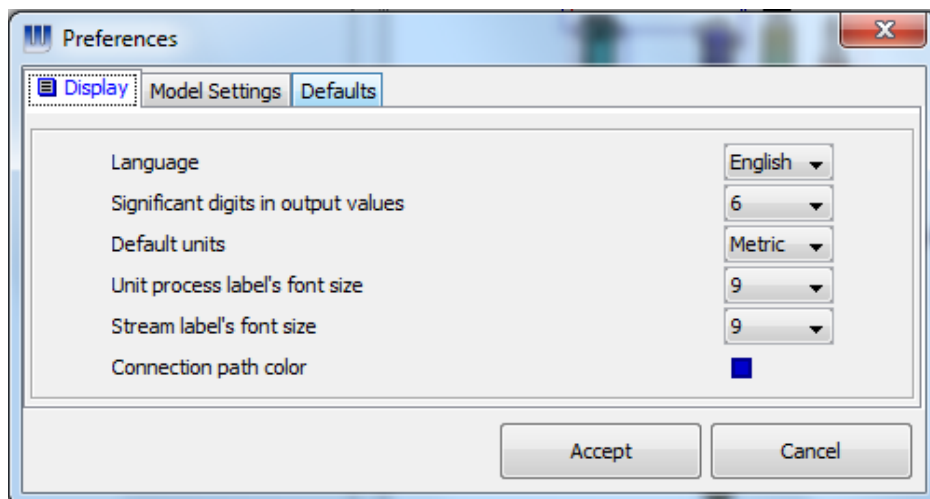


If the facility final treated water exceeds the maximum allowable concentrations for disinfection by-products (total THMs, HAA<sub>5</sub>, chlorite, chlorate), disinfectant residuals, (chlorine, chloramine, chlorine dioxide) or turbidity, the water is considered to be out of compliance. The Final Effluent Summary table discussed previously will reveal the non-compliant parameters.

WatPro determines a plant’s requirements for *Giardia* and virus inactivation based on the influent water *Giardia* cyst concentration as specified by the EPA’s Surface Water Treatment Rule. These requirements can be superseded by checking the box.

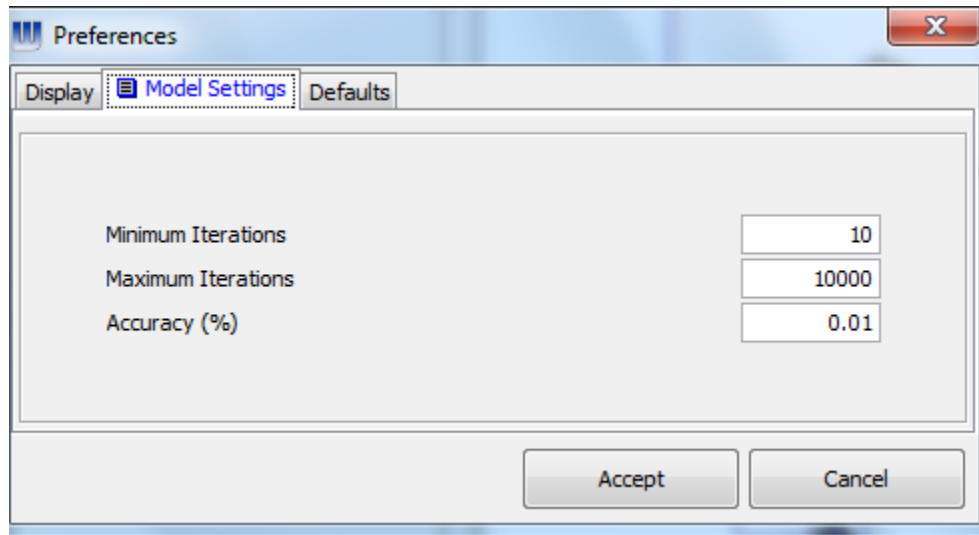
### 6.4 How to Change the System Preferences

WatPro allows customization of the display, and the selection of default units (metric or U.S.) for output on the display and on the printed reports. These options are found in **View→Preferences**. The figure below shows the customizations available in WatPro.



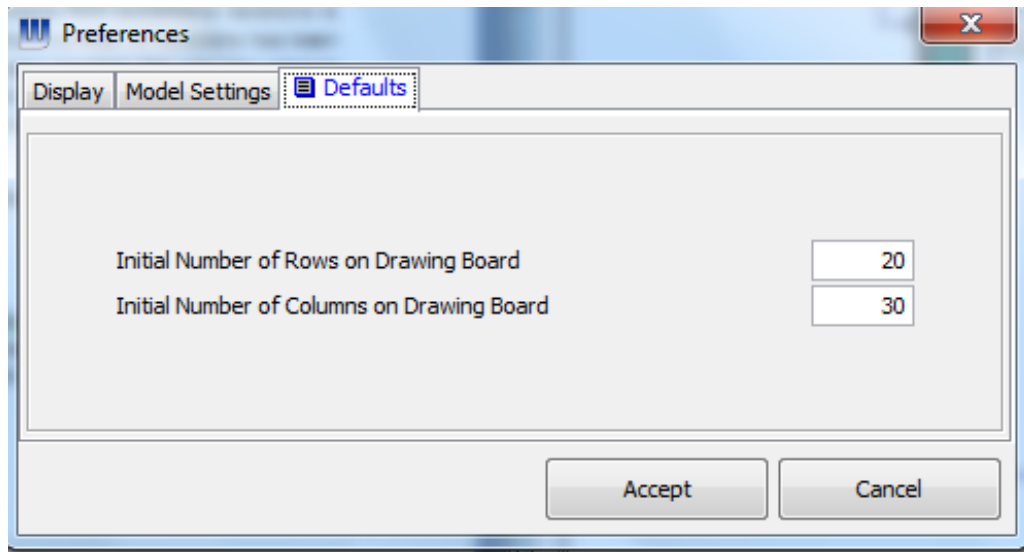
**Display Settings:** This setting determines the language, significant digits in output values, default units, font size, connection path color display for all of the data entry screens, the model report screens, as well as the units in all of the reports. This setting should be set to the preference of the user of the software.

**Model Settings:** The model settings feature is used by the model to determine the length and accuracy of model iterations;



Certain models in WatPro use an iterative procedure to arrive at a numerical solution. The opportunity for the model to arrive at an iterated solution is determined by the number of iterations performed, and by the specified precision of the solution. The model stops the iteration procedure if the difference between numerical solutions from successive iterations is less than or equal to the specified accuracy, or if the maximum number of iterations has been reached without arriving at a solution. If a solution has not been reached, the user may elect to change either the number of iterations or solution accuracy to enable the model to reach a solution. By default, WatPro uses 1000 as the maximum number of iterations, and a solution accuracy of 0.001 %.

**Defaults Settings:** This setting is used when new schematic configurations are created. The default number of trains (rows) for a drawing is 20. The basic default number of processes (columns) for a drawing is 30. These values can be changed when more appropriate values for the number of rows or columns are required.



## 6.5 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.

The following steps 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. Click-and-drag to move the line in indicated direction.
- (2) To create a break-point, right-click the line at the point where the break point is desired. From the pop-up menu, select "Create breakpoint".

## 6.6 How to View Stream Properties Quickly

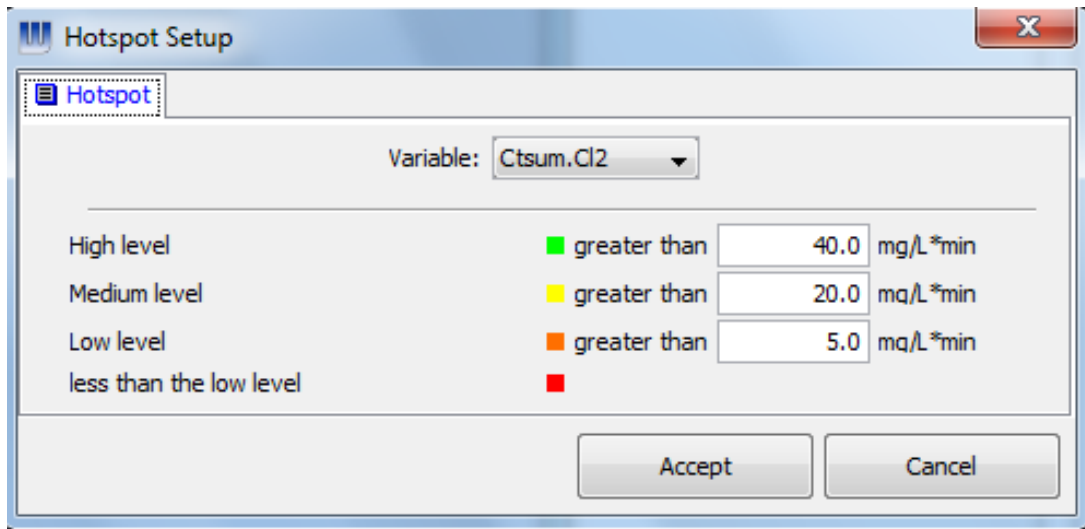
To view the properties of a stream, right-click on the stream and select "View Stream States". The pop-up window will show the calculated values of the stream properties.

## 6.7 How to use Hotspots

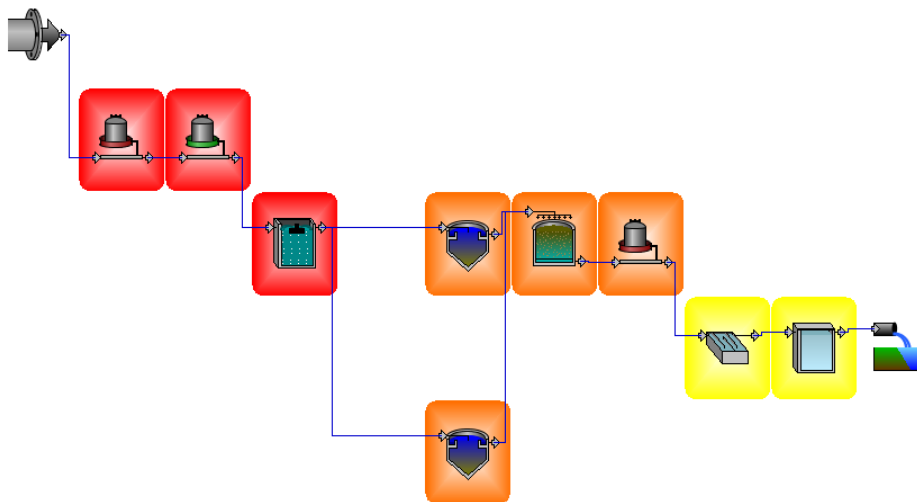
With the hotspots feature, after a model has been successfully run, the background of the various unit processes is assigned a color coded display depending on the predicted concentration. Thus, the display can quickly indicate where "hotspot" concentrations are located. The Hotspots feature can be used to follow the progression of modeled parameters through the water treatment plant.

The hotspot toolbar must be displayed for this feature to take effect (accessed through the **View→Toolbars** menu). A legend is displayed on the toolbar along with a dropdown list to select the desired variable and a settings button to access the range settings for each variable.

The hotspots display can be de-activated by hiding the Hotspots toolbar.



An example of the model configuration after a run with the Hotspots feature activated is shown below.

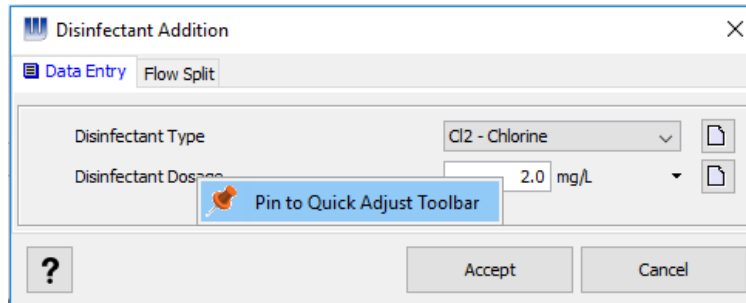


### 6.8 How to Add Parameters to the Quick Adjust Toolbar

The Quick Adjust Toolbar is a handy place to isolate certain parameters that you'd like to adjust in a readily accessible location so that they can be quickly modified and the layout can be re-calculated.

To place a parameter on the quick adjust toolbar, open the Data Entry form by right clicking on the object and selecting Edit Parameters. Then right-click on the parameter that needs to be placed on the quick adjust toolbar and select the "Pin to Quick Adjust Toolbar".





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”. 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.