2.1 Developing a Design Case

In this chapter, we will guide you through the steps of creating a design case. We do that by first describing how to create a simple example process. This example will illustrate the key initialization steps involved with the creation of any type of flowsheet. Regardless of which industry you are in, you should read through this example to become familiar with the basic steps of modeling processes using either SuperPro or EnviroPro Designer.

In addition to this simple example, three other example processes will be described in this chapter. These other examples – listed below – are more complex than the first and they are better representations of what a "real" process modeled with Pro-Designer would look like.

- *Synthetic Pharmaceuticals*. This example deals with a synthetic pharmaceutical process. It is recommended for users in the pharmaceutical and specialty chemical industries.
- *Biotech Processing*. This example deals with the production of β-galactosidase and it is recommended for users in the bioprocessing industries.
- *Wastewater Treatment*. The third additional example deals with an industrial wastewater treatment plant and it is recommended for users that target water purification and wastewater treatment applications.

Table 2.1a provides a brief description of other examples that are included with your copy of SuperPro/EnviroPro Designer.

Table 2.1a: Examples shipped with SuperPro / EnviroPro Designer
(in addition to those described in this chapter)

Subdirectory	Available In	Description
CHEESE	SuperPro	This example analyzes a highly integrated dairy plant that produces cheese, butter, WPC, and ethanol. It is recommended for users with interests in food processing.
MAMMCELL	SuperPro	This example analyzes the production of a therapeutic monoclonal antibody using animal cell culture. It is recommended for users with interests in animal cell culture and high value biopharmaceuticals.
INSULIN	SuperPro	This example analyzes the production of biosynthetic human insulin (a variation of Eli Lilly's process for Humulin). It is recommended for users with interests in bioprocessing and biopharmaceuticals.
PHTABLET	SuperPro	This example deals with a process for making pharmaceutical tablets. It is recommended for people that deal with secondary manufacturing (dosage formulation and fill-finish) of pharmaceuticals and related products.

MISC	SuperPro	A set of small examples demonstrating special features of the software. (a) "BKinFerm" focuses on modeling of Batch Kinetic Fermentor and demonstrates how to generate composition profiles of reactants and products. (b) "BKinRxn" explains how to model batch kinetic reactions. (c) "EquilRxn" explains how to use an equilibrium reaction to estimate extent of precipitation and crystallization. (d) "BtchDist" explains how to model a batch distillation step and generate composition profiles. (e) “PulOp” explains how to use Pull In and Pull Out operations. (f) “FedBR” explains how to model a fedbatch kinetic reaction. (g) “MxPrp” explains how to use the Mixture Preparation procedure.
MUNWATER	SuperPro EnviroPro	This example focuses on the modeling and retrofit design of a municipal wastewater treatment plant. It addresses issues of nutrient removal and it is recommended for users with interests in industrial and municipal wastewater treatment.
UPWATER	SuperPro	This example deals with water purification (ultra-pure water production) and wastewater treatment at a Semiconductor Manufacturing Facility. Evaluation of recycling options for minimizing city water use and wastewater disposal is included.
GE	SuperPro EnviroPro	This example analyzes an effort to minimize generation of hazardous sludge and wastewater at a manufacturing facility of General Electric. It is recommended for users with interests in waste minimization, water recycling, and pollution control.
INCINRTR	SuperPro EnviroPro	This example describes a simple process (a single unit) for analyzing the combustion of sludge in an incinerator. It is recommended for users with interests in incineration and pollution control.
AIRCONTR	SuperPro EnviroPro	This example analyzes a three-step process for removing dust particles and acetone (a VOC molecule) from an air stream. It is recommended for users with interests in air pollution control processes.

After you have installed SuperPro/EnviroPro on your computer, you can access these examples in the EXAMPLES subdirectory. In addition, each example has its own detailed Read-Me file (in MS Word format).

2.1.1 Getting Started

The first example of this chapter demonstrates the key initialization and analysis steps for modeling a process with Pro-Designer. The fundamental steps and analysis features used in this example are the same as the steps and features that would be used during the creation of any other type of flowsheet. Therefore, regardless of which type of process you intend to model, reading through the following example should provide you with the knowledge required to model processes on your own. In addition, since this example is a batch process, it serves as a medium for discussing several scheduling issues. Note: in continuous processes, the initialization steps related to scheduling of operations within unit procedures (described in Section 2.1.5) do not need to be performed.

The steps listed below summarize the process of developing a design case with Pro-Designer. These steps are explained in much greater detail in the remainder of this chapter.

1. Initialize the flowsheet using the first three items of the **Tasks** menu: **Set Mode of Operation, Register Components & Mixtures,** and if the mode of operation is batch, **Recipe Scheduling Information**.
2. Build a flowsheet by selecting the desired procedures from the **Unit Procedures** menu. Switch to **Connect Mode** to draw the streams and connect the process steps.
3. Add operations, such as **Charge, Agitate, Heat, React,** etc. to each unit procedure (this applies to batch procedures only). Different unit procedures have different operations available to them. After the desired operations have been added, initialize all operations and streams.
4. Complete the analysis of the flowsheet using the remaining items of the **Tasks** menu: **Solve M&E Balances,** input **Stream Classification** data, **Perform Economic Calculations,** etc. Other analyses may be optionally performed.
5. Generate and view reports using items from the **Reports** menu. Use the **View** menu to see the results of the analyses and charts.

Starting Pro-Designer

To begin working on a new flowsheet, simply open Pro-Designer either by selecting it from your Start Menu or by double-clicking the Designer.exe application file in the Pro-Designer folder of your hard drive. After the program boots up, the following dialog box will appear:

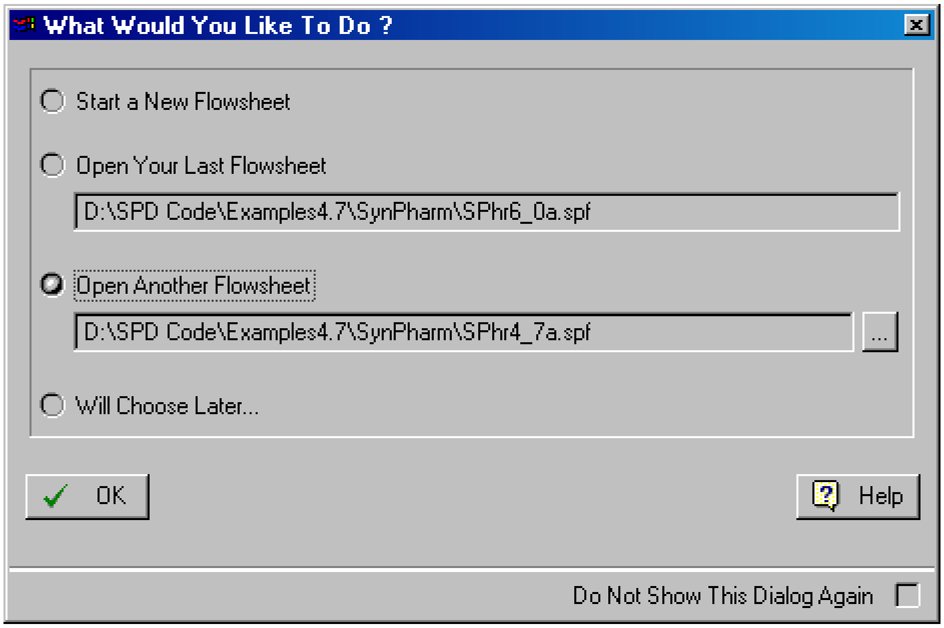


Figure 2.1-a Opening Dialog

Select the option entitled *Start a New Flowsheet.*

2.1.2 Specifying the Mode of Operation for the Entire Plant

After you choose to start a New flowsheet, the new design case dialog (Figure 2.1-b) will appear. This dialog box allows you to set the primary mode of operation and the annual operating time for the new flowsheet. Pro-Designer can model process plants that operate in batch, continuous, or mixed modes. You can also use the **Tasks: Set Mode of Operation...** menu item to change the mode of operation at any time. Please note that Pro-Designer allows you to have continuous unit procedures in a batch flowsheet as well as batch (cyclical) procedures in a continuous flowsheet. Furthermore, when the operating mode of the entire plant is set to batch, all stream flows are displayed on a per-batch basis, as opposed to on a per-hour basis. For plants operating continuously, no scheduling information is necessary. At this point, please select “Batch” as the Plant Operation Mode for the example process, which you will create.

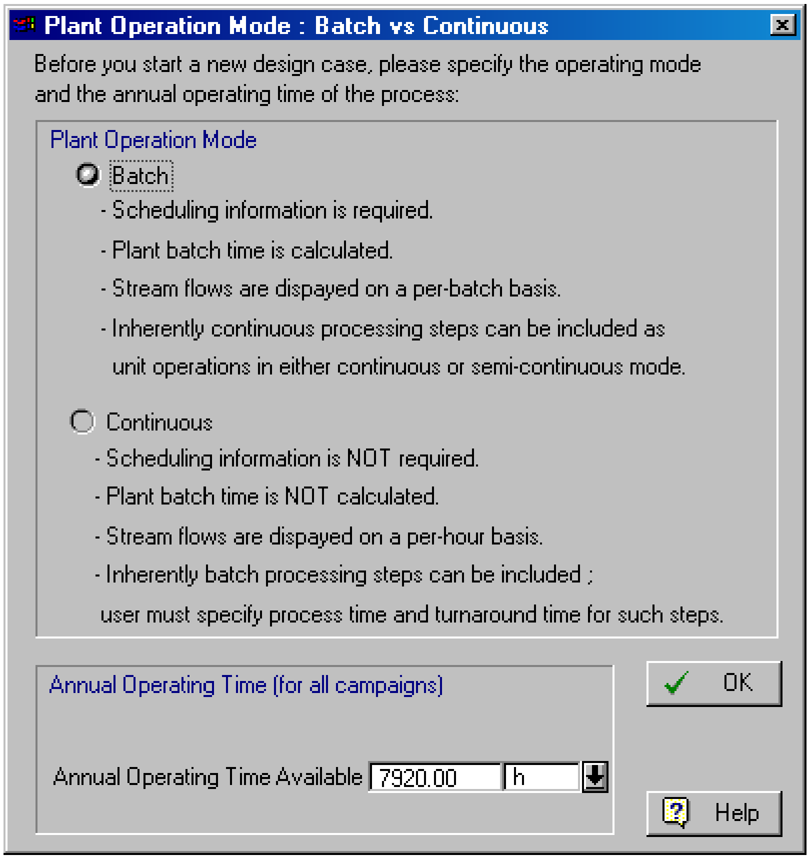


Figure 2.1-b: Specifying the operating mode for the entire flowsheet

2.1.3 Setting the Default Physical Units

Pro-Designer provides a variety of options for units of measure for the entry and display of data. You may use the **Edit: Flowsheet Options: Preferences: Physical Units Options…** menu item to view or modify the default units.

2.1.4 Registering Components and Mixtures

Databanks. Pro-Designer provides for the use of multiple component databases. The default databank shipped with Pro-Designer, entitled “Designer,” provides data for a number of commonly used compounds. If you use the DIPPR database you may use it with Pro-Designer. There is also an empty databank entitled “User” than may be used to store data for user-defined components. Use **Databanks: Edit Databank Location** to change or add component databanks. See section 3.8 in the manual for details.

Registering Components. All the components that will be used in a design case must be specified. Many of these components may be selected from the component library in Pro- Designer. To register components (in other words, to add them to your design case), choose the menu command **Tasks: Edit Pure Components**. This will activate the dialog shown below (Figure 2.1-c).

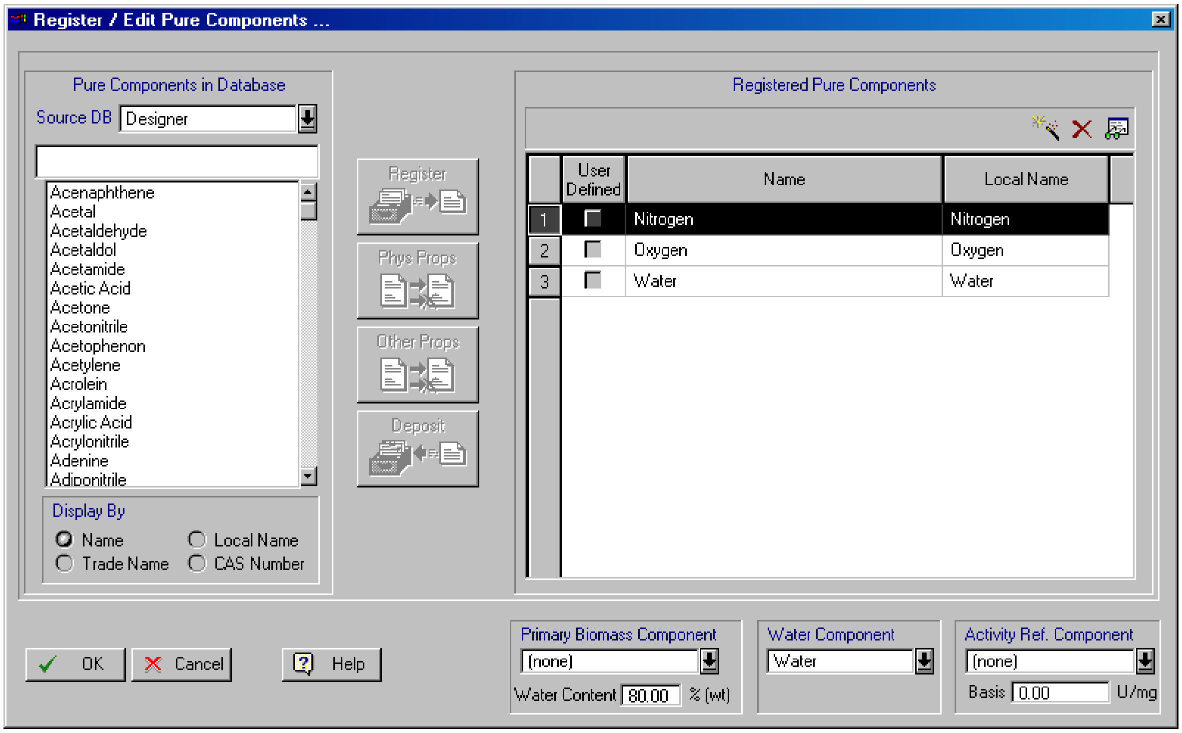


Figure 2.1-c: The Component Registration dialog

By default, nitrogen, oxygen, and water are always registered as pure components in new processes. For this example process, you will need to add heptane to the list of registered components as well. To add heptane, you can either scroll down to it in the pure component database list on the left, or you can begin typing “heptane” in the box above the list and the database will automatically scroll to the correct location. Next, use the **“Register”** button to add heptane to the Registered Components list for this flowsheet. Alternatively, you may double click on heptane in the database listing and it will be added to your list of Registered Components.

If a component does not appear in the library, you should use the "New..." button to add it. For this process, you will need to create three new components: A, B, and C. These components will represent the reactants and products of a simple reaction. To add component A to your database, click the “New…” button () and fill in the letter “A” for the Name, CAS Number, etc. (Note – as far as the program is concerned, you do not have to have correct CAS Numbers, Formulas, etc. You just need to have something written in each of these six fields. The Local name is the one that appears in the reports and all the input/output dialog windows of the program.) Notice that at the bottom of this dialog box, you can choose to either initialize the physical properties to zero or copy them from some other component (see Figure 2.1-d).

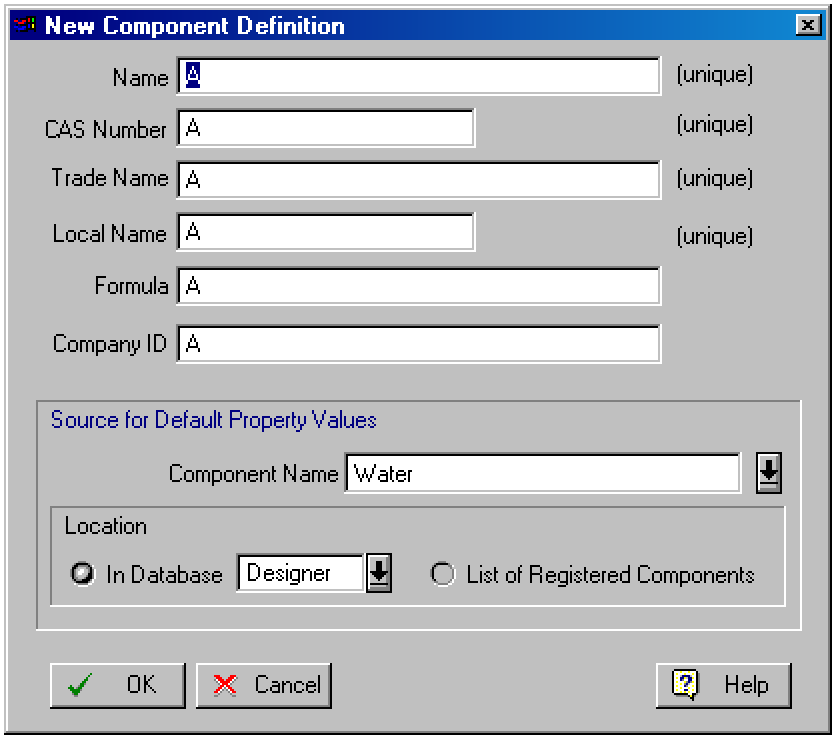


Figure 2.1-d: The New Component Definition dialog

For this example, simply click “OK” to copy the property values for component A from water.

After you have added component A to your list of registered components, follow the same steps to add components B and C. When you have completed this, you should edit some of the properties of these components. To access the basic properties of component A, select its line by clicking on the corresponding number on the left-most column of the table (e.g., number 1 for component A in Figure 2.1-e) and then click on the “Properties...” button ( ). This brings up another dialog window which allows you to view and edit the physical and environmental properties of component A as well as its cost data and regulatory information.

For the purposes of this example, the only physical parameter we will be concerned with is the molecular weight (MW). For component A, please change the MW to 150 (as shown in Figure 2.1-f). In addition, please go to the Economics tab, specify a purchase price of \$10/kg, and press “OK”.

Next, please visit the Properties dialog for component B (by clicking on line 2 and then clicking the “Properties…” button) and enter a MW of 25 and a purchase price of \$15/kg. Finally, enter a MW of 175 and a selling price of \$300/kg for component C. This completes your initialization of components for our simple example.

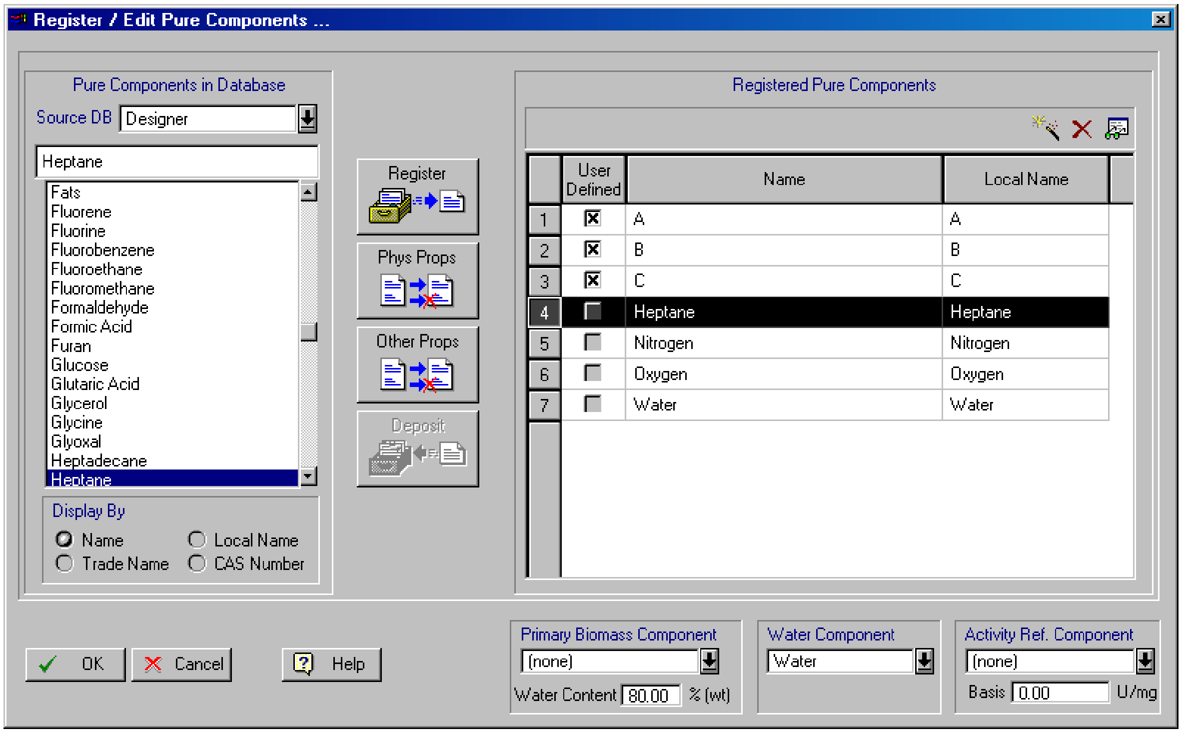
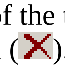


Figure 2.1-e: Selecting a component to edit its properties

Notes:

1) If you need to delete a component from the Registered Components listing, click on the corresponding number on the left-most column of the table (e.g., number 1 for component A) and then click the “Delete” button ().
2) If you wish to add components which you have edited or created to the User database (so that you can access these components in future design case files), select the User database (from the Source Databank drop-down menu), highlight the component by clicking on the corresponding number on the left-most column of the table (e.g., number 1 for A) and then click the “**Deposit**” button.
3) The current version of Pro-Designer does not make use of the normal freezing point of chemicals components. As a result, the value of that field can be ignored.
4) Mixtures are used to facilitate initialization of input streams in cases where certain raw materials (e.g., buffers) are consumed as mixtures. Mixtures are registered by selecting **Tasks: Edit Stock Mixtures.**

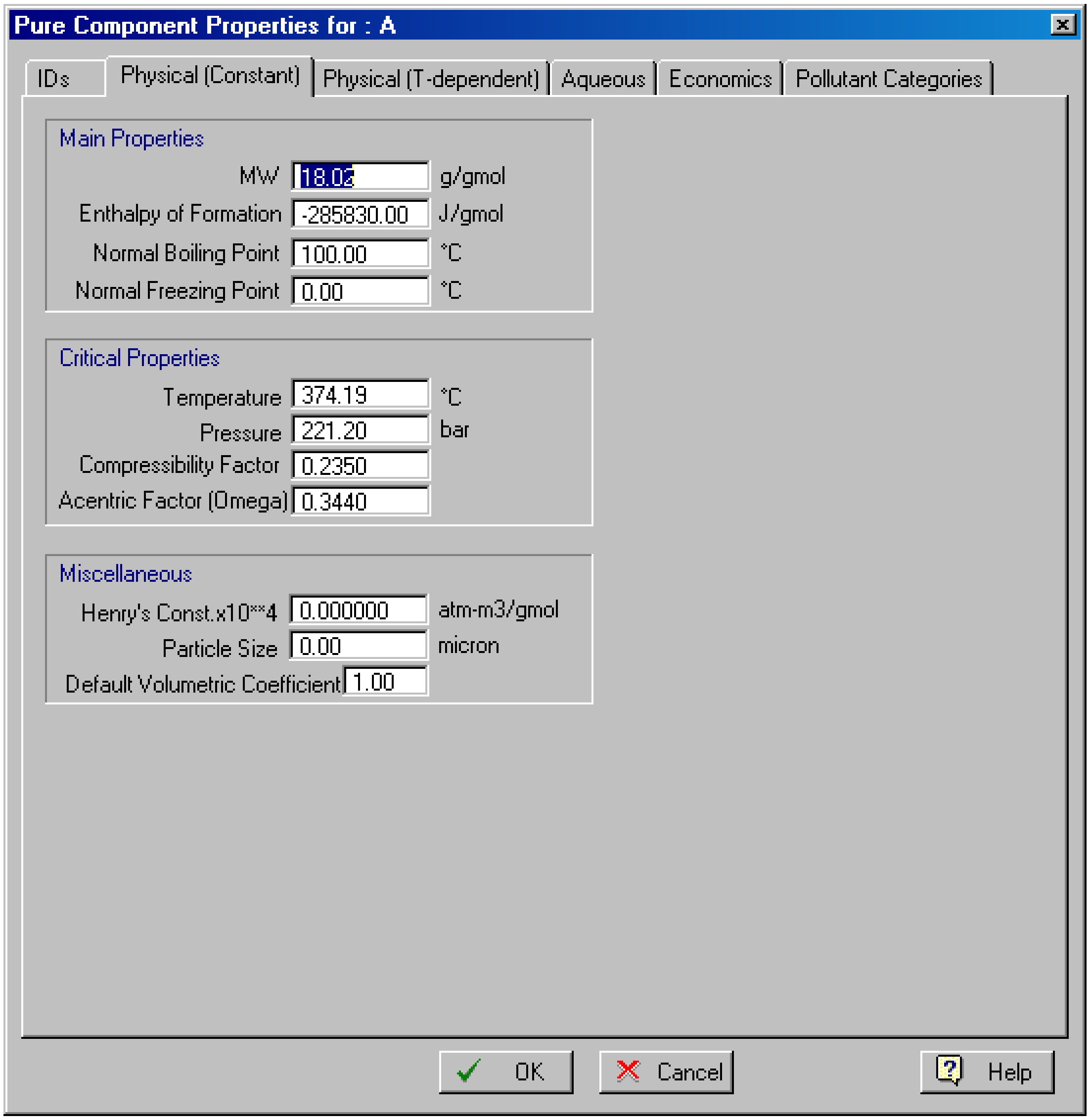


Figure 2.1-f: Editing the properties of component A

At this point in time, you should probably save your file by choosing **File: Save As…** and giving your flowsheet a descriptive name. In general, it is a good idea to save your work often in order to avoid having to redo work in the event of a program crash. If the program does crash, there is sometimes a possibility that you will not be able to reopen the file you were most recently working on. In that case, you should try opening the backup versions of your file. Anytime you save a newer version of your file, Pro-Designer changes the previous version to a ".sp~" file (as opposed to a normal ".spf" file.) If there is already a ".sp~" backup file, Pro-Designer changes this older file to a ".s~~" file as a second backup. To open a backup file, simply go to the directory where you saved your original file and look for the ".sp~" backup (select "All Files" for file types). Then double-click this file to open it. The file extensions for EnviroPro are {.epf, .ep~, .e~~}, respectively.

Tip: When working with larger design cases, include the date or some other version indicator in the case name.

2.1.5 Building the Flowsheet

The first step in building a flowsheet is to add processing steps (unit procedures) to the flowsheet. A unit procedure is defined as a series of operations that take place within a piece of equipment. The types of operations available depend on which type of unit procedure you are using. Please note that continuous unit procedures are equivalent to unit operations.

To Add a Unit Procedure...

First select the desired unit procedure from the **Unit Procedures** menu. For our example, please select **Unit Procedures \ Vessel Procedure \ in a Reactor**. Notice that after you select this unit procedure, the mouse cursor changes to:

indicating that your next mouse click on the flowsheet will lay down the reactor unit procedure in that location. Please click near the left side of the flowsheet to place the Vessel Procedure icon.

After you have added the Vessel Procedure to the flowsheet, please add a Plate and Frame filtration procedure by selecting **Unit Procedures \ Filtration \ Plate and Frame Filtration**, and then clicking somewhere to the right of the Vessel Procedure icon. Your flowsheet should now look something like this:

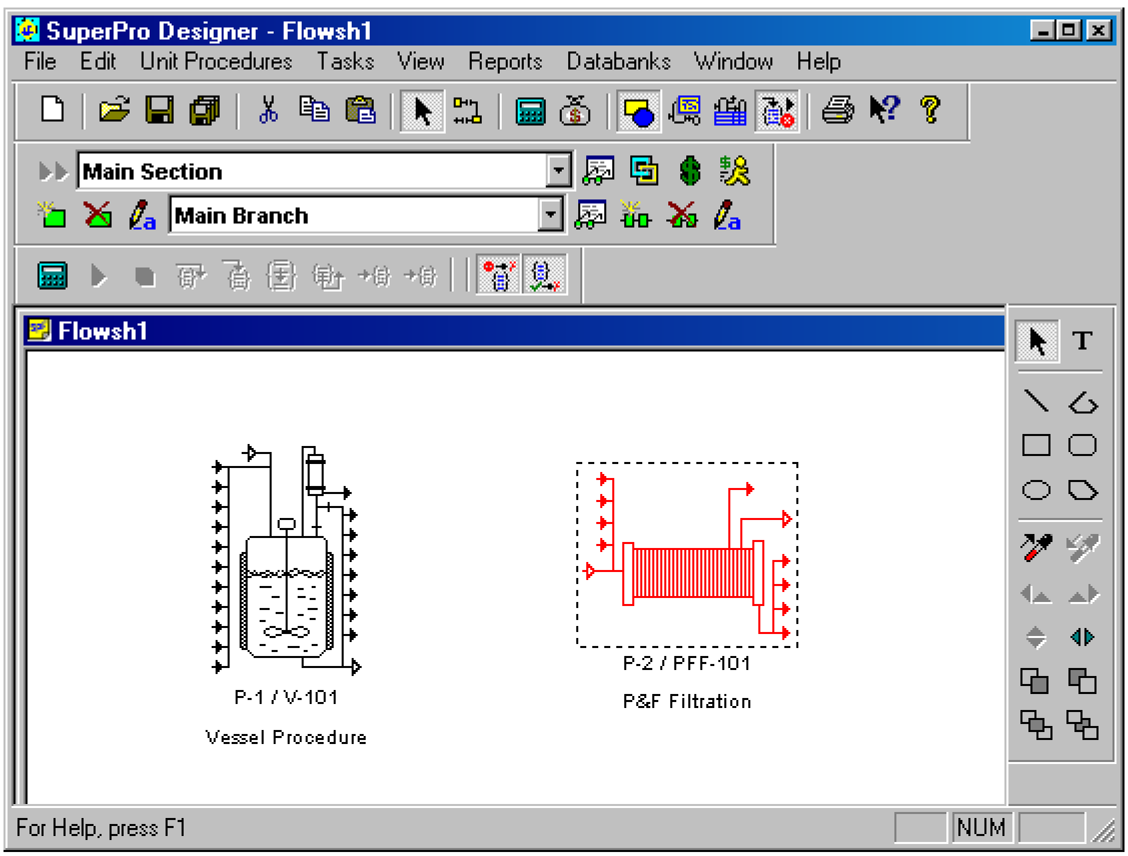


Figure 2.1-g: The example flowsheet with the Vessel Procedure and Plate and Frame Filtration icons added

Note: If you decide to abort the addition of the new unit procedure, you can simply hit the **ESC** key. If you intend to introduce the same unit procedure several times, you can use the following shortcut: after you have laid down the first unit procedure icon, hold down the **Ctrl** and **Shift** keys and click where you want the next copy of the process step to be located.

Note: If you wish to modify the default equipment prefixes, e.g. "V" for vessel and "PFF" for plate and frame filtration, use the **File: Application Settings...** menu item and select the prefixes tab.

If You Wish to Move a Unit Procedure...

1. Select the desired unit procedure icon by clicking on it with the mouse. If more than one icon needs to be moved at the same time, you can either group-select them by dragging an enclosing rectangle around them, or you can edit the selected icon set by adding or removing icons one by one. To add an icon to the selection set, click on it while holding down the **Ctrl** key. Note that if the icon was already in the selection set, it will be de-selected if you **Ctrl+Click** on it.

2. Drag the selected icon to the new location. If the selection set has more than one icon, drag any member of the selection set and all icons will move simultaneously. If you want to move the selected set of icons one pixel at a time, you can use the arrow keys.

NOTE: When you move a unit procedure icon, which has streams, attached to it, all streams will move with it. If the destination and source icons of a stream move, then the stream will keep its structure intact and move with them. If one of the stream's ends remains anchored while the other end is being moved, then the stream will adjust its first and/or last elbow to accommodate the change of location. You can also manually edit the location of the stream's elbows (see Chapter 4). Adding and moving stream lines will also be explained later in this example.

If You Wish to Delete a Unit Procedure...

1. Select the unit procedure icon you wish to delete by clicking on it with the mouse. If desired, you can delete multiple procedures at once (see "To Move a Process Step" above to learn how to select multiple unit procedures).

2. Hit the **Delete** key or select the **Edit : Clear** option from the main menu. The selected unit procedure(s) will be erased.

NOTE: When you delete a unit procedure, all streams attached to it will be deleted with it.

If You Wish to Cut/Copy and Paste a Unit Procedure...

Pro-Designer allows you to place a selection of unit procedures and streams into the clipboard by cutting or copying them and later pasting them into another area of the same flowsheet. In addition, you can use the Cut/Copy and Paste features of the program to copy whole sections from one flowsheet to another. To do this, select the desired unit procedure icon(s), and then select **Edit: Cut** (or **Ctrl+X**) to cut the icons or **Edit: Copy** (or **Ctrl+C)** to copy the icons. Next, paste the unit procedures onto another area of the flowsheet, or onto different flowsheet by selecting **Edit: Paste (**or **Ctrl+V**).

NOTES:

a. If you want to paste the copied icons into another application (e.g., a word processing application), please consult Chapter 14.

b. You cannot copy and paste streams alone. Streams are placed onto the clipboard only if their source and destination unit procedures (when they exist) are also placed on the clipboard.

c. When pasting unit procedures from the clipboard into a flowsheet, you should be aware that certain features of the original unit procedures are *not transferred* into the newly created copy:

1. Stream connections to any unit procedures not included in the pasted set.

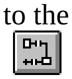
2. If the start time of the first operation of the pasted unit procedure was defined on a relative basis (e.g., with respect to the start or end of another operation in some other procedure), then the scheduling of the pasted procedure is reset to remove the coupling.

3. If the original unit procedure was sharing equipment with another procedure, the pasted procedure is reset to be executed in its own equipment.

d. Pasting streams and certain processing steps with component-related specifications from one flowsheet to another is not possible unless all components of the source flowsheet exist in the destination flowsheet as well. If that is not the case, the program will automatically expand the set of registered components in the destination flowsheet to include the missing ones.

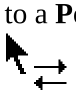
Adding Streams to the Flowsheet:

After you have placed unit procedures on your flowsheet, you may add stream connections to the icons. There are three types of streams: feed streams, intermediate streams, and product (output) streams. Feed streams do not have a source unit procedure and in batch processing they are mainly utilized by charge operations. Intermediate streams connect two unit procedures, and they are used to transfer material from the source to the destination unit procedure. Product streams do not have a destination unit procedure. All streams are automatically identified with a stream tag.

In order to add streams to the flowsheet, you much first enter **Connect Mode** by clicking on the **Connect Mode** button  of the main toolbar. When you do this, the cursor icon changes to the following: 

to indicate that you are in Connect Mode. Then add the feed, intermediate, and product streams as follows:

1. <u>Adding a Feed Stream:</u> Click any unoccupied area on the open screen to initiate drawing of the stream and then click on the appropriate inlet port of the destination unit procedure to terminate the stream. Notice that as the cursor moves over the inlet and outlet ports, it changes to a **Port Cursor**:



You must make sure the cursor looks like this before you click to attach the stream to a port. Otherwise the computer will simply add a stream elbow at this point and will not actually terminate the stream. If you accidentally miss the stream port, you can simply hit ESC to cancel the stream-drawing process. Then you can restart the stream-drawing process by clicking the Connect Mode button again.

Between initiation and termination of the feed stream, the mouse may (optionally) be clicked at intermediate points to create right angle bends; this permits customization of the stream route and flexibility in flowsheet design. Pro-Designer automatically draws the feed stream symbol and labels the stream.

2. Adding an Intermediate Stream: Click on the appropriate outlet port of the source unit procedure and then on the appropriate inlet port of the destination unit procedure to terminate the stream. Be sure to wait until the **Port Cursor** icon (explained above) is displayed before attempting to begin or terminate a stream on a port. As before, you can create specific routing by clicking the mouse wherever a right angle bend is desired.

3. Adding a Product Stream: Click on the appropriate outlet port of the source unit procedure and then *double-click* somewhere to terminate the stream line. When you double-click, the cursor should be close to the last drawn horizontal or vertical line segment. Note that Pro-Designer automatically draws the product stream symbol.

At this point, please add feed, intermediate, and product streams to your example process. Your flowsheet should now look something like this:

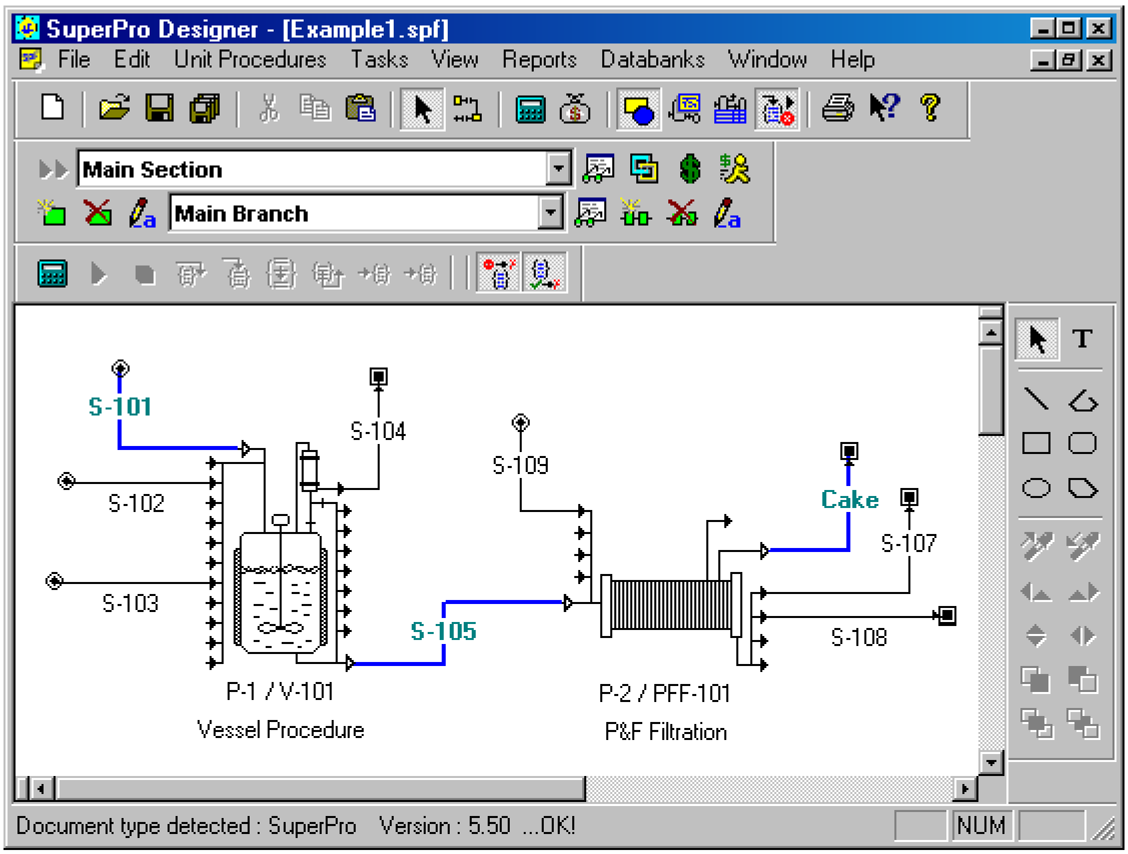


Figure 2.1-h: The example flowsheet with streams added

Notes:

1) Hitting ESC while drawing a stream terminates the stream drawing process. To get back into stream mode after hitting ESC, simply hit the Connect Mode button again.

2) In many unit procedures, there are dedicated ports, such as feed, vent, cake removal or filtrate removal. To see which ports are dedicated to each function, you can look up the desired unit procedure in the Help menu. As a shortcut to the Help for any procedure, you can click the Help icon (the one with a question mark and an arrow on it) and then click on the unit procedure icon you are interested in. Alternatively, you can click on the unit

procedure icon to highlight it, and then hit the F1 key. A portion of the Help for the Plate and Frame Filtration unit procedure appears below. Notice that the dedicated ports are labeled next to the filter icon. The Help facility also contains a general description of each procedure, links to its operation models, and much more.

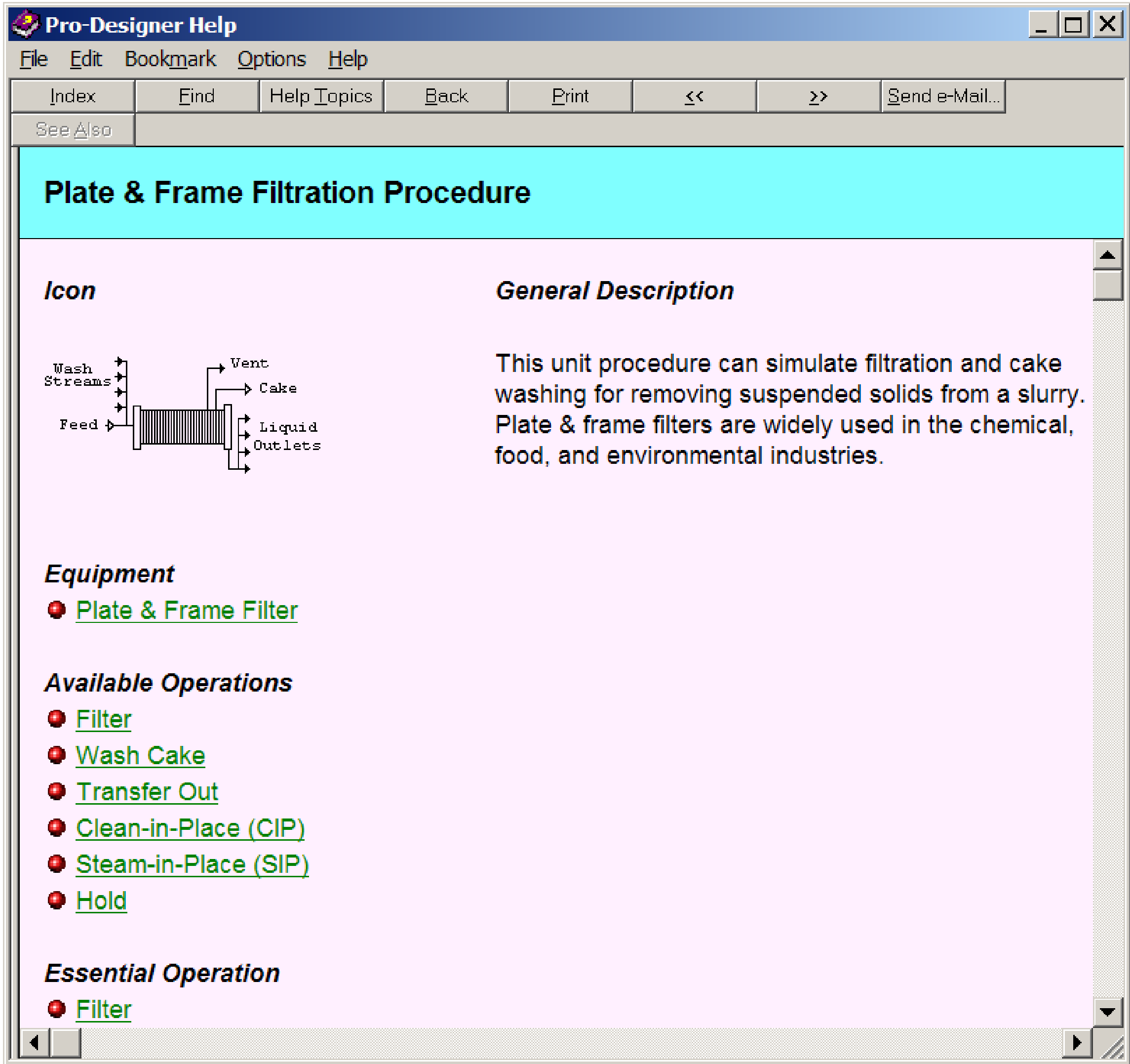


Figure 2.1-i: A Portion of the Help file for Plate and Frame Filtration

When you are finished drawing streams, you should exit Connect Mode and return to **Select Mode**. This is done by hitting ESC or clicking on the toolbar button that looks like: 

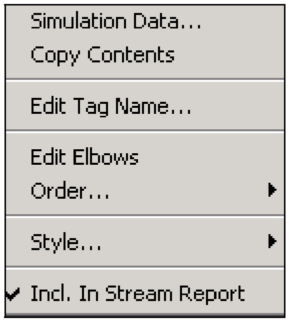


Figure 2.1-j: The stream context menu

When Pro-Designer is in Select Mode and the mouse is over a stream line, the arrow will change to indicate the availability of a stream context menu (see Figure 2.1-j), which may be activated by clicking the right mouse button. Through this menu you can view and edit (for input streams only) the composition, flowrate, and other stream properties. You may also change the Tag Name (label), adjust the Elbows, and edit the Style (e.g., label and line color, line thickness, etc.) of any stream. Note that double-clicking on a stream line with the left mouse button is equivalent to selecting the **Simulation Data...** menu item.

At this point, please right-click on the Vessel Procedure input stream “S-101” and choose Edit Tag Name. Change the name of this stream to “Heptane” and click OK. Then right-click the Heptane stream line, select **Style: Edit Style…**, and Click on the **Name Tag** tab (see below).

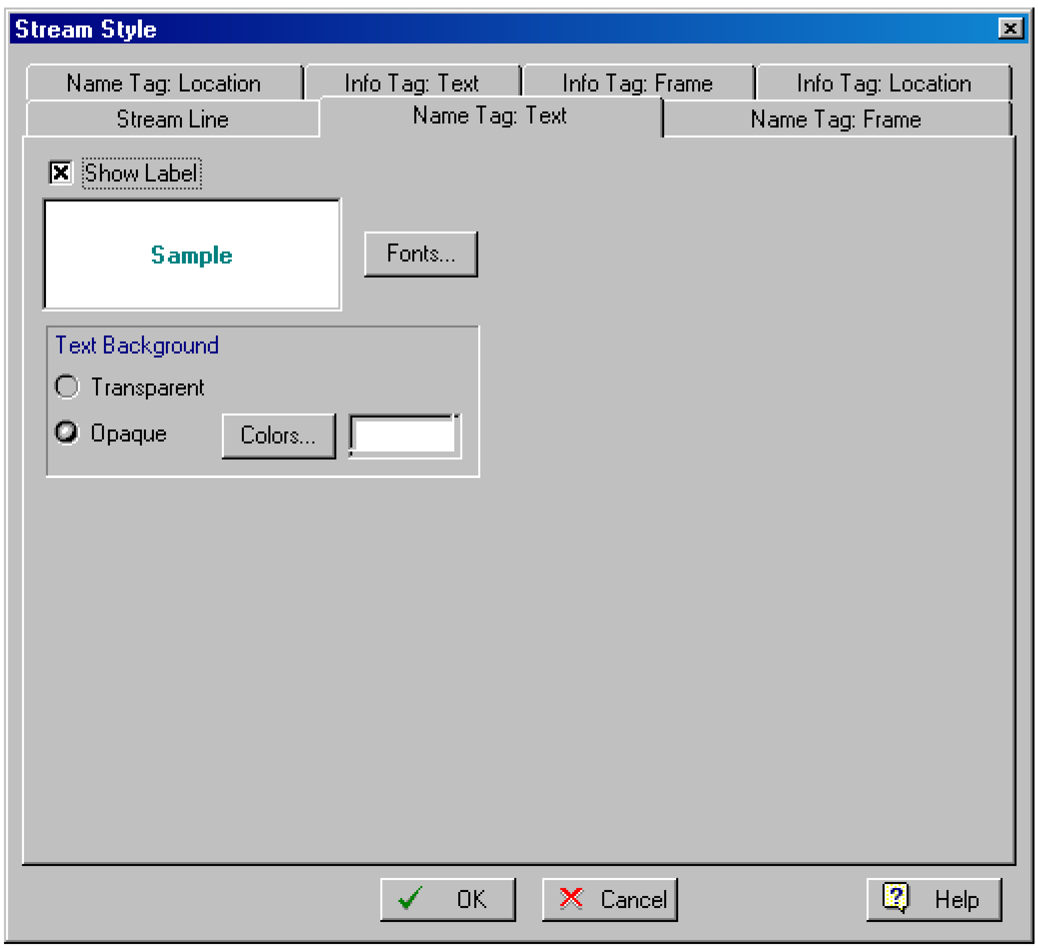


Figure 2.1-k: The Stream Style dialog

Now click the **Fonts…** button to change the style, size and color of this stream tag name. After clicking OK, your flowsheet should look something like this:

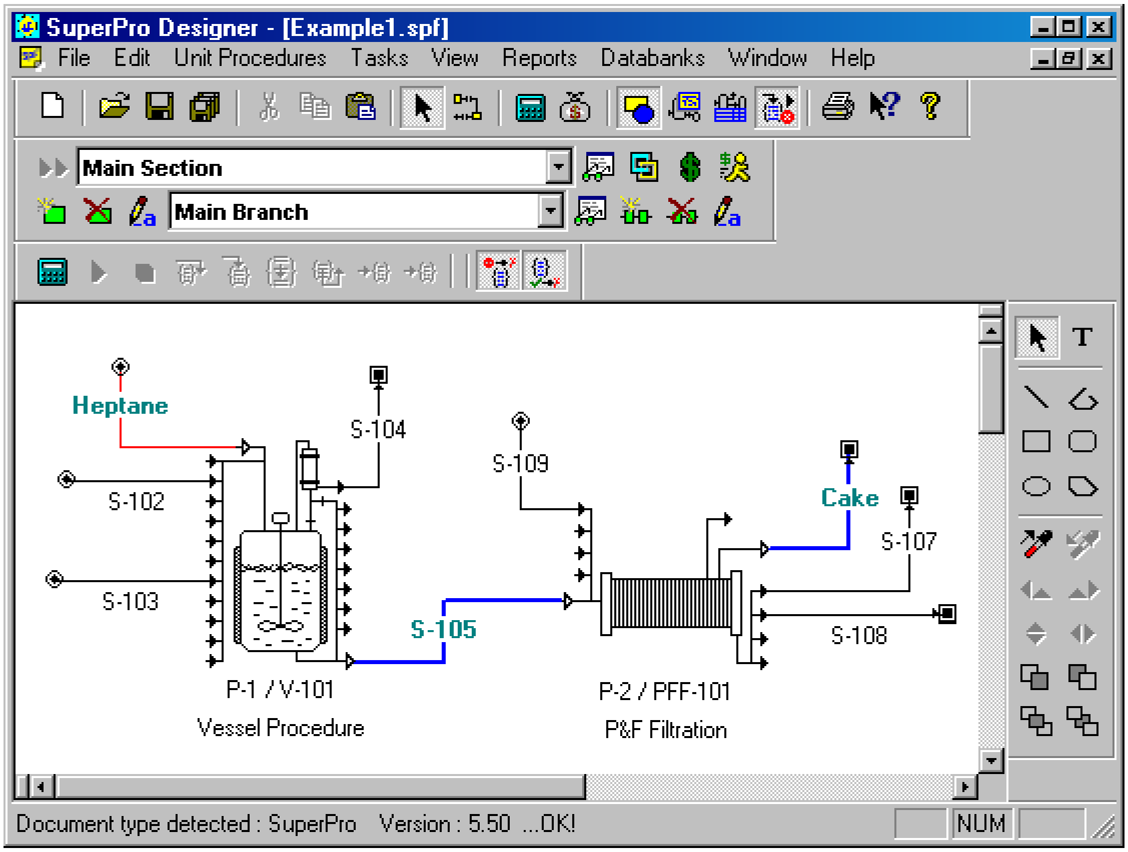


Figure 2.1-l: The example flowsheet after the name and style for one of the input streams have been changed.

Please see Chapter 4 or the on-line Help facility for more information on stream-drawing.

2.1.6 Initializing Unit Procedures

Adding Operations to the Unit Procedures:

The first step toward initialization of unit procedures is to add relevant operations to each unit procedure. This can be done by either 1) double-clicking a unit procedure icon or 2) right clicking on the unit procedure icon and selecting **Add: Remove Operations**. Either action will bring up the following dialog box:

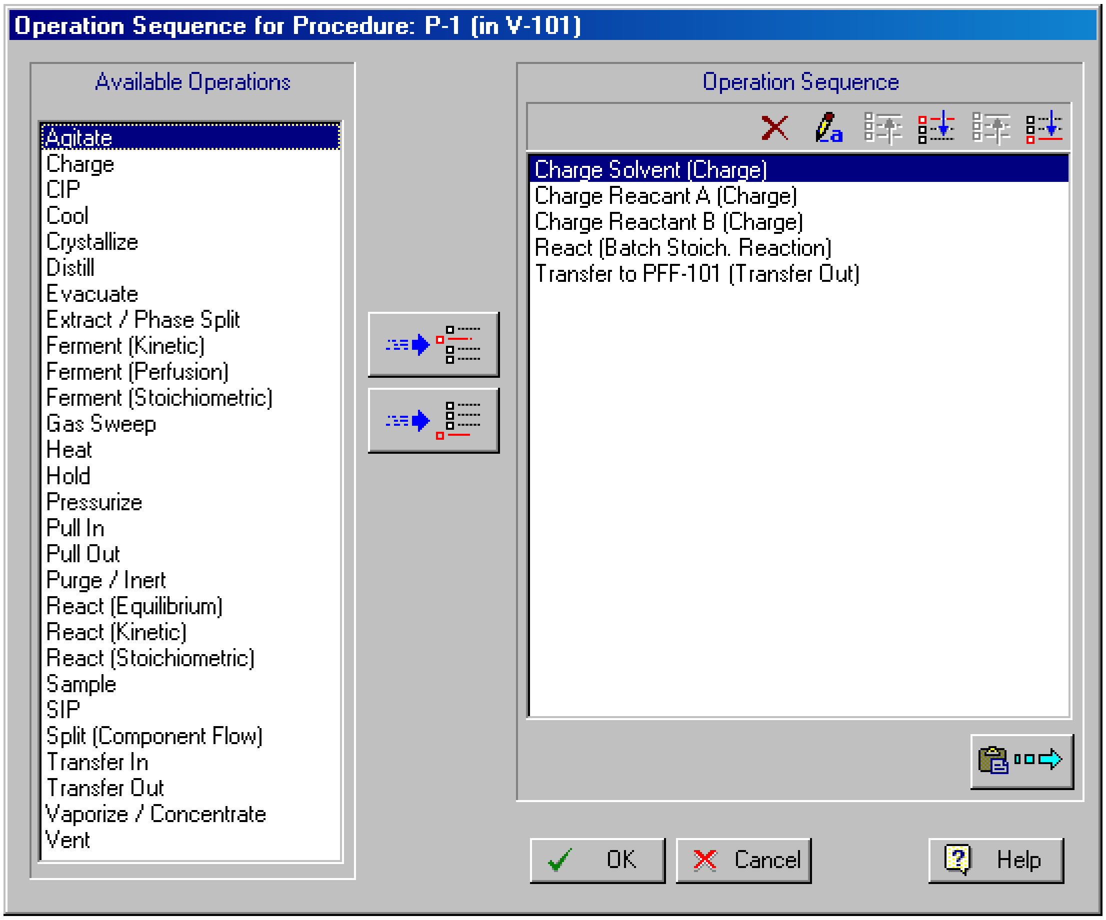
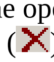


Figure 2.1-m: Adding Operations to the Vessel Procedure in the example process

At this point, please add a charge operation to the Operation Sequence in your Vessel Procedure by double-clicking the word “Charge” in the list on the left. Alternatively, you can add the operation by highlighting the word “Charge” and clicking the **Add** or **Insert** buttons. The **Add** button (the bottom button in the middle) will add the new operation at the end of the list, while the **Insert** button (the top button in the middle) will add the new operation *before* the currently selected operation.

Now add two more Charge operations, a React (Stoichiometric) operation, and a Transfer Out operation (so that your dialog box looks like Figure 2.1-m above). Then click **OK** to return to the flowsheet.

Note: If you make a mistake while adding operations, you can delete the operation by selecting it in the Operation Sequence list and hitting the **Delete** button (). If you add an operation in the wrong order, you can move it to a different position in the Operation

Sequence list using the Move Up/Down buttons. To change the name of an operation, select it and hit the **Rename** button ( ).

After you have added operations to the Vessel Procedure, double-click the Plate and Frame filter icon to add operations to it. Notice that by default, this unit procedure has an operation (Filter-1) assigned to it. Use the same method as before to add a Cake Wash operation and a Transfer Out operation to this unit procedure (in addition to the Filtration operation which is already present).

Note: Double clicking on a continuous procedure (e.g., a Centrifugal Pump) that is present in a continuous flowsheet brings up the dialog window of its essential operation instead of the dialog of Figure 2.1-m. Essentially, a unit procedure in a continuous flowsheet behaves like a unit operation.

Initializing the Operations:

Reactor Vessel

The next step is to initialize each of the operations that have been added to the unit procedures. To do this, please right-click the mouse over a unit procedure icon to bring up its context menu (see Figure 2.1n).

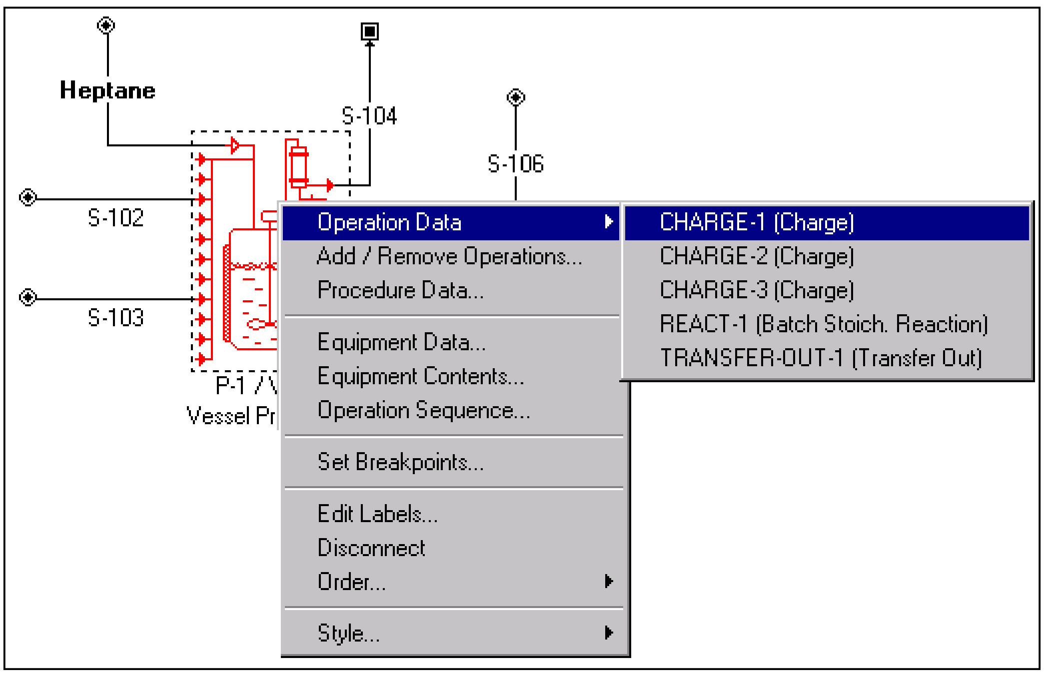


Figure 2.1-n: The context menu for the vessel procedure in this example process

The meaning of each portion of the context menu in Figure 2.1-n is explained below:

- The “**Operation Data**” menu allows the user to access and modify the simulation parameters for each operation in this unit procedure. (Note – the Operation Data menu will not appear until at least one operation has been added. Furthermore, if only one operation is present in the unit procedure, no drop-down list will appear to the right of the context menu. In this case, simply click on the Operation Data line of the context menu to bring up the parameters for the operation).

- The "**Add / Remove Operations…**" menu allows the user to add new operations to the procedure, delete existing ones, rename them, and rearrange their order. This is the same dialog that is brought up when you double-click on a batch unit procedure.
- The "**Procedure Data**" menu item allows the user to view and set some scheduling and throughput analysis data. You may change the mode of operation for the entire procedure from batch to continuous and vice versa (if the procedure can operate in both modes).
- Through "**Equipment Data…**" the user can select the equipment sizing mode (Design or Rating), specify equipment sharing information, and parameters related to size and purchase cost. Information related to staggered pieces of equipment and consumables are also specified through this dialog.
- Through "**Equipment Contents…**" the user can view the contents (and their state) of the equipment after each operation.
- Through "**Operation Sequence…**" the user can view a summary of information for each operation, including start/end time, material transferred in /out with each operation, and batch contents after each operation.
- The "**Set Break Points…**" allows the user to place a stop in the sequential solution of material and energy balances. This is normally used for troubleshooting in large or complicated flowsheets.
- Through "**Edit Labels…**" the user can change the name of the procedure (e.g., P-1 in the above procedure), the name of the equipment (V-101 in the above case), and the description of the procedure ("Vessel Procedure" in the above case).
- The "**Disconnect**" menu item deletes all the streams connected to the unit procedure.
- The "**Flip (reverse flow direction)"** option from the context menu changes the flow direction, which is left-to-right by default, to right-to-left. Note that the Flip icon option is only available when the unit procedure is not connected to other steps via material streams. You can also flip the icon by selecting it and clicking on the Flip Horizontal button of the Visual Object Toolbar (see chapter 12).
- The "**Order…**" option of the context menu allows you to force the unit procedure icon to appear behind or in front of other icons, text, etc.
- The "**Style…**" option allows you to edit such things as the icon color, the name tag color and font, etc.

At this point, please select **Operation Data: Charge-1** from the vessel procedure context menu. This will bring up the following dialog:

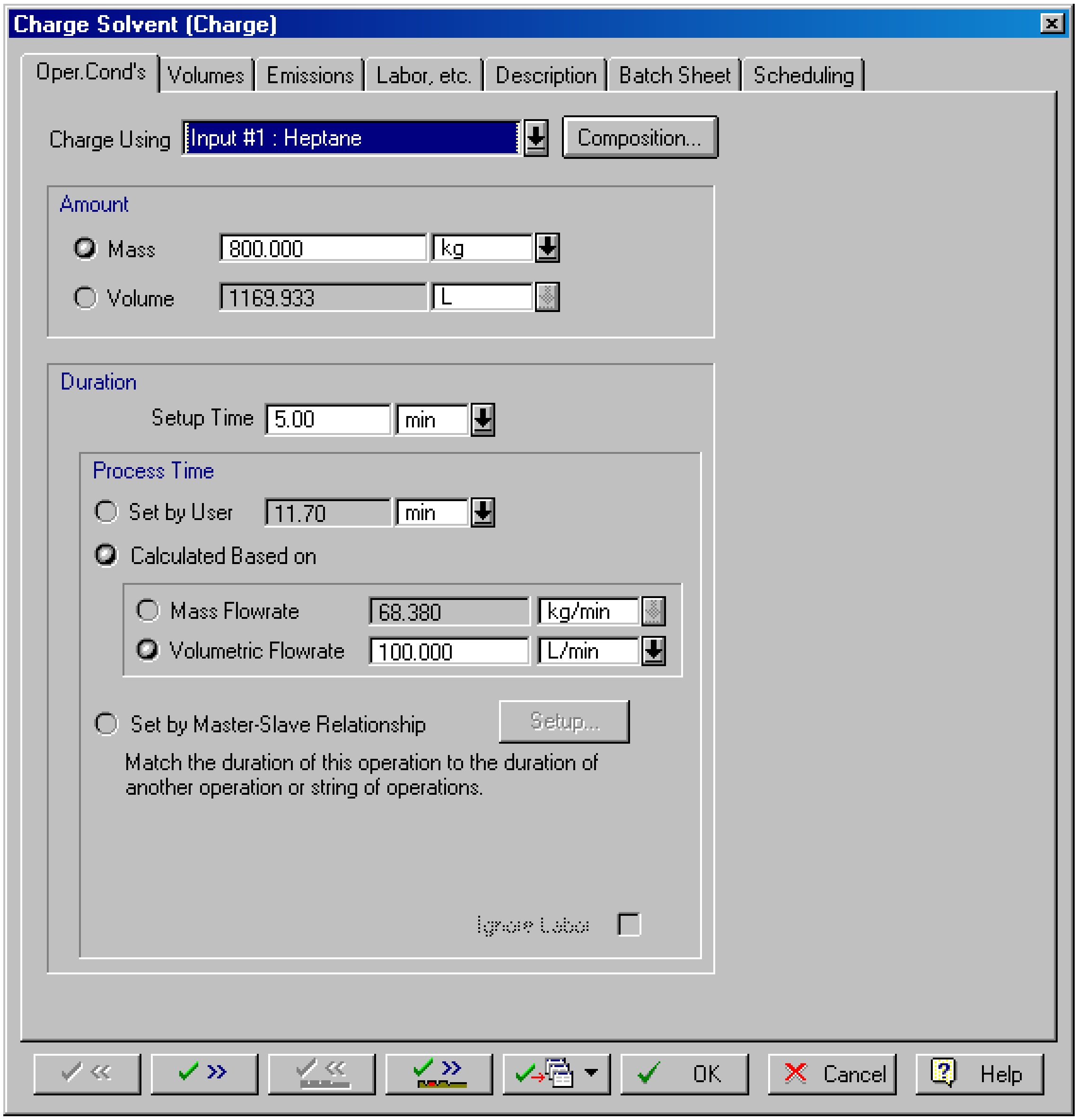


Figure 2.1-o: The Operating Conditions dialog for the first Charge operation in the Vessel Procedure.

The Operating Conditions dialog allows you to specify the operating conditions, emissions data, labor, scheduling, etc. for each operation. Different tabs of input fields are available for different operations. To initialize the Operating Conditions tab for the first charge operation in this example, you begin by specifying the amount of material that is going to be charged (800 kg). To specify its composition, use the drop-down menu at the top of the Operation Data dialog box to select the stream which you renamed “Heptane” earlier in this chapter. Click on the **Composition…** button to access the stream data for this stream (see Figure 2.1-p). To add heptane to the stream, double-click its name in the Registered Ingredients list on the left side of the dialog box.

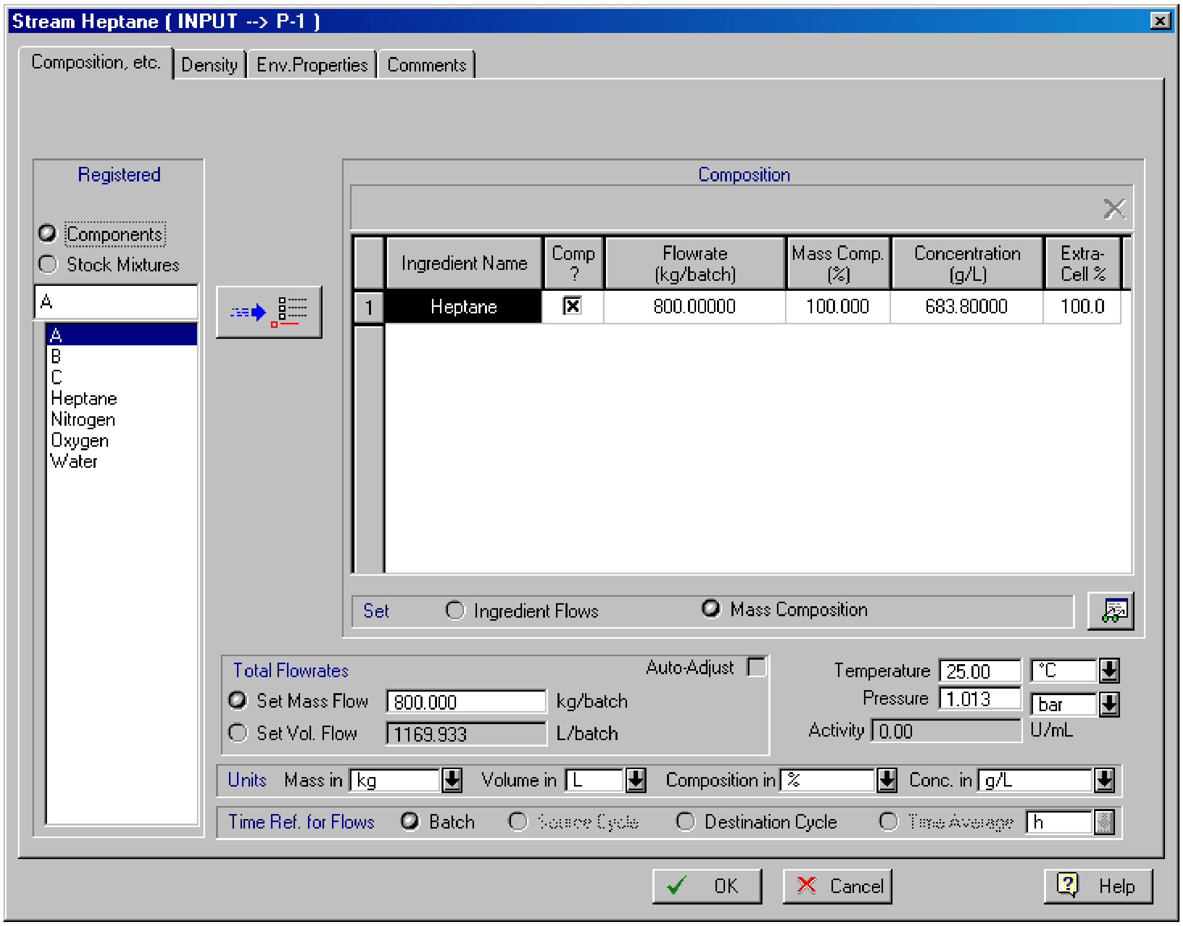


Figure 2.1-p: The Heptane stream dialog.

Notes:

1) You can charge multiple components in the same stream if you wish. To do this, simply add additional component names from the Registered Ingredients (Pure Components or Stock Mixtures) list and specify their amounts. The computer will automatically calculate the mass % and concentration (g/L or mole/L) of each ingredient, the stream's density (if it is not set by the user), the volumetric flowrate and the activity of the stream. Alternatively, you can click on "Mass Composition" and specify the total mass or volume flow and the mass % of each component. You may also select units for entry and display.

2) As an alternative to going through the Operation Data dialogs to edit stream properties, you can initialize and edit input streams directly from the flowsheet itself. To do this, open the stream context menu by clicking the right mouse button over a stream line and selecting **Simulation Data**. This will bring up the same dialog box as the one shown in Figure 2.1-p. You could also double-click the left mouse button on a stream line to generate this dialog box. Note that only the **feed** streams to the flowsheet need to be specified. The flowrates and compositions of intermediate and output streams are calculated by the program. However, the user can specify the density and volumetric contribution coefficients of such streams (see Chapter 4 for more detailed information on streams and their properties).

3) In addition to pure components, mixtures can be fed (or “charged”) into a process step using an input stream.
4) For biotech processes, the extracellular percentage (Extra-Cell %) of an ingredient represents its fraction that is in the bulk solution (as opposed to inside the cell). For more information on this topic, please refer to the β–Galactosidase example in Section 2.3.
5) If the operating mode of a flowsheet is batch, all flowrates are reported on a per batch basis (or per cycle of source or destination process step). If the process is set to continuous mode, then all flowrates are reported on a per hour basis. The choice for mass units can be made from each stream’s dialog. This choice overwrites the default choice made by the specification at the **Edit: Flowsheet Options: Preferences: Stream Report Options...** dialog.
6) The **Env.Properties** tab of a stream dialog displays the concentrations and daily throughputs of the environmental and aqueous properties of the stream (TOC, $CaCO_3$, TP, TKN, COD, ThOD, BOD5, BODu, etc.) All values are for display only and cannot be edited by the user through this dialog box. However, the environmental properties of the pure components (that contribute to the above stream properties) can be edited through the **Tasks: Edit Pure Components** dialog.

For more information on stream properties, please refer to Chapter 4.

After you have specified the charge amount of Heptane, click **OK** to return to the Operation Data dialog for Charge-1 (Figure 2.1-o). Notice that there are several ways that the duration of this operation can be specified. For this example, change the setup time of your charge to 5 minutes and set the Volumetric Flowrate to 100 L/min. Please also visit the **Volumes, Emissions**, **Labor etc**, and **Scheduling** tabs to see what they contain. A brief description of each of these tabs follows:

Volumes tab: here the user can specify the maximum and minimum allowable working / vessel volume for this operation (i.e., by the end of the Charge operation the vessel should not be more than 90 % full). In Design mode this is taken into account for sizing the equipment. In Rating mode, the program makes sure that a vessel is not overfilled or the level does not drop below the agitator level.

Emissions tab: here the user can specify which volatile organic compounds (VOCs) will be emitted, whether a sweep gas will be used (for emissions associated with reaction and crystallization operations), and what temperature the vent condenser should be set at. Pro-Designer is equipped with VOC emission models that are accepted by EPA. Please see Chapter 10 or consult the on-line Help Facility for more info on emission calculation models. For the heptane charge in your example process, please click in the Perform Emission Calculations box. Then Click in the Emitted box next to the Heptane component. After the simulation, please remember to visit the dialog of stream S-104 and check the amount of emitted Heptane. For particulate and other components for which emission models are not available, the user can specify the Emission %.

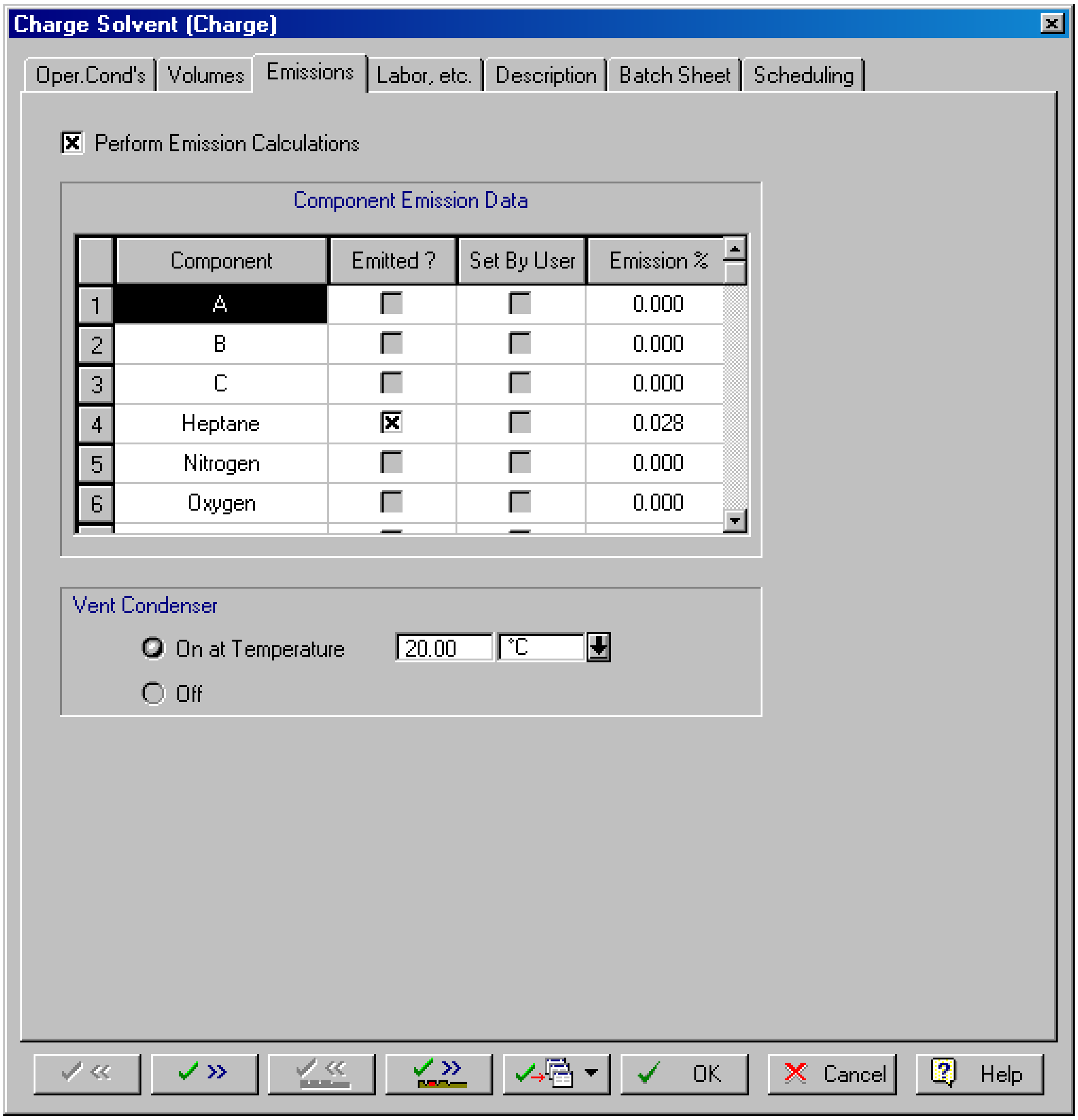


Figure 2.1-q: The Emissions tab for the heptane charge.

Labor tab: here the user can specify labor requirements and auxiliary utilities.

Scheduling tab: The right-most tab of a batch unit procedure is always the Scheduling tab. Through this tab, the user specifies the start time of an operation relative to the start or end of other operations in the same or different procedures. For unit procedures in continuous mode, no scheduling information is required.

Note: Depending on the complexity of an operation, additional tabs may be employed to display other pertinent variables.

For this operation, leave all the default values for the **Labor etc** and **Scheduling** tabs.

Next, click the **OK >>** button on the Operation Data dialog to move to the second charge operation in this unit procedure. For this operation, use stream S-102 to add 50 kg of material A to the reactor. Also specify a 5 minute setup time and a 20 kg/min charge rate. Leave the default values for the other tabs.

Then click the **OK >>** button to move to the final charge operation. Initialize this similarly, but use stream S-103 to add 40 kg of material B. Also change the setup time to 5 minutes and the charge rate to 20 kg/min.

Once again, click the **OK >>** button to move to the next operation (the Batch Stoichiometric Reaction). Notice that the Operating Conditions tab is different for this operation than it was for the Charges, and that several other tabs are present.

Starting with the Operating Conditions tab, change the Final Temp to 50 C, the Heat Transfer Agent to Steam, and the Process Time to 6 hours. Leave all the other default values on this tab as they are.

Next, referring to the Volumes tab, notice that you can specify a maximum and minimum working to vessel volume ratio. Change the Max Allowable working/vessel volume to 80%. Then move to the Reactions tab (see Figure 2.1-r).

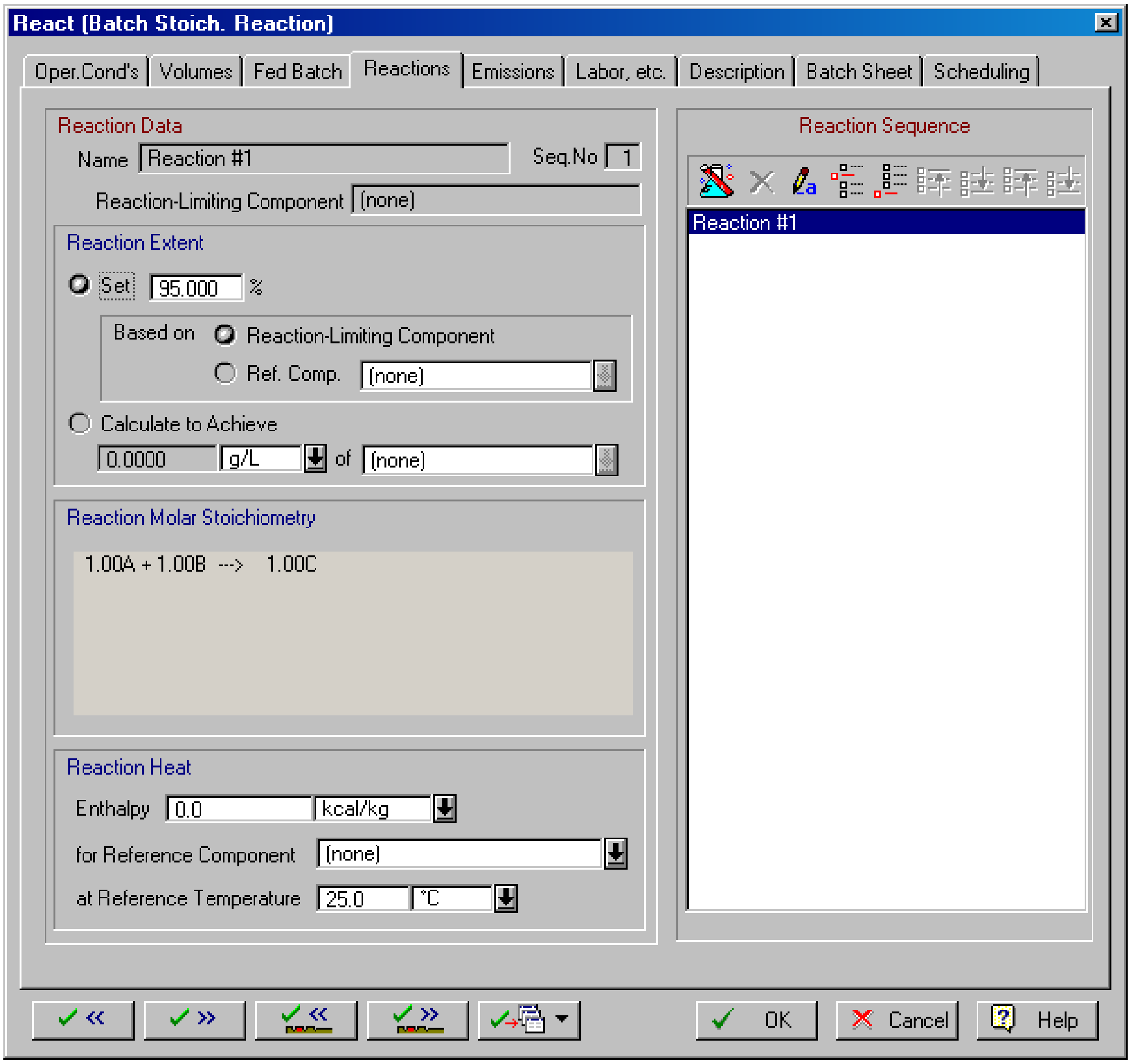
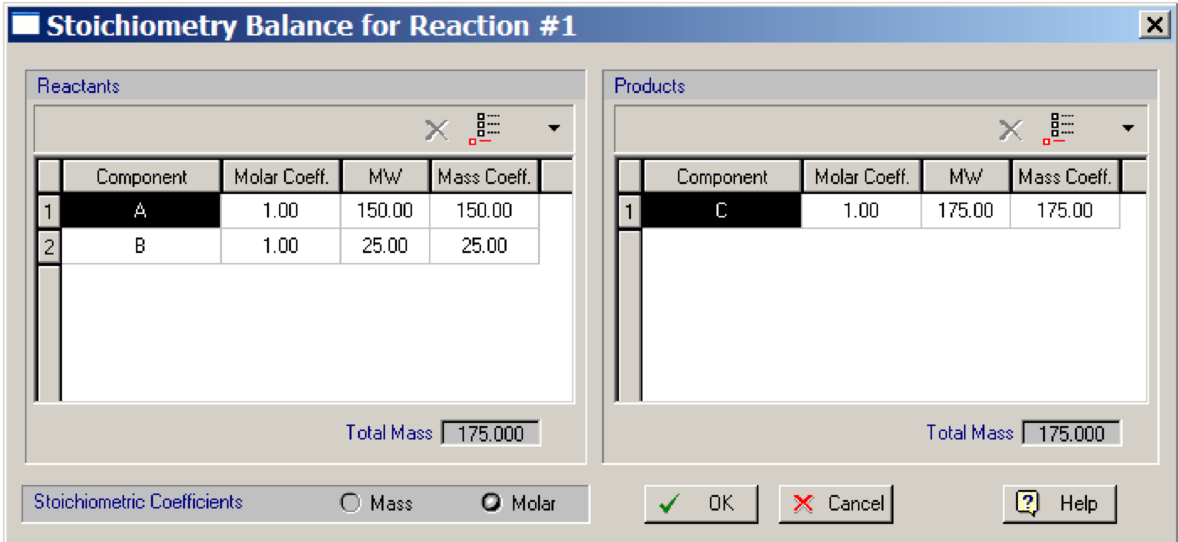


Figure 2.1-r: The Reactions tab.

In this tab, you will need to specify the parameters describing a reaction in which 1 molecule of reagent (A) combines with 1 molecule of reagent (B) to form a molecule of product (C):

$$A + B \rightarrow C$$

To enter this, bring up the "**Edit Stoichiometry**" dialog (see below) by clicking on the button that looks like a shake flask (at the top of the Reaction Sequence box). Introduce the reactants {A and B} and the product {C} using the "**Add Reactant**" and "**Add Product**" buttons (located above the reactant and product tables). Select "Molar" for stoichiometric coefficients option and enter "1" for everything. For more information on specifying reaction coefficients, please see Chapter 2.2. Now close the "Edit Stoichiometry" dialog. In addition to specifying the stoichiometric coefficients, you will need to specify the extent of reaction. For this example, set the Extent to 95%, as was done in Figure 2.1-r. Next, click the **OK** >> button to move to the Transfer Out operation (leave all the default values for the **Emissions**, **Labor etc**, and **Scheduling** tabs.)



In the Transfer Out dialog (Figure 2.1-s), use the drop-down menu at the top of the screen to specify which stream line will be used for the transfer operation. In addition, in order to accurately capture the time required for this operation, set the duration to be the same as the filtration duration in P-2 (see below). To do that, select the **Set By Master Slave Relationship** duration option and then click the **Setup** Button. Through the dialog that comes up, select “P2 (in PFF-101)” as the Master Procedure (through the Another Procedure drop down menu), and “FILTER-1 (Cloth Filtration)” as the Master Operation (through the Match a Single Operation drop down menu).

This will ensure that the reactor will be considered “utilized” during filtration, since the reactor will not be completely emptied until the filtration is complete. You can leave the default values for the other tabs in this dialog.

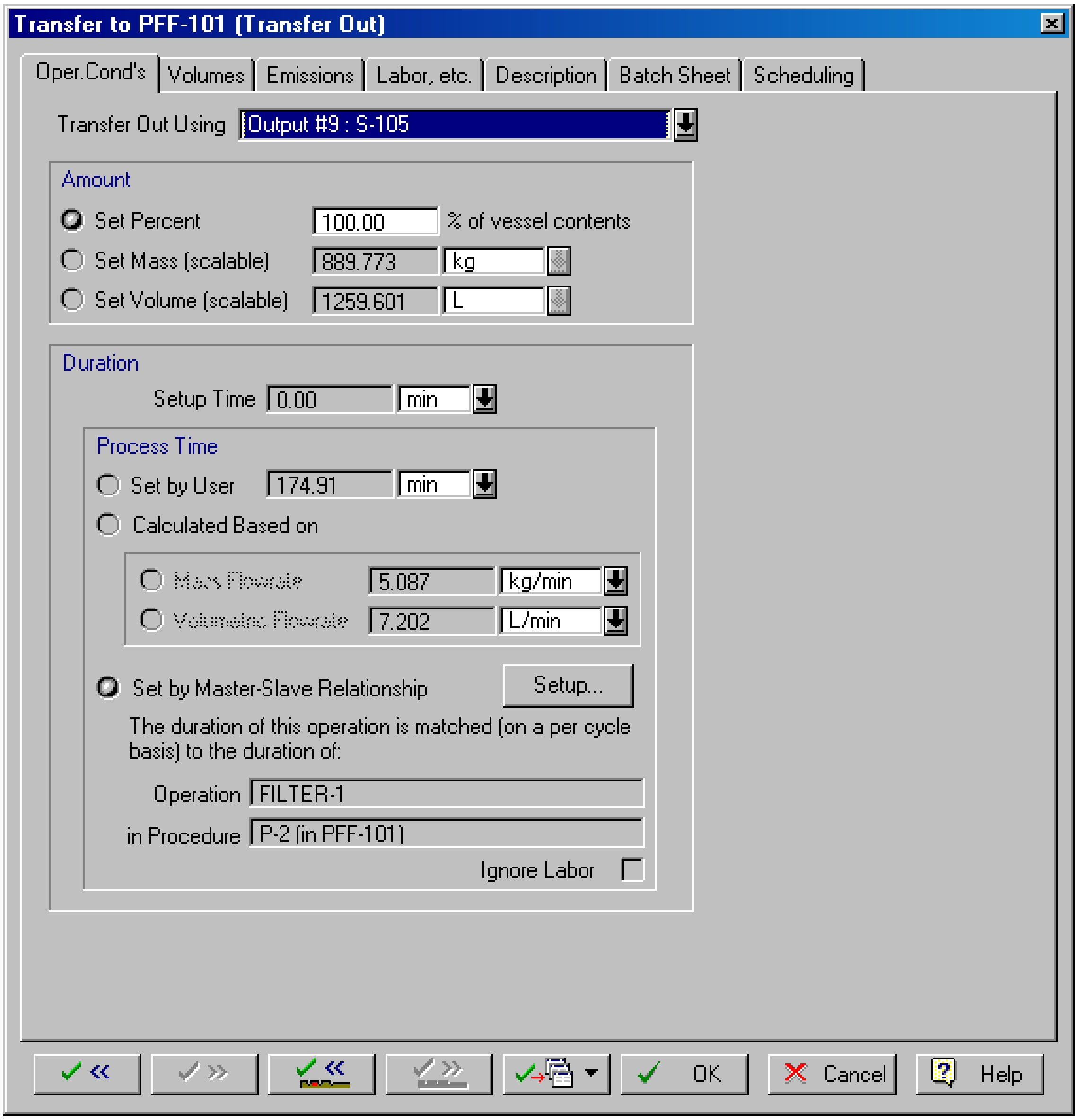


Figure 2.1-s: The Transfer Out operation dialog.

Plate and Frame Filter

Next, you will need to initialize the operations in the Plate and Frame Filtration unit procedure. To do this, right-click on the filtration procedure and choose **Operation Data: Filter-1**. For this example, assume that components A and B are completely soluble in Heptane, and component C is virtually insoluble. Therefore, in the Particulate Component Removal section of this dialog box, please specify that 95% of your product C will remain on your filter, but the other components will not be preferentially retained (they will end up in the filtrate). Also notice that you can specify a Cake Dryness based on LOD (loss on drying) or Cake Porosity. Please change the LOD for your filtration to 35%. This value will cause a portion of the Heptane (and any soluble components) to be held in your wet cake. By specifying a LOD of 35%, you are telling the program that only 65% of wet cake is the insoluble product C.

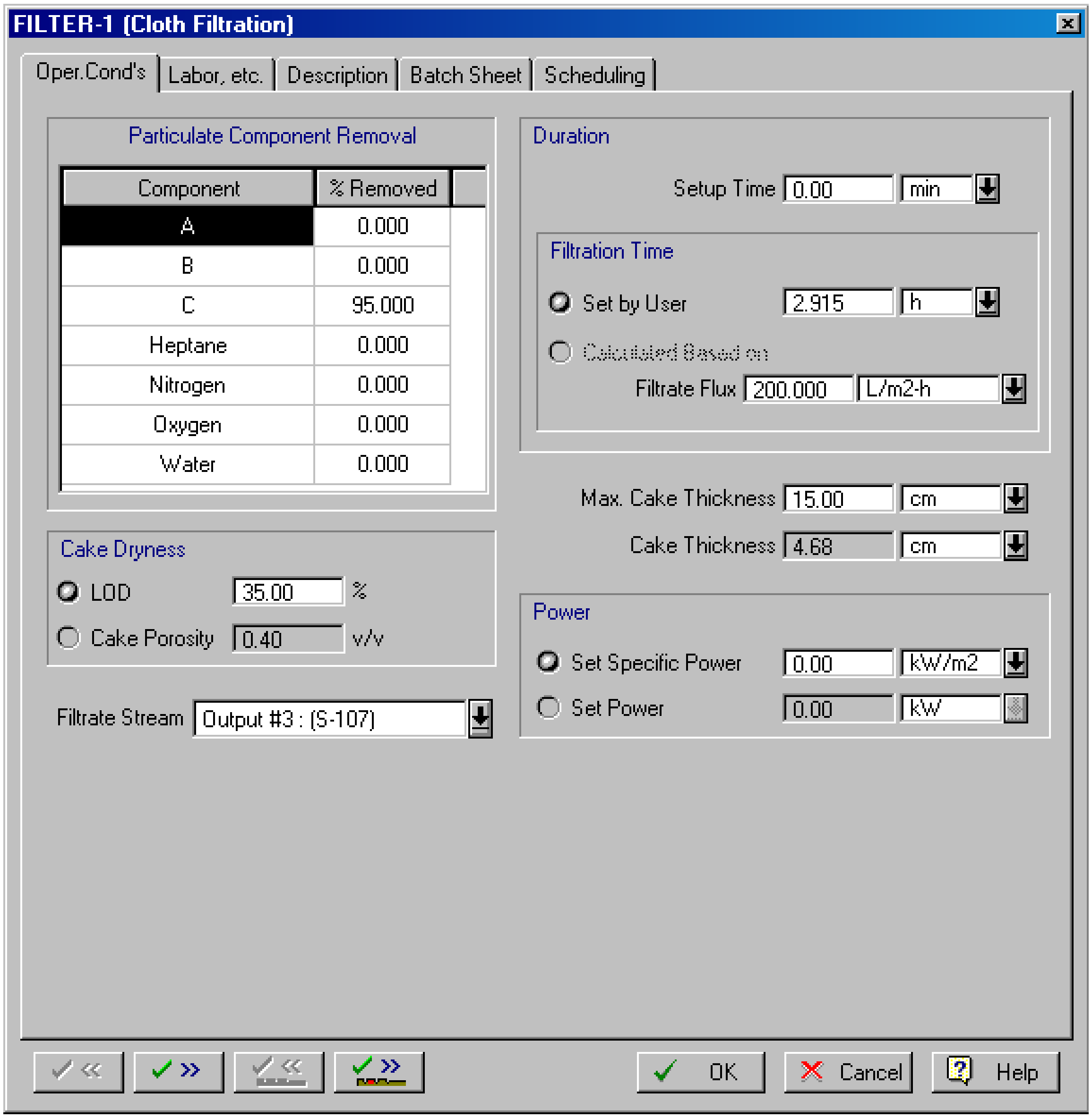


Figure 2.1-x: The Filtration operation dialog.

Next, please visit the Scheduling tab of the filtration operation. This tab is common to all operations. By default, the first operation in any batch unit procedure is scheduled to start relative to the beginning of the batch. In order to accurately schedule your filtration, you will need to change the Start Time to be relative to the start of the Transfer Out operation in procedure P-1 (see Figure 2.1-y).

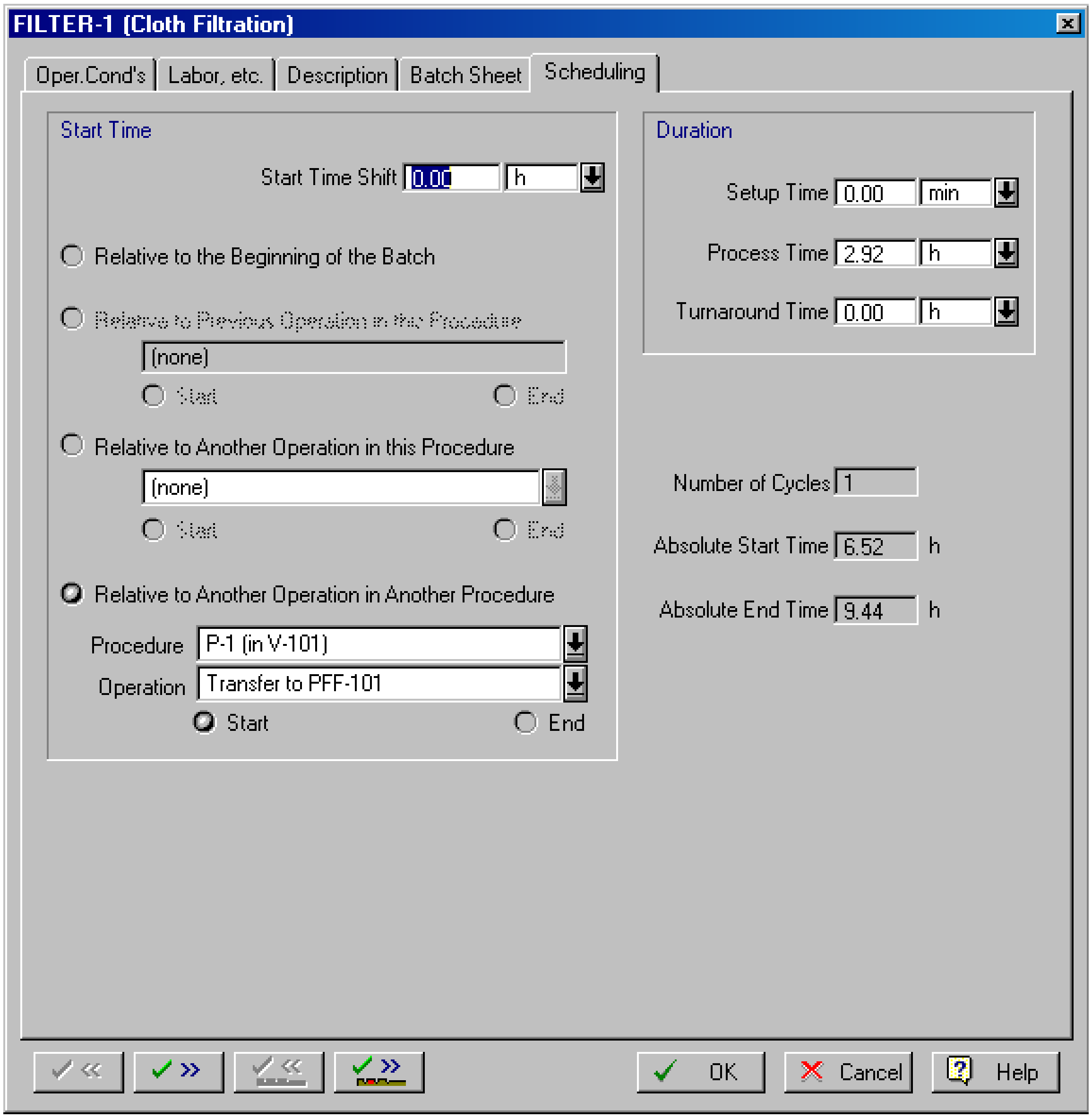


Figure 2.1-y: The Scheduling tab of the filtration operation.

Next, click **OK** >> to move to the Cake Wash operation (see Figure 2.1-z). Here you will need to specify which stream will provide the wash solvent and which one will remove the waste (S-109 and S-108 in this case). In addition, you will need to specify what solvent is used for the wash. To do this, press the **Composition** button and select Heptane. Then click OK to return to the Cake Wash dialog. Notice that from this dialog you can specify the volume of wash to use based on the cake volume or a set value. Please keep the wash amount as 1 L/L of cake, use a wash time of 30 minutes, and change the wash type to slurry from displacement. A "slurry" wash will essentially dilute the soluble components trapped in the cake and remove most of them in the wash stream, whereas a "displacement" wash will remove the soluble components from the cake in a plug-flow fashion.

Finally, click the **OK** >> button to initialize the Transfer Out operation in this unit procedure (Figure 2.1-aa). In this operation, you will need to specify that you are going to transfer out the cake using a specific stream (S-107 is the only one available in this case) and the transfer will be done at a certain rate (10 kg/min in this case). Then Press **OK**.

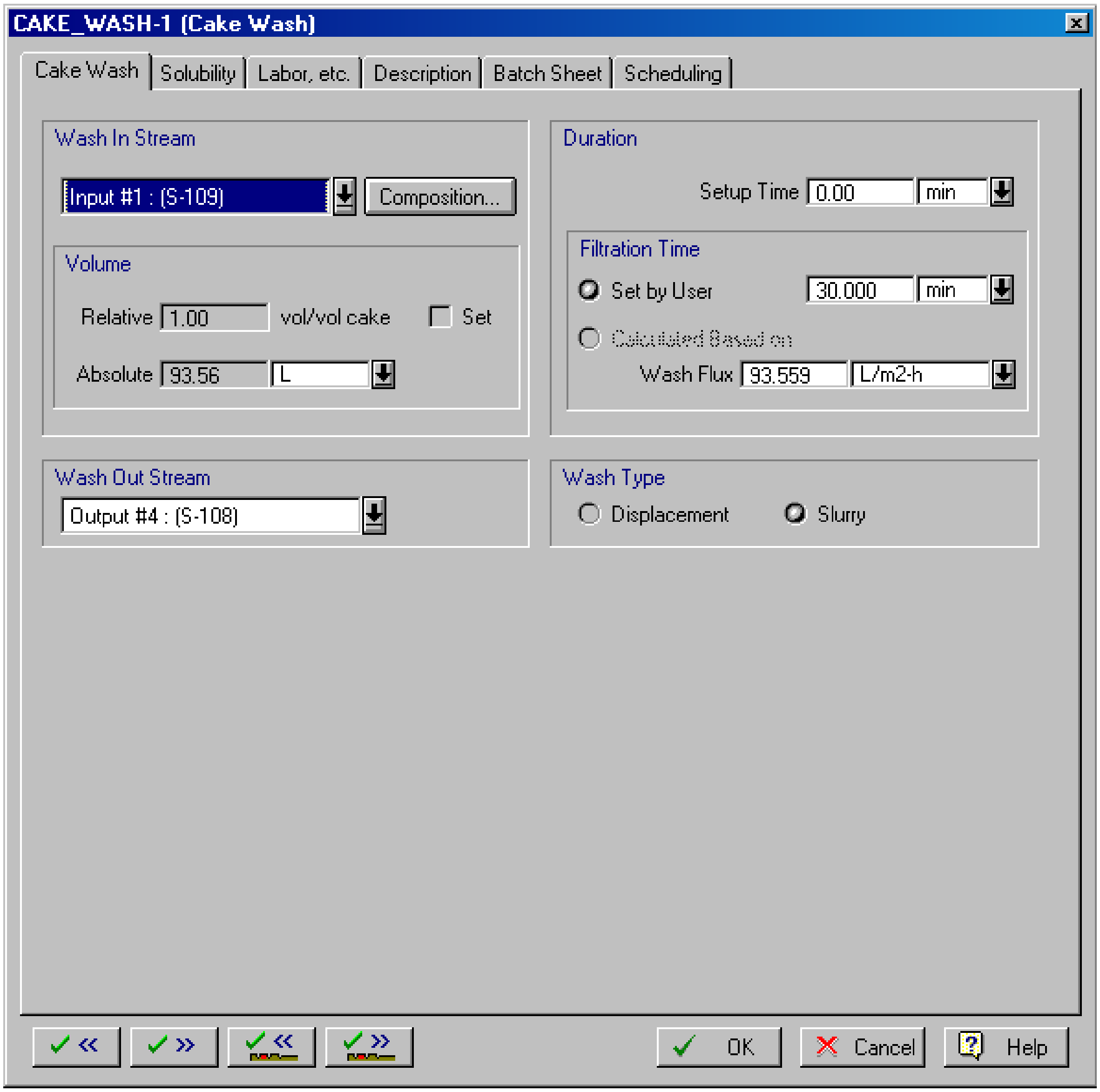


Figure 2.1-z: The Cake Wash dialog.

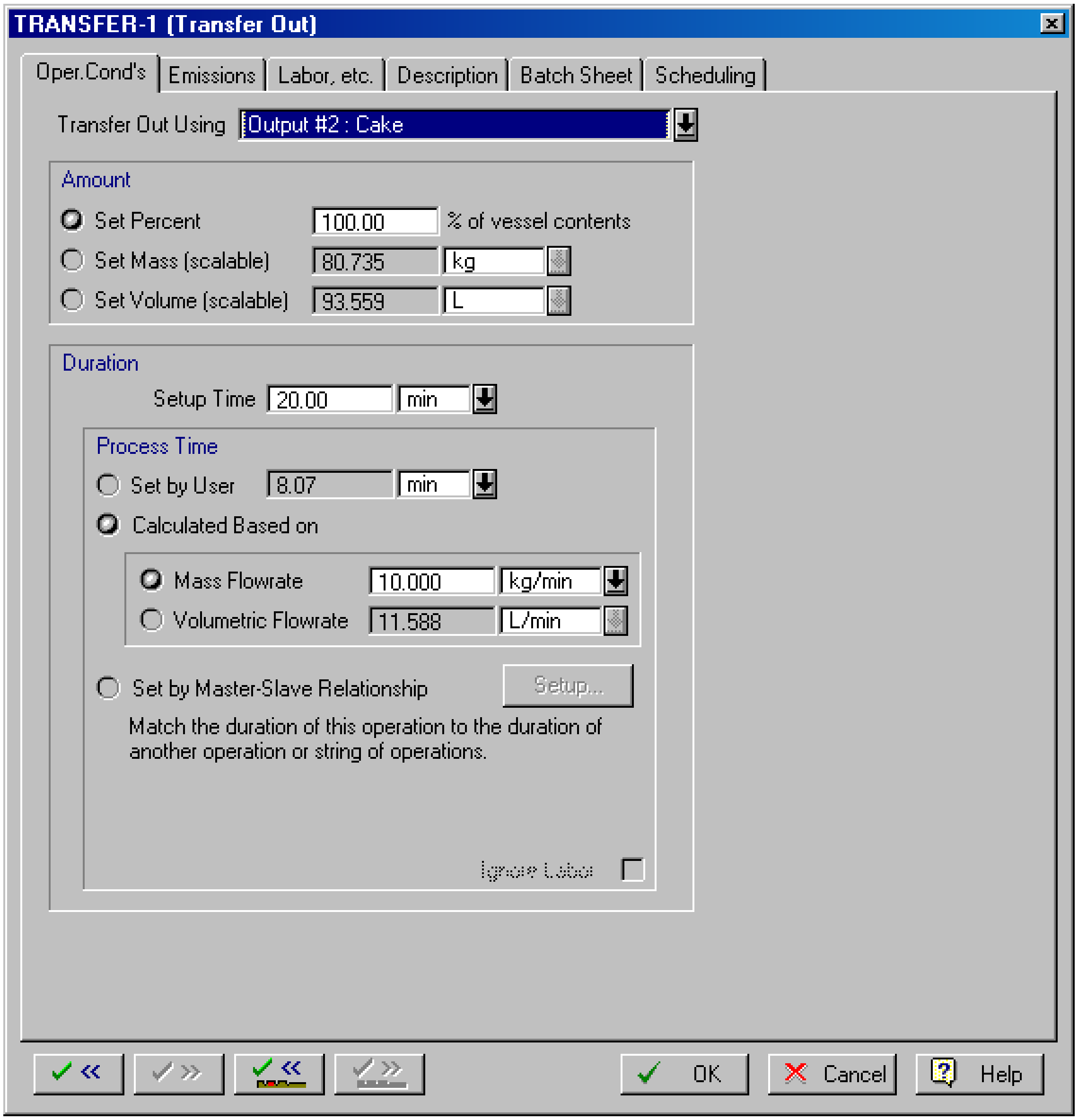


Figure 2.1-aa: The Transfer Out dialog.

You have now finished initializing the operations and streams for this example flowsheet. Use the **File: Save** menu item to save your work.

2.1.7 Simulating the Process and Viewing the Simulation Results

At this point, you can use the **Tasks: Solve M&E Balances** option from the main menu to perform the simulation. This will cause the program to perform the mass and energy balances for the entire flowsheet, estimate the sizes of all pieces of equipment in Design Mode, and model the scheduling of each piece of equipment. As a short-cut for performing simulations, you may hit **Ctrl+3** or simply click on the following toolbar button:  that looks like a calculator.

The simulation results can be viewed in the following ways:

1. The calculated output variables for each operation can be viewed by revisiting the corresponding **Operation Data** dialog windows (right-click on the desired Unit Procedure icon, then choose the operation you are interested in). For instance, you can see how long each of the Charge operations takes (recall that their durations were based on a given mass to be charged and a flowrate).

2. The calculated flowrates and compositions of intermediate and output streams can be viewed by revisiting the **Simulation Data** dialog windows of each stream (double-click on any stream line to see its **Simulation Data** dialog).

3. The contents of a piece of equipment as a function of time can be viewed by right clicking on a unit procedure and selecting **Equipment Contents** or **Operation Sequence**.

4. A report containing information on raw material requirements, stream compositions and flow rates, as well as an overall material balance, can be generated and displayed by selecting the **Reports: Streams & Material Balance...** option from the main menu. This report has tables that include an overview of the process, a listing of the raw material requirements, a listing of the compositions of each stream, and an overall component balance. Please generate and view this report now. To see more comprehensive stream reports, please refer to the examples in Chapters 2.2, 2.3, or 2.4. If you wish to customize the stream report, use the menu item **Reports / Options: Stream (tab)**.

5. To see the calculated equipment sizes, right-click on a unit procedure icon and choose the **Equipment Data…** option. All unit procedures have two options for equipment sizing: **Design** and **Rating**. By default, all equipment starts in **Design Mode**. In this mode, Pro-Designer will determine the required equipment sizes based on operating conditions and performance requirements. Usually, there are physical limitations on the available size of processing equipment. For example, a Plate & Frame filter may not be available with a cloth area greater than 80 m^2.

   When you are in **Design Mode**, you must specify the maximum available size for the equipment involved. If the calculated equipment size exceeds the maximum allowable size, Pro-Designer will employ multiple pieces of equipment (sized equally) with sizes that do not violate the maximum available size. For your example flowsheet, a filter size of roughly 2 m^2 should have been calculated. This number was calculated from the volume of material that is processed per cycle, the filtrate flux, and the filtration time.

   If you change the equipment sizing method to **Rating Mode** (Figure 2.1-bb), you can specify the size and number of units. Pro-Designer will then take this information into account in the simulation calculations (equipment size and number of units may affect the material and energy balances, the process time, etc.). Switching to Rating Mode may also affect the interface of some operations of that procedure. To experience this, please change the size of the filter to 4 m^2 and revisit the dialog of the filtration operation (Figure 2.1-cc). In this case, you need to specify either the filtration time or the average filtration flux (in Design Mode, you specify both).

Please set the filtrate flux to 150 L/m^2 hr and redo the calculations. This will calculate a new filtration time. In general, most batch operations have the capability of calculating their cycle time when the equipment size is specified (Rating Mode).

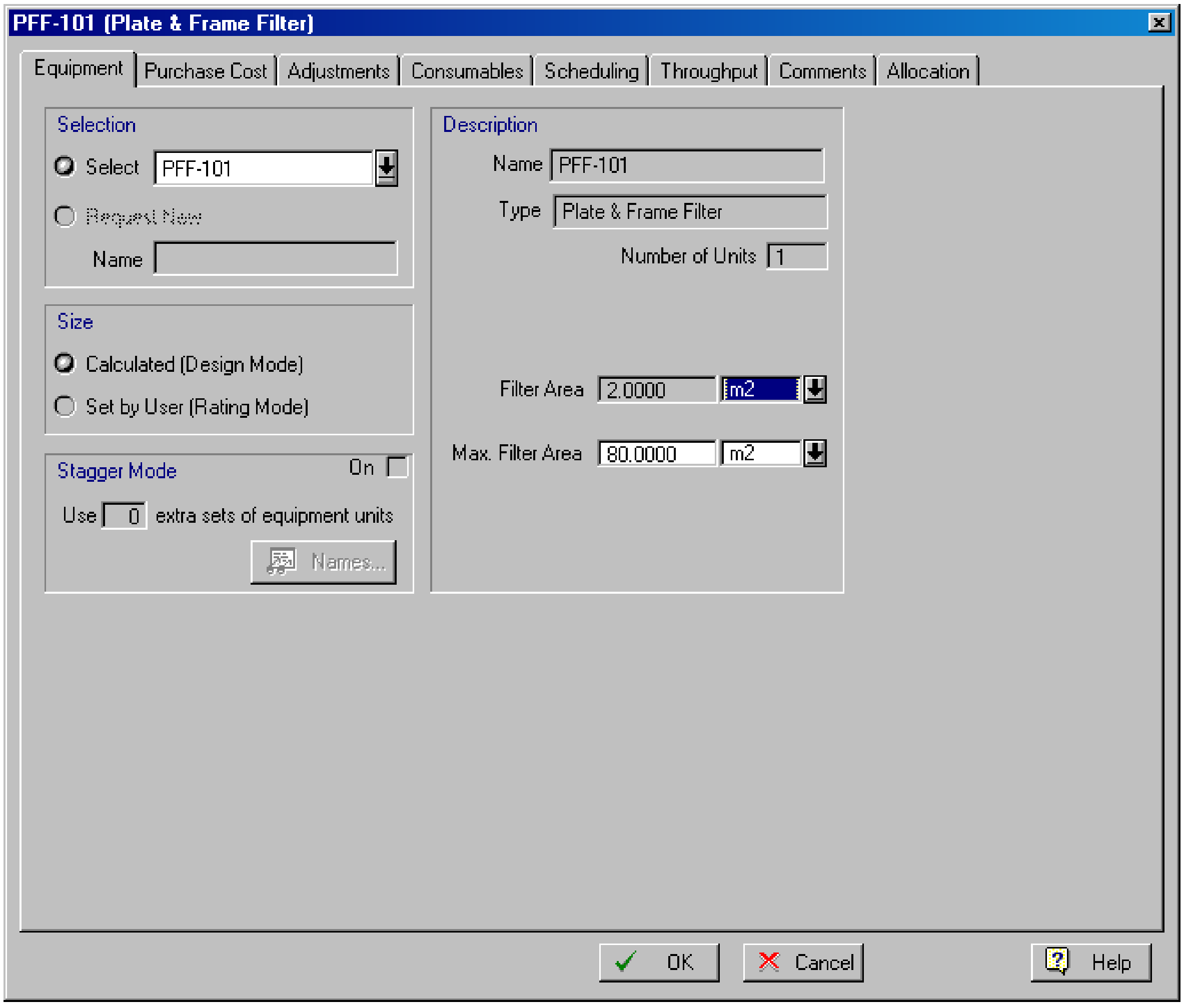


Figure 2.1-bb: The Equipment Data tab of the Plate & Frame Filter.

Through the equipment tab, you can also select the specific piece of equipment that is going to carry out the processing step. By default it is assumed that each unit procedure is carried out in its own (exclusive) equipment. However, two (or more) different procedures can share equipment if they are in batch operating mode and the entire flowsheet is also in batch mode. For more information on equipment sharing as well as allocation, please see Chapter 5 and the two detailed examples that follow or consult on-line Help Facility (search for "Equipment Sharing").

At this point you have completed the basic initialization steps for the streams, operations, and equipment. As you become more familiar with Pro-Designer, it will take much less time to do these activities. For instance, all the steps that we have done thus far in this chapter could be performed in about 15 minutes if you were already familiar with how to use Pro-Designer.

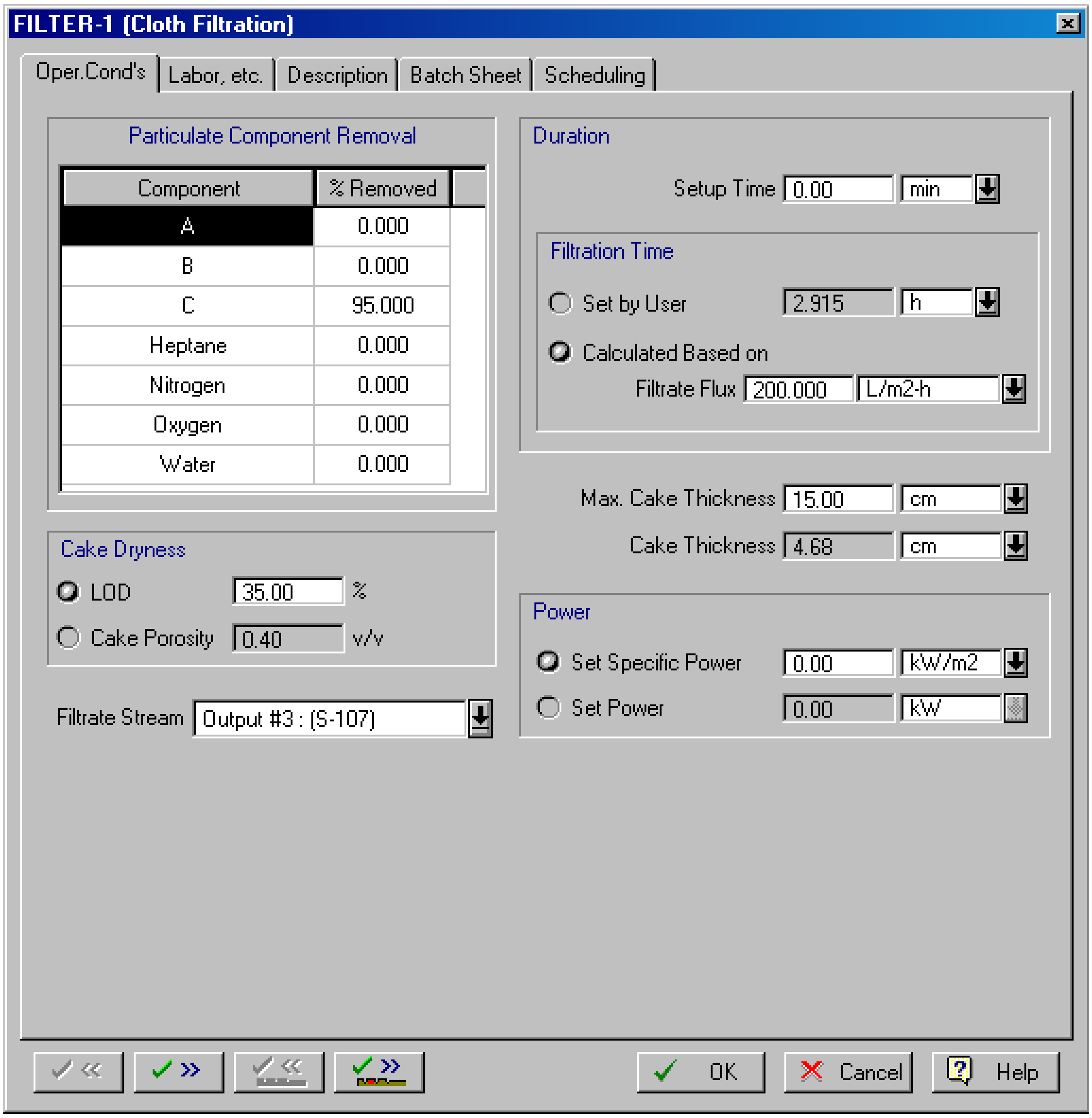


Figure 2.1-cc: Dialog of the Filtration Operation (when the Equipment is in Rating Mode).

Important note about building and initializing large flowsheets – when you design complex flowsheets, keep in mind that you don't have to add all the unit procedures at once. You can always add or remove procedures as desired at a later stage of the design. For complex flowsheets, it is highly recommended that you begin your design with just a few unit procedures (two is a good number) and add more of them only after you have simulated the first unit procedures and determined that the streams and operations have been initialized correctly and your mass balances make sense.

Using Break Points

When simulating large flowsheets it is sometimes useful to solve only part of the process. Setting breakpoints tells the simulator to halt calculations at a certain point. A brief description of this facility is given below.

You can place a breakpoint, and force the M&E balance execution sequence to pause either right before, or right after the solution of a unit procedure. You may even place a breakpoint inside the unit procedure's solution sequence of unit operations. Use the following steps to place a breakpoint on a unit procedure:

- Right click on a unit procedure to bring up the command menu:
- After selecting the "Set Breakpoint" option, a dialog will appear asking where to break the simulation. Check the place(s) where you wish the simulation to pause and exit this dialog, notice a red sign,  , is shown above the procedure's icon to indicate that one or more breakpoints are set on this procedure. The position of the sign indicates whether the break is on the entry, operations or exit of the procedure.
- Once a breakpoint is set, next time the "Solve M&E Balances" command is issued, the simulation calculation sequence will pause at that location. When the simulation sequence is paused, some of the "Solve" Toolbar's buttons become active. Also notice that while the simulation has been paused, all unit procedure display another icon underneath that has indicates the simulation state of each procedure at that time (as the simulation is paused):

   has not been visited yet

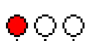
   has been successfully simulated already

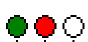
   is being solved recursively (as part of loop convergence)

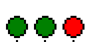
   solution ended unsuccessfully (as part of an un-converged loop)

   solution ended unsuccessfully (an error was encountered)

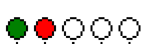
  The following sequences of images, indicate the state of the unit procedure that is CURRENTLY BEING SOLVED (i.e. when the breakpoint was encountered):

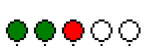
   Break on entry

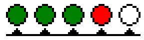
   Break in an operation

   Break on exit

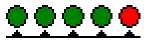
   Break on entry

   Break on material pull in/push out (applies to operations with auto adjust material streams)

   Break in an operation



Break on material pull in/push out (applies to operations with auto adjust material streams)



Break on exit

Notes:

You can toggle the visibility of the breakpoint icons (above the UP) as well as the simulation status icon (below the UP) from the Solve Toolbar (last two buttons).

Also note, that you can temporarily deactivate breakpoints (without removing them). Simply visit the Set Breakpoints interface dialog of a unit procedure, and click once more on the checked breakpoint location. Notice how the checkmark now is still there, but looks faded (grayed out). The breakpoint sign above the UP's icon will look faded as well.

When the "Solve M&E Balances" sequence is paused, you may visit any stream or procedure or operation's simulation dialog to inspect or even modify values of operating conditions. If you modify the values of streams and/or operations belonging to unit procedures that have already been solved (i.e., the check mark icon appears underneath) or to the unit procedure that is being currently solved but the operations whose value has been modified has already been solved, then the new values will not be taken into account until the next "Solve M&E Balances" command is issued.

2.1.8 Setting the Process Scheduling Information:

The following terms are used for batch process scheduling:
Operating Time: The number of hours per year the plant is devoted to making a specific product.
Campaign: An uninterrupted run of batches.
Batch Time: The start to finish time for one batch.
Cycle Time: The time between batch starts. Sometimes called the recipe or plant cycle time.
Minimum Cycle Time: The minimum time between batch starts based on the time (scheduling) bottleneck.
Cycle Time Slack: The difference between the actual and minimum cycle times.

If the process is in batch mode, which is the case for your example flowsheet, you should provide process scheduling information before performing a simulation. Pro-Designer allows you to specify the following scheduling data:

1. For each operation:

a. the process time,

b. the setup and turnaround times,

c. the starting time, and

d. the number of cycles (at the procedure level).

2. **For the entire plant:**

e. the annual operating time,

f. the number of campaigns per year,

and either:

g1. the number of batches per year, or

g2. the cycle time, or

g3. the cycle time slack.

Scheduling of operations was explained in Section 2.1.5. Figure 2.1-y in that section showed the Scheduling tab of a filtration operation. Through the Scheduling tab, you can specify the starting time relative to the beginning of the batch or relative to the start or end of other operations in the same or different procedures. You may also specify the process time (if it is not calculated by the model), the setup and turnaround time.

To specify the number of cycles per batch of a procedure (the same number applies to all operations of the procedure), simply right-click on the unit procedure's icon and choose **Procedure Data**. By default, all procedures start with one cycle.

To specify scheduling information for an entire process, select **Tasks: Recipe Scheduling Information...** (see Figure 2.1-dd below).

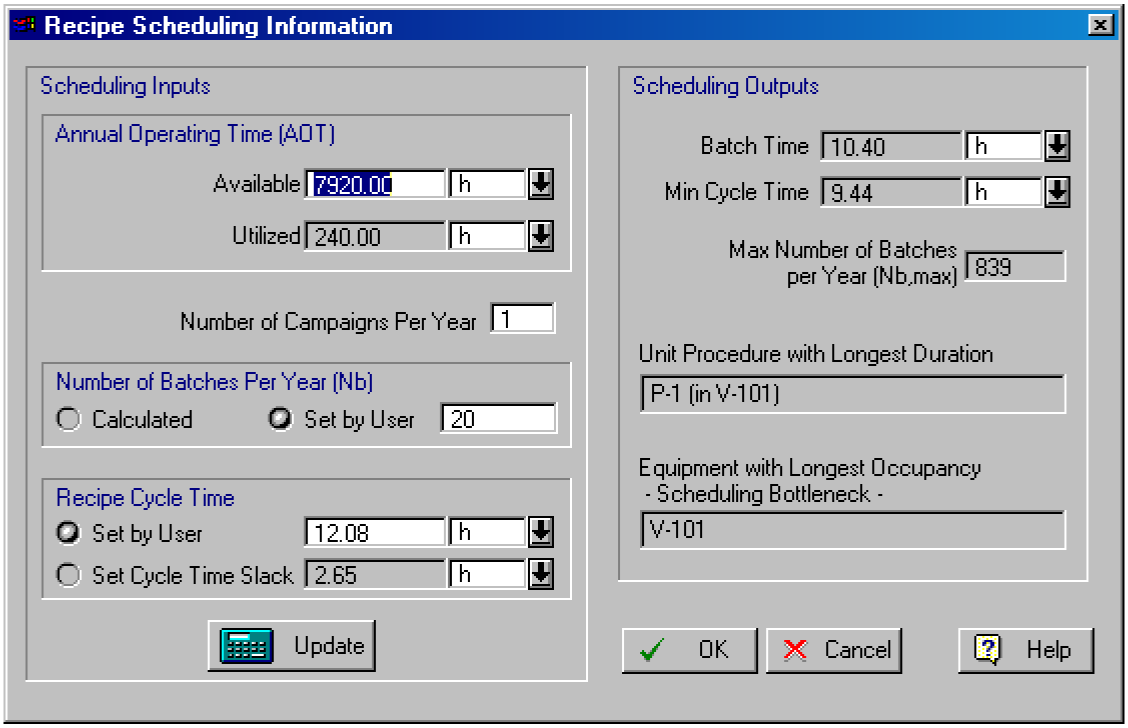


Figure 2.1-dd: Specifying the scheduling information for a batch process

For your example process, please change the "Number of Batches per Year" to 20. This implies that your example process will be run in a pilot plant 20 times this year (it is assumed that the equipment used by this process is used by other processes the rest of the year.) In addition, please change the annual operating time for this process to 240 hours to reflect the completion of one batch during every 12-hour shift.

Based on the scheduling information and the annual operating time specified for the plant, the system will do the following:

1. Make sure there is no conflict created by the specified start time and end time of processing steps. Conflicts can be created if the cycle times of procedures that share equipment overlap.
2. Make sure there is no conflict between the specification of annual operating time, the number of batches, and the plant cycle time (as calculated from all the procedures).

3. Calculate the plant's batch time, the plant's cycle time, the plant's minimum cycle time (with maximum batch overlapping), the maximum number of batches possible, the longest procedure (i.e., the procedure with the longest total cycle time) and the scheduling bottlenecking equipment (the equipment with the longest occupancy time).

2.1.9 Viewing Scheduling, Equipment Utilization and Resource Tracking Results

A variety of scheduling, equipment utilization and resource tracking tools are included in Pro-Designer. These include Operations and Equipment Gantt Charts, Main and Auxiliary (CIP skids & SIP panels) Equipment Occupancy Charts, and Resource Demand and Inventory Charts.

Gantt Charts

Please generate the Operations Gantt Chart for your example process by selecting **Tasks: Gantt Charts: Operations GC** from the main menu. It should look similar to Figure 2.1-ee below. The left view (spreadsheet view) displays in each line: the name, duration, start and end time for each activity whose bar line is shown straight across on the chart (all information is presented for viewing purposes only). You use the left view to expand and/or collapse activity summaries by clicking on the + or – rectangle showing at the left of the name of the activity. The right view (chart view) displays a bar for each activity participating in the overall scheduling and execution of the recipe.

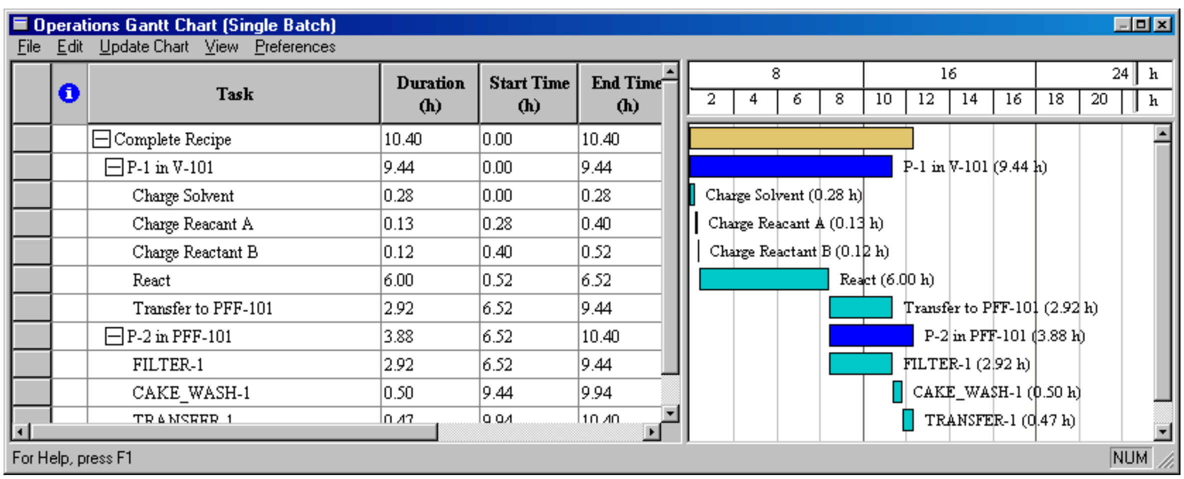


Figure 2.1-ee: The Operations Gantt Chart.

Note: If you wish to modify the appearance of the chart, including the bar width and time-scale use the **Preferences: Styles: Gantt Chart** menu item on the chart's menu bar.

From the Gantt Chart interfaces you can modify the scheduling parameters of each procedure and operation as well as the scheduling parameters for the entire process (i.e., annual operating time, number of batches per year, etc.). In fact, anything you can accomplish with the scheduling interfaces described in Section 2.1.7, you can also accomplish from the Gantt chart interface. In order to edit scheduling parameters from this interface, right-click on the bar of the desired procedure or operation. This will bring up the **Procedure Data** dialog (in the case of procedures) or the **Operation Data** dialog (in the case of operations.) To view and edit the scheduling information for the entire batch, right-click on the bar which corresponds to the Complete Recipe (at the top of the chart) and choose **Recipe Scheduling Info**. After you have edited a scheduling parameter, you must click the Update Chart button on the Gantt chart main menu. As you can see, these Gantt Charts present you with a graphical way to set the scheduling parameters of each processing step and immediately visualize the effects on the entire batch production. Please refer to the examples in Chapter 2.2 and 2.3 to see Gantt Charts for more complex processes.

Equipment Occupancy Charts

Another way of visualizing the execution of a batch process as a function of time is through the Equipment Occupancy chart (select **View: Equipment Occupancy Chart: Multiple Batches**). By default two batches are shown. To add more, right-click on the chart and select **Set Number of Batches**. Figure 2.1-ff displays the equipment occupancy chart for three consecutive batches of the process of this example. White space represents idle time. The equipment with the least idle time between consecutive batches is the **time (or scheduling) bottleneck** (V-101 in this case) that determines the maximum number of batches per year. Its occupancy time (9.44 hours in this case) is the minimum possible time between consecutive batches (also known as Min. Cycle Time). The actual time between consecutive batches (also known as Cycle Time) is 12 hours.

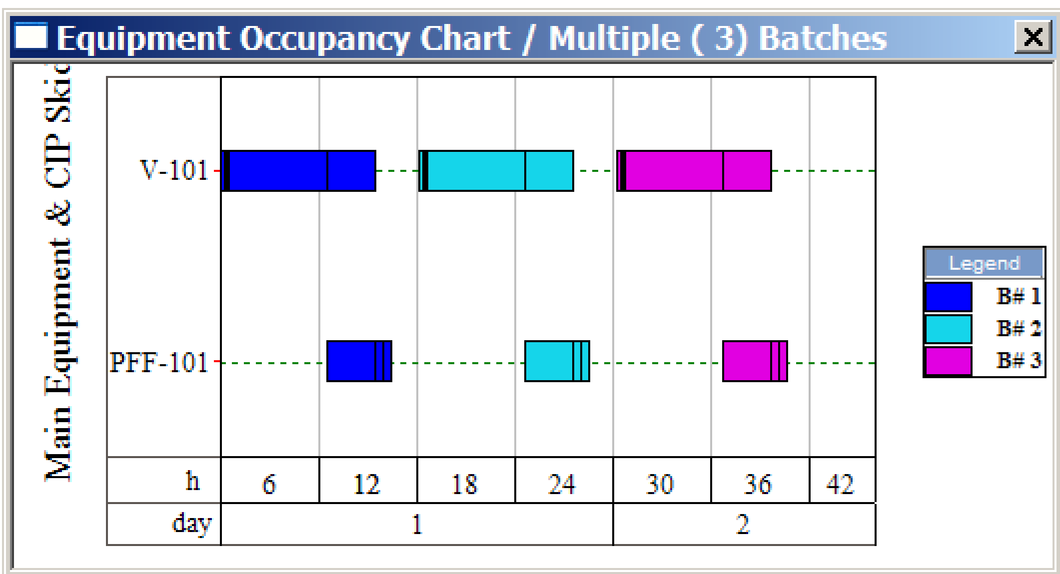


Figure 2.1-ff: Equipment Occupancy Chart (three consecutive batches).

Resource Tracking

In addition to creating Gantt charts for equipment utilization and operations, Pro-Designer automatically generates graphs of resource demand as a function of time for such things as heating and cooling utilities, power, labor, and raw materials. To view these graphs, select **View: Resource Consumption Tracking Chart: Labor (Multiple Batches)**. Figure 2.1-gg displays the labor requirement resource demand graph for two consecutive batches. As can been, three operators are required to handle this process.

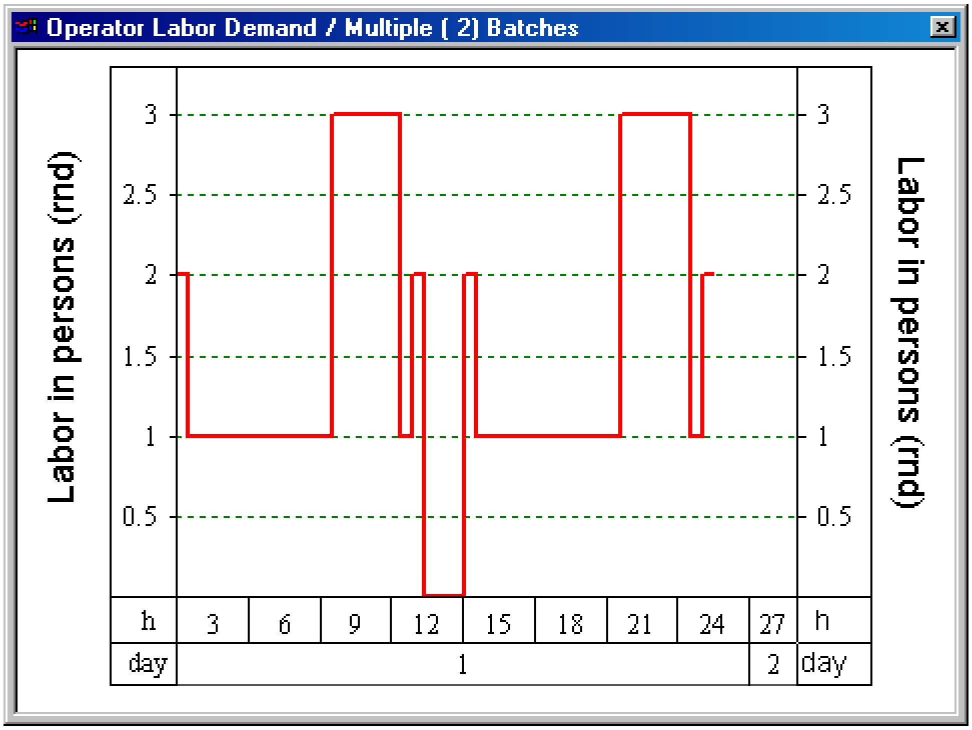


Figure 2.1-gg: The Labor Resource Tracking Chart for the example process

Inventory Tracking

Pro-Designer can also analyze and display inventory information for material resources. Recall that 50 kg of material ‘A’ are used in each batch. Suppose there is a 300kg storage capacity for ‘A’ and an opening inventory of 100kg. Suppose further that the loading rate of ‘A’ into storage is 200kg/hr. How often should shipments of ‘A’ be scheduled?

Select the menu item **View \ Resource Inventory Chart \ Ingredient (Multiple Batches)**. Select ‘A’ and select the **Supply Info** button. Fill out the dialog as shown in figure below.

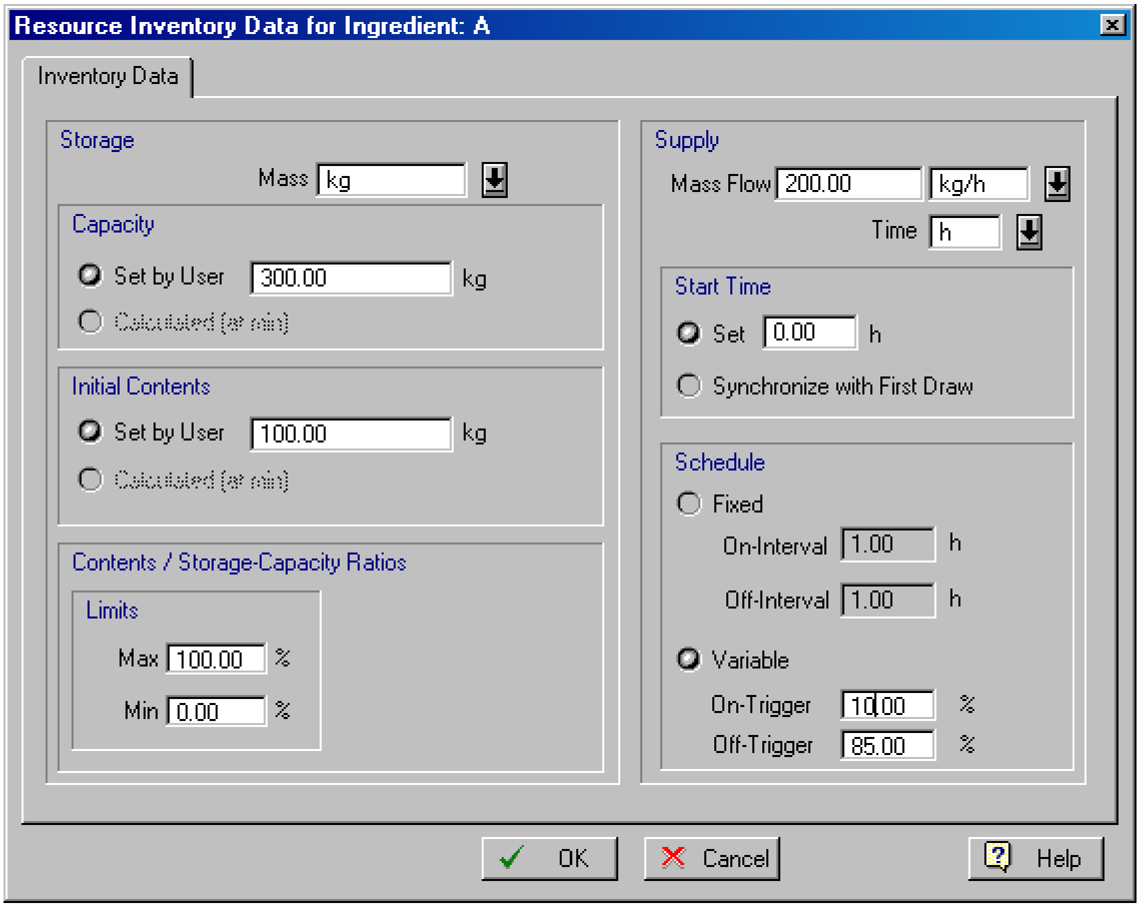


Figure 2.1-hh: The Ingredient Resource Supply Dialog

This will tell Pro-Designer that the supply of 'A' should be replenished when the inventory falls to 10% of the capacity. The replenishment should be halted when the inventory reaches 90% of storage capacity. Click OK.

Next, select the **Chart Style** button and select the Contents tab. Under the Inventory heading check the boxes for *amount* and *limits*. Deselect everything else and click OK. Click OK to continue and the chart will be displayed with two batches. Set the number of batches to 12 by right-clicking and selecting **Set Number of Batches**. The resulting chart will look something like the following figure. The increases in inventory indicate the replenishment schedule suggested by Pro-Designer. It is also possible to set the replenishment schedule and allow Pro-Designer to calculate the minimum inventory capacity required.

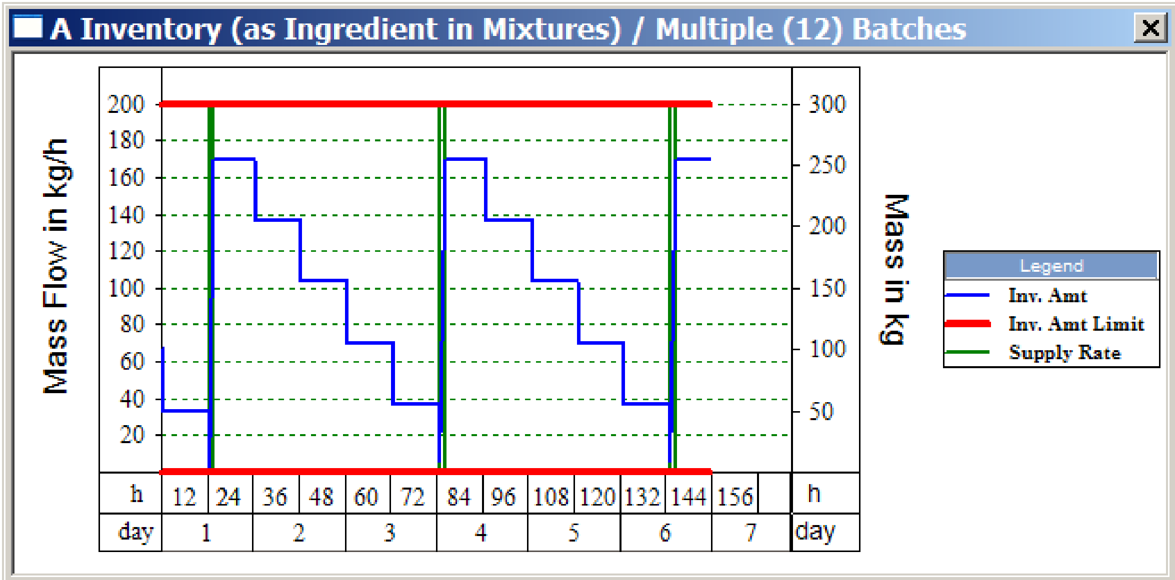


Figure 2.1-ii: The Inventory Profile of Component A

Throughput Analysis and Debottlenecking

Pro-Designer is equipped with powerful throughput analysis and debottlenecking capabilities. The objective of these features is to allow the user to quickly and easily analyze the capacity and time utilization of each piece of equipment, and to identify opportunities for increasing throughput with the minimum possible capital investment. The most important utilities are:

- The throughput potential chart, which indicates opportunities for increased production per batch
- The utilization charts

For a detailed throughput analysis example (based on the process of the second example), please see Chapter 9 or search for Debottlenecking in the Help Facility. A brief description is given here.

Since throughput calculations are based on fixed equipment, set the equipment calculation mode to **User Defined (Rating)** for all the items to be evaluated (specify 1600 L for the reactor and 2 m2 for the filter). Solve the model and select **View: Throughput Analysis Charts: Utilization**. The utilization chart below will appear.

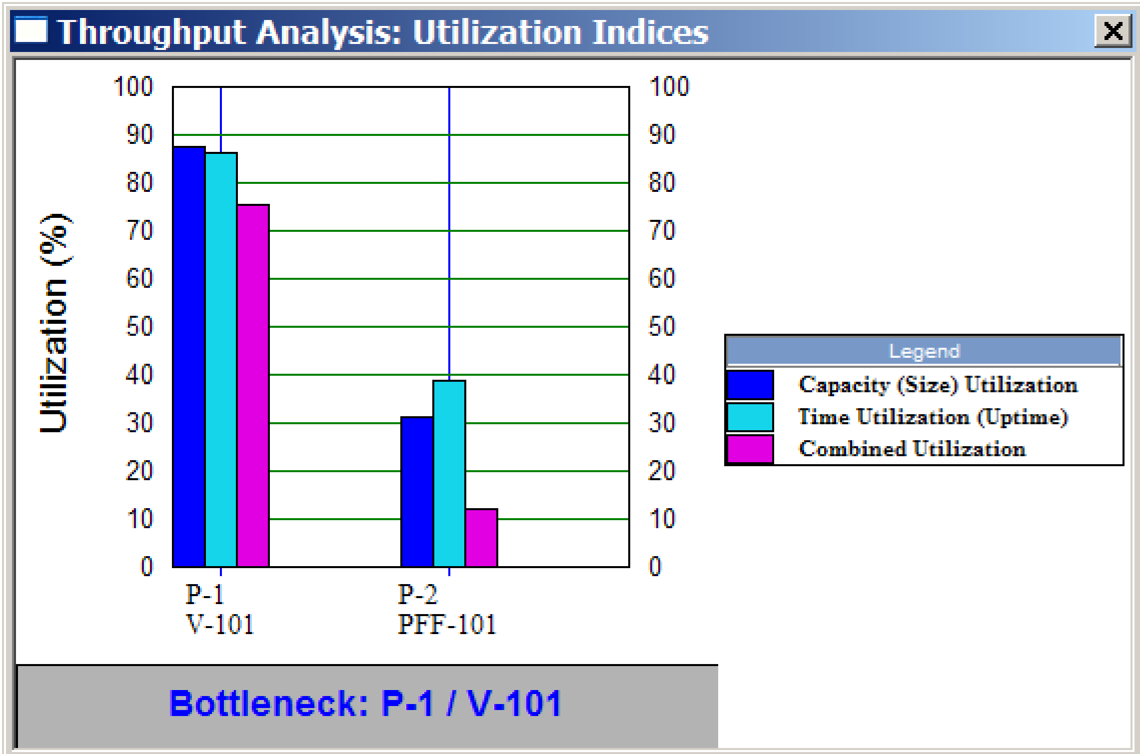


Figure 2.1-jj: Equipment Capacity/Time Utilization Chart

The chart shows, for each piece of equipment, the capacity utilization (how "full" the equipment is) and the time utilization (it's "uptime"). The combined utilization is the product of the two. Also the time utilization is somewhat low because some slack time was introduced.

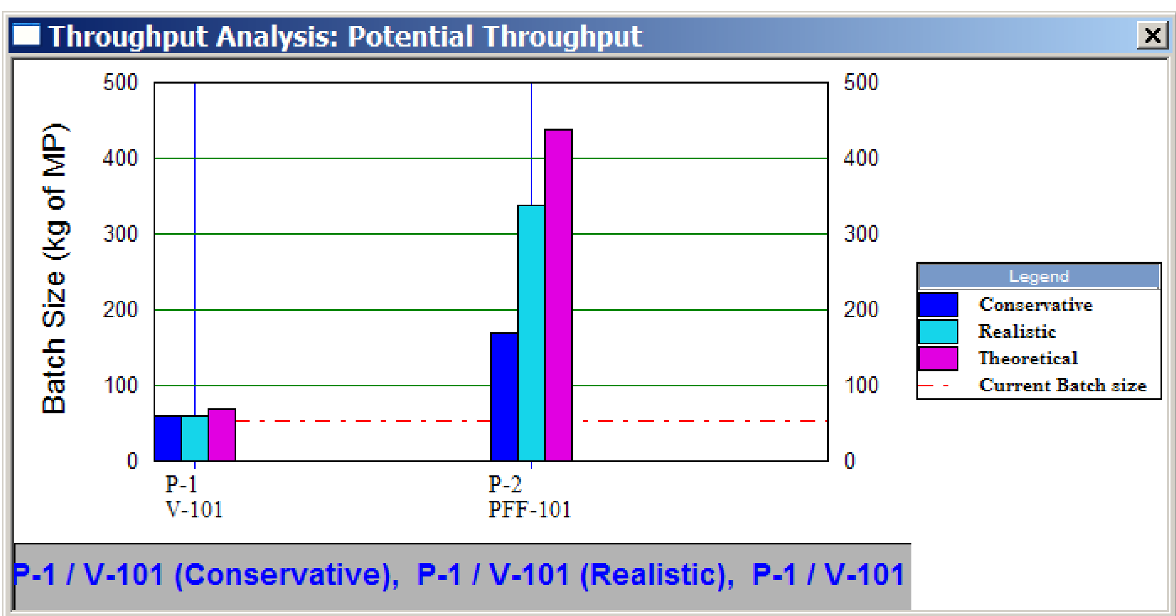


Figure 2.1-kk: Throughput Potential Chart.

Select **View: Throughput Analysis Charts: Potential** to view the throughput potential chart (Figure 2.1-kk). This chart shows the potential and actual (red dotted line) batch sizes based on each piece of equipment.

2.1.10 Cost Analysis and Economic Evaluation

Pro-Designer performs thorough cost analysis and economic evaluation calculations and generates three pertinent reports. The key initialization steps are described below.

Supplying Revenue, Raw Material, and Waste Stream Data

This step must precede economic evaluation, throughput analysis, and environmental impact assessment calculations. To supply this data, first select the **Tasks: Stream Classification...** item from the main menu. You will be presented with a dialog window (see below) where you can classify all input and output streams as raw materials, revenues or wastes (solid, aqueous, organic, or gaseous) and supply any cost data associated with the classification. By default, the system estimates a purchase or selling price for a stream based on the price of each component and the composition of the stream. The price of a pure component or stock mixture is part of its Properties, which can be edited when Registering Components as described earlier in this chapter. In this example process, please classify the output streams and set costs for the two liquid waste streams (as was done in Figure 2.1-ll). Notice that the Selling Price of the Revenue stream is calculated automatically, based on the stream's composition (recall that there is still heptane and small amounts of impurities in our product cake, so the price per kg of cake is less than the $300/kg price of pure component C.) Next, click on the **Set By User** boxes next to the two liquid waste streams and type in $0.10/kg for the Disposal Cost of each. Also be sure to classify them as liquid waste.

Finally, select your revenue stream (S-107 below) from the Main Product Rate drop-down list, and specify that the unit cost for this process will be reported based on the Component Flow of product C (see below).

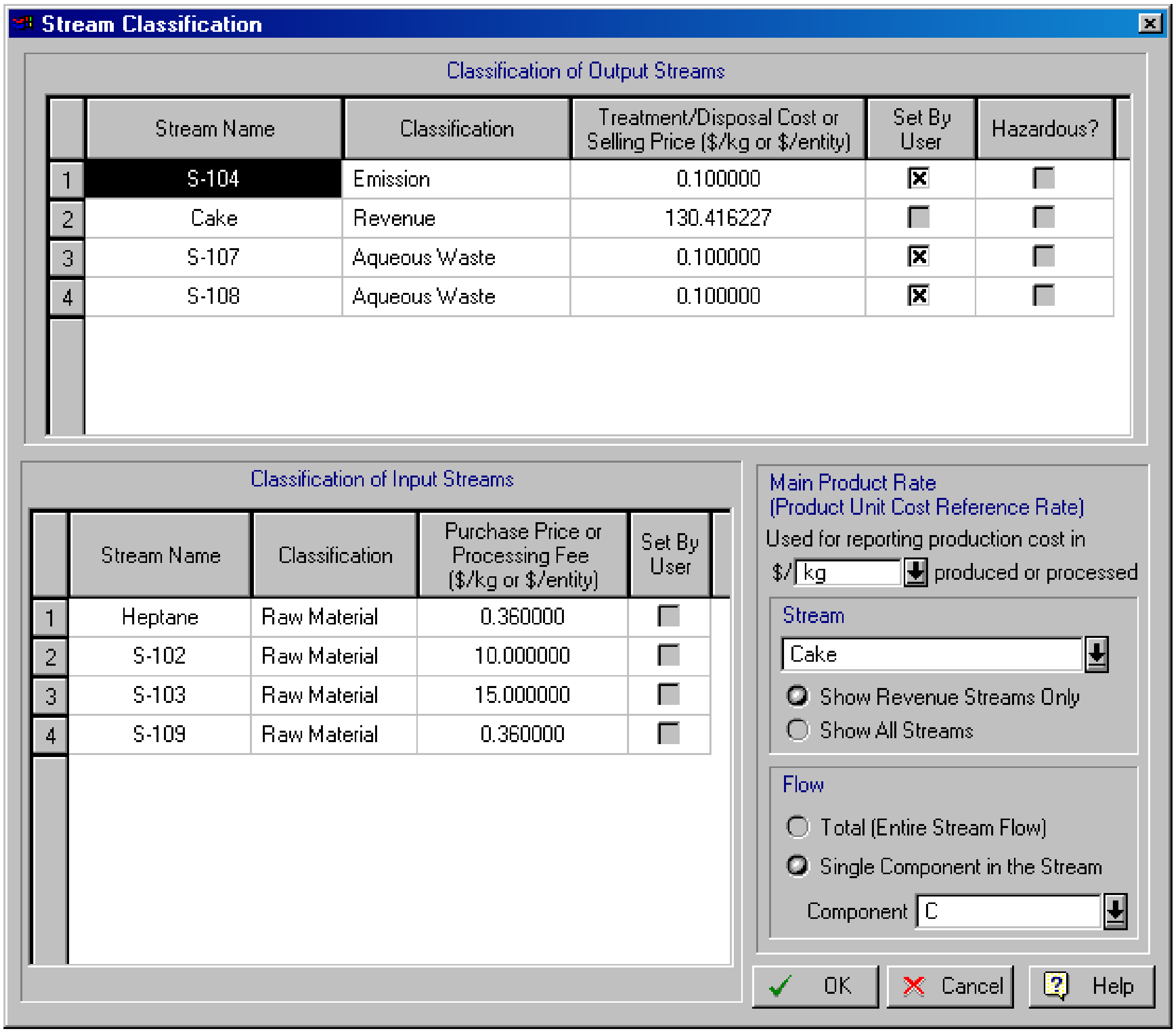


Figure 2.1-ll: The Revenue, Raw Material and Waste Stream dialog box

Note: Classification of a stream as a solid, aqueous, organic, or gaseous waste will cause it to be reported in dedicated sections of the **Environmental Impact Report**, where a detailed bookkeeping is kept on all chemicals that end up in each waste category. The environmental impact report allows you to evaluate the burden of the process on the environment. Such an assessment assists the designer to focus his/her attention on the most troublesome streams and the processing steps that generate them. A related report, the **Emissions Report** provides information on emissions of volatile organic compound (VOC) and other regulated compounds.

Adjusting the Cost Factors

The user can specify economic evaluation parameters at three levels: the Operation, Equipment, Section, and Flowsheet (Design Case) level. Please note: the economic evaluation parameters from each of the three levels have a significant impact on the cost calculations. Therefore, the parameters at all three levels should be examined by the user and edited if necessary.

Economic Parameters at the Operation Level

Parameters that affect demand for Labor and Utilities are specified at the operation level. For instance, the labor requirement for an operation can be specified through the **Labor, etc.** tab of an operation's dialog. Through the same dialog you can specify auxiliary utilities, which have no impact on material and energy balance calculations (they do not affect output stream temperatures). They are only considered in costing and economic evaluation calculations. Auxiliary utilities offer a convenient way to associate utility consumption with generic boxes and other operations that do not calculate utility demand.

Economic Parameters at the Equipment Level

All unit procedures have two common dialog tabs through which the user can provide information that affects the capital investment and certain items of the operating cost of that particular step.

Information about equipment purchase costs and various adjustments can be provided through the Purchase Cost and Adjustments tabs of the Equipment Data dialog (right click on the vessel procedure and select Equipment Data). By default Pro-Designer uses a built-in model to estimate purchase costs for each piece of equipment (Figure 2.1-mm). However, you can override this estimate by either using your own model (click on User-Defined Model) or specifying an exact purchase cost (from a vendor quote, for instance.)

Now please click on the Adjustments tab of this dialog to view the % depreciated, material factor, # of standby units, etc. for the reactor. The fields on this tab are described in detail below:

Already Depreciated Portion

Oftentimes, a piece of equipment has already been either fully or partially depreciated. This can be captured using this variable. Any values other than 0.0% reduce the cost of depreciation but have no impact on the maintenance cost because that cost depends on the full purchase cost and not just the undepreciated portion.

Installation Cost

This factor is used to estimate the installation cost for each piece of equipment as a fraction of their purchase cost. The most common value is 0.5, meaning that the installation cost is 50% of the equipment purchases cost.

Material Factor

The purchase cost that is estimated using the built-in model corresponds to a certain material of construction that is displayed on this tab. Selecting a different material will affect the equipment purchase cost. Note – the material cost factors for each type of equipment can be viewed by choosing **Databanks \ Construction Materials…** from the menu bar. Additional materials and material factors can be added to the User database.

Maintenance Cost

This factor is used to estimate the annual maintenance cost for each piece of equipment. The most common value is 0.1, meaning that the annual maintenance cost is 10% of its purchase cost.

Usage and Availability Rates

These factors represent the equivalent of equipment rental rates. They are used only when the Facility-Dependent (overhead) cost is estimated in a certain way (not the default way). More information on this subject can be found in Chapter 8 (Economic Evaluation).

Standby Units

For pieces of equipment that are critical to the operation of a process, you may choose to have one or more standby units (in case the regularly used pieces of equipment go down for scheduled or unscheduled maintenance). The number of standby units affects the capital investment but has no impact on maintenance and labor cost.

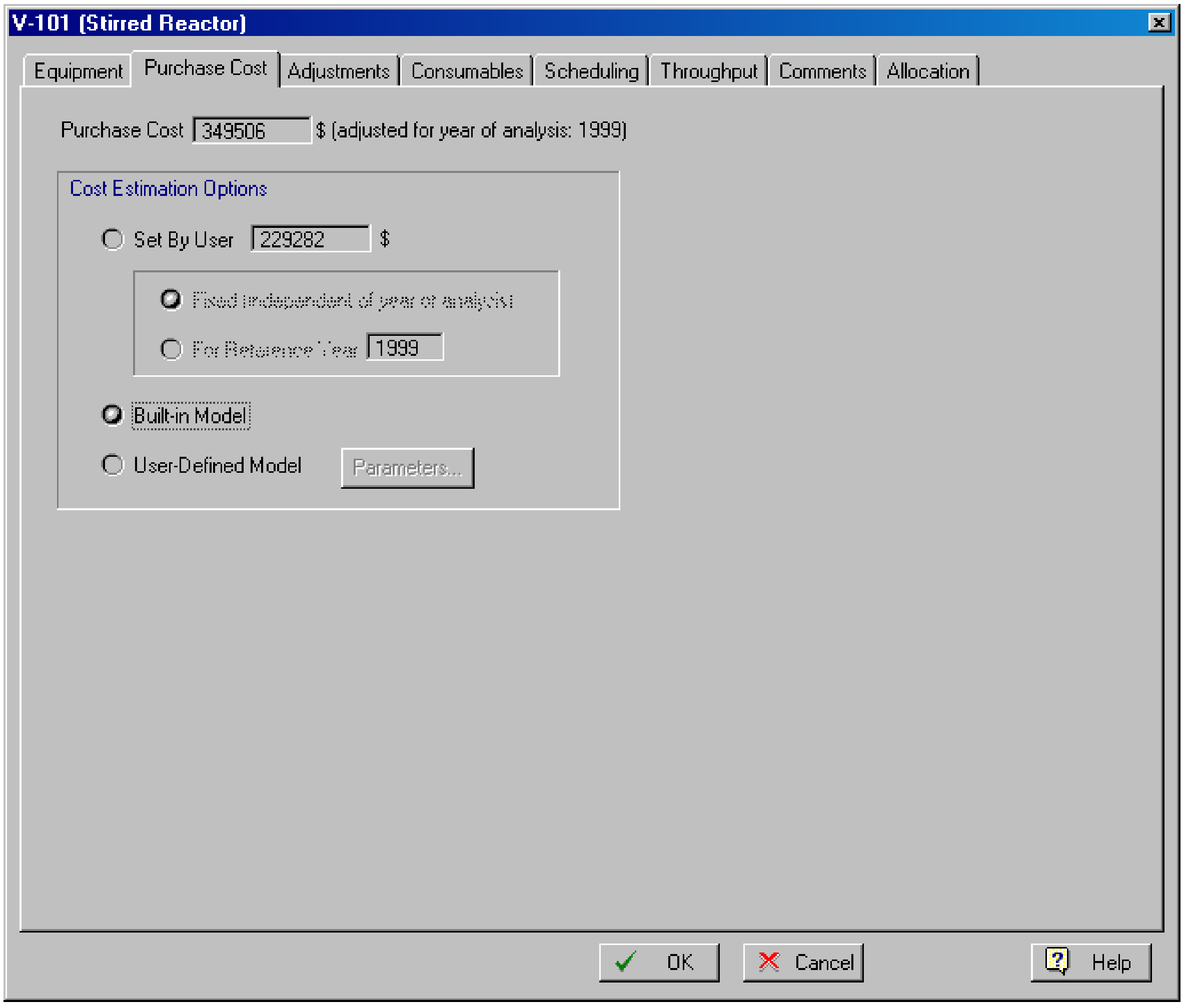


Figure 2.1-mm: The Purchase Cost tab of the Equipment Data dialog box

Notes:

a) If a piece of equipment is shared by multiple unit procedures, its purchase-cost-dependent expenses (e.g., depreciation, maintenance, etc.) are distributed to its hosting steps based on the occupation time of each step.

Cost of Consumables

Consumables include materials and items that need to be replaced periodically, such us chromatography resins, cartridges of membrane filters, lubricants of equipment, etc. Disposable equipment, such as plastic bags, plastic bioreactors, roller bottles, etc. that are used once and thrown away belong to this category too. Parameters related to consumables are specified through the Consumables tab of the Equipment Data dialog. Starting with version 6.0, SuperPro features a Consumables database where users can store information for all the consumables that they utilize. The information in the Consumables database is accessible through the Consumables tab of an equipment.

Economic Parameters at the Section Level

Division of a flowsheet into sections facilitates reporting of results for economic evaluation, raw material requirements, and throughput analysis of integrated processes. A flowsheet section is a group of unit procedures that have something in common. All flowsheets initially contain one section (called the “Main Section” by default). For information on how to create flowsheet sections and edit their properties, please read Chapter 5 or consult the Help Facility (look up the keyword “Sections” in the Help index).

Section Capital Investment Factors

Pro-Designer uses a factor-based method to estimate the capital investment associated with each section of a flowsheet. These factors have been assigned default values that should be reasonable for most cases. However, you should still check these factors to ensure that they are accurate for your situation. You can then adjust the factors to better suit your particular design case. Figure 2.1-nn shows the dialog box that allows you to edit factors used to estimate the direct fixed capital (DFC) of a section. This dialog box is brought up by selecting the appropriate section (“Main Section” in this case) from the Section drop-down menu, and then clicking on the **Capital Cost Adjustments** button of the section toolbar (the button with the green dollar sign on it). This dialog box can also be accessed by right-clicking on a blank area of the flowsheet and selecting **Section (section name): Capital Cost Adjustments**.

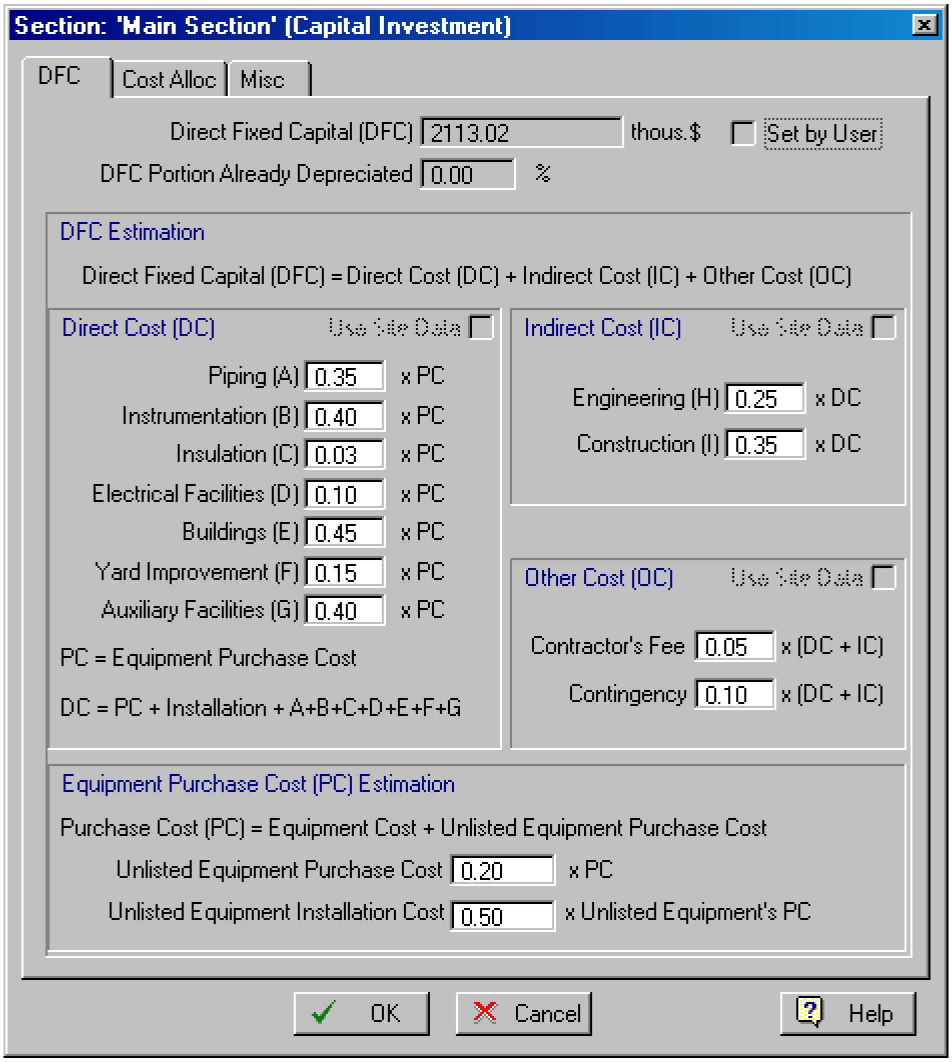


Figure 2.1-nn: The dialog box for Capital Cost Adjustments.

If an entire section or certain equipment items of a section are utilized by multiple projects (this is quite common for batch processes), the user can specify either the fraction of DFC or the equipment purchase cost that should be allocated to the present project through the **Cost Allocation** tab of the above dialog. In the Cost Allocation tab specify a “Section Wide” cost allocation factor of 0.5.

Through the **Miscellaneous** tab of the Capital Cost Adjustments dialog, you can adjust parameters that affect the calculation of the Working Capital, Startup and Validation Cost, Up Front R&D, and Royalties.

Note:

The above parameters also can be retrieved from a database site by allocating a flowsheet section to a database site. That is the best way to utilize meaningful parameters for different industries around the globe. That is also the recommended way for standardizing cost analysis assumptions. For more information on how to take advantage of the database capabilities for cost analysis, please consult the “SynPharmDB” read-me file in the “Examples \ SynPharm” directory of SuperPro.

Section Operating Cost Factors

Pro-Designer calculates and reports nine cost items for each flowsheet section: *Raw Materials, Labor-Dependent, Facility-Dependent, Laboratory/QC/QA, Consumables, Waste Treatment/Disposal, Utilities, Transportation, and Miscellaneous*. Figure 2.1-oo displays the options available for calculating the facility-dependent operating cost.

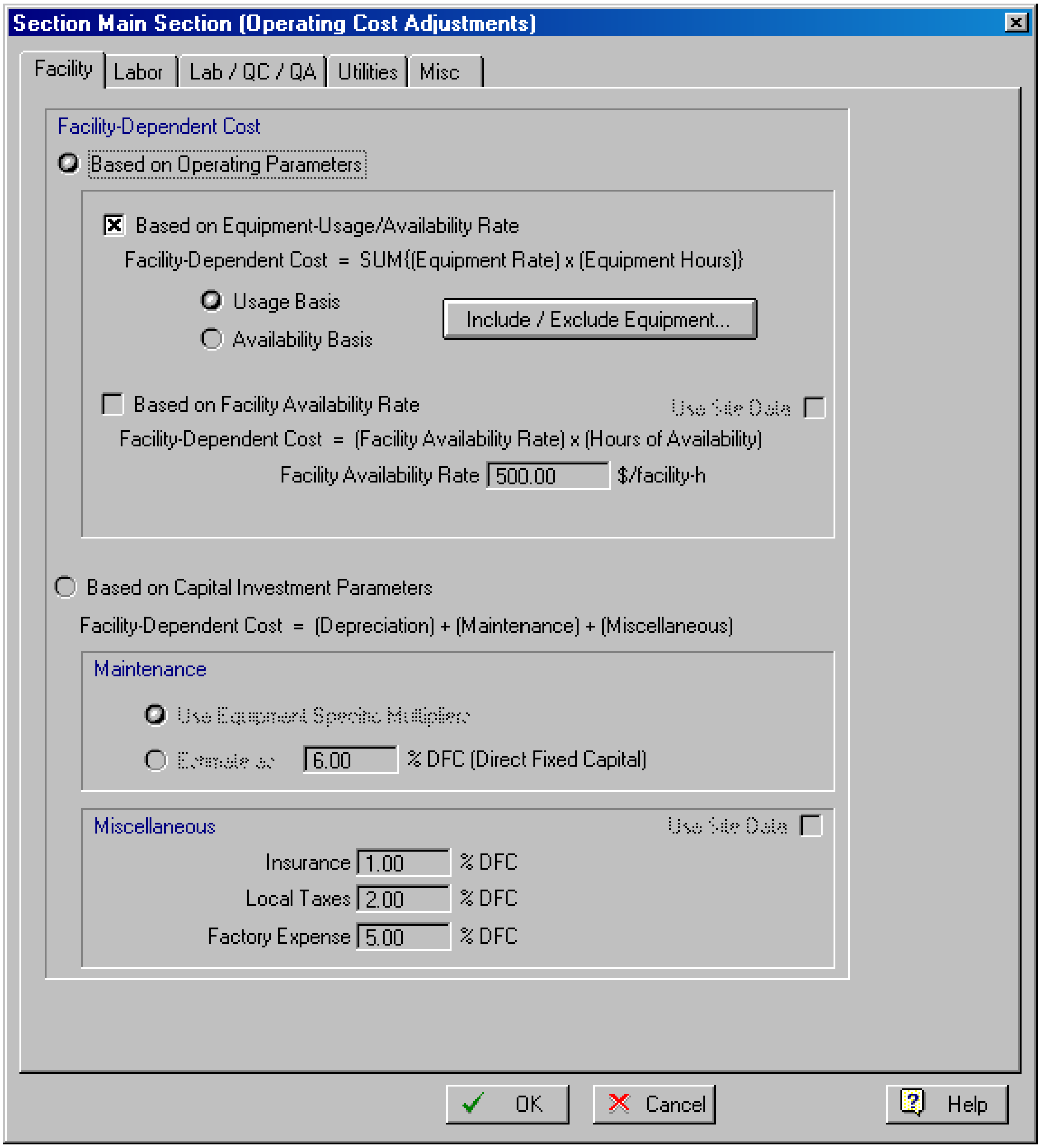


Figure 2.1-oo: The dialog box for Operating Cost Adjustments.

This dialog is brought up by selecting the appropriate section ("Main Section" in this case) from the Section drop-down menu and then clicking on the **Operating Cost Adjustments** button of the section toolbar (the button with the small dollar sign and the runner). This dialog box could also be accessed by right-clicking on a blank area of the flowsheet and selecting **Section (section name): Operating Cost Adjustments**.

Through the Operating Cost Adjustments interface, the user can adjust parameters that affect the Facility, Labor, Lab/QC/QA, Utilities, and Miscellaneous costs of a section. For your example process, please change the Facility Cost to be based on an Equipment Usage Rate. This will account for depreciation, maintenance, and miscellaneous equipment expenses. The equipment usage or availability rates are equipment-dependent, are initialized to $100/hr and can be edited though the **Adjustments** Tab of the Equipment Data dialog.

Next, please visit the other tabs on the above dialog to familiarize yourself with their functions. Notice that in the **Labor** tab there are various options for specifying the labor costs of your process, including lumped and itemized estimates for both the number of hours required and the labor rate. Furthermore, the **Lab/QC/QA** tab of the above dialog allows you to specify information for detailed calculation of laboratory, quality control, and quality assurance expenses (see Chapter 8 for more details.)

Economic Evaluation Factors at the Flowsheet Level

Finally, there are parameters at the flowsheet level that affect the results of project economic evaluation. Through the dialog of Figure 2.1-pp, for instance, the user can specify various time parameters as well as the interest levels for calculating the net present value (NPV) of the project. This dialog box is brought up by selecting the **Edit: Flowsheet Options: Economic Evaluation Parameters...** option from the main menu. It can also be brought up by right-clicking on a blank area of the flowsheet and selecting the **Economic Evaluation Parameters...** option.

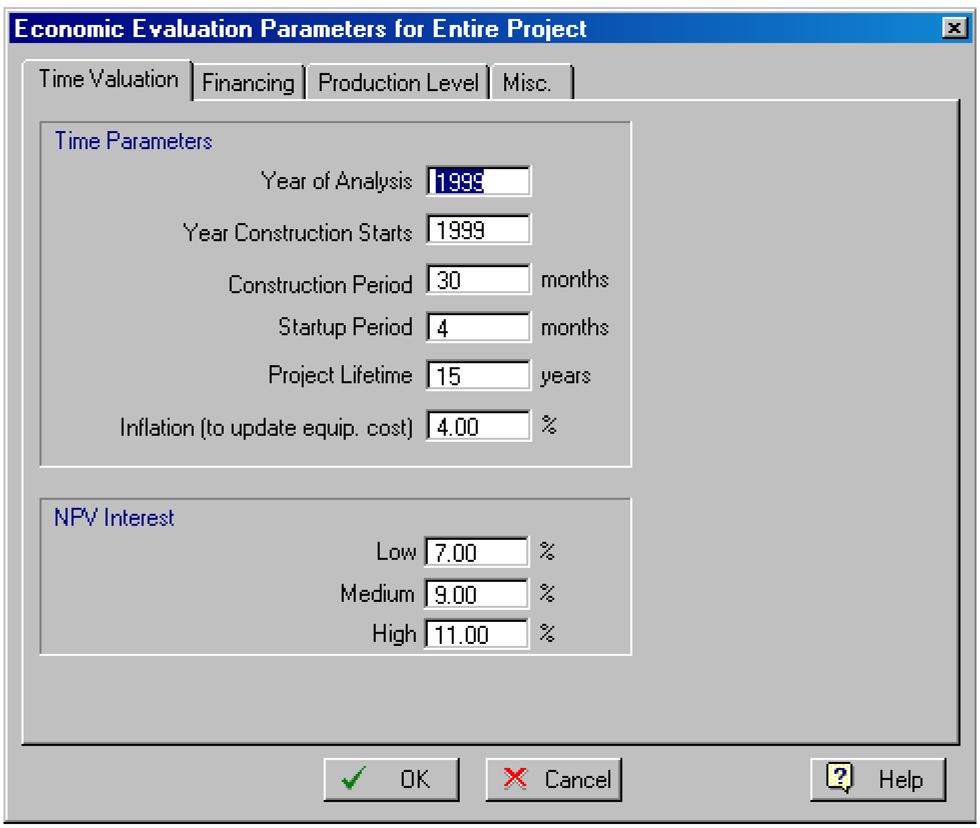


Figure 2.1-pp: Adjusting the economic evaluation parameters at the flowsheet level.

Through the **Financing** tab of the above dialog, the user can provide information on the financing of the project (e.g., equity versus borrowed money for DFC, working capital, etc.), the method of depreciation, the depreciation period, the salvage value, and the DFC outlay (the spending of direct fixed capital as a function of time).

Through the **Production Level** tab of the above dialog, the user can specify the capacity utilization profile (production level) for the expected lifetime of the project and provide information for product failure rate and disposal cost of scrapped product. Please note that the production level only affects the Cash Flow Analysis calculations. It has no impact on other project economic evaluation variables.

Through the **Miscellaneous** tab of the above dialog, the user can provide information for estimation of income tax, advertising and selling expenses, and running royalties.

For detailed definitions of economic evaluation parameters and information on calculation methods, please consult Chapter 8.

2.1.11 Performing Economic Calculations and Viewing the Results

After simulating the process, you can carry out the economic calculations by selecting **Tasks: Perform Economic Calculations**. The same can be accomplished by clicking on the “Perform Economic Calculations” button that looks like a bag of coins and is located to the right of the calculator button. Depending on your interest, you may then do the following:

1. View the equipment purchase cost for each process step by right-clicking the corresponding procedure icon and selecting the **Purchase Cost** tab of the **Equipment Data** dialog. Remember that the displayed purchase cost is for a single piece of equipment. If the requirements to carry out the specific processing task are such that more than one equipment item (of the same size) is needed, the total cost is the indicated cost times the number of equipment items. The number of equipment items is displayed on the first tab of the Equipment Data dialog.
2. Select **View: Executive Summary** to view the essential economic evaluation results for the whole process. Please view the Executive Summary of your example process now. It should look similar to Figure 2.1-qq below:
3. To view the detailed results which were used to produce the Executive Summary, you will need to generate the **Economic Evaluation Report** (EER). To generate and view this report, select **Reports: Economic Evaluation (EER)**. Any report can be created in different file formats. You can set the format and many other settings from the dialog that comes up if you select **Reports: Option**. For more information on the reports see Chapter 11. The EER contains tables which give an overview of the process costs, a listing of the cost of each piece of equipment, a breakdown of the fixed capital estimate, summaries of labor, raw material, consumable, waste treatment, and utility costs, a summary of the annual operating cost, and profitability analysis. Please generate and view the Economic Evaluation Report now.

4. Another useful economic report is the **Itemized Cost Report** (ICR). This report breaks down the costs per flowsheet section. For more information on the contents of the economic reports, please read through the examples in Chapter 2.2, 2.3, and 2.4 or consult Chapters 8 and 11.

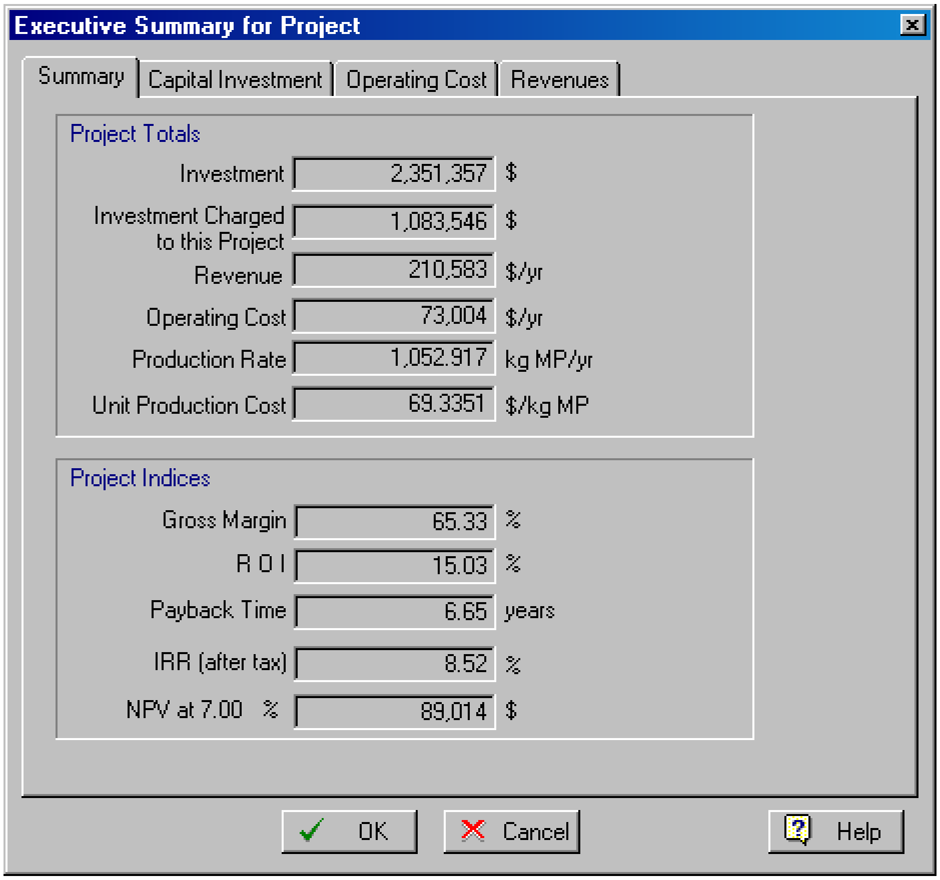


Figure 2.1-qq: The executive summary for the example flowsheet.

2.1.12 Convergence of Recycle Loops

The material of this paragraph is only relevant to flowsheets that include recycle loops. Pro-Designer default convergence parameters for flowsheets that include loops (which result in iterative calculations) have been tuned in order to be adequate for most situations. However, occasionally (especially in cases involving highly non-linear models) they may fail to converge. In these cases, you may fine-tune the convergence characteristics for a particular application. To change the convergence parameters, select **Edit: Flowsheet Options: Recycle Loop Options** (or right-click on a blank area of the flowsheet and select **Recycle Loop Options**). This will bring up the dialog of Figure 2.1-rr. Below is a list of actions that you can take to improve the system's performance in converging iterative calculations:

1. Adjust the convergence tolerance (relative tolerance). The convergence tolerance is defined as: (New Value - Old Value) / Old Value. Setting the relative tolerance to a larger value may speed up the convergence (but may lead to less accurate simulation results).

2. Switch from convergence based on the total flow to convergence based on individual component flows. This may slow down the convergence process but it will yield more accurate simulation results. This is especially important for design cases that deal with components that are in trace amounts, but whose accurate balance is of utmost importance (e.g., hazardous and/or toxic chemicals).

3. Increase the maximum number of iterations.

4. Request that tear streams be initialized to zero flow (for all components) before every new simulation. Normally, in cases where the flowsheet has been converged once, the initially guessed state for tear streams is their current state at the end of the previous (converged) simulation. In most cases, this leads to a faster convergence the next time the mass and energy balances are solved. However, after a convergence failure, it may be better to start with zero values.

5. Adjust the Wegstein algorithm parameters (q_{min}, q_{max}, and q). If the convergence procedure seems to be unstable, raising the value of q_{min} (i.e., making it less negative) may improve convergence; if it is converging very slowly but monotonically, you might lower q_{min}; and if it is converging in an oscillatory manner, try raising q_{max}. You also have the option of adjusting the value of q. If q is between zero and 1, the procedure is a modified successive substitution; if q is negative then the convergence is accelerated.

6. Switch from Wegstein acceleration to successive substitution. This may slow down the convergence calculations but will increase the likelihood of convergence.

7. Select a different tear stream for a recycle loop by right clicking on a specific stream (that is part of the loop) and selecting “Preferred Tear”. The current tear streams are identified on the flowsheet (with two red slashes) if you check the “Show Tear Streams” box.

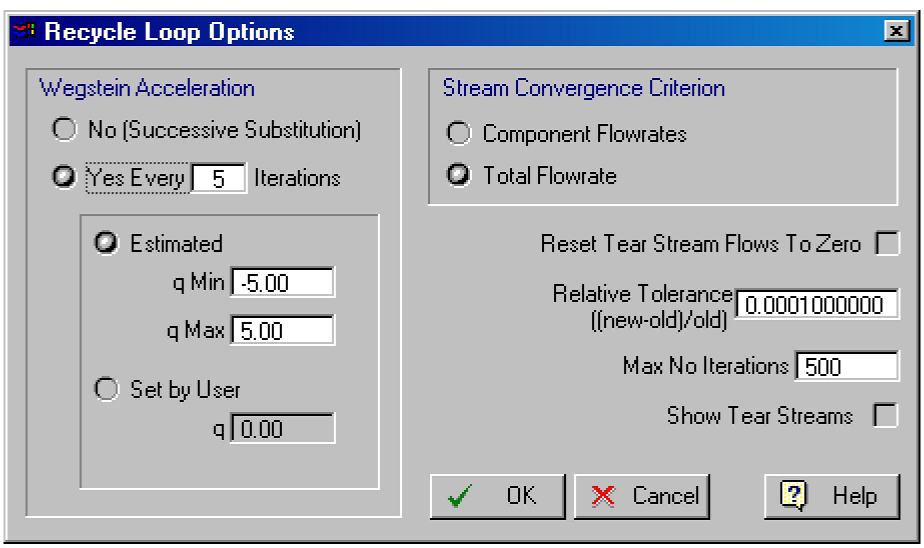


Figure 2.1-rr: Adjusting the convergence parameters for design cases with recycle loops.

2.2 The Synthetic Pharmaceutical Design Case

This example analyzes the production of a synthetic pharmaceutical intermediate, which is formed by condensation of quinaldine and hydroquinone. This example is recommended for users in the pharmaceutical, agrochemical, and specialty chemical industries.

2.2.1 Process Description

Several reaction and separation steps are required to synthesize and purify this product. The generation of the flowsheet was based on information available in the patent and technical literature. The seven Pro-Designer files that are included in this example can be found in the **Examples \ Synpharm** subdirectory:

File SPhr6_0L: This process is based on lab-scale data which has been scaled up to pilot plant production volumes. At this point all equipment is in Design Mode. In other words, the equipment sizes have not yet been fixed.

File SPhr6_0a: This process was designed based on pilot plant volumes of reagents in manufacturing scale equipment. It is the same as SPhr6_0L except that the calculation mode for all process steps has been switched to Rating Mode. In addition, the reactors and filter are used for multiple unit procedures. Two 1000 gal reactors, one 4 m^2 filter and one 10 m^2 tray dryer are utilized.

File SPhr6_0b: This process is the same as SPhr6_0a, but the throughput has been scaled to 100% capacity utilization of the limiting-size reactor (R-102).

File SPhr6_0c: This process is the same as SPhr6_0b, except that THREE reactors are used in order to decrease the plant's effective batch time (so that more cycles can be run per year).

File SPhr6_0d: This process is the same as SPhr6_0c except that a second filter (NFD-102) has been added.

File SPhr6_0e: This is the same as SPhr6_0d except that procedure P-11 in R-103 (and subsequent procedures) have been split into two cycles, and the batch throughput has been increased to 100% in the new capacity-limiting piece of equipment (R-102).

File SPhr6_0f: This is the same as SPhr6_0e except that the utilization of several reactors has been rearranged. Specifically, the reactors for procedures P-5 and P-7 have been switched. This allows more cycles to be run per year because the batch cycle time of reactor R-103 is decreased. The SPhr6_0f file is described in more detail below.

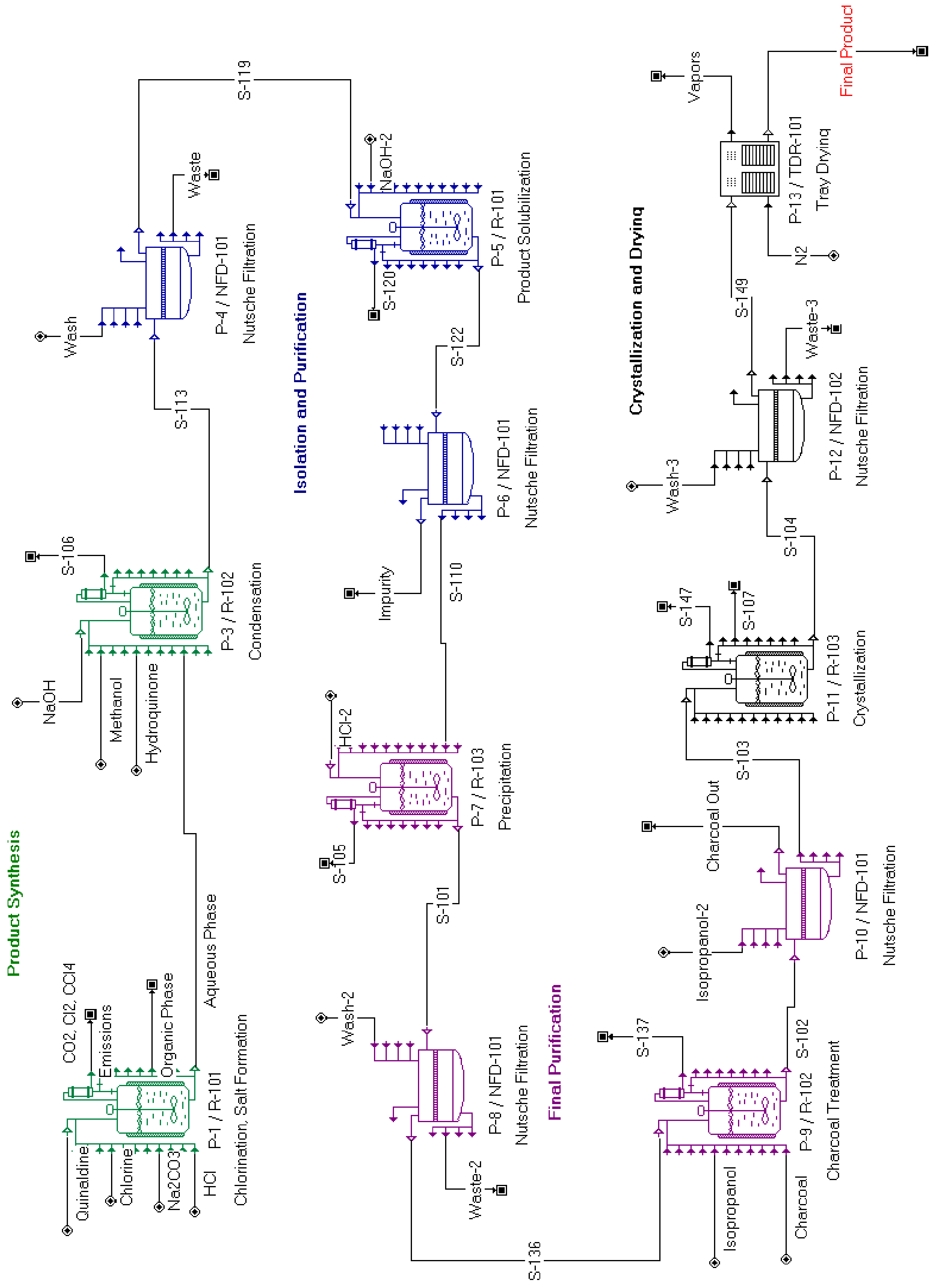
The description that follows corresponds to SPhr6_0f (see Figure 2.2-a). Please open this file now. The objective is to produce at least 33,000 kg of this intermediate per year in a plant that has the following equipment items:

1) three stirred-tank reactors each having a total volume of 1000 gallons,

2) two nutsche filters each with an area of 4 m^2, and

3) a tray dryer with a total tray area of 10 m^2.

Figure 2.2-a: Synthesis of a Pharmaceutical Intermediate Compound



Chlorination Reaction and Salt Formation Steps (P-1/R-101)

The first reaction step involves the chlorination of quinaldine. Quinaldine is dissolved in carbon tetrachloride (CCl_4) and reacts with gaseous Cl_2. The yield of the reaction is around 98%. The generated HCl is neutralized using Na_2CO_3. The stoichiometry and yield of the three reactions follows:

```
Quinaldine + Cl2  ===>  Chloroquinaldine + HCl    Yield = 98 %

Na2CO3    +  HCl  ===>  NaHCO3  +  NaCl           Yield = 100 %

NaHCO3   +  HCl   ===>  NaCl  + H2O + CO2         Yield = 100 %
```

Small amounts of unreacted Cl_2, generated CO_2, and volatilized CCl_4 are vented. The above three reactions occur sequentially in the first reactor vessel (R-101).

The second reaction step involves the formation of Chloroquinaldine.HCl. The added HCl first neutralizes the remaining $NaHCO_3$ and then reacts with chloroquinaldine to form its salt. The stoichiometry and yield of the two reactions follows:

```
NaHCO3   +   HCl         ===>  NaCl  + H2O  + CO2         Yield = 100 %
Chloroquinaldine  + HCl  ===>  Chloroquinaldine.HCl      Yield = 100 %
```

Small amounts of generated CO_2 and volatilized CCl_4 are vented. The presence of water (added with HCl as hydrochloric acid solution) and CCl_4 leads to the formation of two liquid phases. The small amounts of unreacted quinaldine and chloroquinaldine remain in the organic phase while the salts Chloroquinaldine.HCl and NaCl move to the aqueous phase. After the reactor contents have been allowed to settle, the aqueous phase is transferred to R-102 for further processing. The organic phase is then discharged as waste. Approximately 15.8 hours are required for the chlorination and salt formation reactions above, along with all associated charges and transfers. (Note – the times given for other procedures below also include associated material transfers, etc.)

Condensation Reaction Step (P-3/R-102)

The third reaction step involves the condensation of chloroquinaldine and hydroquinone. First, the salt chloroquinaldine.HCl is converted back to chloroquinaldine using NaOH. Then, hydroquinone reacts with NaOH and yields hydroquinone.Na. Finally, chloroquinaldine and hydroquinone.Na react and yield the desired intermediate product. Along with product formation, a small amount of chloroquinaldine dimerizes and forms an undesirable by-product (Impurity) that needs to be removed from the product. The stoichiometry and yield of the four reactions follows:

```
Chloroquinaldine.HCl + NaOH  ===> NaCl + H2O  + Chloroquinaldine  Yield = 100 %

2Chloroquinaldine  +  2NaOH  ===> 2H2O + 2NaCl + Impurity         Yield =   2 %

Hydroquinone  +  NaOH        ===>  H2O + Hydroquinone .Na         Yield = 100 %
Chloroquinaldine + Hydroquinone.Na  ===>  Product  +  NaCl        Yield = 100 %
```

This step takes a total of 16.3 hours to complete.

Filtration Step #1 (P-4/NFD-101)

Both the product and impurity molecules formed during the condensation reaction precipitate out of solution and are recovered using a nutsche filter. The product recovery yield is 90%. The total filtration and cake discharge time is 5.4 hours assuming an average filtrate flux of 200 L/m^2-h.

Solubilization Reaction Step (P-5/R-101)

The Product/Impurity cake recovered by filtration is added into a NaOH solution. The Product molecules react with NaOH forming Product.Na which is soluble in water. The Impurity molecules remain in solid phase. The stoichiometry and yield of the solubilization reaction follows:

Product + NaOH ===> H_2O + Product.Na   Yield = 100 %

This step takes a total of 10.9 hours.

Filtration Step #2 (P-6/NFD-101)

Next the Impurity is removed using another filtration step (NFD-101). The total filtration and cake discharge time is 3.5 hours assuming an average filtrate flux of 200 L/m^2-h.

Precipitation Reaction Step (P-7/R-103)

The excess NaOH is neutralized using HCl and then Product.Na is converted back to Product. The stoichiometry and yield of the two reactions follows:

HCl + NaOH ===> H_2O + NaCl   Yield = 100 %

HCl + Product .Na ===> NaCl + Product   Yield = 100 %

The Product, which is insoluble in water, precipitates out of solution. This step takes around 8.1 hours.

Filtration Step #3 (P-8/NFD-101)

Next the Product is recovered using another filtration step. The Product cake is washed with water to remove impurities. The product recovery yield is 90%. The filtration and cake discharge time is 4.8 hours assuming an average filtrate flux of 200 L/m^2-h.

Charcoal Treatment (P-9/R-102)

The recovered Product cake is dissolved in isopropanol and treated with charcoal for discoloration. This step takes a total of 17.6 hours.

Filtration Step #4 (P-10/NFD-101)

After charcoal treatment, the solid carbon particles are removed using another filtration step. The filtration and cake discharge time is around 14.8 hours assuming an average filtrate flux of 200 L/m^2-h, and a hold time of 10.4 hours (to account for the extra time spent waiting for the second filtration cycle to get underway).

Crystallization Step (P-11/R-103)

In this step, the product solution is distilled to one third of its initial volume. Then it is crystallized with a yield of 97%. Crystallization is represented by the following reaction:

Product ===> Product-Cryst   Yield = 97 %

In other words, a new component (Product-Cryst) is used to represent the crystalline form of product. This step is performed in two 12.1 hour cycles.

Filtration Step #5 (P-12/NFD-102)

The crystalline product is recovered using another filtration step with a yield of 90%. The filtration and cake discharge takes place in two 12.1 hour cycles, assuming an average filtrate flux of 50 L/m^2-h, and an 8.5 hour hold time (the hold time is necessary to synchronize these cycles with the P-11 crystallization step cycles).

Drying Step (P-13/TDR-101)

The recovered product crystals are dried in a tray dryer. The drying is done in two 12.1 hour cycles, which includes a 3.02 hour hold time (to synchronize these cycles with P-11 and P-12). Approximately 246 kg of dried product is produced per batch.

2.2.2 Flowsheet Sections

A flowsheet section is a group of processing steps that have something in common. The flowsheet of this example was divided into four sections: 1) Product Synthesis, 2) Isolation and Purification, 3) Final Purification, and 4) Crystallization and Drying. All unit procedure icons of the Product Synthesis section are displayed in green. The icons in the Isolation and Purification, Final Purification, and Crystallization and Drying sections are displayed in blue, purple, and black, respectively.

Many economic factors in SuperPro are section-dependent and that is one reason to break-up your flowsheeet into more than one sections. Another reason is that you can allocate sections to different physical sites declared in the databank and thus make use of equipment and resources of specific sites. To use this feature you will first need to declare the sites in the databank through the **Databanks/Sites and Resources…** menu option from the main menu. There you are able to define new sites in a parent-child hierarchy (i.e. sites with their sub-sites or facilities) and declare their equipment, utility and labor resources as well as site-related economic data (see Chapter 5 and Chapter 16 for details.)

To allocate a section to a databank site, first select the section through the drop-down menu of the section toolbar and then click on the "Edit Section" button (), select the 'Allocated' option in the dialog that comes up and select the desired site from the drop-down tree of available sites. Once you allocate a section to a site, you can allocate equipment of this section to site equipment and also make use within each operation of site utilities and labor. Following the instructions in Chapters 5 & 16, the Help Facility, or the User's guide, you might want to go through the exercise of declaring new site in the User databank and allocating one or more sections of this example.

In the same dialog that comes up when you press the "Edit Section" button you can also define and see the main starting material and product of the section along with the calculated yields. If you go to the Yields tab, you can see the molar yields of the Product Synthesis, Isolation and Purification, Final Purification, and Crystallization and Drying sections are 93.9%, 89.9%, 90.0%, and 87.3%, respectively.

Note:
For more info on how to allocate sections and equipment to database entities, please consult the "SynPharmDB" read-me file in the "Examples \ SynPharm" directory of SuperPro.

2.2.3 Equipment Sharing

In a batch plant, it is common to utilize the same piece of equipment for carrying out multiple processing steps. For instance, in this example process, vessel R-101 handles steps P-1 and P-5. By default, whenever a unit procedure is introduced in the flowsheet, the system assumes that the procedure is carried out in its own piece of equipment. However, you also have the option of selecting one of the existing equipment items that are compatible with this procedure through the Equipment Data dialog (right-click on a unit procedure icon and choose the **Equipment Data**… option).

Figure 2.2-b displays the equipment data dialog of procedure P-5. Instead of using a unique vessel for this procedure, the user decided to reuse R-101, which also handles procedure P-1. Starting with version 4.0, equipment sharing is available in Design as well as in Rating mode. Equipment sharing is also implied when two or more procedures use equipment allocated to the same databank site equipment. The site equipment databank, therefore, provides you the means to declare that the same equipment is used for multiple tasks not only in the same recipe but across recipes as well.

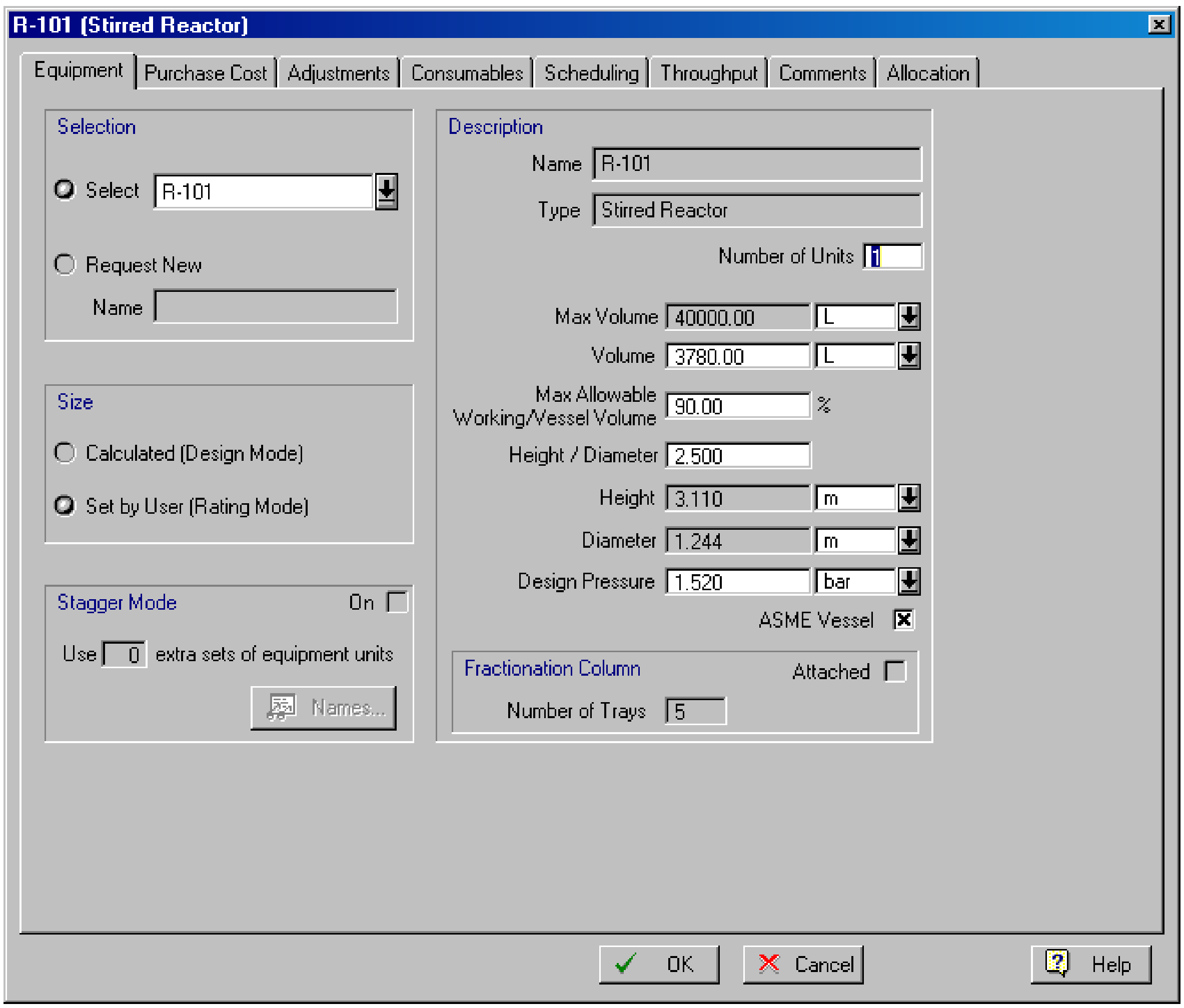


Figure 2.2-b: Equipment Data Dialog of a Stirred-Tank Reactor.

When multiple procedures share a piece of equipment that is in Design mode (unspecified size), each procedure recommends its own sizing and Pro-Designer selects the maximum. If the calculated equipment size exceeds the maximum possible value, then Pro-Designer assumes multiple (identical) equipment items with a total size equal to the calculated total capacity requirement and an individual size that is smaller than or equal to the maximum. For example, if the maximum size of an individual filter in Design mode is 5 m^2, and your process requires 12 m^2 of filter area to achieve the necessary throughput, three 4 m^2 filters will be used by Pro-Designer. In Rating mode, the user specifies the equipment size as well as the number of equipment items employed by a unit procedure. In other words, in Pro-Designer a single unit procedure icon may correspond to multiple equipment items that operate in parallel, or multiple unit procedure icons may correspond to a single piece of equipment (if the flowsheet is in Batch mode and those procedures share equipment).

When the equipment is allocated, its mode is set by default to Rating (with the Design Mode option deactivated), all its data are set according to the corresponding site equipment and become non-editable. This signifies the fact that the equipment shown in the recipe is actually the one declared in the site databank and has therefore fixed specifications that cannot be changed unless you visit the site databank and change them from there.

Equipment sharing reduces the number of equipment items required for a batch process and consequently saves money in terms of capital expenditures. However, it also introduces scheduling constraints that may reduce the number of batches that can be processed per year. Information on visualization of equipment sharing can be found in section 2.2.5. For detailed information on the impact of equipment sharing on plant throughput please see Chapter 10 or search for Debottlenecking in the Help Facility.

2.2.4 Initialization of Reaction Operations

Batch reactions constitute the most common operation in synthetic pharmaceutical processes. Pro-Designer is equipped with three different batch reaction operation models: stoichiometric, kinetic, and equilibrium. The stoichiometric is used if no kinetic and equilibrium data are available. If kinetic data are available, the kinetic model can be used to calculate composition, temperature, and utility profiles as a function of time. All reaction operations share the same “Oper.Cond’s” tab (see Figure 2.2-c) through which the user can specify the duration of the operation, the thermal mode, the power consumption, etc.

Similarly, all reaction operations share the same “Volumes” tab (see Figure 2.2-d). In Design Mode (equipment size unspecified), the Maximum Allowable Working / Vessel Volume (%) value is used for sizing the vessel. If multiple operations in the same unit procedure require different capacity values, the maximum capacity requirement of these operations is selected as the equipment size. In Rating mode (equipment size specified), the Maximum Allowable (%) acts as a constraint that generates a warning when it is violated. The Minimum Allowable (%) value also acts as a constraint. The same logic applies to other vessel operations.

Starting with version 5.5, all batch reactions also have fed-batch capability for supply of additional reactants during the reaction operation. This is common practice in cases of highly exothermic reactions. Slow addition of one of the reactants controls the reaction rate and the need for cooling. Feb-batch operation is also common in bio-processing to maintain a certain level of media concentration during fermentation. For an example of a fed-batch reaction model, please consult the FedBR.spf example in “Examples \ Misc”.

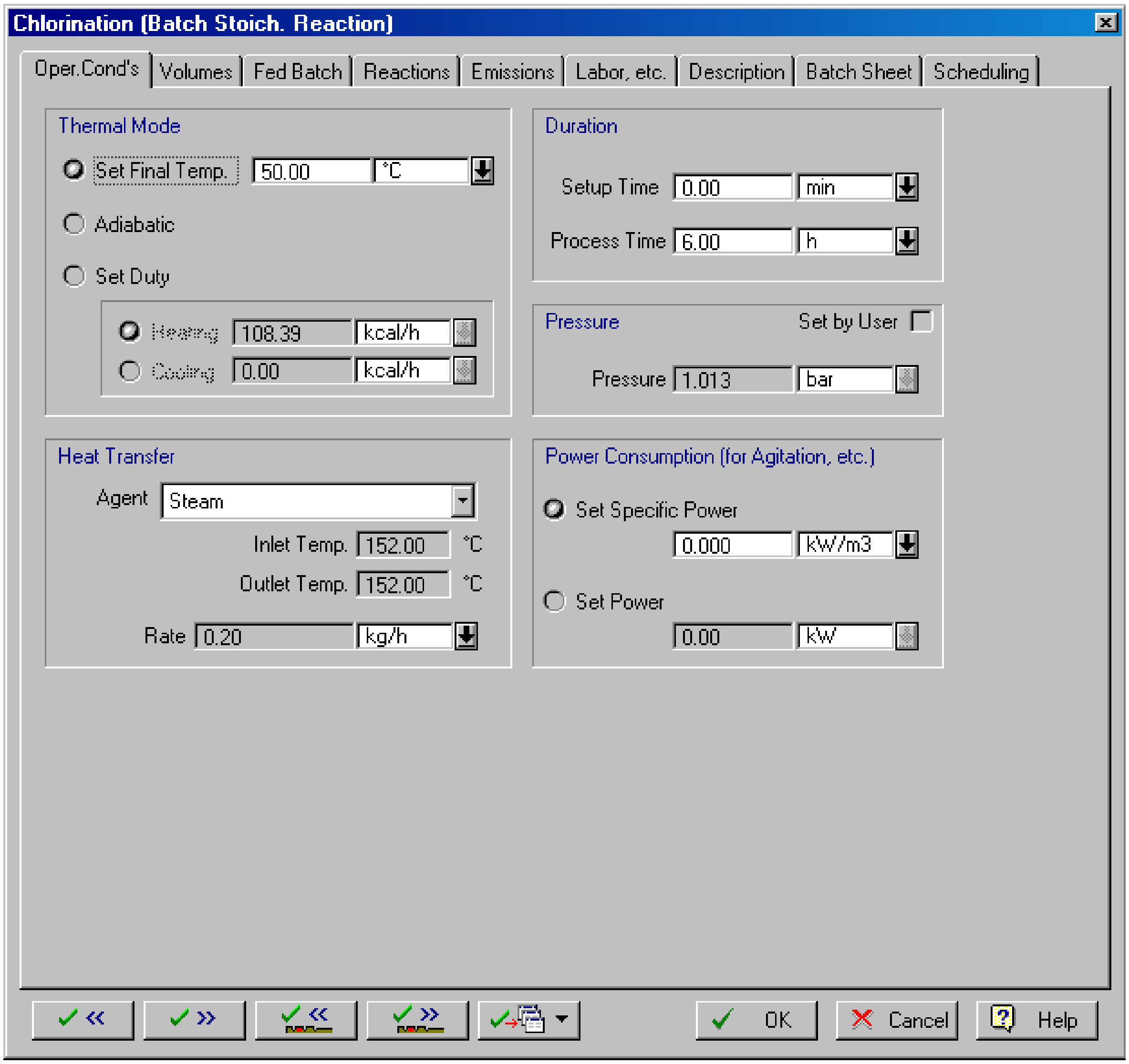


Figure 2.2-c: Oper. Cond’s tab of a reaction operation.

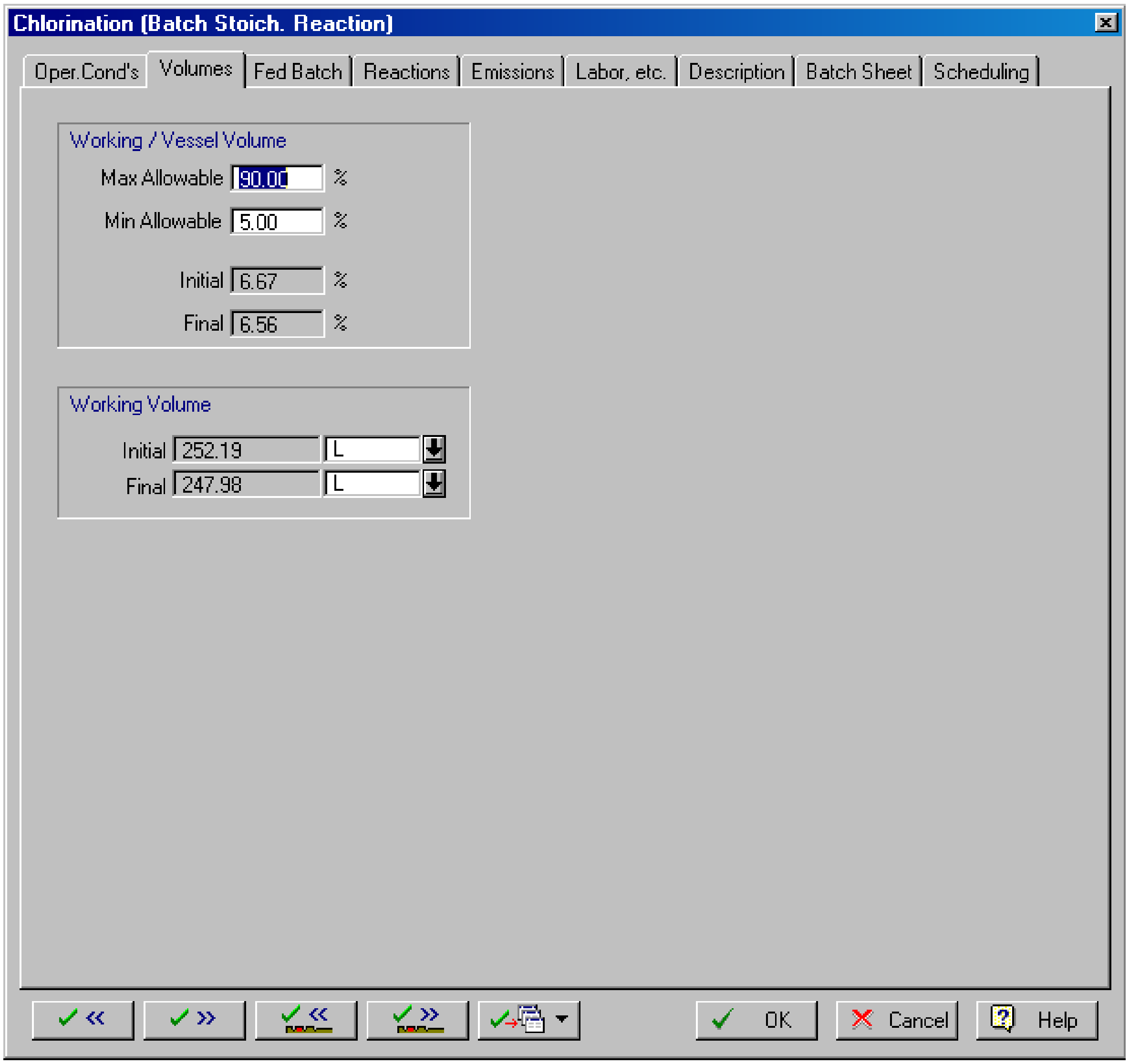


Figure 2.2-d: Volumes tab of a reaction operation.

Figure 2.2-e displays the “Reactions” tab of a stoichiometric reaction operation. Through this tab the user specifies the stoichiometry and other data associated with the various reactions in this operation. Please note that a reaction operation can handle any number of reactions. The stoichiometry of a reaction is specified by selecting a reaction and clicking on the “Edit Stoichiometry” button (the button that looks like a shake flask and is located at the top of the Reaction Sequence box).

The “Extent” of a stoichiometric reaction represents the fractional conversion of its limiting component. By default, the limiting component is identified by the model based on the stoichiometric coefficients and the feed composition. The user has the option to specify a reference component for the extent of reaction. In that case, if the specified value of the extent of reaction is not feasible, the model adjusts its value to the maximum possible. The user also has the option to specify the desired final concentration of a reactant or product and have the model estimate the extent of reaction. Again, in this case if the specified concentration is not feasible, the model adjusts its value to the maximum (or minimum) possible.

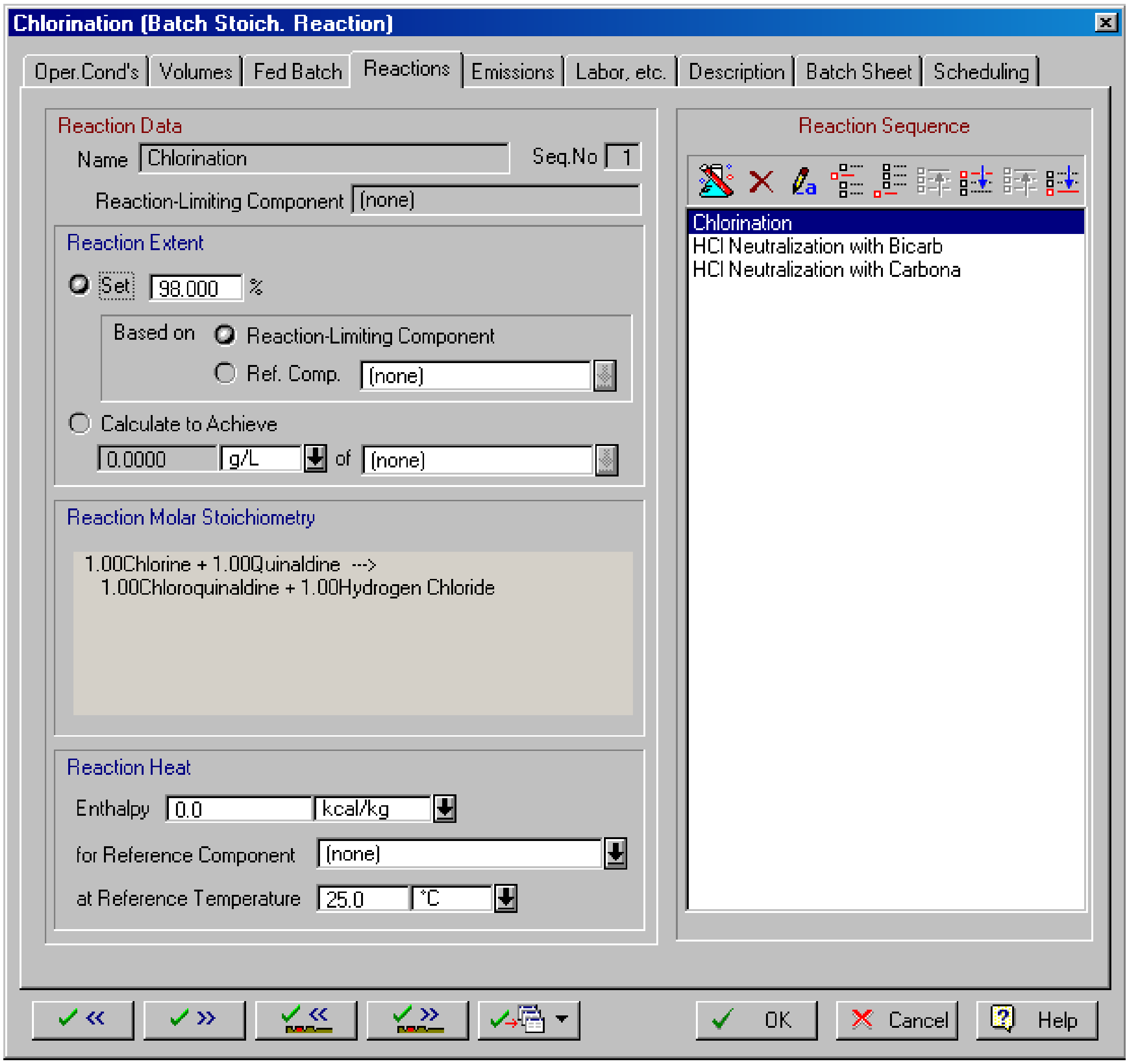


Figure 2.2-e: Reactions tab of a stoichiometric reaction operation.

The "Reactions" tab of kinetic and equilibrium batch reactions is quite similar to that of Figure 2.2-e. The main difference is that instead of the extent of reaction variables, it has a button through which the user can bring up the kinetic data dialog of a reaction. Through this dialog the user specifies the kinetics of a reaction. Furthermore, clicking on the "Start/End Criteria" buttons brings up other dialogs through which the user can specify when or under what conditions a reaction is initiated or terminated. For more info on kinetic reactions, please consults the following examples in the "Examples \ Misc" directory: BKinRxn, BKinFerm, and FedBR.

Important Note about Stoichiometric Reactions

Several different methods can be used to specify multiple reactions within a single Reaction Operation. For instance, each reaction could be written individually (as was done for the Chlorination and HCL Neutralization listed in the Reaction Sequence box of the above dialog.) In this case, mass balances for each reaction are performed sequentially. In other words, first the Chlorination Reaction proceeds to its specified Extent of Reaction. Then the first Neutralization proceeds to its specified Extent of Reaction. Finally, the second Neutralization occurs. In other situations, you may wish to specify reactions that occur simultaneously. This can be done in several ways. In the first method, you can specify all stoichiometric coefficients in one reaction. Consider the following example: 90% of your Starting Material reacts with your Reagent to produce the Desired Product, while the other 10% dimerizes to form a Byproduct (made of two reagent molecules):

1) Starting Material + Reagent → Desired Product (90% yield)
2) Starting Material + Starting Material → Byproduct

These two scenarios would happen simultaneously, and the extent of reaction for this system would be 100% (100% of the Starting Material would react). In this situation, the relative stoichiometric coefficients (on a molar basis) of Starting Material, Reagent, Desired Product, and Byproduct would be: 1, 0.9, 0.9, and 0.05, respectively. In other words, for every 1 mole of Starting Material used, 0.9 moles of Reagent are used, 0.9 moles of Desired Product is produced, and 0.05 moles of Byproduct is produced.

Sometimes it is clearer to specify stoichiometric coefficients on a mass basis (as opposed to molar.) In the above example, let's assume that the molecular weights of Starting Material, Reagent, Desired Product, and Byproduct are: 200, 50, 250, and 400 g/mole, respectively. Assuming a 200 kg basis for the amount of Starting Material and a 50 kg basis for the amount of Reagent, the mass of Reagent consumed would be 45 kg (50*0.9), and the masses of Desired Product and Byproduct generated would be 225 kg (250*0.9) and 20 kg (400*0.05). Notice that the mass balance here is complete: initially there is 200 kg of Starting Material and 50 kg of Reagent (250 kg total). After the reactions are complete, there are 225 kg of Desired Product, 20 kg of Byproduct, and 5 kg of unreacted Reagent (250 kg total).

Another method that could have been used to model these simultaneous reactions is the following: Create two distinct reactions within your Reaction Operation (similar to the three distinct reactions shown in Figure 2.2-e). Then specify the following:

1) Starting Material + Reagent → Desired Product (90% extent of reaction)
2) Starting Material + Starting Material → Byproduct (100% extent of reaction)

When modeled as <u>separate</u> reactions, the computer will first calculate the results for Reaction 1 above. In other words, it will determine that 180 kg (200*0.9) of Starting Material and 45 kg (50*0.9) of Reagent have been consumed, and 225 kg (250*0.9) of Desired Product has been generated. Next, the computer will simulate the second reaction, in which <u>all</u> of the <u>remaining</u> 20 kg of Starting Material is transformed into 20 kg of Byproduct.

2.2.5 Process Analysis

At this point you may return to the synthetic pharmaceutical example.

Do not hesitate to change the values of certain parameters and redo the calculations (by selecting **Tasks/Solve M&E Balances**). The calculated flowrates and compositions of intermediate and output streams can be viewed by revisiting the input/output dialog windows of each stream (double click on a stream line or click with the right mouse button and select **Simulation Data…).** In addition, a report containing information on raw material requirements, stream compositions and flowrates, as well as an overall material balance, can be generated and displayed by selecting the **Reports: Stream and Mat. Balance (SR)...** option from the main menu. To select the file format of the report select the **Reports: Options** from the main menu. For more information on the reports see Chapter 11. Tables 2.2a,b, and c display portions of the stream report. These tables were extracted from the .rtf version of the Stream Report.

The detailed equipment contents during a processing step can be viewed by right clicking on the appropriate unit procedure and selecting **Equipment Contents**. Right clicking and selecting **Operation Sequence** displays related information.

Table 2.2a: OVERALL PROCESS DATA

Annual Operating Time	7,890.54	h
Annual Throughput	35,185.06	kg MP
Batch Throughput	246.05	kg MP
Recipe Batch Time	100.77	h
Recipe Cycle Time	54.86	h
Number of Batches per Year	143.00	
MP = Main Product = Total Flow in Final Product		

Table 2.2b: STARTING MATERIAL REQUIREMENTS

Section	Starting Material	Active Product	Amount Needed (kg Sin/kg MP)	Molar Yield (%)	Mass Yield (%)	Gross Mass Yield (%)
Product Synthesis	Quinaldine	Product	0.86	93.94	164.87	164.87
Isolation and	Product	Product.Na	1.41	89.90	97.74	97.74
Final Purification	Product.Na	Product	1.38	90.00	82.78	82.78
Crystallization and Drying	Product	Product_crys	1.14	87.30	87.30	87.30
Sin = Section Starting Material, Aout = Section Active Product						

Table 2.2c: BULK RAW MATERIAL REQUIREMENTS – ENTIRE PROCESS

Raw Material	kg/yr	kg/batch	kg/kg MP
Chlorine	18,184	127.167	0.517
Na2CO3	21,342	149.245	0.607
Water	602,443	4,212.888	17.122
HCl (20% w/w)	72,613	507.786	2.064
NaOH (50% w/w)	41,547	290.542	1.181
Methanol	112,393	785.965	3.194
Hydroquinone	34,829	243.561	0.990
Carb. TetraCh	101,027	706.485	2.871
Quinaldine	30,194	211.151	0.858
Sodium Hydroxid	15,065	105.355	0.428
Isopropanol	403,267	2,820.055	11.461
charcoal	3,220	22.519	0.092
HCl (37% w/w)	44,199	309.087	1.256
Nitrogen	225,592	1,577.568	6.412
TOTAL	1,725,920	12,069.376	49.053

Scheduling, Equipment Utilization, and Resource Demand Graphs

Pro-Designer generates **Operations** and **Equipment Gantt charts** for single and multiple batches. Figure 2.2-g displays a portion of the operations Gantt chart for a single batch of this example process.

The left view (spreadsheet view) displays the name, duration, start time, and end time for each activity (e.g. each operation, unit procedure, cycle, batch, etc). You can use the left view to expand or collapse the activity summaries by clicking on the + or – signs in the boxes to the left of the activity names.

The right view (chart view) displays a bar for each activity in the overall process recipe. To edit the scheduling data (or any other data affecting an activity), simply right-click on a bar and a relevant command menu will appear. Selecting the uppermost entry on this menu will bring up a dialog that will allow you to edit the information associated with that particular activity bar. In fact, anything you can accomplish with the other scheduling interfaces, you can also accomplish from the Gantt chart interface. Furthermore, you can redo the M&E balances and have the Gantt chart updated to reflect the new (calculated) scheduling settings for the recipe by clicking on the Update Chart entry in the main menu of the interface.

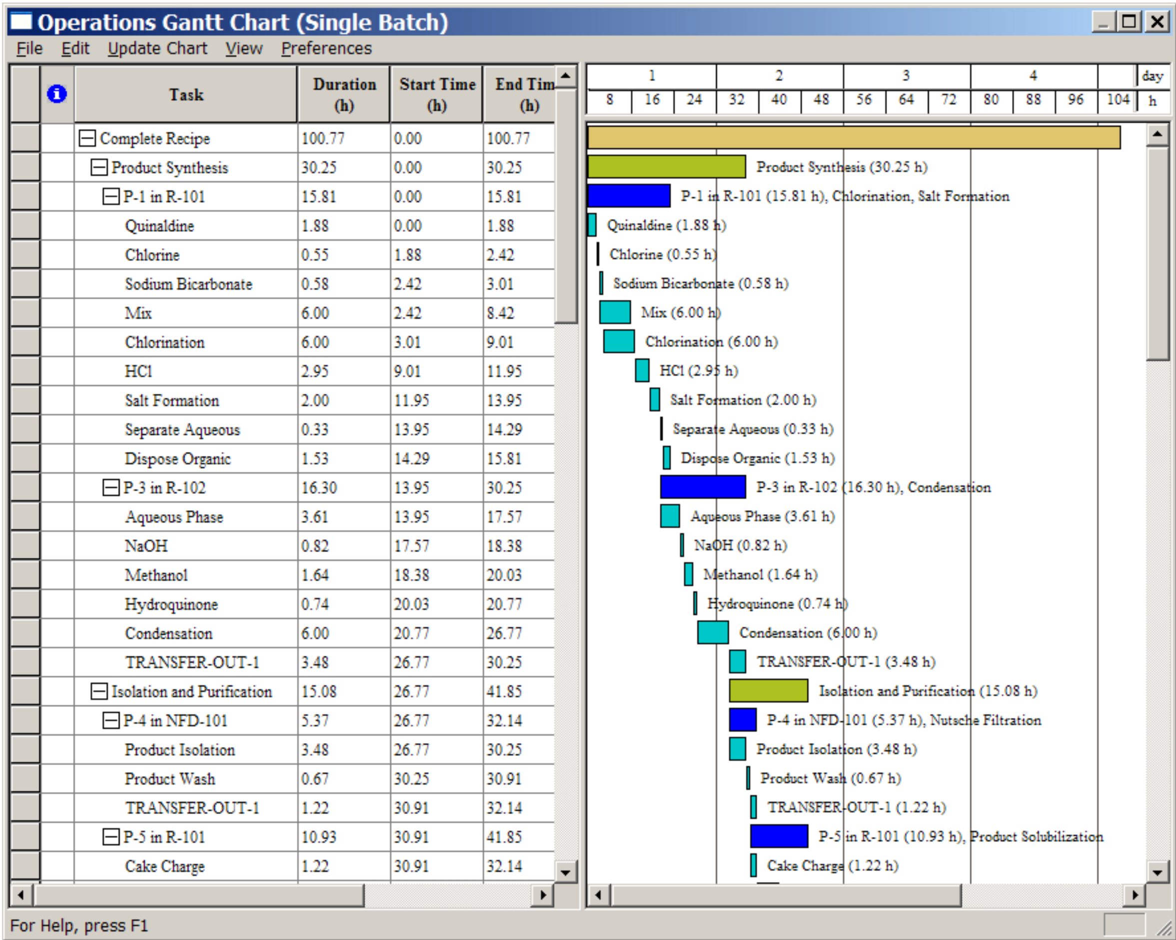


Figure 2.2-g: Operations Gantt Chart for a Single Batch.

Note: If your Gantt chart does not appear exactly as shown, you may want to change some of its display options. Select **Preferences: Styles: Gantt chart**. The resulting dialog will allow you to display or hide the branch and section bars and to configure the text displayed with the bars.

Another way of visualizing the execution of a batch process as a function of time is through the Equipment Occupancy chart (select **View : Equipment Occupancy Chart**). Figure 2.2-h displays the equipment occupancy chart for two consecutive batches of this example process. Multiple bars on the same line (e.g., for R-101, R-102, NFD-101, and R-103) represent reuse (sharing) of equipment by multiple procedures. White space represents idle time. The equipment with the least idle time between consecutive batches is the **time (or scheduling) bottleneck** (R-102 in this case) that determines the maximum number of batches per year. Its occupancy time (approximately 54 hours) is the minimum possible time between consecutive batches (also known as Min. Effective Cycle Time). The actual time between consecutive batches (also known as Recipe Cycle Time) is approximately 55 hours. The recipe batch time (the time required to complete a single batch) is roughly 101 hours.

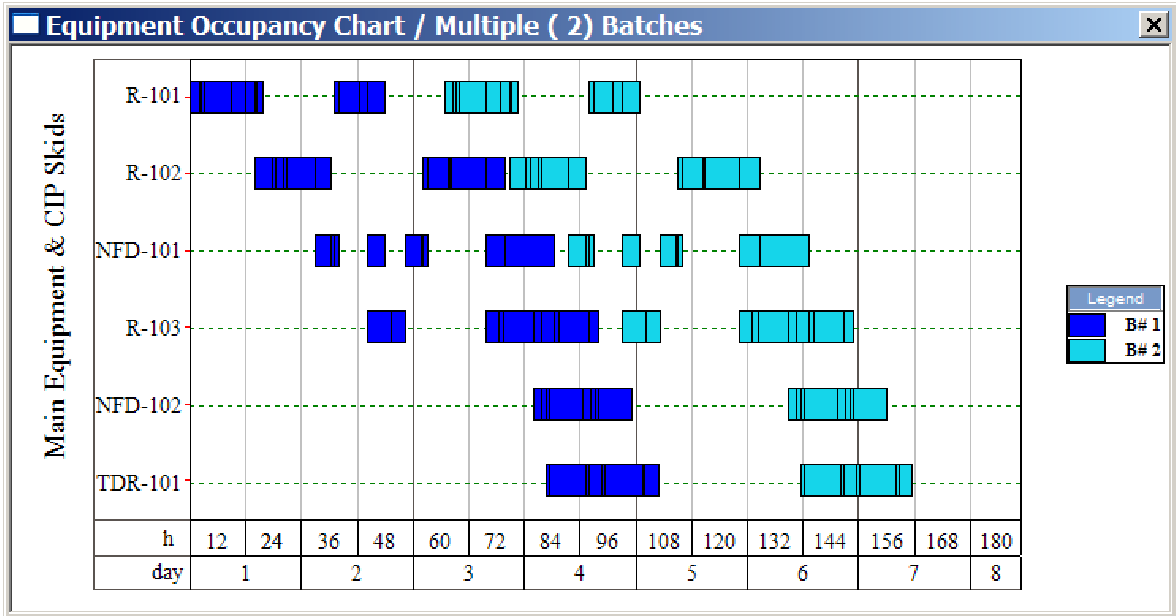


Figure 2.2-h: Equipment Occupancy Chart (two consecutive batches).

Pro-Designer also generates charts of resource demand as a function of time for raw materials, heating and cooling utilities, power, and labor. To view the total labor demand, select **View: Resource Consumption Tracking Chart** \ L**abor** \ **Multiple Batches** from the main menu and from the pop-up dialog select the desired labor type (**total labor**). Figure 2.2-i displays the total labor demand for eight consecutive batches. Note that for short periods of time there is a need for up to eight operators. If this exceeds the actual number of operators available, then certain operations will need to be delayed to accommodate the labor constraint. Inventory graphs for raw materials also can be generated in a similar way by using the **View: Inventory Chart** menu item.

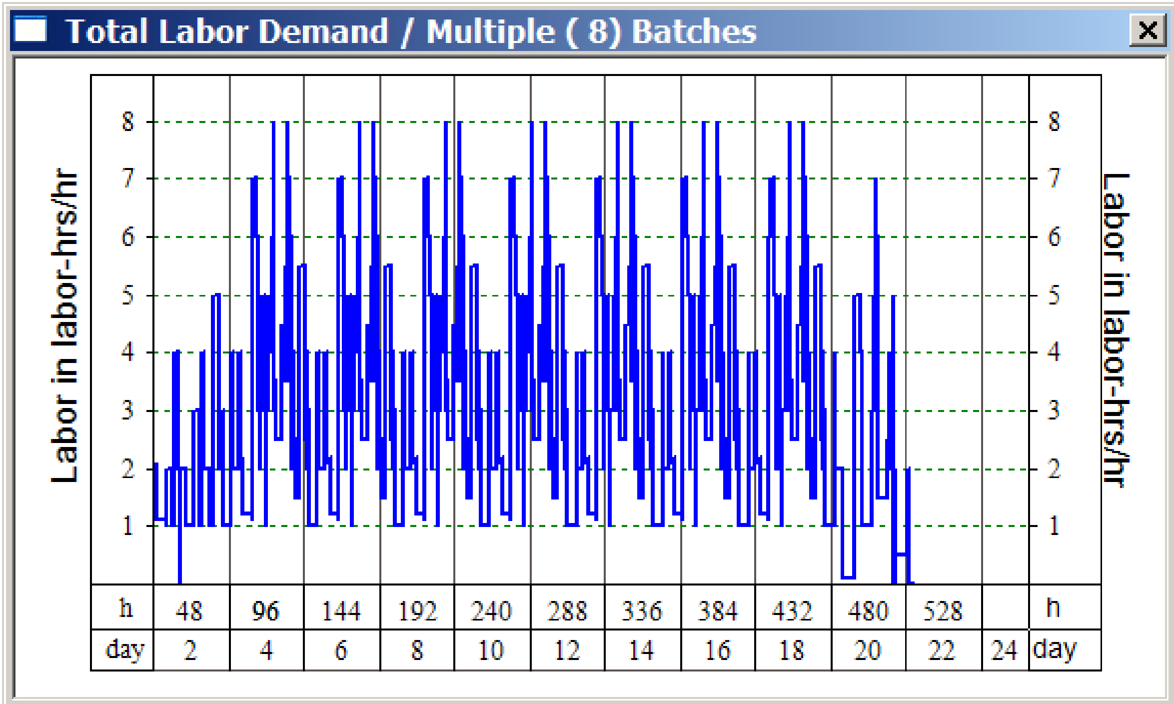


Figure 2.2-i: Labor Demand Chart (eight consecutive batches).

Throughput Analysis and Debottlenecking

Pro-Designer is equipped with powerful throughput analysis and debottlenecking capabilities. The objective of these features is to allow the user to quickly and easily analyze the capacity and time utilization of each piece of equipment, and to identify opportunities for increasing throughput with the minimum possible capital investment. For a detailed throughput analysis example (based on this process), please see Chapter 9 or search for Debottlenecking in the Help Facility.

To see the analysis results for this example, select **View: Throughput Analysis Charts: Utilization**. The utilization chart will appear showing the capacity, time, and combined utilizations for each procedure. If the equipment is shared, the time utilization is based on the entire time the equipment is used.

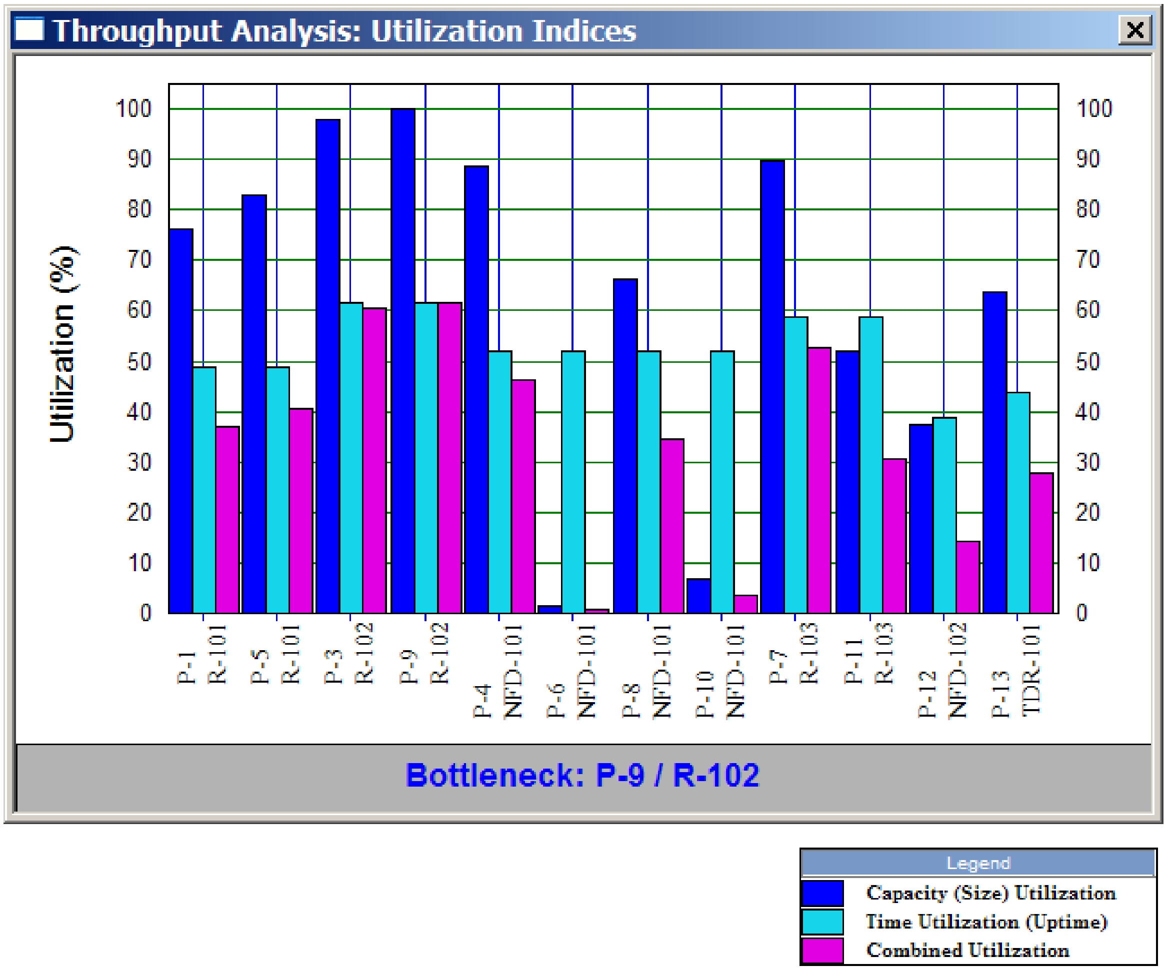


Figure 2.2-j Utilization Analysis Chart

Select **View: Throughput Analysis Charts: Potential** to view the throughput potential chart below. This chart shows the potential batch size increase for each unit procedure. The actual batch size is indicated by the red dashed line behind the bars.

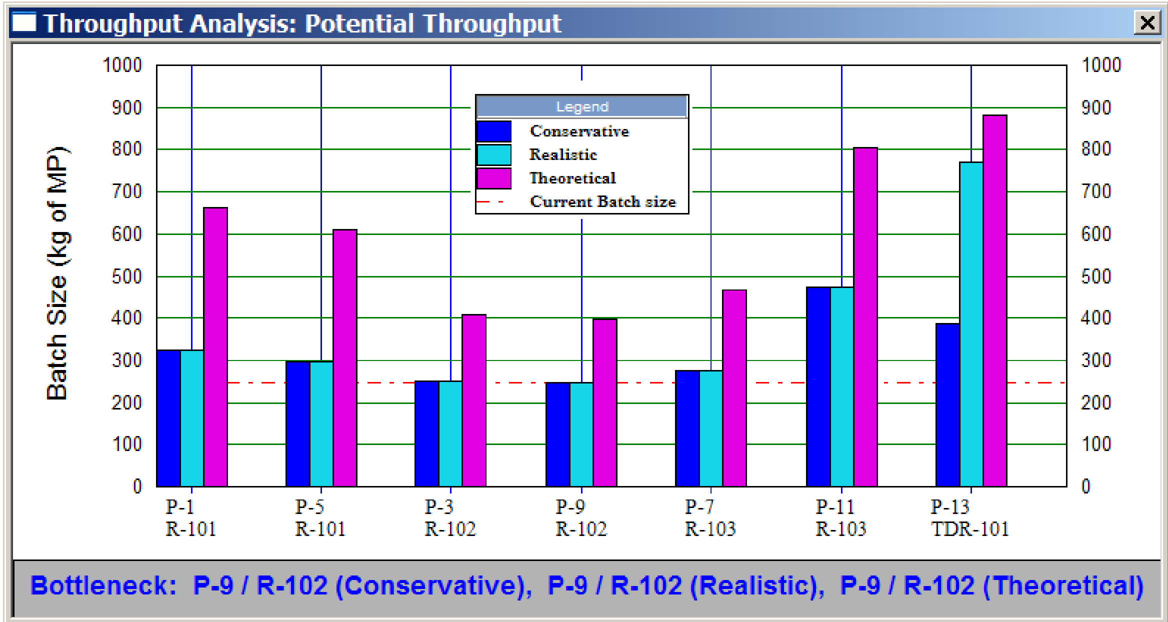


Figure 2.2-k Throughput Potential Chart

2.2.6 Cost Analysis and Economic Evaluation

Below are the key results of cost analysis for a plant producing 35,200 kg of this intermediate per year. The Table 2.2d gives an overview of the total economic impact of the plant, including the total capital investment, yearly revenues, and rate of return. This table was extracted from the RTF version of the Economic Evaluation Report (EER). The full EER can be generated by selecting **Reports** : **Economic Evaluation Report (EER)...** from the main menu.

Table 2.2d: Executive Summary

Total Capital Investment	19,643,000	$
Capital Investment Charged to This Project	19,643,000	$
Operating Cost	8,537,000	$/yr
Production Rate	35,185.06	kg of MP/yr
Unit Production Cost	242.64	$/kg of MP
Total Revenues	17,593,000	$/yr
Gross Margin	51.47	%
Return On Investment	36.50	%
Payback Time	2.74	years
IRR (After Taxes)	26.02	%
NPV (at 7.0% Interest)	26,301,000	$
MP = Total Flow of Stream Final Product		

Tables 2.2e and 2.2f provide breakdowns of the annual operating and raw materials costs. They were extracted from the RTF version of the Itemized Cost Report (ICR). The full

ICR can be generated and viewed by selecting **Reports: Itemized Cost Report (ICR)...** from the main menu. The ICR enables the user to readily identify the cost sensitive sections of a flowsheet – the economic hot-spots. For instance, a quick look at Table 2.2e reveals that in this example the largest cost is the Facility-Dependent expenses, which account for roughly 40% of the operating cost. Increased equipment sharing may reduce this cost but may also reduce the annual throughput. Another large item is cost is associated with raw materials (25.8%), which is mainly caused by quinaldine (that info is available in the full report). If a lower-priced quinaldine vendor could be found, the overall process cost would be reduced significantly. Labor and Waste Treatment/Disposal occupy the 3rd and 4th positions, respectively. Labor can be reduced through increased automation. The environmental cost can be reduced through solvent recovery, purification, and reuse.

Table 2.2e: Summary of Operating Costs

SUMMARY PER ITEM (Entire Process)				
Cost Item	**$/kg MP**	**$/batch**	**$/year**	**%**
Raw Materials	62.622	15,408	2,203,358	25.81
Facility	96.026	23,627	3,378,667	39.58
Labor	50.675	12,468	1,782,991	20.89
Consumables	0.000	0	0	0.00
Lab/QC/QA	7.601	1,870	267,448	3.13
Utilities	0.009	2	305	0.00
Waste Trtmt/Disp	25.703	6,324	904,375	10.59
Transportation	0.000	0	0	0.00
Miscellaneous	0.000	0	0	0.00
TOTAL	242.636	59,700	8,537,146	100.00

The above analyses show how the economic reports can be used not only for estimation of the total cost of a process, but also as a tool to optimize the process through "what-if" scenarios. Would it make economic sense to use two reactors instead of three? It depends on how much the throughput would decrease if two reactors were used, and how much the third reactor adds to the total cost. Would a radically modified purification scheme be better than the current scheme? It depends on what equipment, reagents, etc. would be required for the modified purification, and what the overall yield of the product would be. This type of what-if analysis is quickly and easily done using SuperPro Designer.

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2.2.7 Environmental Impact

Pro-Designer generates two different reports that provide information on the environmental impact of a process. The **Emissions Report** provides information on emissions of volatile organic compounds (VOC's) and other regulated compounds. The **Environmental Impact Report** provides information on the amount and type of waste generated by a manufacturing facility. It also provides information on the fate of a compound that enters an integrated manufacturing facility.

2.2.8 Product Formulation and Packaging

Pro-Designer contains a variety of formulation, packaging, and transportation unit procedures in order to capture the cost associated with such processes.

Product formulation and packaging processes often involve formation and use of discrete entities, such as tablets, bottles, boxes, etc. The flow of such entities is represented by discrete streams, which by default are displayed in blue. For more information on discrete streams and entities, please see Chapter 4 and/or consult the Help Facility.

To familiarize yourself with the formulation and packaging models and the concepts of discrete streams and entities, please open the **Bgal6_0c** design case and visit the simulation data and operation data dialog windows. As usual, you can open these dialogs by right-clicking on the various packaging unit procedure icons and their corresponding streams. Notice the different interface of discrete streams, which display the flow of discrete entities as well as the equivalent bulk flow (based on the bulk ingredients that compose the discrete entities.

Another good example for dosage formulation and discrete processing can be found in the “Examples \ PhTablet” directory. That example deals with a process that manufacturers pharmaceutical tablets.

2.3 The β-Galactosidase Design Case

This example analyzes the production of β–Galactosidase, an intracellular enzyme produced by *E.coli*. This example is recommended for users in the biotech and food industries. In addition, since this example is a batch process, it serves as a medium for discussing several scheduling issues.

At this point, we suggest that you open the β-Galactosidase design case file and examine it briefly. To open this file, simply select the **File: Open...** option from SuperPro Designer's main menu. Then find the file named BGal6_0b in the **Examples\BGal** folder, select it, and click **OK**.

We suggest that you keep the design case flowsheet window open as you read the remainder of Chapter 2.3. However, you should not edit the flowsheet file until after you have finished reading through this chapter.

2.3.1 Process Description

Figure 2.3a shows the entire flowsheet for the β-Galactosidase process (for a better quality printout of Figure 2.3a, please use the printing capabilities of SuperPro).

β-Galactosidase is mainly used in the utilization of cheese whey. More specifically, immobilized reactors with β-Gal have been developed to convert lactose found in cheese whey to glucose and galactose, yielding a sweetened product which can be used as an additive to ice cream, egg-nog, yogurt, and other dairy products. Another application of β-Gal is in the treatment of milk products. A significant number of people are lactose intolerant and cannot digest milk or milk products. Production of lactose-free milk products (using β-Gal reactors) allows those people to digest them.

The β-Galactosidase enzyme is normally produced by *E. coli* up to 1-2% of total cell protein under conditions of induction of the lac operon. Using genetic engineering, the level can go up to 20-25% of total protein. In this example, an easily attainable level of 10% is assumed. This example analyzes a plant that produces 11,500 kg of β-Gal per year in 134 batches. Several files have been included with this example:

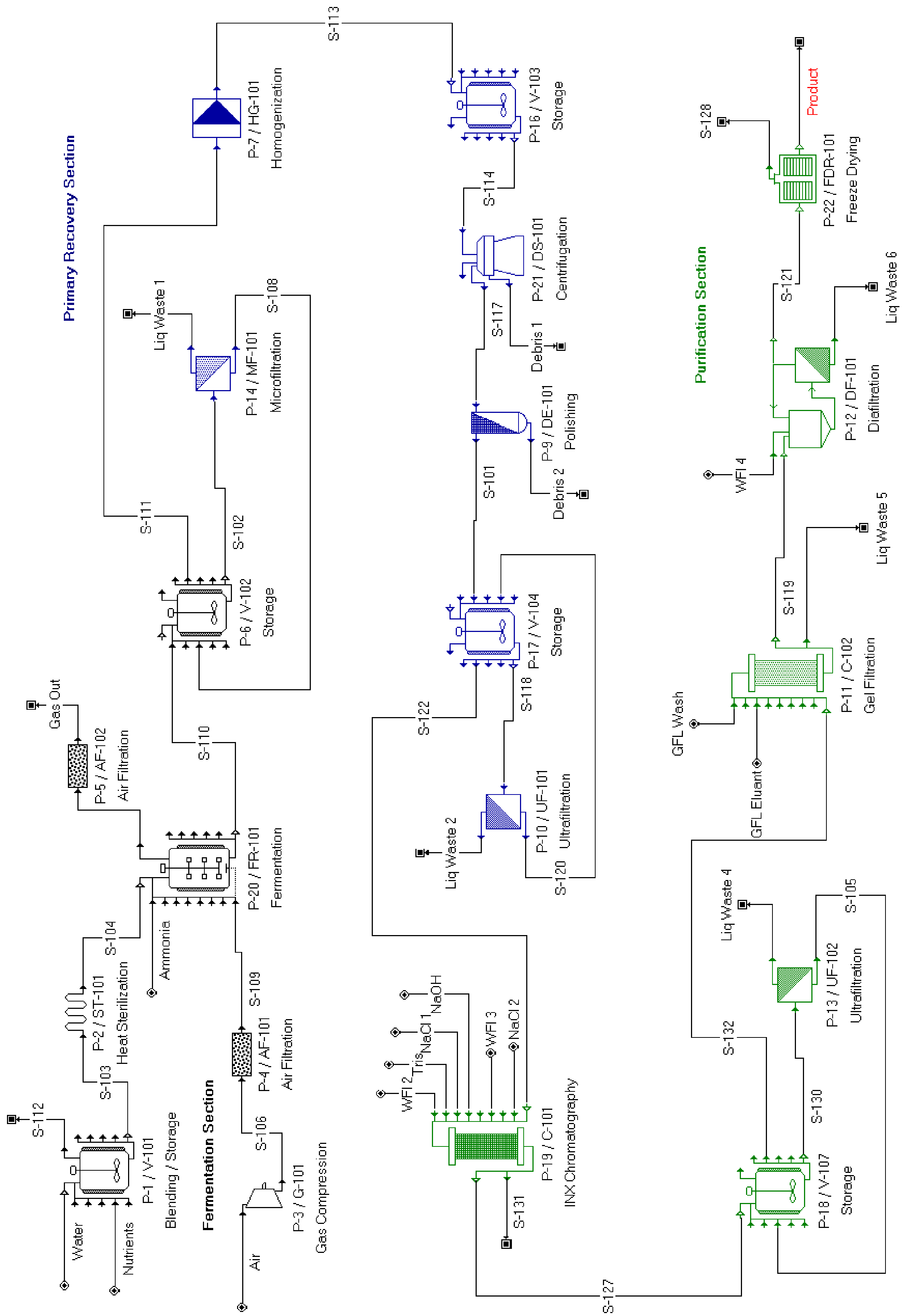
BGal-a: This file represents the process at an early stage of plant design. All equipment is in Design Mode, meaning that all equipment sizes and throughputs are calculated as opposed to being specified by the user.

BGal-b: This file represents the process after equipment sizes have been specified for key pieces of equipment. The BGal-b file was used to produce the tables and graphs in the rest of Chapter 2.3.

BGal-c: This file is the same as BGal-b, except that final product formulation and packaging unit procedures have been added.

We will focus on the BGal-b file for the rest of our process description.

Figure 2.3-a :Beta-Galactosidase Process Flowsheet



General note about Flowsheet Sections

The concept of flowsheet sections was introduced as part of release 3.0 to facilitate reporting of results for costing, economic evaluation, raw material requirements, and throughput analysis of integrated processes. A flowsheet section is a group of unit procedures that have something in common. For instance, the ß-galactosidase flowsheet has been divided into three sections: 1) Fermentation, 2) Primary Recovery, and 3) Purification. All the procedure icons of the Fermentation section are displayed in black, while the icons of the Primary Recovery and Purification sections are displayed in blue and green, respectively. If you wish to add unit procedures to a specific section, select the section in the drop-down menu that displays the list of available section, highlight the desired unit procedure icons on the flowsheet, and then click the "Add to Section" button (the one with two blue triangles on it) on the left end of the **Sections Toolbar**. To specify the default color for icons in a specific section, click the "Edit Section" icon () of the **Sections Toolbar**. This brings up a dialog box, which allows you to specify a Starting Material and Active Product for the section. If you click on the "Icon Color" tab of this dialog, you can edit the section's default unit procedure icon color. These dialogs can also be reached by choosing **Edit: Flowsheet Options: Section: Properties**. For additional information on how to specify flowsheet sections and edit their properties, please see Chapter 13 or consult the Help Facility (look up the keyword "Sections" in the Help index).

Fermentation Section

Fermentation media are prepared in a stainless steel tank (V-101) and sterilized in a continuous sterilizer (ST-101). A compressor (G-101) and an absolute air filter (AF-101) provide sterile air to the fermentor (FR-101). Gaseous ammonia is used as a nitrogen source.

Primary Recovery Section

The first step of the downstream section is cell harvesting to reduce the volume of the broth and remove extracellular impurities; it is carried out by a membrane microfilter (MF-101). Since ß–galactosidase is an intracellular product, the next important step is cell disruption, performed in a high-pressure homogenizer (HG-101). After homogenization, a disk–stack centrifuge (DS-101) is used to remove most of the cell debris particles. A dead-end polishing filter (DE-101) removes the remaining cell debris particles. The resulting protein solution is concentrated by an ultrafilter (UF-101), and stored in V-103.

Purification Section

Next the product stream is purified by an ion exchange chromatography column (C-101), further concentrated by a second ultrafiltration step (P-13/UF-101), and polished by a gel filtration column (C-102). Finally, a diafiltration unit (DF-101) exchanges the gel filtration buffer, and the protein solution is lyophilized in a freeze dryer (FDR-101).

Important information on Staggered Equipment

To cut the cycle time of a batch process, it is common to utilize multiple equipment items operating in staggered mode (i.e., alternating from batch-to-batch) for steps (procedures) that have long cycle times. That's the case with steps P-17 and P-18 of this process. Those steps (involving storage tanks) have long cycle times because they receive material from previous steps and feed subsequent steps. If we employ two tanks for each of those steps that alternate from batch to batch, we can cut their cycle times in half. This is specified through the "Stagger Mode" box of the Equipment Data dialog. Figure 2.3b displays that for tank V-104 used by step P-17. If one equipment item was employed before, specifying "1" extra sets of units is equivalent to creating a pool of two equipment items that can alternate in use. Specifying "2" extra sets is equivalent to having a pool of three equipment items.

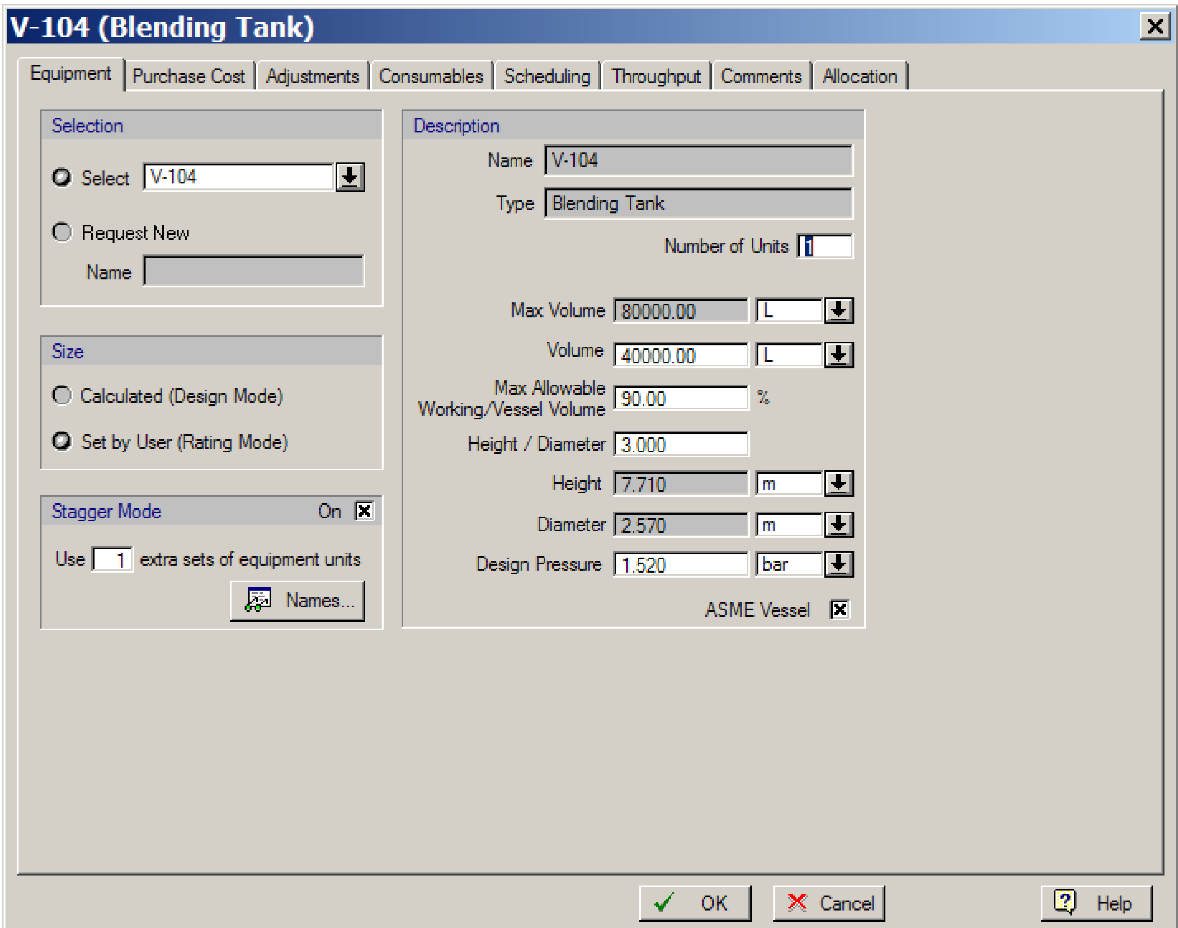


Figure 2.3b: Equipment Data Dialog of a Storage Vessel.

The impact of the use of staggered equipment can be visualized by looking at Figure 2.3c. V-104b is the alternate of V-104. The first batch (blue color) is handled by V-104 whereas the second (cyan color) by V-104b. The two tanks continue to alternate in subsequent batches. The same happens with tanks V-107 and V-107b for step P-18. The staggered equipment items do not appear on the flowsheet at all. They are kind of hidden equipment resources. Their names can be edited by clicking on the "Names…" in the "Stagger Mode" box of the Equipment data dialog (see Figure 2.3b). Staggered equipment items, however, are fully considered in cost analysis.

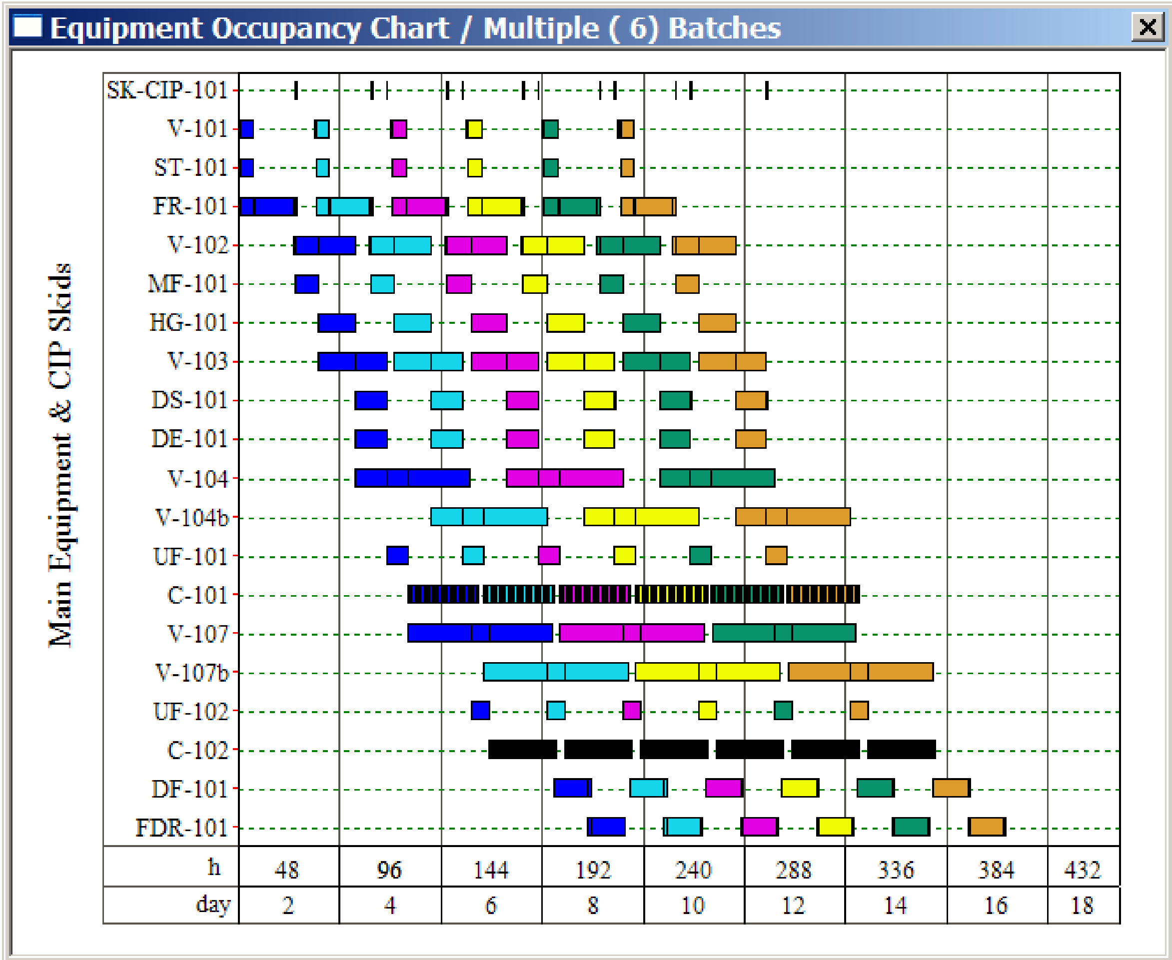


Figure 2.3c: Equipment Occupancy Chart (six consecutive batches).

2.3.2 Initializing Data Specific to Biotech Processes

The Primary Biomass Component and Extra-Cellular Percentage

In bioprocessing, we have formation of intracellular (remain inside the cell) as well as extracellular (released into the solution) products. To capture this as well as the fact that biomass is usually reported on a dry-cell-mass basis, we use the concept of **Extra-Cell %** in streams and fermentation reactions. The “Extra-Cell %” of a component in an input stream (something fed into the system) or a product of a fermentation reaction (something generated in the system) can be specified only if the **Primary Biomass Component** is identified.

This is accomplished through the Pure Component Registration dialog (select **Tasks: Edit Pure Components**) shown in Figure 2.3d. The primary biomass component is selected among components whose “Is Biomass ?” flag has been set to true on the ID’s tab of the **Properties** dialog. The Properties dialog is displayed by clicking on a component's line number (# 3 for Biomass in Figure 2.3d) on the left-most column of the 'Registered Components' table and then clicking on the **Properties** button.

If the Primary Biomass Component is identified, its **Water Content** is specified (through the same dialog) and there is formation of Primary Biomass (as a fermentation product), the program will automatically associate intracellular water with biomass in order to satisfy its water content as specified during component registration. This is displayed using an "Extra-Cell %" value of less than 100 in the stream dialogs (see Figure 2.3e). This has an impact on material balances in separation procedures (e.g., centrifugation, clarification, filtration, etc.). If a removal percentage is assigned to Primary Biomass, the program will use the same removal percentage for the intracellular portion of all components. This results in solids streams (e.g., retentate, concentrate, etc.) with concentrations closer to reality.

Please note that a fermentation product can be identified as intracellular by specifying an "Extra-Cell %" value of less than 100 in the Stoichiometry tab of a fermentation operation dialog. That component can become extracellular (released into the solution) using a cell disruption procedure (e.g., high pressure homogenization or bead milling).

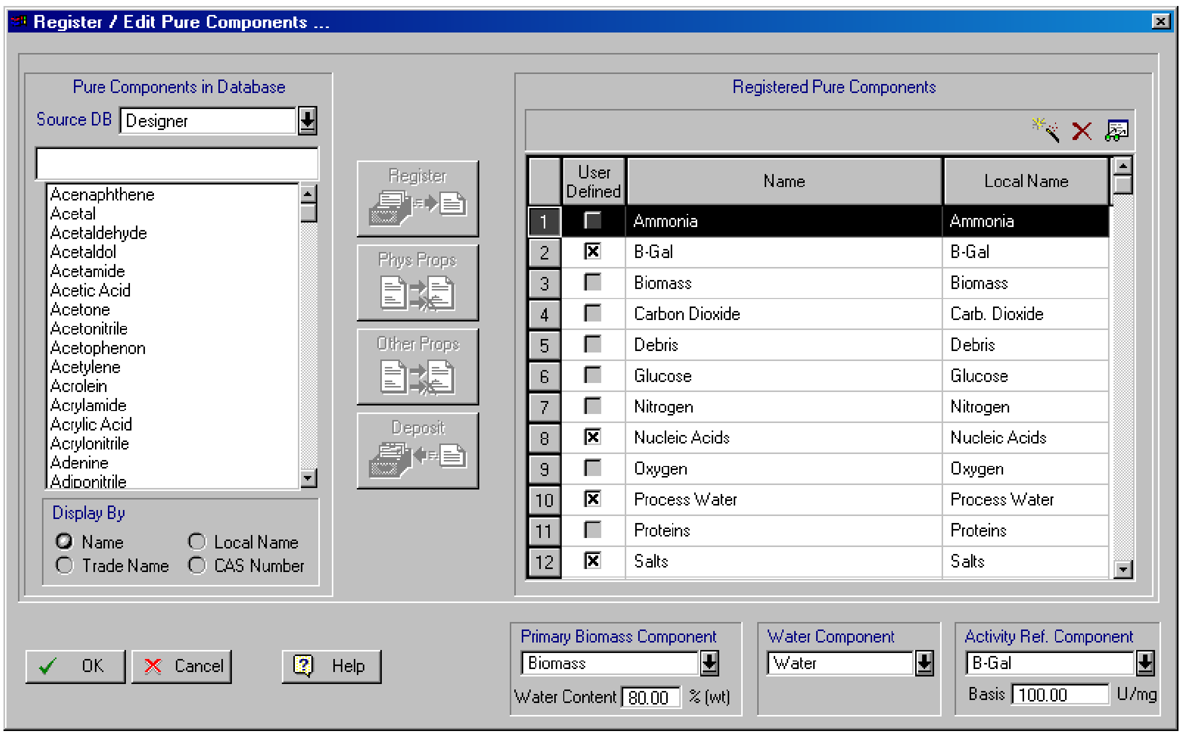


Figure 2.3d: The Pure Component Registration dialog.

The Stream Activity Reference Component

In bioprocessing, the concentration of a product or undesired impurity is often reported as activity measured using a certain assay. In SuperPro this is represented using the **Stream Activity Reference Component** and its **Activity Basis**, expressed in U/mg (see Figure 2.3d). The activity basis represents how many (arbitrary) units of activity (U) correspond to each mg of the reference component present in a stream. This information is used to calculate and report the activity of a stream in U/mL (see Figure 2.3e).

This concept is also applicable to other industries. For instance, in treatment of nuclear waste, the calculated stream activity may represent radioactivity.

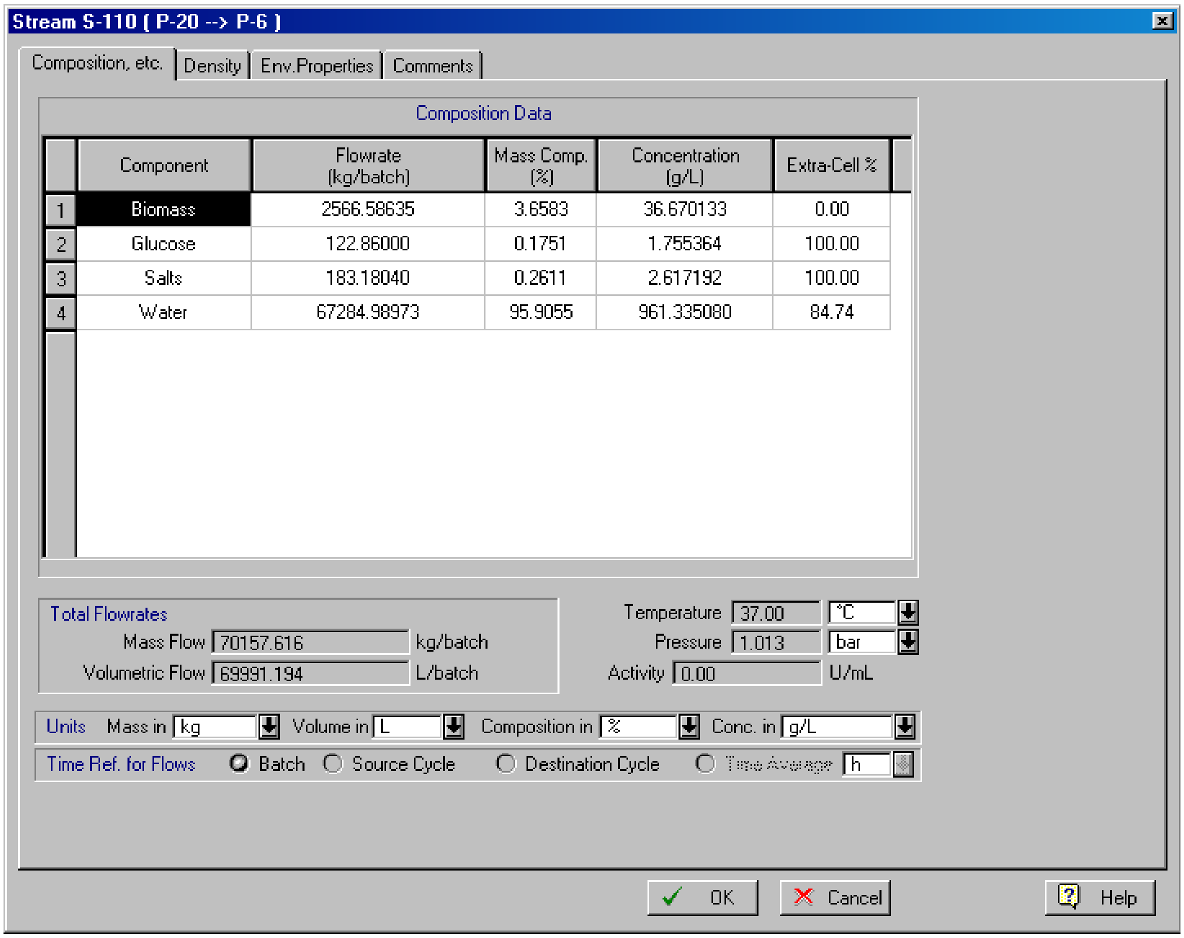


Figure 2.3e: Dialog of stream S-110 (fermentation outlet).

Initializing Fermentation Operations

Correct modeling of fermentation operations is important in biotech processes. SuperPro is equipped with two different types of fermentation models: stoichiometric and kinetic for batch as well as continuous fermentation reactions. The stoichiometric model is used if no kinetic data are available or if simplicity is desired, which is the case in this example. If kinetic data are available, the kinetic model can be used to calculate composition, temperature, and utility profiles as a function of time. Initialization of a stoichiometric fermentation is essentially identical to initialization of a stoichiometric chemical reaction, except that there is an option on the Fermentation Oper. Cond's tab for fermentor aeration. Please refer to Chapter 2.2.4 for information on initialization of stoichiometric chemical reactions. The same chapter section provides information on initialization of kinetic reactions and generation of profiles as a function of time.

Starting with version 5.5 all batch reactions have fed-batch capabilities. Starting with version 6.0, a Perfusion fermentation operation became available. Examples of kinetic and fed-batch reaction models can be found in “Examples \ Misc”. Look for the following SuperPro files: BKinRxn, BKinFerm, and FedBR.

2.3.3 Process Analysis

At this point, you may want to change the values of certain parameters and redo the calculations (by selecting **Tasks: Solve M&E Balances**). The calculated flowrates and compositions of intermediate and output streams can be viewed by revisiting the input/output dialog windows of each stream (double click on a stream line or click with the right mouse button and select **Simulation Data…).** In addition, a report containing information on raw material requirements, stream compositions and flowrates, as well as an overall material balance, can be generated and displayed by selecting the **Reports: Stream and Mat. Balance (SR)...** option from the main menu. The 2.3a that follows provides info on the overall material balance and was extracted from the Stream & Material Balance report.

Stream related information also can be displayed on the screen using the “Stream Summary Table” pane that is activated through “**View \ Stream Summary Table**”. Figure 2.3f displays a portion of the Stream Summary Table. The pane is empty when it is brought up the first time. To populate it, you right-click on the pane and select “Edit Contents”. The Contents Selection dialog allows you to specify which streams to monitor. You also have the option to exclude certain component from the list by clicking on “**Incl / Excl Comps**…”. The unit cells of the Stream Summary Table are editable. Also, the table has printing capabilities and can be easily exported to Excel. Finally, the Stream Summary Table can be floated by right-clicking on it and delecting the “Dock” option and be printed along with the flowsheet. Printing with the flowsheet is available only when the table is floating and the “Include in Printing” option (through right-click) is selected.

Table 2.3a: Raw Material Requirements – Entire Flowsheet

Raw Material	kg/yr	kg/batch	kg/kg MP
Process Water	14,463,999	64,000.000	754.200
Glucose	1,388,318	6,143.000	72.391
Salts	231,876	1,026.000	12.091
Ammonia	89,269	395.000	4.655
Water	2,034,000	9,000.000	106.059
WFI	44,425,983	196,575.147	2,316.516
Tris Buffer	38,780,906	171,596.929	2,022.163
NaCl (0.1 M)	31,676,504	140,161.526	1,651.716
NaOH (0.5 M)	18,854,907	83,428.793	983.156
NaCl (0.5 M)	2,641,892	11,689.791	137.757
TOTAL	154,587,657	684,016.185	8,060.706

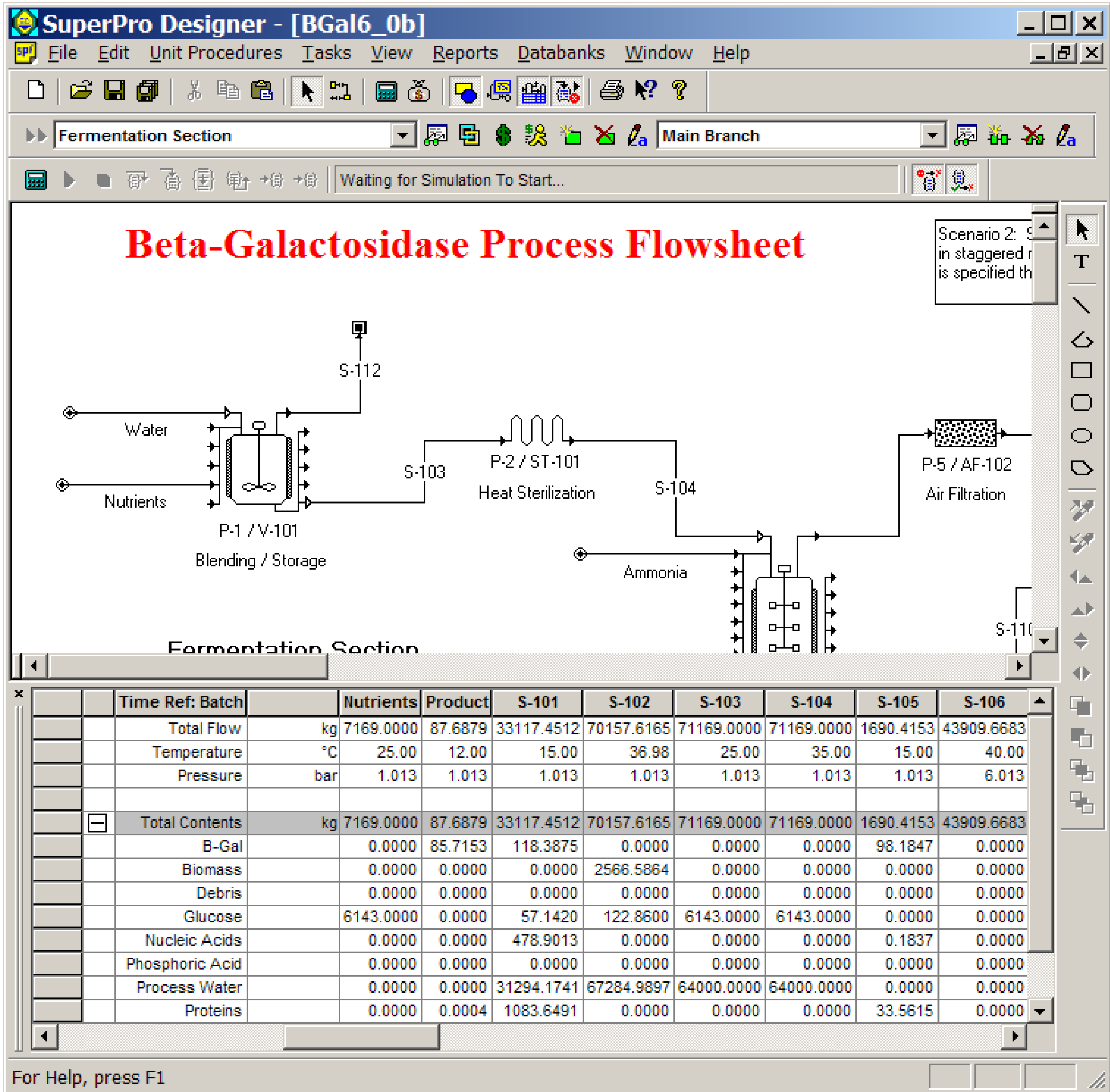


Figure 2.3f: Stream summary table displayed on the flowsheet.

Scheduling and Equipment Utilization

SuperPro generates **Operations** and **Equipment Gantt charts** for single and multiple batches. Figure 2.3g displays a portion of the operations Gantt chart for a single batch of this example process. The left view (spreadsheet view) displays the name, duration, start time, and end time for each activity (e.g. each operation, unit procedure, cycle, batch, etc). You can use the left view to expand or collapse the activity summaries by clicking on the + or – signs in the boxes to the left of the activity names.

The right view (chart view) displays a bar for each activity in the overall process recipe. To edit the scheduling data (or any other data affecting an activity), simply right-click on a bar and a relevant command menu will appear. Selecting the uppermost entry on this menu will bring up a dialog that will allow you to edit the information associated with that particular activity bar. In fact, anything you can accomplish with the other scheduling interfaces, you can also accomplish from the Gantt chart interface. Furthermore, you can redo the M&E balances and have the Gantt chart updated to reflect the new (calculated) scheduling settings for the recipe by clicking on the Update Chart entry in the main menu of the interface. You may also export the Gantt chart to MS Project through the File menu of the chart or the File menu of the application.

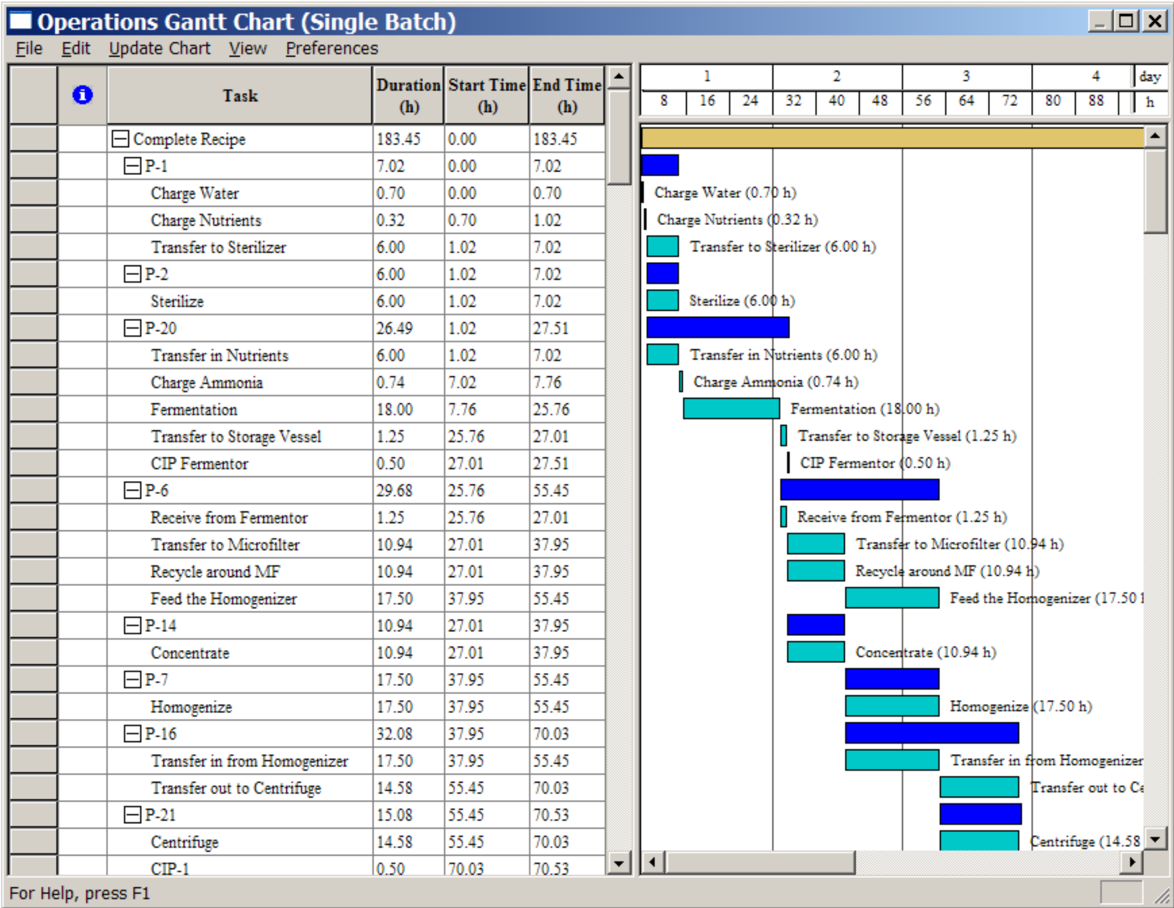


Figure 2.3g: Operations Gantt Chart for a Single Batch.

Another way of visualizing the execution of a batch process as a function of time is through the Equipment Occupancy chart (select **View: Equipment Occupancy Chart**). Figure 2.3c displays the equipment occupancy chart for six consecutive batches of this example process. White space between bars represents idle time. The equipment with the least idle time between consecutive batches is the **time (or scheduling) bottleneck** (V-107 in this case) that determines the maximum number of batches per year. Its occupancy time (approximately 68.48 hours) would be the minimum possible time between consecutive batches (also known as Min. Cycle Time). However in this example we chose to operate the procedure in stagger mode, that is, to have an extra piece of equipment for V-107. (Right Click on Procedure P-18 and choose **Equipment Data**). Having an extra piece of equipment reduces the Minimum Cycle Time by a factor of two to 34.24 h. The actual time between consecutive batches (also known as Recipe Cycle Time) was set to 36 hours. Staggered equipment is also used for V104. The recipe batch time (the time required to complete a single batch) is 183.45 hours.

Tracking of Resource Demand and Inventory

SuperPro Designer calculates and displays graphically the demand for resources, such as heating and cooling utilities, power, labor, and raw materials. To view these graphs, select **View: Resource Chart**, and then choose the desired resource from the drop-down menu. Figure 2.3h displays the water for injection (WFI) demand graph for six consecutive batches. The red lines (spikes) represent the instantaneous demand, the blue line represents the averaged demand (averaged over a period of a day), and the green line represents the cumulative demand and corresponds to the y-axis on the right hand side. The cumulative demand is reset to zero every seven days. If you move the cursor close to the peak of a red line, SuperPro displays the operations that create that peak.

Notes:

1) To change the number of batches, right-click on the chart and select **Set Number of Batches**.
2) To change the contents (variables displayed) and the style (e.g., color, thickness, etc.) of the various lines, right-click on the chart and select Edit Style.
3) To print the chart, right-click, select Copy, and then paste the contents of the clipboard into any MS Office application (e.g., Powerpoint, Excel, Word). You may even paste the clipboard contents into SuperPro itself. To print the chart along with its window frame, press “Alt + Prt Scrn” when the window is active and then follow the above strategy.
4) The demand data for a resource may also be exported into a file in Excel format with a discretization time interval that can be specified by the user. This is a useful feature if you wish to combine in Excel demand for a certain resource from multiple flowsheets.

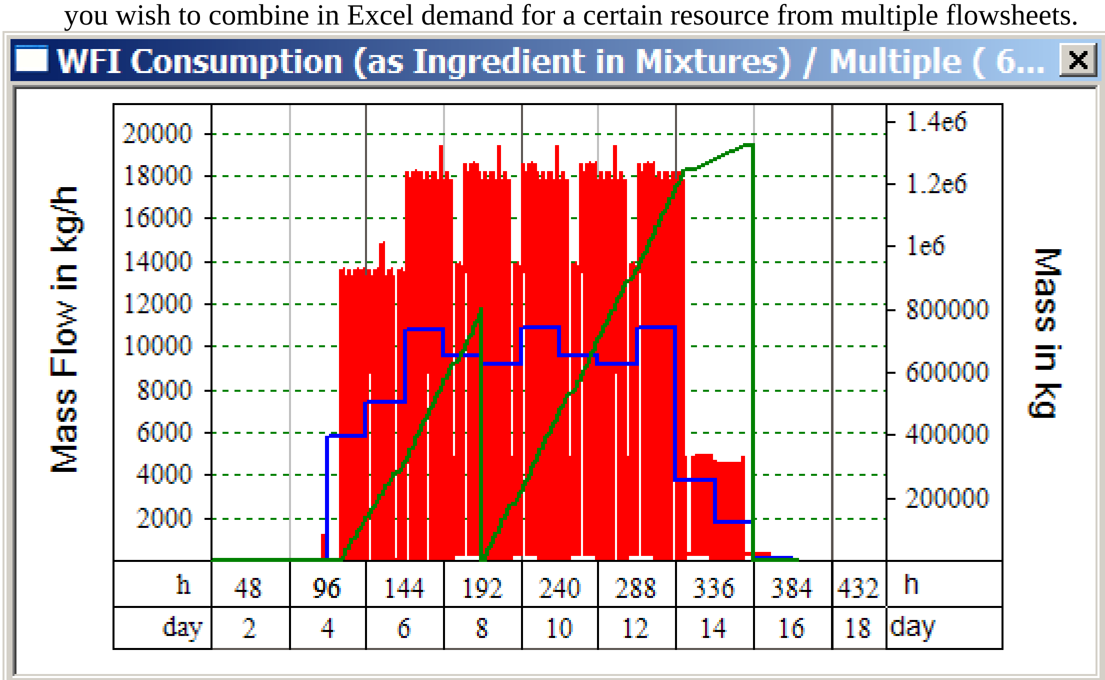


Figure 2.3h: WFI Demand Chart (three consecutive batches).

SuperPro can also analyze and display inventory information for material resources and utilities. Suppose there is a 40,000 kg WFI storage tank. Suppose further that the WFI still has a rate of 20,000 kg/h and it is turned on when the level in the tank drops below 30% and off when it exceeds 85%. To visualize the liquid level in the tank for a single batch, do the following.

Select the menu item **View \ Resource Inventory Chart \ Ingredient**. Select 'WFI' and select the **Supply Info** button. Fill out the dialog as shown in Figure 2.3i. Then click OK and on the next dialog click OK again. This will bring up the graph of Figure 2.3j that shows the WFI level in the storage tank. This graph and the associated calculations are very useful in judiciously sizing WFI stills and storage tanks.

Notes:

1) The inventory graph by default displays the inventory level, the rate of supply, and the inventory limit. To change the contents of the graph, right click on the graph and select Edit Style.
2) If you wish to print the chart or export its data in Excel format, please read the notes for resource demand tracking.

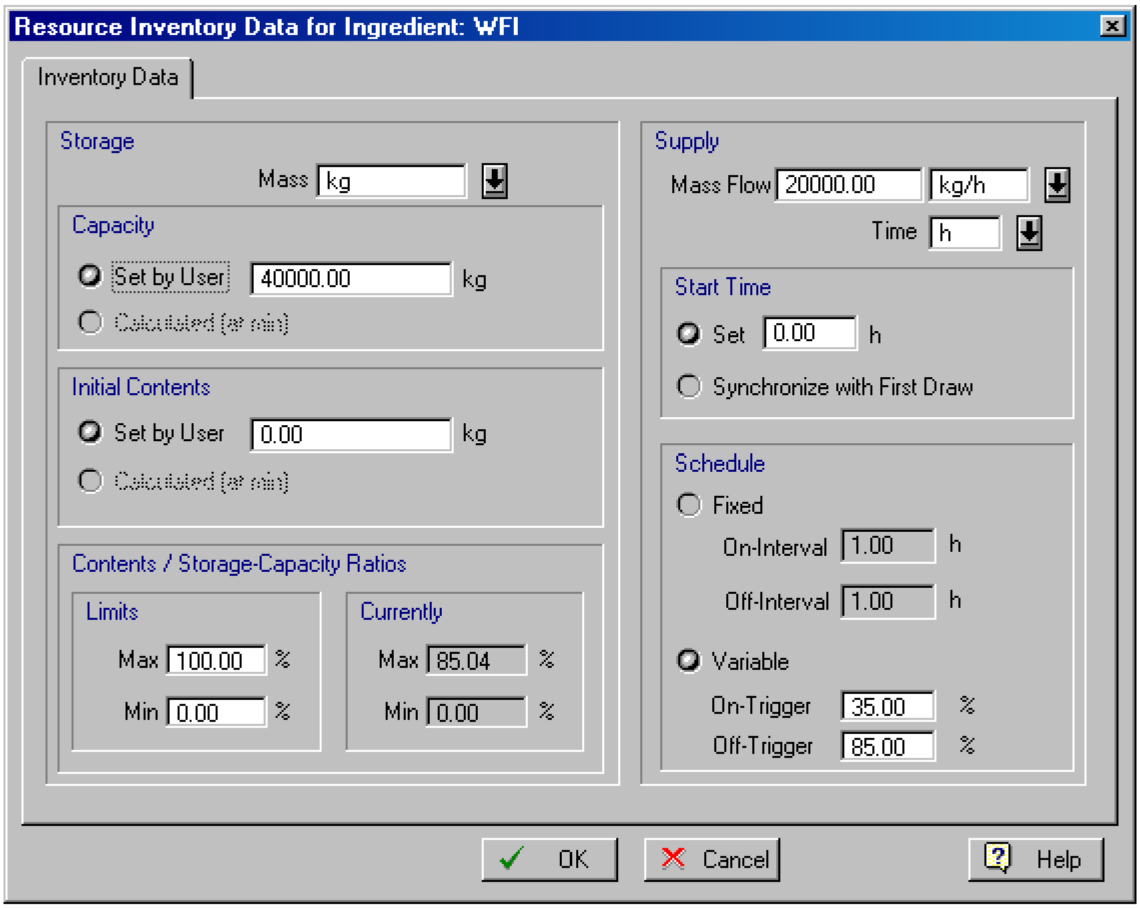


Figure 2.3i: The resource supply info dialog.

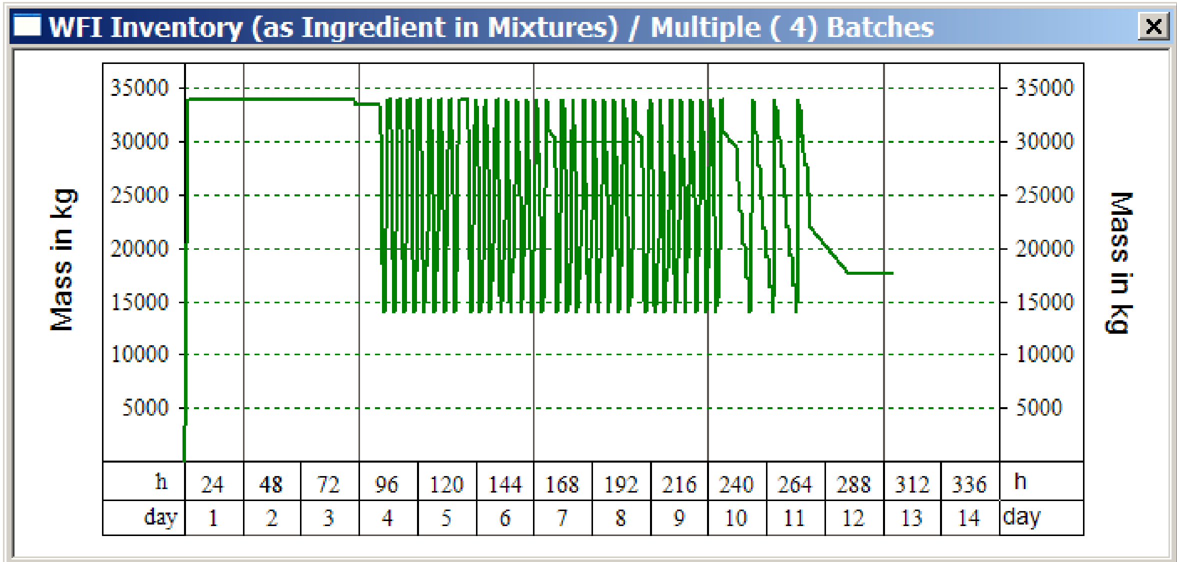


Figure 2.3j: WFI liquid level in its storage tank during four consecutive batches.

Throughput Analysis and Debottlenecking

SuperPro is equipped with powerful throughput analysis and debottlenecking capabilities. The objective of these features is to allow the user to quickly and easily analyze the capacity and time utilization of each piece of equipment, and to identify opportunities for increasing throughput with the minimum possible capital investment. For a detailed throughput analysis example, please see Chapter 9 or search for Debottlenecking in the Help Facility.

Select **View: Throughput Analysis Charts** to view the utilization and throughput potential charts. Both charts indicate that procedure P-19 that utilizes chromatography column C-101 is the bottleneck. It has the highest combined utilization and the lowest throughput potential.

2.3.4 Cost Analysis and Economic Evaluation

Several different economic reports can be generated from SuperPro Designer. To view the essential economic evaluation results for the whole process, please select **View: Executive Summary**. You will need to generate the **Economic Evaluation Report** (EER) and the **Itemized Cost Report** (ICR) if you wish to view the detailed results. Portions of the EER and ICR appear on the following pages. For more information on the economic evaluation calculations, please consult Chapter 8. For more information on report generation and formatting see Chapter 11.

The Economic Evaluation Report (EER)

This report provides information on the capital investment and operating costs for the entire flowsheet. It also includes profitability and cash-flow analysis tables. Additional cost data, broken down per section, is available in the Itemized Cost Report (which follows the EER tables).

To generate and view the EER, select **Reports: Economic Evaluation (EER)**. The EER for the β-Galactosidase design case begins on the next page.

Economic Evaluation Report (EER) for the "Bgal6_0b" Design File

The EER provides summaries and detailed breakdowns of various factors, which affect the overall capital investment and the operating cost. Additional cost data, broken down per section, are available in the Itemized Cost Report (which follows the EER tables).

1. EXECUTIVE SUMMARY (2004 prices)

Total Capital Investment	94,713,000	$
Capital Investment Charged to This Project	94,713,000	$
Operating Cost	108,665,00	$/yr
Production Rate	19,177.93	kg of MP/yr
Unit Production Cost	5,666.14	$/kg of MP
Total Revenues	191,779,00	$/yr
Gross Margin	43.34	%
Return On Investment	60.65	%
Payback Time	1.65	years
IRR (After Taxes)	44.92	%
NPV (at 7.0% Interest)	296,690,00	$

MP = Flow of Component B-Gal in Stream Product

2. MAJOR EQUIPMENT SPECIFICATION AND FOB COST (1999 prices)

Quantity/ Stand-by	Name	Description	Unit Cost ($)	Cost ($)
1/0	ST-101	Heat Sterilizer Size/Capacity = 17.24 m3/h	426,000	426,000
1/0	V-101	Blending Tank Size/Capacity = 80000.00 L	322,000	322,000
1/0	G-101	Centrifugal Compressor Size/Capacity = 1331.05 kW	1,131,000	1,131,000
***				
1/1	V-104	Blending Tank Size/Capacity = 40000.00 L	256,000	512,000
1/0	UF-102	Ultrafilter Size/Capacity = 20.00 m2	47,000	47,000
		Unlisted Equipment		2,377,000
			TOTAL	11,887,000

**** To keep this manual concise, most of the equipment listed in the EER was deleted from this table. If you wish to see the entire table, please open the BGal4_0b.spf example and generate the EER.*

3. FIXED CAPITAL ESTIMATE SUMMARY (2004 prices in $)

3A. Total Plant Direct Cost (TPDC) (physical cost)	
1. Equipment Purchase Cost	11,887,000
2. Installation	4,612,000
3. Process Piping	4,160,000
4. Instrumentation	4,755,000
5. Insulation	357,000
6. Electrical	1,189,000
7. Buildings	11,887,000
8. Yard Improvement	1,783,000
9. Auxiliary Facilities	4,755,000
TPDC	45,385,000

3B. Total Plant Indirect Cost (TPIC)	
10. Engineering	11,346,000
11. Construction	15,885,000
TPIC	27,231,000

3C. Total Plant Cost (TPC = TPDC+TPIC)	
TPC	72,615,000

3D. Contractor's Fee & Contingency (CFC)	
12. Contractor's Fee	3,631,000
13. Contingency	7,262,000
CFC = 12+13	10,892,000

3E. Direct Fixed Capital Cost (DFC = TPC+CFC)	
DFC	83,507,000

4. LABOR COST - PROCESS SUMMARY

Labor Type	Unit Cost ($/h)	Annual Amount (h)	Annual Cost ($)	%
Operator	59.80	168,97	10,105,00	93.61
QC Analyst	69.00	10,000	690,000	6.39
TOTAL		178,97	10,795,00	100.0

5. RAW MATERIALS COST - PROCESS SUMMARY

Bulk Raw Material	Unit Cost ($/kg)	Annual Amount (kg)	Annual Cost ($)	%
Process Water	0.010	14,464,000	145,000	0.76
Glucose	1.000	1,388,318	1,388,000	7.27
Salts	1.600	231,876	371,000	1.94
Ammonia	0.500	89,270	45,000	0.23
Water	0.000	2,034,000	0	0.00
WFI	0.100	44,425,983	4,443,000	23.27
Tris Buffer	0.150	38,780,906	5,817,000	30.47
NaCl (0.1 M)	0.130	31,676,504	4,118,000	21.57
NaOH (0.5 M)	0.120	18,854,907	2,263,000	11.85
NaCl (0.5 M)	0.190	2,641,892	502,000	2.63
TOTAL		154,587,657	19,091,000	100.0

6. VARIOUS CONSUMABLES COST (2004 prices) - PROCESS SUMMARY

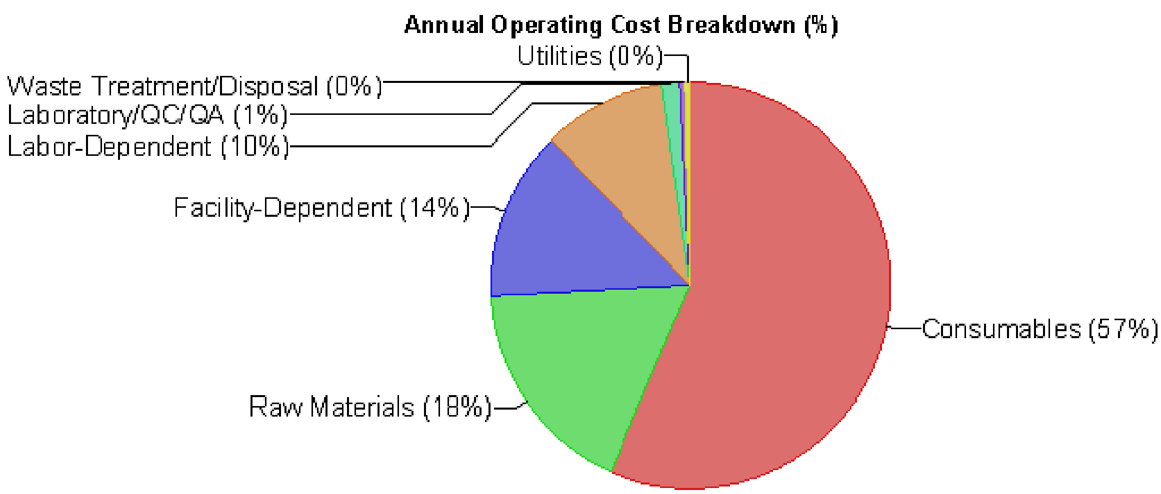
Consumable	Units Cost ($)	Annual Amount		Annual Cost ($)
Dft DEF Cartridge	600	226.000000	0	136,000.00
MF Membrane (Biotech)	600	723.200000	0	434,000.00
UF Membrane (Biotech)	800	587.600000	0	470,000.00
INX Biotech Resin	1,500,000	18467.098117	0	27,701,000.00
Gel Filtration Resin	800,000	40704.295849	0	32,563,000.00
TOTAL				61,304,000.00

Economic Evaluation Report (continued)

9. ANNUAL OPERATING COST SUMMARY (2004 prices)

Cost Item	$	%
Raw Materials	18,162,00	17.62
Labor-Dependent	10,303,00	9.99
Facility-Dependent	13,980,00	13.56
Laboratory/QC/QA	1,484,000	1.44
Consumables	58,320,00	56.57
Waste Treatment/Disposal	448,000	0.43
Utilities	406,000	0.39
Transportation	0	0.00
Miscellaneous	0	0.00
Advertising/Selling	0	0.00
Running Royalties	0	0.00
Failed Product Disposal	0	0.00
TOTAL	103,102,0	100.00

The chart that follows is also from the same report. It is obvious that the consumables are the most important cost item. They account for the expensive chromatography resins that need to be replaced periodically.



Economic Evaluation Report (continued)

10. PROFITABILITY ANALYSIS (1999 prices)

A.	Direct Fixed Capital	83,507,000	$
B.	Working Capital	2,855,000	$
C.	Startup Cost	8,351,000	$
D.	Up-Front R&D	0	$
E.	Up-Front Royalties	0	$
F.	Total Investment (A+B+C+D+E)	94,713,000	$
G.	Investment Charged to This	94,713,000	$
H.	**Revenue Stream Flowrates**		
	B-Gal (in Product)	19,177	kg/yr
I.	**Production Unit Cost**		
	B-Gal (in Product)	5,666.14	$/kg
J.	**Selling / Processing Price**		
	B-Gal (in Product)	10,101.01	$/kg
K.	**Revenues**		
	Product	191,779,000	$/yr
L.	Annual Operating Cost	108,665,000	$/yr
M.	Gross Profit (K-L)	83,114,000	$/yr
N.	Taxes (40%)	33,246,000	$/yr
O.	Net Profit (M-N + Depreciation)	57,444,000	$/yr
	Gross Margin	43.34	%
	Return On Investment	60.65	%
	Payback Time	1.65	years

Itemized Cost Report (ICR)

The Itemized Cost Report (ICR) provides detailed operating cost data, broken down per flowsheet section and cost item. It enables the user to readily identify the cost sensitive sections of a process – the economic hot-spots. For instance, a quick look at the SUMMARY PER SECTION table (see below) reveals that the Purification section is the most expensive part of this process. Thus it would be wise to allocate resources to optimize this section, as opposed to using those same resources elsewhere where optimization would have little effect on the overall project cost.

The above analysis shows how the economic reports can be used not only for estimation of the total cost of a process, but also as a tool to optimize the process through "what-if" scenarios. Would it make economic sense to use a less expensive chromatography resin if it required more cycles to be run and more buffer solution to be used? It depends on how many more cycles are needed, and how much cheaper the new resin is. Would a radically modified purification scheme be better than the current scheme? It depends on what equipment, reagents, etc. would be required for the modified purification, and what the overall yield of the product would be. This type of what-if analysis is quick and easy to perform using SuperPro Designer.

To generate and view the Itemized Cost Report, select **Reports: Itemized Cost (ICR)**.

SUMMARY PER SECTION				
Section	**$/kg MP**	**$/batch**	**$/year**	**%**
Fermentation Section	468.571	39,762.00	8,548,831	8.29
Primary Recovery Section	464.265	39,396.68	8,470,287	8.22
Purification Section	4,718.301	400,386.11	86,083,013	83.49
TOTAL	5,651.137	479,544.80	103,102,131	100.00

2.3.5 The Environmental Impact Report (EIR)

The Environmental Impact Report provides information on the amount and type of waste generated by a manufacturing or waste treatment facility. It also provides information on the fate of a compound that enters an integrated manufacturing or waste treatment facility. To create and view the environmental impact report select **Reports: Environmental Impact (EIR).**

2.3.6 Product Formulation and Packaging

SuperPro Designer contains a variety of formulation, packaging, and transportation unit procedures in order to capture the cost associated with such processes.

Entities

Most material flows in SuperPro designer are *bulk material* flows. Discrete parts (e.g. bottles or boxes) are termed entities. A discrete operation converts a bulk stream into an entity stream (e.g. bulk liquid product to filled bottles) or one entity stream to another (e.g. unlabeled bottles to labeled bottles). Discrete procedures may be placed on the flowsheet and connected like any other procedure. Connection points for entity streams are indicated by an open connection point.

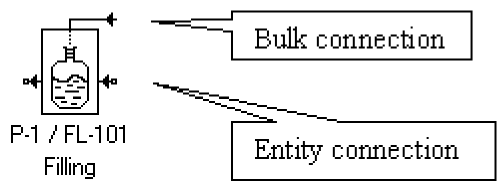


Figure 2.3k Bulk and Entity Connections

To familiarize yourself with the formulation and packaging models and the concepts of discrete streams and entities, please open the **BGal6_0c.spf** design case in the EXAMPLES\BGAL folder and visit the simulation data dialog windows of those operations. As usual, you can open these dialogs by right clicking on the various packaging unit procedure icons and their corresponding streams. Notice the different interface of discrete streams, which display the flow of discrete entities as well as the equivalent bulk flow (based on the bulk ingredients that compose the discrete entities). For more information on discrete streams and entities, please consult the Help Facility.

Another good example for dosage formulation and discrete processing can be found in the “Examples \ PhTablet” directory. That example deals with a process that manufacturers pharmaceutical tablets.

2.4 The Industrial Wastewater Treatment Design Case

This example analyzes an industrial wastewater treatment plant and demonstrates how to track the fate of chemical components (constituents) in an integrated facility. The design case file, **IWWT6_0,** can be found in the **Examples\Indwater** subdirectory. This example is suitable for users with interest in biological wastewater treatment. Other pertinent examples that are provided with SuperPro Designer include the following:

Subdirectory	**Description**
MUNWATER	This example focuses on the modeling and retrofit design of a municipal wastewater treatment plant. It addresses issues of nutrient removal and is recommended for users with interests in industrial and municipal wastewater treatment.
UPWATER	This example deals with water purification (ultra-pure water production) and wastewater treatment at a Semiconductor Manufacturing Facility. Evaluation of recycling options for minimizing city water use and wastewater disposal is included.
GE	This example analyzes an effort to minimize generation of hazardous sludge and wastewater at a polymer manufacturing facility of General Electric. It is recommended for users with interests in waste minimization, water recycling, and pollution control.

Each of these examples has a detailed ReadMe file associated with it. The ReadMe files can be found in the corresponding example subdirectories

2.4.1 Chemical Components

Figure 2.4a displays a flowsheet that represents a simplified version of an industrial activated sludge treatment plant. The flowrate and composition of the influent stream is shown below:

Component	**kg/h**	**g/l**
Water	156,600.00	995.99
Glucose	783.00	4.98
Benzene	100.00	0.64
Biomass	15.66	0.10
Heavy Metals	0.10	0.00064

This corresponds to a relatively small plant with an average throughput of 1 million gallons per day (MGD). Glucose represents the easily biodegradable components while benzene represents the recalcitrant (not easily biodegradable) and volatile components.

Please visit the component registration dialog (select **Tasks \ Edit Pure Components**), to view the physical and environmental properties of the various components. Some of the environmental properties of Glucose are shown below.

Property	Value	Units
COD	1.066	g O2/g
ThOD	1.066	g O2/g
BODu / COD	0.732	g/g
BOD5 / BODu	0.900	g/g
TOC	0.400	g C/g
TP	0.000	g P/g
TKN	0.000	g N/g
NH3-N	0.000	g N/g
NO3-N	0.000	g N/g

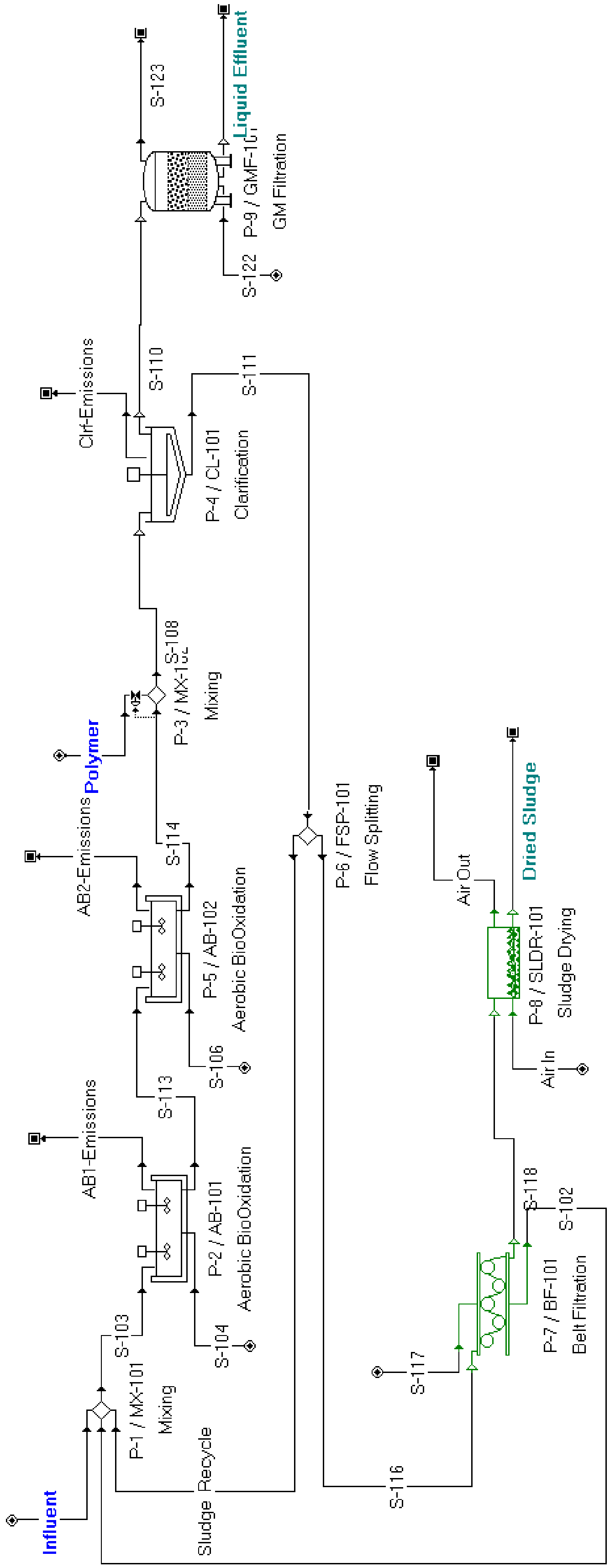
Please note that the above values are displayed when you select the Glucose component by clicking on its line number (# 5) on the left hand side of the 'Registered Components' table and then click on the **Properties** button. Values for such properties are available in the component database for many components. Whenever you enter a new component, you should visit its Properties dialog box to enter appropriate values for the important properties. Note that these values, along with the stream compositions, are used to calculate the lumped environmental stream properties (BOD, COD, TKN, TSS, etc.). More information on component and environmental stream properties can be found in Chapters 3 and 4.

2.4.2 Process Description

The influent stream is combined with the sludge return stream (Sludge Recycle) and is sent to a sequence of two aeration basins (AB-101 and AB-102) for biological oxidation of the organic material. Each aeration basin operates at an average hydraulic residence time of 6 hours and an average sludge residence time of 17.2 hours. A surface aeration system is used to maintain a minimum dissolved oxygen (DO) concentration of 2 mg/l. A clarifier (CL-101) is used to remove the biomass and thicken it to around 10 g/L solids content. The liquid effluent from the clarifier is further treated using a granular media filter (GMF-101) to remove any remaining particulate components. The withdrawn sludge (S-116) is concentrated to a 15% (wt/wt) solids content using a belt filter press (BF-101). The removed water (S-102), which contains small amounts of biomass and dissolved solids, is sent back to the aeration basin. The concentrated sludge stream is dewatered to a final solids concentration of 35% (wt/wt) using a sludge dryer (SLD-101).

At this point, please visit the interface dialogs of the various operations to check the specified parameter values. The bioconversion reaction parameters are explained in detail later in this section.

Figure 2.4 a: Biological Treatment of Industrial Wastewater



Flowsheet Sections

A flowsheet section is a group of unit procedures that have something in common. For instance, the flowsheet of this example has been divided into two sections: 1) BioOxidation and 2) Sludge Treatment. All procedures of the Sludge Treatment section are displayed in green. For information on how to specify flowsheet sections and edit their properties, please see Chapter 15 (Menus & Palettes).

Stoichiometry and Kinetics of Biotransformations

You may view the stoichiometry and kinetics of the various reactions by visiting the reaction dialog window of the aeration basin (see Figure 2.4b). This dialog is displayed by first visiting the “Reactions” tab of the Aerobic BioOxidation procedure and then clicking on the “View\Edit Kinetic Rate” button (the button that looks like an italic R at the top of the Reaction Scheme box). The stoichiometry of a reaction can be edited by clicking on the “Edit Stoichiometry” button (the button that looks like a shake flask).

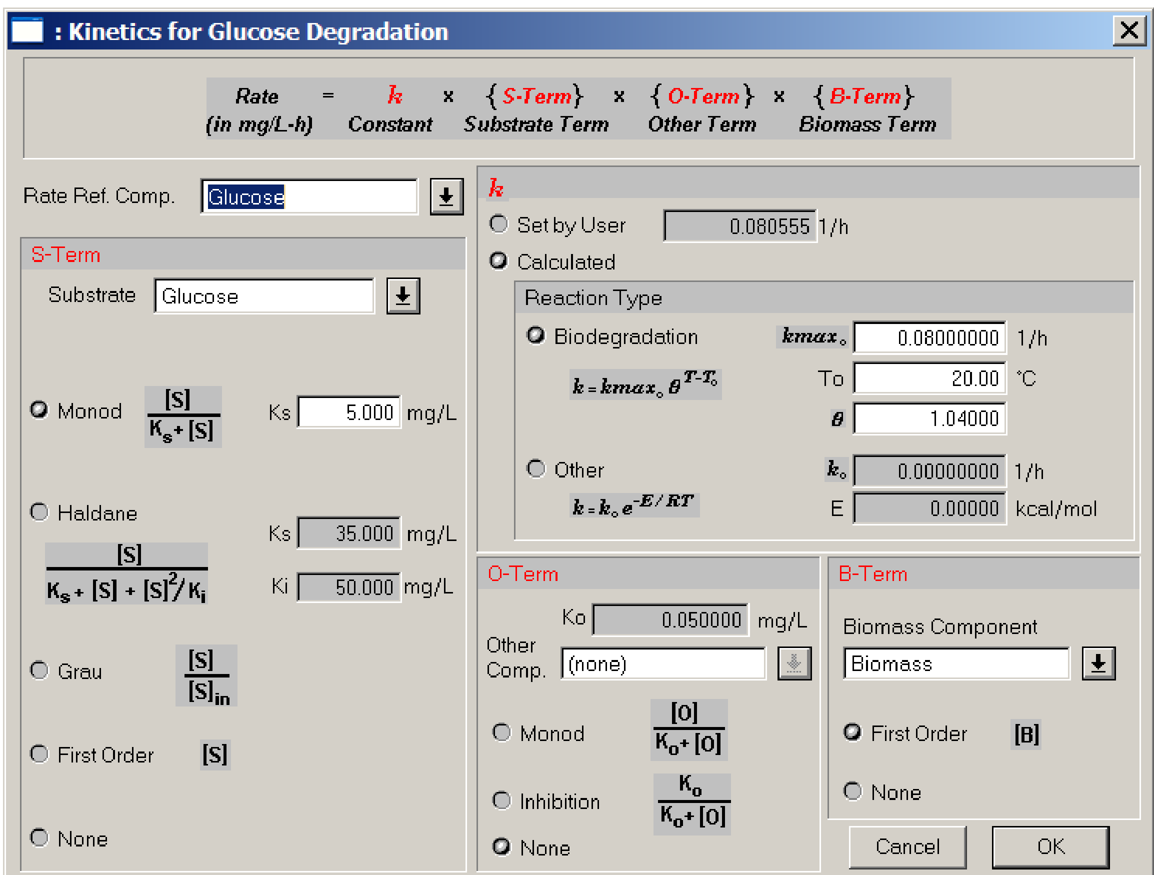


Figure 2.4b: The Kinetics dialog of the Reactions tab of Aerobic BioOxidation.

As can be seen, the model offers great flexibility in specifying the kinetics of a bio-reaction. A bio-reaction operation (e.g., aerobic bio-oxidation) can handle any number of such reactions. Make sure you look at the MUNWATER example if you wish to distinguish between autotrophic and heterotrophic biomass and its impact on oxidation and nitrification / denitrification reactions.

The stoichiometry and kinetics of the bioconversion reactions of this example are described below. The stoichiometry is on a mass basis.

a. Glucose degradation - stoichiometry on a mass basis

Glucose ===> Biomass + H_2O + CO_2

1 g 0.4 g 0.3 g 0.3 g

For those of you who are used to thinking in terms of yield coefficients, the above stoichiometry is equivalent to the following yield coefficient.

Y = 0.4 mg Biomass / mg Glucose

Note that in SuperPro the user never specifies yield coefficients since that information can be extracted from the reaction stoichiometry.

$kmax_o$ = 0.08 1/h at T = 20 deg C

theta = 1.04 (to account for the impact of temperature variations).

Ks = 5 mg Glucose/ L

Note that we express the kinetic constants in terms of Glucose concentration and not BOD5 because BOD5 is not a component in SuperPro but a stream property. We treat BOD5 as a stream property and not as a component because many different components (e.g., Glucose, Benzene, etc.) may contribute to BOD5.

b. Benzene degradation - stoichiometry is on a mass basis

Benzene ===> Biomass + H_2O + CO_2

1 g 0.3 g 0.4g 0.3 g

$kmax_o$ = 0.019 1/h at T = 20 deg C

theta = 1.04 (to account for the impact of temperature variations).

Ks = 13.571 mg Benzene / L

c. Biomass decay

Biomass ===> DeadBiomass

1 g 1 g

k = 0.005 1/h

Note that in SuperPro biomass decay is handled through a separate reaction. In other words, you do not specify a decay coefficient but instead you specify a decay reaction with its own kinetic constants. This is a richer representation compared to the traditional way because it enables the user to distinguish between active and inert biomass.

In the above reactions we ignored the consumption of oxygen and nitrogen for the sake of simplicity. If you wish to consider it, simply modify the stoichiometry of the reactions and make sure that those components are available in the feed streams of the reactors.

VOC Emissions

Volatile organic compounds (VOC's) in influent streams tend to volatilize from open tanks and end up in the atmosphere. Current US EPA regulations limit VOC emissions from treatment plants to no more than 25 tons per year (Van Durme, Capping Air Emissions from Wastewater, *Pollution Engineering*, pp. 66-71, Sept. 1993). SuperPro Designer can be used to predict VOC emissions using models that are accepted by the EPA. A detailed description of the models is available in Chapter 10 (Emissions).

In this example, emissions occur from the two aeration basins and the clarifier. Please double-click on the emission streams to see the amount of benzene that is emitted. Around 17.4% of the total incoming benzene is emitted from the first aeration basin. A much smaller amount (around 0.04% of the total incoming) is emitted from the second aeration basin and essentially none is emitted from the clarifier.

Sorption on Biomass (Sludge)

In activated sludge plants, certain compounds (e.g., heavy metals) adsorb on biomass and follow its path. In the current version of SuperPro, you can account for that by specifying the sorption (%) for each component that adsorbs on biomass through the "Sorption" tab (see Figure 2.4c) of the biological reaction operations. In this case, it was assumed that 90% of heavy metals adsorb on biomass.

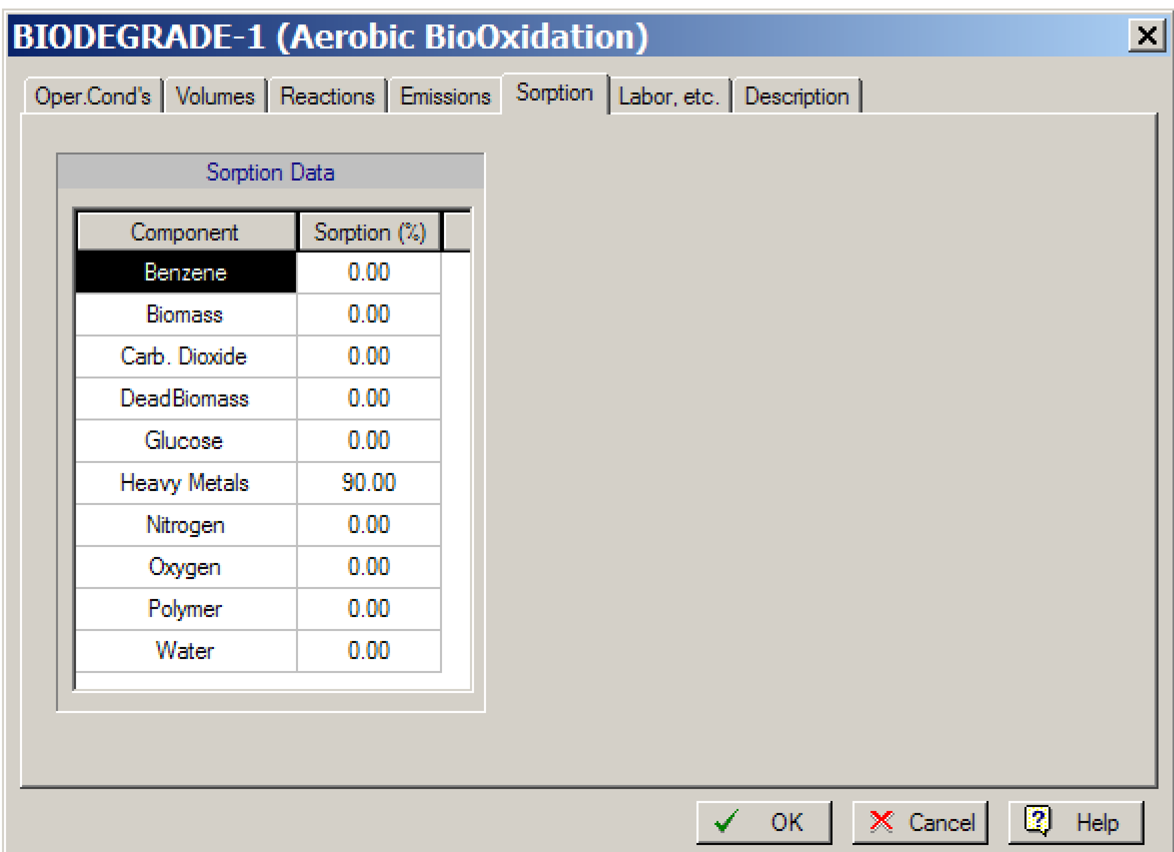


Figure 2.4c: The Sorption tab of Aerobic BioOxidation.

For the sorption specifications to have an impact, you also need to identify the Primary Biomass component through the component registration dialog (select **Tasks \ Edit Pure Components**…). If you use more than one biomass component (e.g., heterotrophic, autotrophic, etc. as in the MUNWATER example), you should identify the heterotrophic bacteria (the most abundant) as your primary biomass.

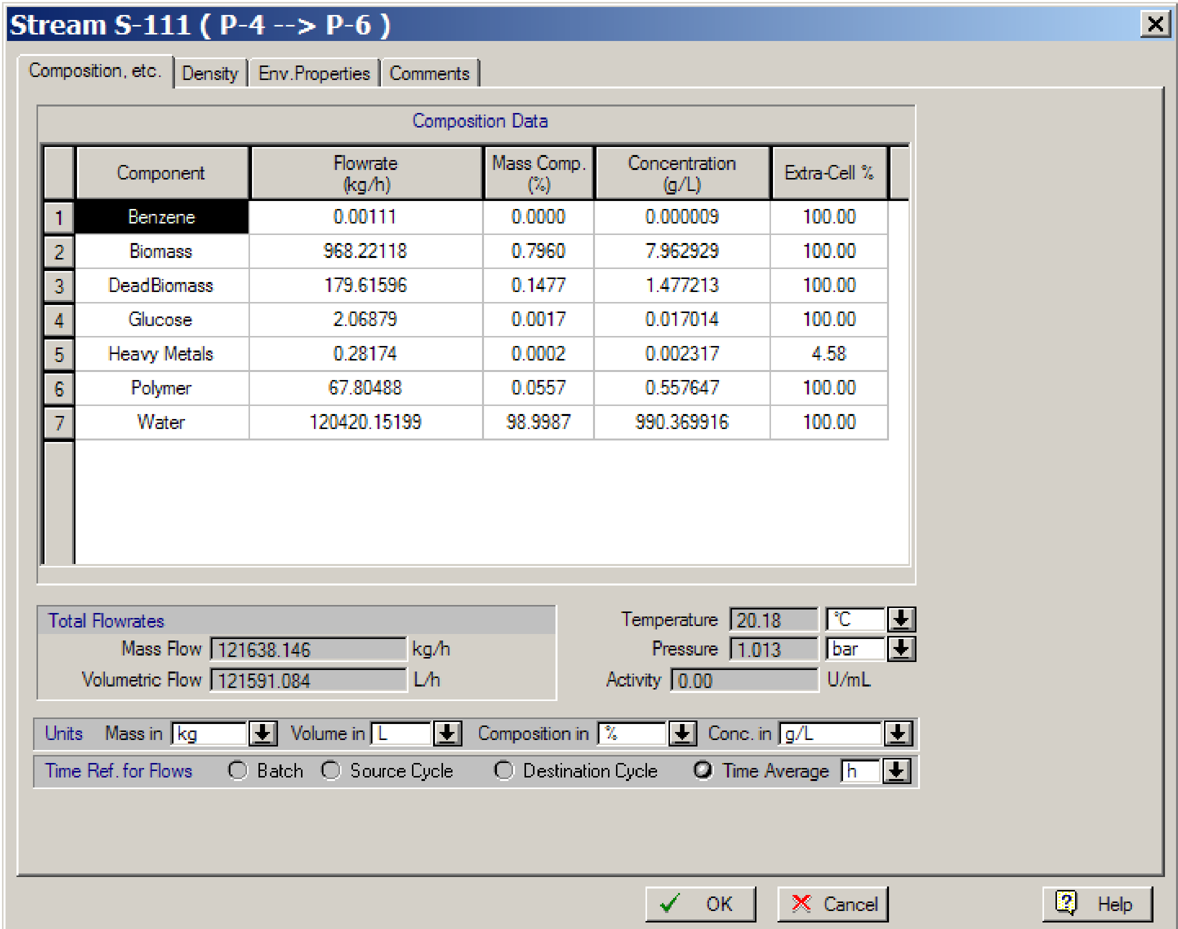


Figure 2.4d: Dialog of an intermediate stream.

In a stream, the percentage of a component that is not associated with primary biomass is displayed on the stream dialog (see Figure 2.4d) with the “Extra-Cell %” variable. In the above case, 4.58% of the total amount of Heavy Metals is extracellular (in solution) and consequently 94.42% is associated with primary biomass (the above stream represents the sludge stream of the clarifier). This information is utilized in the material balances of separation operations. For instance, if the removal percentage of the primary biomass in a clarifier is 98%, then 98% of an adsorbed component will follow the primary biomass component. Please visit the “Liquid Effluent” and “Dried Sludge” streams to see how the Heavy Metals are distributed between the two output streams (the vast majority end up in the Dried Sludge stream).

2.4.3 Process Analysis

At this point, you may want to change the values of certain operating parameters and redo the calculations (be selecting **Tasks \ Solve M&E Balances**). The calculated flowrates and compositions of intermediate and output streams can be viewed by revisiting the input/output dialog windows of each stream (double click on a stream line or click with the right mouse button and select **Simulation Data…)**.

Clicking on the “Env. Properties” tab of a stream dialog will bring up the window shown in Figure 2.4e. This dialog window displays the compositions and flowrates of the traditional environmental stream properties (e.g., BOD, COD, TOC, TSS, etc.). The values of these properties are calculated based on the chemical composition of the stream and the contributions of the various stream components to these properties (see section 2.4.1 as well as Chapter 3).

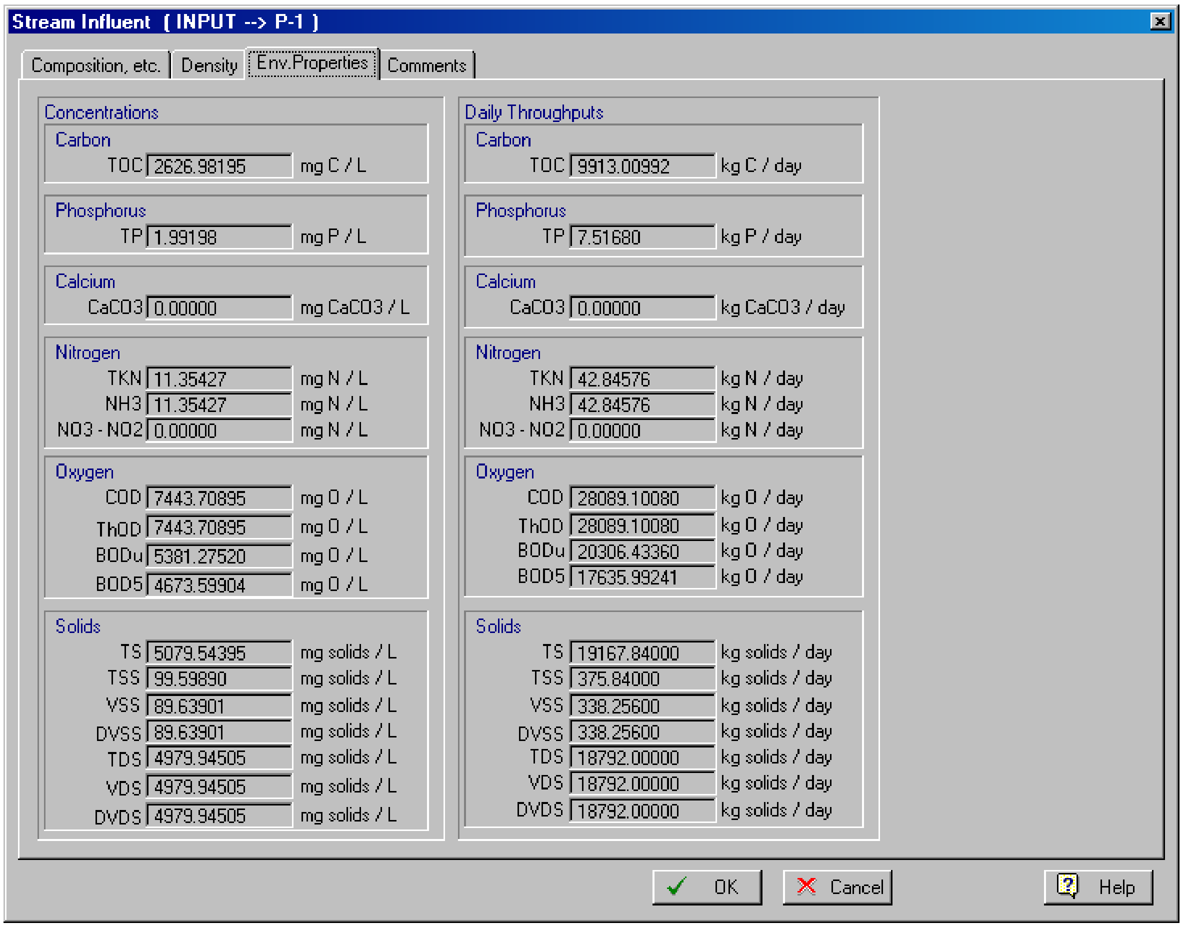


Figure 2.4e: Environmental and Aqueous Stream Properties

Note: Information about water hardness expressed in CaCO3 is used in water purification processes for sizing Ion Exchange columns and characterizing the purity of water. Please check the UPWater (ultrapure water) example for more info on that.

To generate and view the flowrates and compositions of every stream on the flowsheet, you can generate the Stream Report by selecting **Reports \ Stream and Mat. Balance (SR)**.

You may also want to have a look at the environmental impact assessment report (EIR), which contains information on the amount and type of waste that is generated by a manufacturing or waste treatment facility. The EIR also displays the compositions and flowrates of the traditional environmental stream properties (e.g., BOD, COD, TOC, TSS, etc.) for all the input and output streams of a process.

2.4.4 Economic Evaluation

Before looking at the cost analysis and economic evaluation reports, it is useful to visit the Input/Output Stream Classification dialog window by selecting **Tasks \ Stream Classification...** Please note that the “Influent” stream has been classified as a Revenue stream with a unit processing cost of $0.008/kg (or $80/m^3). In other words, we assume that this plant will charge $80/m^3 to the waste generators that use this facility to treat their wastewater. Please also note the unit cost of treatment/disposal that has been assigned to the various output streams.

The table below provides a breakdown of the annual operating cost. The facility-dependent cost is the most important item even when depreciation is ignored. Depreciation can be ignored for very old plants or for plants that were built with public funding. The facility-dependent cost includes Depreciation, Maintenance, Insurance, Local Taxes, and Factory Expense (see Chapter 8 of the manual for more detailed information). To estimate the labor cost, it was assumed that a total of 5 operators (3 in the BioOxidation section and 2 in the Sludge Treatment section) are required to run the plant on a 24-hour basis. The unit labor cost was assumed to be $18/hour. Depending on plant location, this cost may require adjustment. The sludge disposal cost was assumed to be $50/ton. Again this may vary considerably depending on plant location.

	Including Depreciation		Excluding Depreciation	
Cost Item	**$/year**	**%**	**$/year**	**%**
Raw Materials	293,718	3.79	293,718	6.54
Facility	6,516,47	84.05	3,254,14	72.46
Labor	248,400	3.20	248,400	5.53
Consumables	0	0.00	0	0.00
Lab/QC/QA	37,260	0.48	37,260	0.83
Utilities	1,206	0.02	1,206	0.03
Waste	656,458	8.47	656,458	14.62
Transportatio	0	0.00	0	0.00
Miscellaneous	0	0.00	0	0.00
TOTAL	7,753,51	100.0	4,491,18	100.0

To eliminate the cost of depreciation, the value of "Portion of Purchase Cost Already Depreciated" for all the equipment items was set to 100%. The above variable is displayed on the **Adjustments** tab of the **Equipment Data** dialog of each unit procedure (right click on a procedure icon and select Equipment Data...). The material for the above table was extracted from the itemized cost report (ICR) of the base case and the case that excluded depreciation.

If we had to build a plant of this size, the capital investment would be around $33.4 million. Other relevant economic results for this case appear below.

Including Depreciation:

Total Capital Investment	37,906,000	$
Capital Investment Charged to This	37,906,000	$

Operating Cost	8,658,000	$/yr
Processing Rate	1,247,389,387.20	kg of MP/yr
Unit Processing Cost	6.94	$/MT of MP
Total Revenues	9,979,000	$/yr
Gross Margin	13.24	%
Return On Investment	11.10	%
Payback Time	9.01	years

Excluding Depreciation:

Total Capital Investment	37,906,000	$
Capital Investment Charged to This	37,906,000	$
Operating Cost	5,243,000	$/yr
Processing Rate	1,247,389,387.20	kg of MP/yr
Unit Processing Cost	4.20	$/MT of MP
Total Revenues	9,979,000	$/yr
Gross Margin	47.46	%
Return On Investment	7.50	%
Payback Time	13.34	years

The detailed results of the economic evaluation can be produced by selecting **Reports \ Economic Evaluation (EER)**. Note that several multipliers are used to estimate the capital investment of a treatment plant and perform its cost analysis and economic evaluation. Please read the first example of this chapter for more information on how to access and modify those multipliers. Many of the current default multipliers in SuperPro are more appropriate for chemical manufacturing plants than for wastewater treatment plants. If you have better multipliers for wastewater treatment facilities, you may create a template site in the UserDB and deposit them there. Then, if a new process is allocated to that DB site, it utilizes by default the multipliers of the site. For more information on how to take advantage of the database capabilities for cost analysis, please consult the “SynPharmDB” read-me file in the “Examples \ SynPharm” directory of SuperPro.

2.4.5 Modeling Challenges

This example can be used as a good starting point for modeling your own wastewater treatment plants. You may add more components and/or unit procedures to this flowsheet in order to better approximate your own processes. For instance, you may add O_2, NH_3, and PO_4, and introduce appropriate reactions for tracking the consumption and generation of those compounds. The example on municipal wastewater treatment (directory EXAMPLES\MUNWATER) provides information on modeling of nitrogen removal.

Warning! As you increase the number of components, reactions, process steps, and recycle loops, SuperPro will take longer to converge. Consequently, you are strongly advised to increase the complexity of your flowsheets in small steps so that you can be in a position to readily identify the changes that really slow down the convergence. For instance, reactions with very different reaction rates specified in a single unit procedure slow down the calculations considerably and may even cause convergence to fail. In such situations, it may be better to simplify your model by ignoring a slow reaction, at least at the early stages of analysis. Similarly, if you have a very fast reaction, you may want to model it using a generic reaction box (in which you specify the stoichiometry and the extent of conversion) and assume 100% conversion.

A New Way of Thinking. The use of SuperPro, like most other software tools, requires a new way of thinking. This is particularly important for those of you who have little or no previous experience in process simulation. Remember that with simulation we only attempt to approximate the behavior of the real world. It is impossible to completely represent the behavior of a treatment plant on the computer. Consequently, your objective should be to limit the analysis to those variables that are of interest to you from a design (if the objective is to design a new plant or retrofit an existing one) or operations (if the goal is to improve the performance of an existing plant) point of view.

Commonly Asked Questions. Almost all new users that attempt to model biological wastewater treatment processes using SuperPro ask the following question:

“Very often we design and operate wastewater treatment processes based on overall stream properties such as BOD, COD, TKN, SS, etc. We have no information on individual chemicals (constituents) in influent and effluent streams. Since SuperPro performs material balances on constituents, how can we use it to design processes based on traditional stream properties such as BOD, COD, etc.?”

Answers to this and other questions can be found in the Q&A file (a hypertext type of file) that is provided with the software. For this particular question, click on Components and look at the first Q&A. The municipal wastewater treatment example (directory EXAMPLES\MUNWATER) provides additional information related to the above question.

If you have difficulty in using SuperPro to its full potential, please do not hesitate to contact our tech-support office. Our staff will be happy to assist you and provide you with guidance. Also, it may be a good idea to attend one of our training courses or arrange for a training course at your company's site.

GO TO TOP LEVEL CONTENTS