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.
MISC	SuperPro	A set of small examples demonstrating special features of the software. (a) "BKinFerm" focuses on modeling of Batch Kinetic Fermentation 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 batch distillation and generate composition profiles.
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 description 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, Generate Stream Report,** supply **Revenue, Raw Material and Waste Stream** data, **Perform Economic Calculations, Generate Economic Evaluation Report,** etc. Other analyses may be optionally performed. Use the **View** menu to see the results of the analyses.

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:

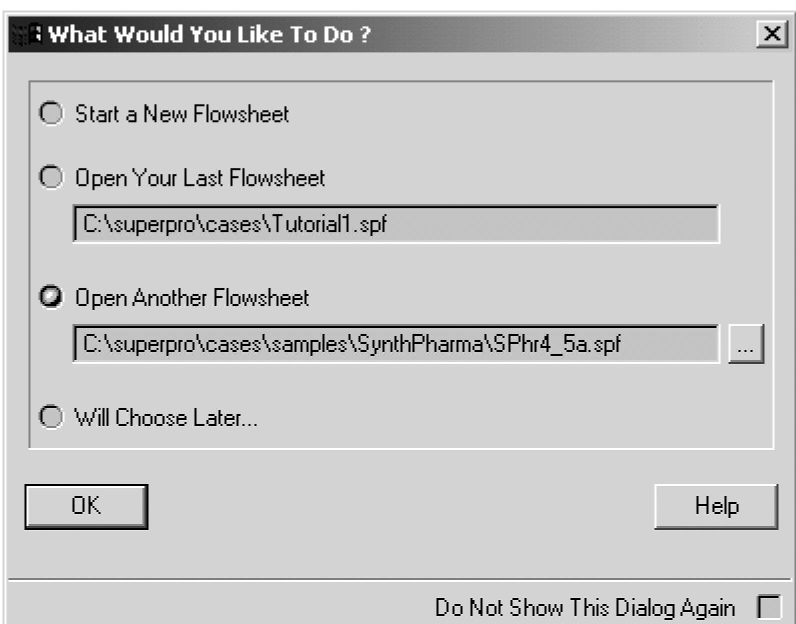


Figure 2.1-a Opening Dialog

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-a) 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.

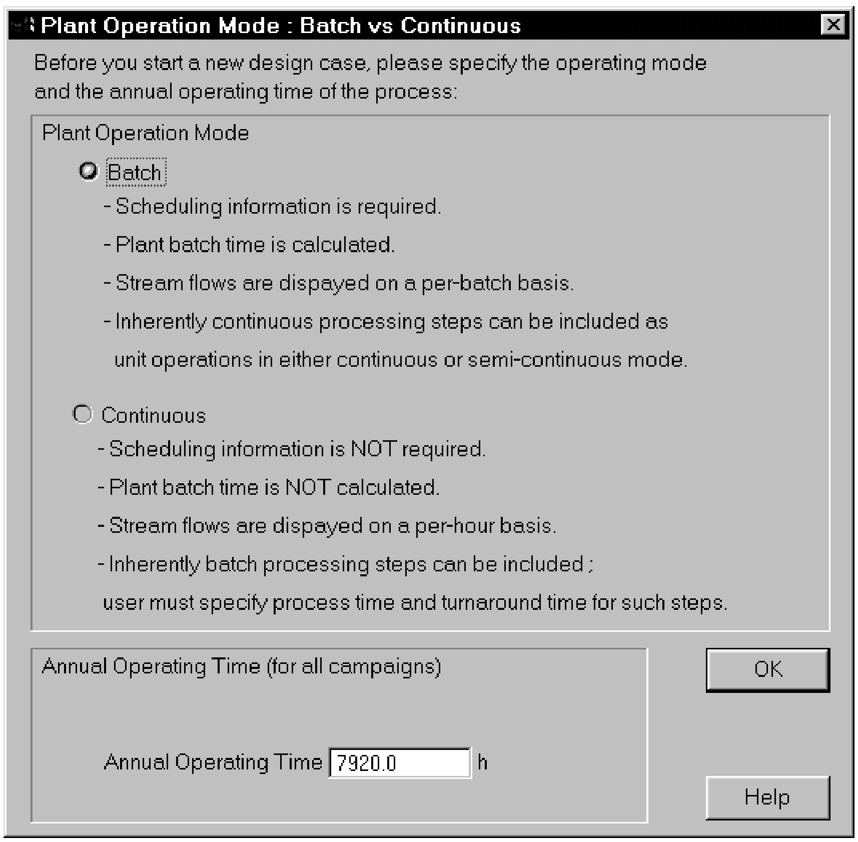


Figure 2.1-b: Specifying the operating mode for the entire flowsheet

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: Register Components & Mixtures: Pure Components**. This will activate the dialog shown below (Figure 2.1-c).

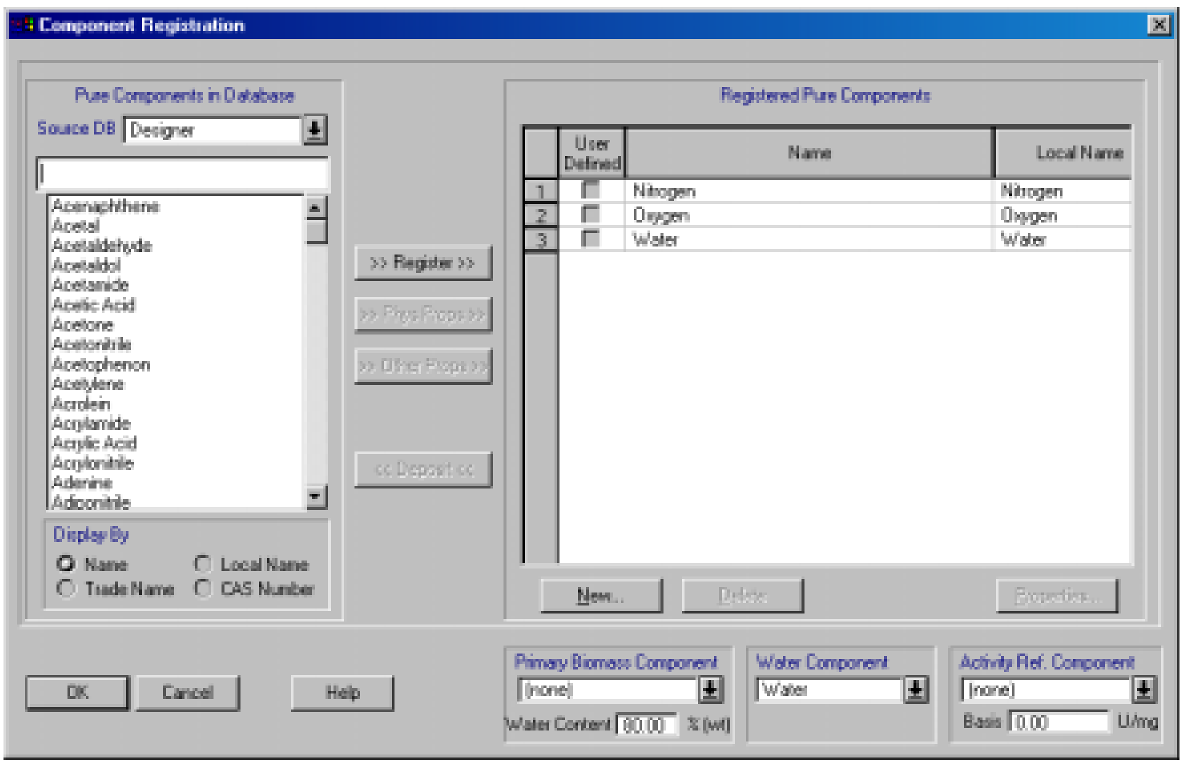


Figure 2.1-c: The Component Registration dialog

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).

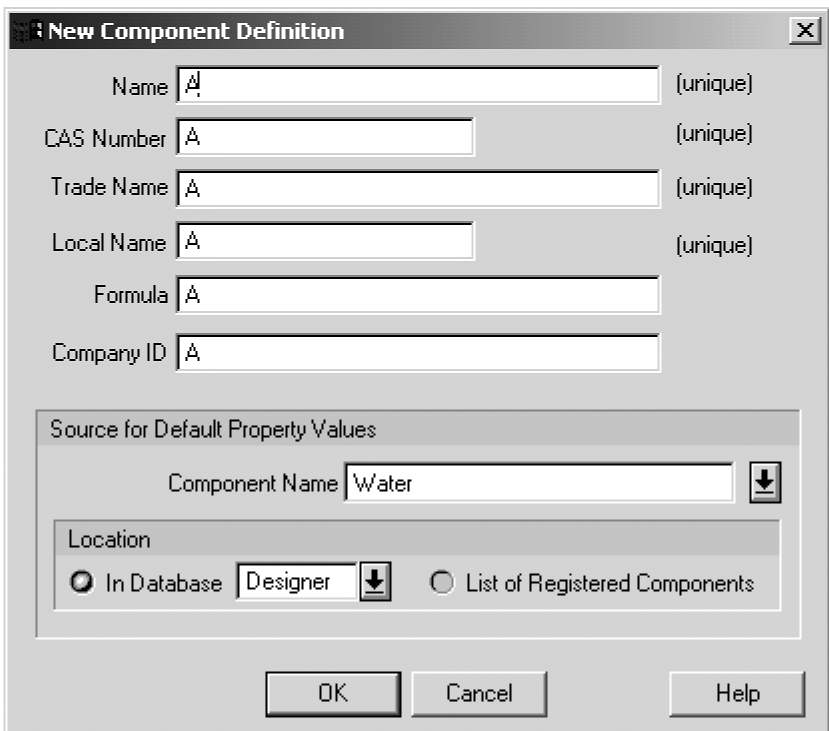


Figure 2.1-d: The New Component Definition dialog

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 \$200/kg for component C. This completes your initialization of components for our example.

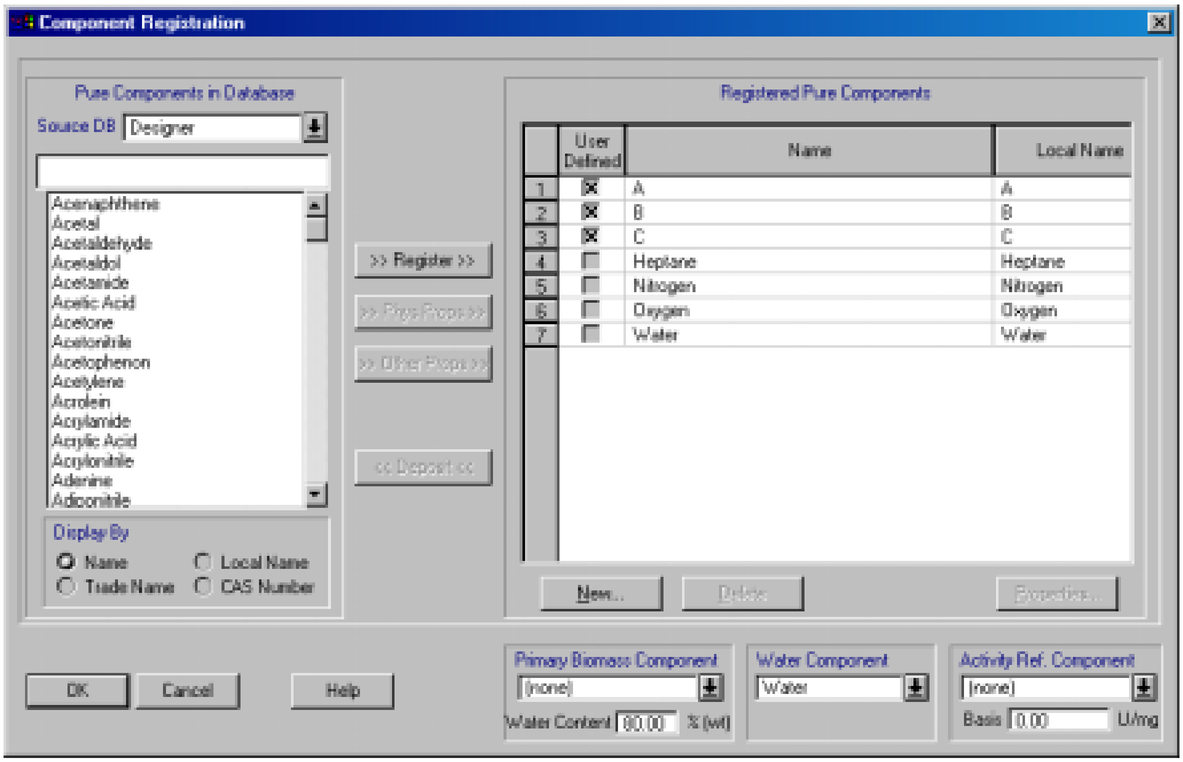


Figure 2.1-e: Selecting a component to edit its properties

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: Register Components and Mixtures: Stock Mixtures.**

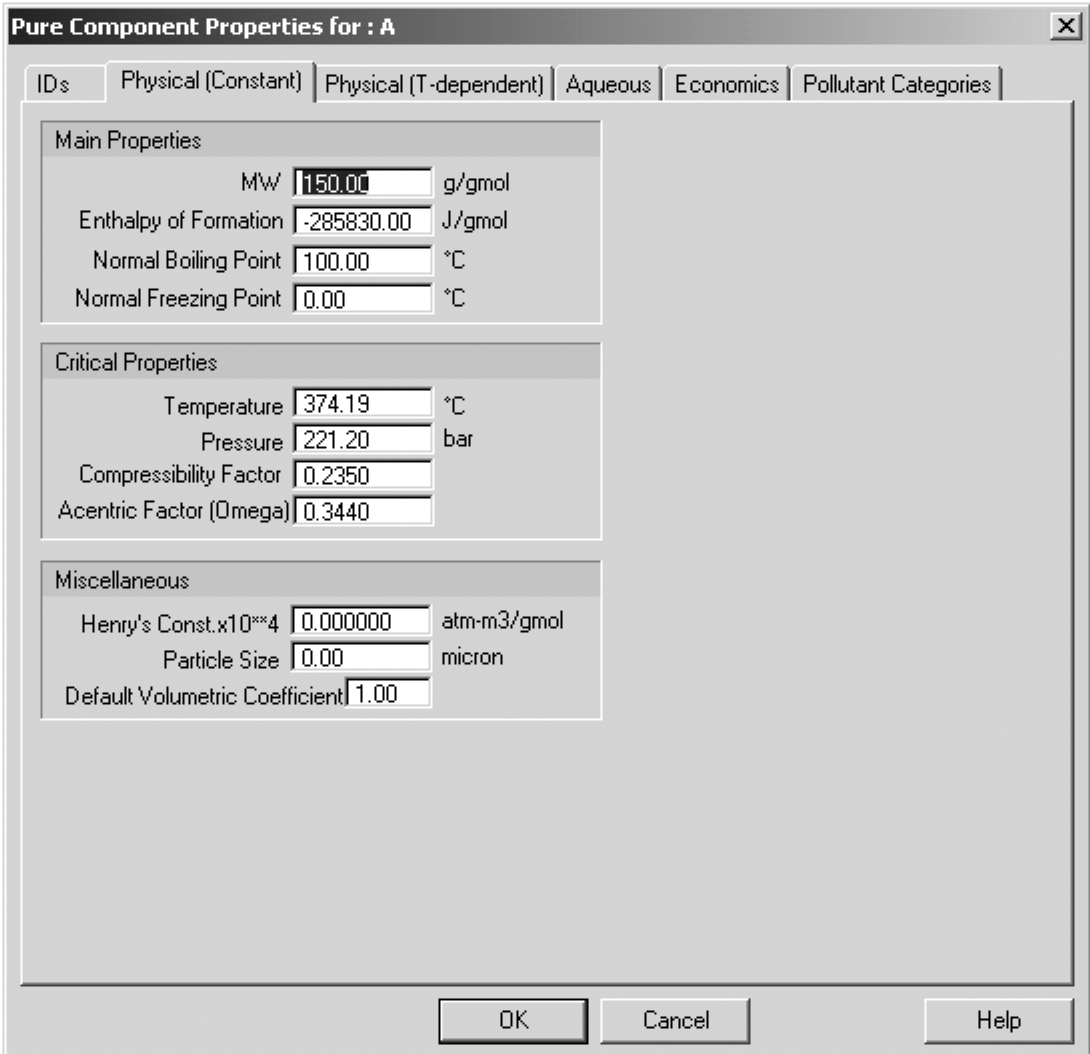


Figure 2.1-f: Editing the properties of component A

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:

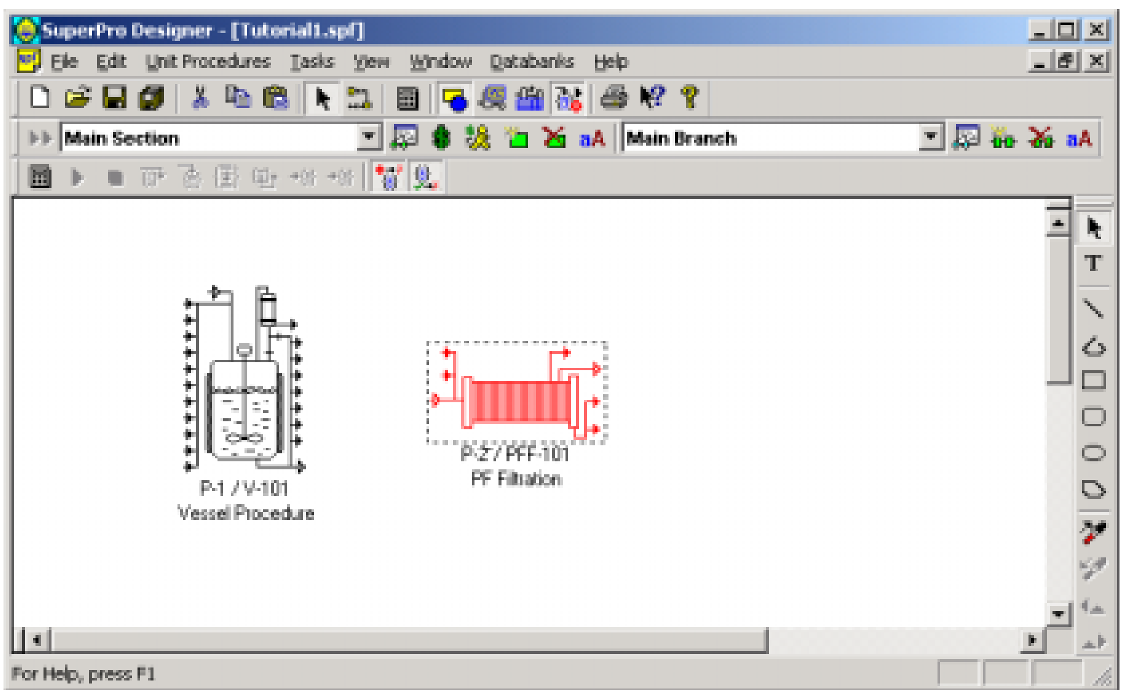


Figure 2.1-g: The example flowsheet with the Vessel Procedure and Plate and Frame Filtration icons added

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.

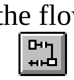
2. If the start time of the first operation of the pasted unit procedure was defined on a relative basis (e.g., with respect to the start or end of another operation in some other procedure), then the scheduling of the pasted procedure is reset to remove the coupling.

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.

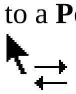
Adding Streams to the Flowsheet:

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:

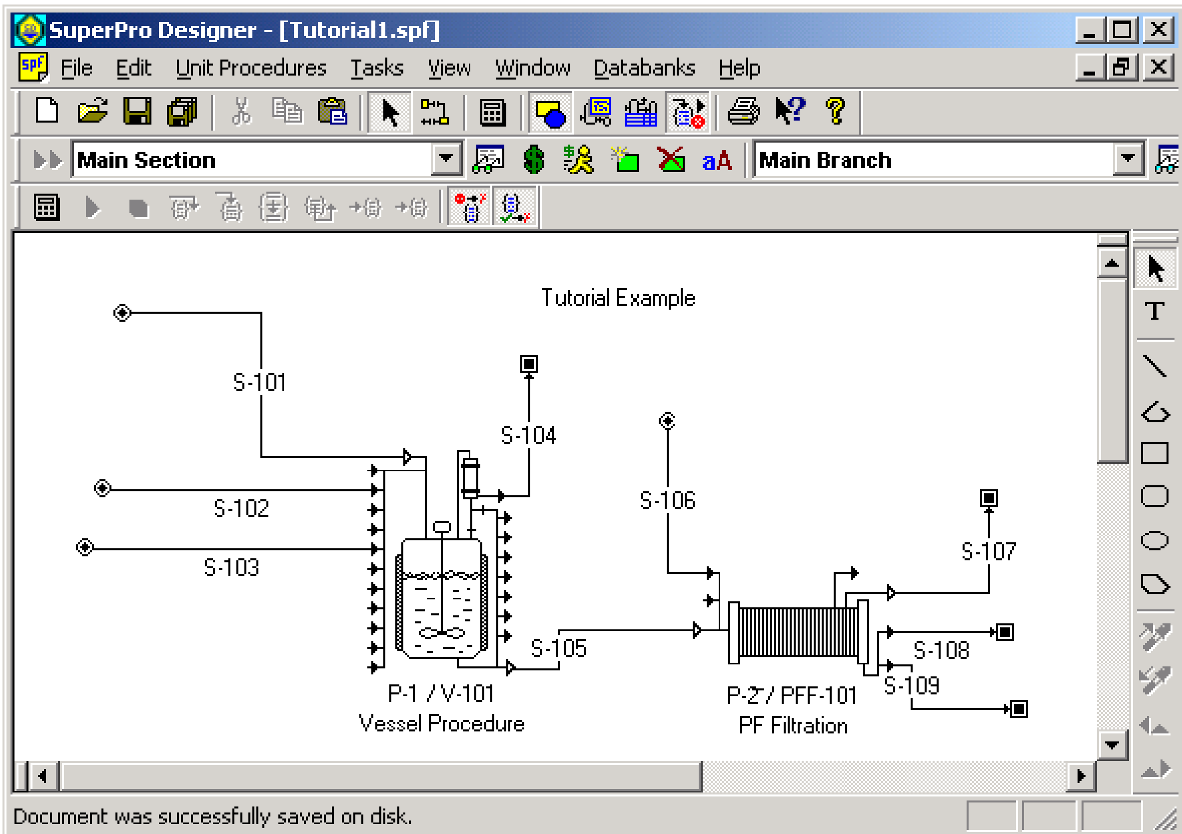


Figure 2.1-h: The example flowsheet with streams added

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.

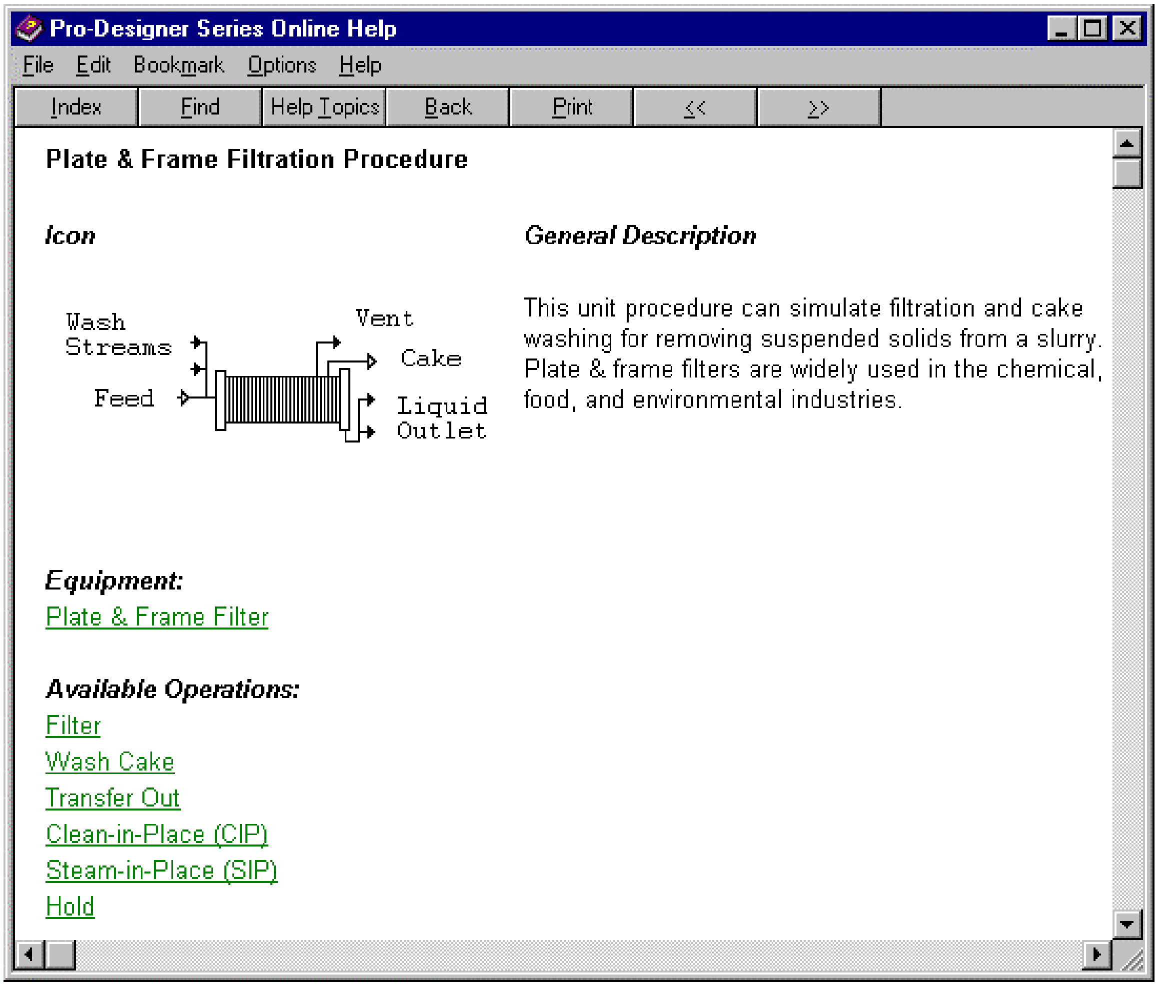


Figure 2.1-i: A Portion of the Help file for Plate and Frame Filtration

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).

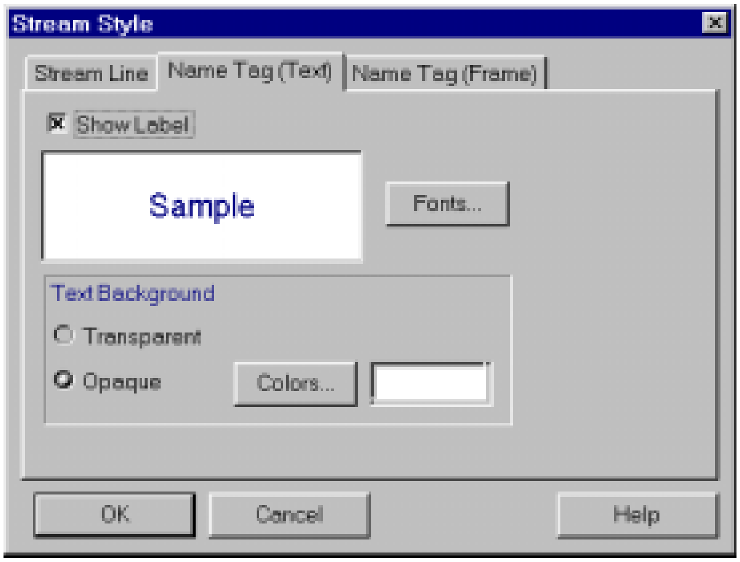


Figure 2.1-k: The Stream Style dialog

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:

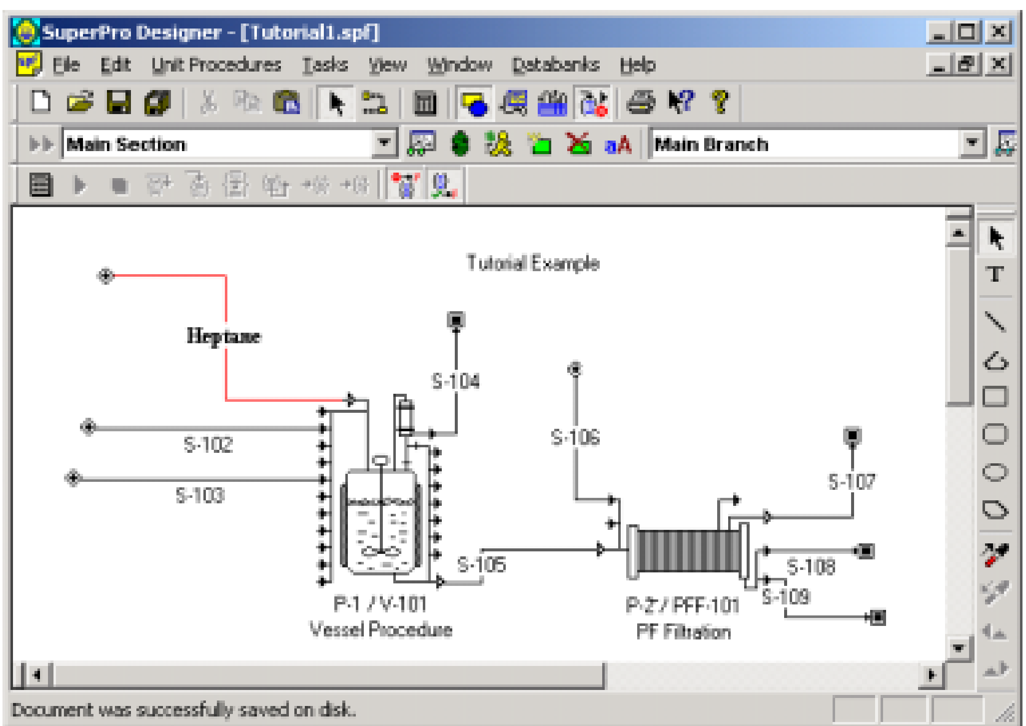


Figure 2.1-l: The example flowsheet after the name and style for one of the input streams have been changed.

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:

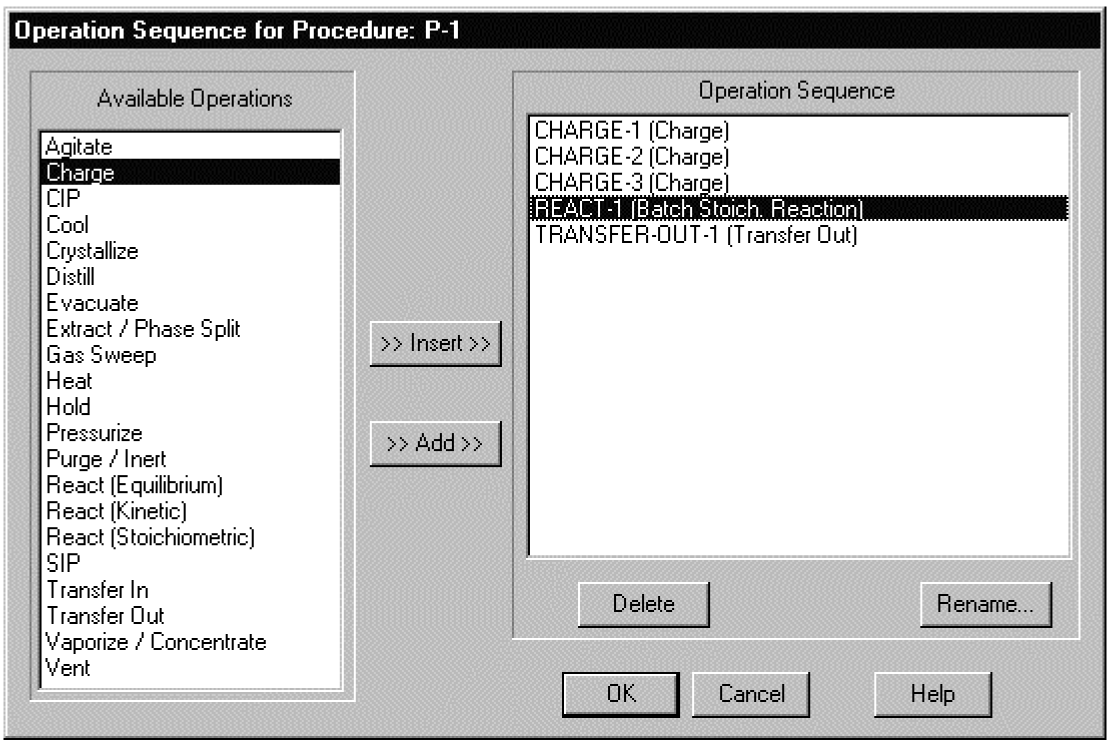


Figure 2.1-m: Adding Operations to the Vessel Procedure in the example process

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 will add the new operation at the end of the list, while the **Insert** button 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 click and drag it to a different position in the

Operation Sequence list. 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 2.1m).

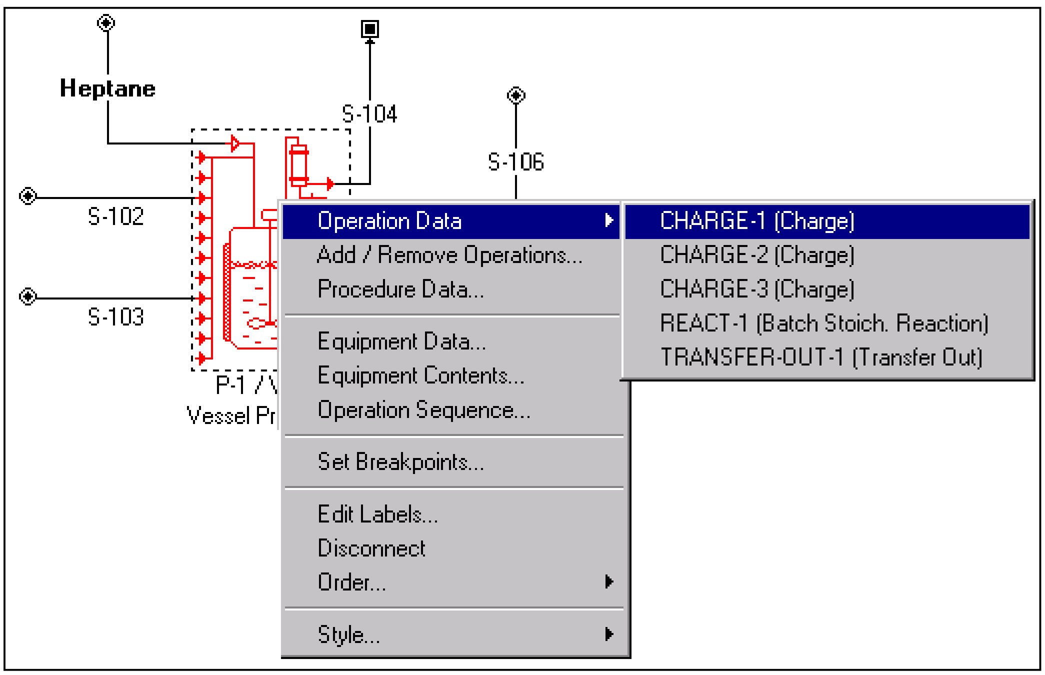


Figure 2.1-n: The context menu for the vessel procedure in this example process

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 also specify staggered pieces of equipment associated with this step and 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) and specify size and purchase cost parameters.
- 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:

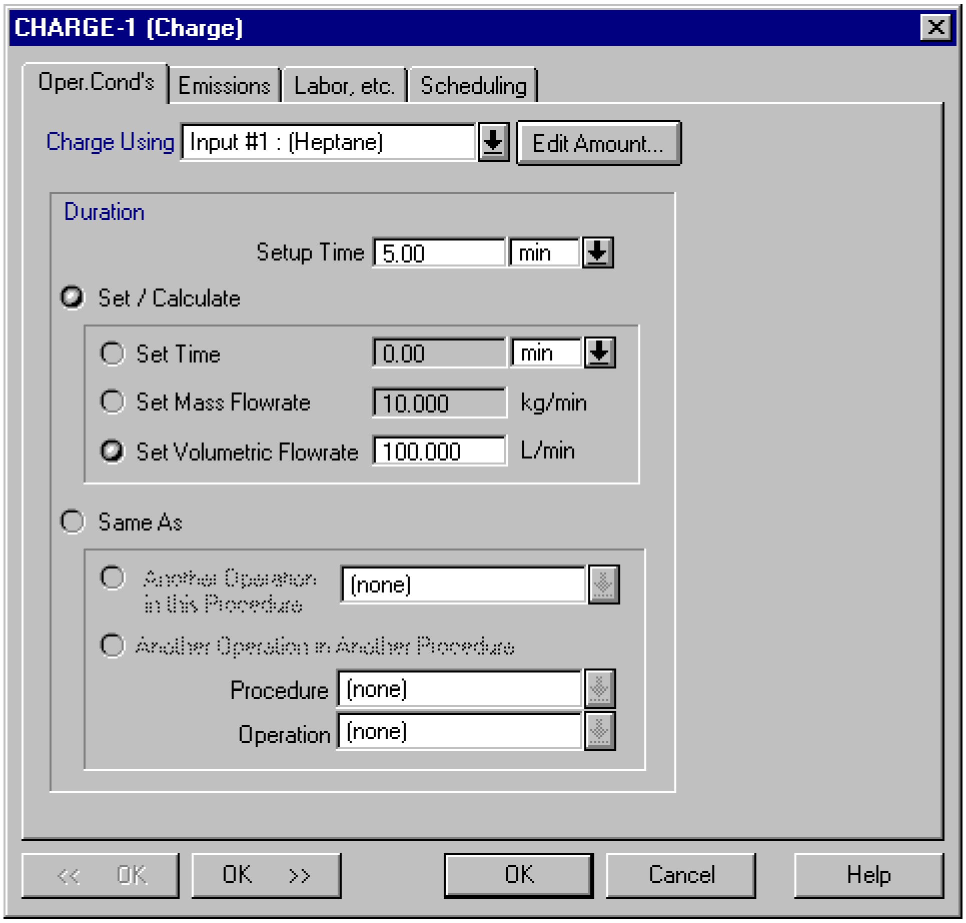


Figure 2.1-o: The Operating Conditions dialog for the first Charge operation in the Vessel Procedure.

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 will first need to specify where the material being charged is coming from. To do this, 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. Then click the **Edit Amount** 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. Then specify the amount to be 800 kg/batch by clicking in the "Flowrate (kg/batch)" box and typing 800 directly in the grid. If you wish to specify the volume of added heptane, select "Mass Composition" (instead of the default Ingredient Flows) and then select "Set Vol. Flow" under Total Flowrates and specify the volume of the added solvent.

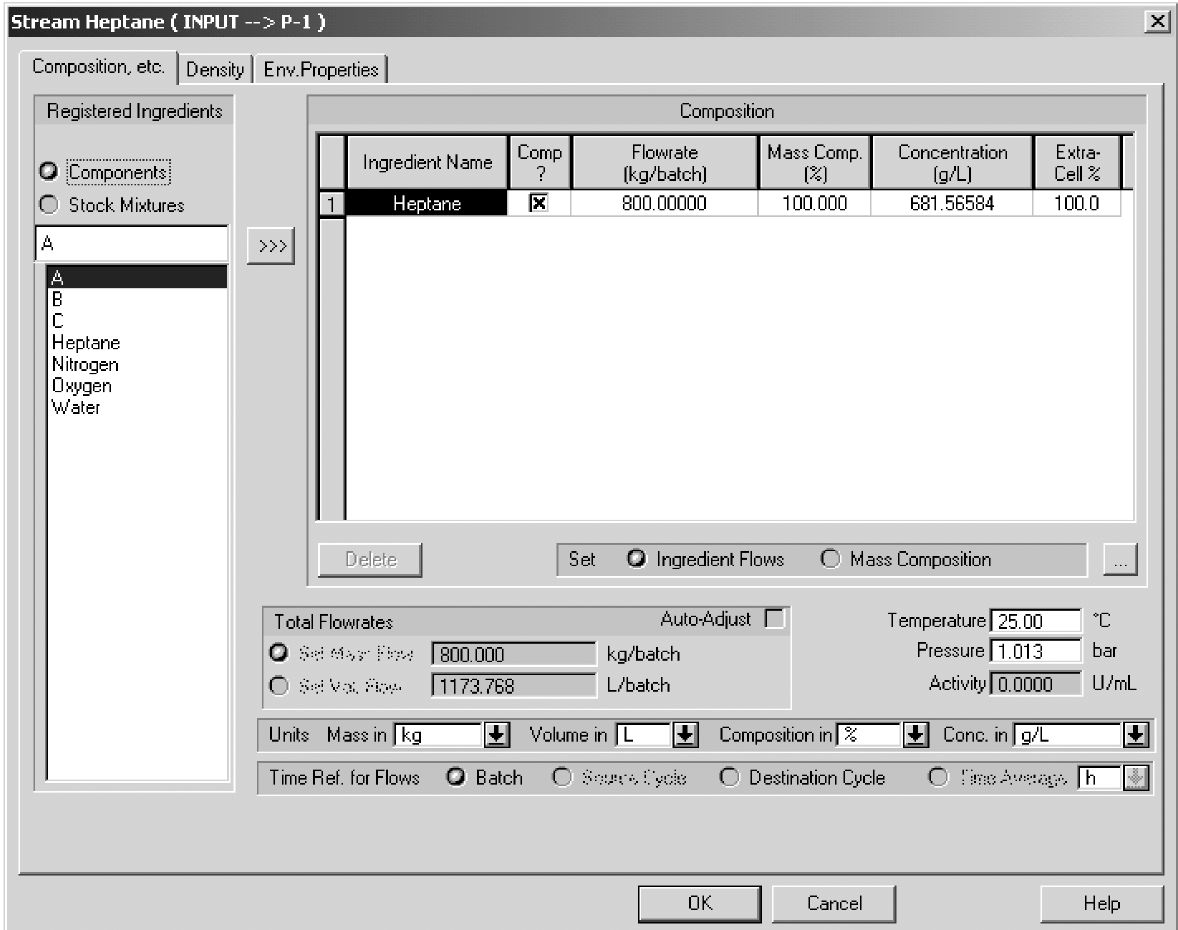


Figure 2.1-p: The Heptane stream dialog.

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) Some operations (e.g., cake wash, column elution, etc.) that utilize input streams automatically calculate the amount of material that they require. In such cases the user only needs to specify the composition of an input stream; its total flow can have any positive value.
4) In addition to pure components, mixtures can be fed (or “charged”) into a process step using an input stream.
5) 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.
6) 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 plant is set in 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.
7) The **Env.Properties** tab of a stream dialog displays the concentrations and daily throughputs of the environmental and aqueous properties of the stream (TOC, CaCO3, 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: Register Components & Mixtures : 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 **Emissions**, **Labor etc**, and **Scheduling** tabs to see what they contain. A brief description of each of these tabs follows:

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 %.

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.

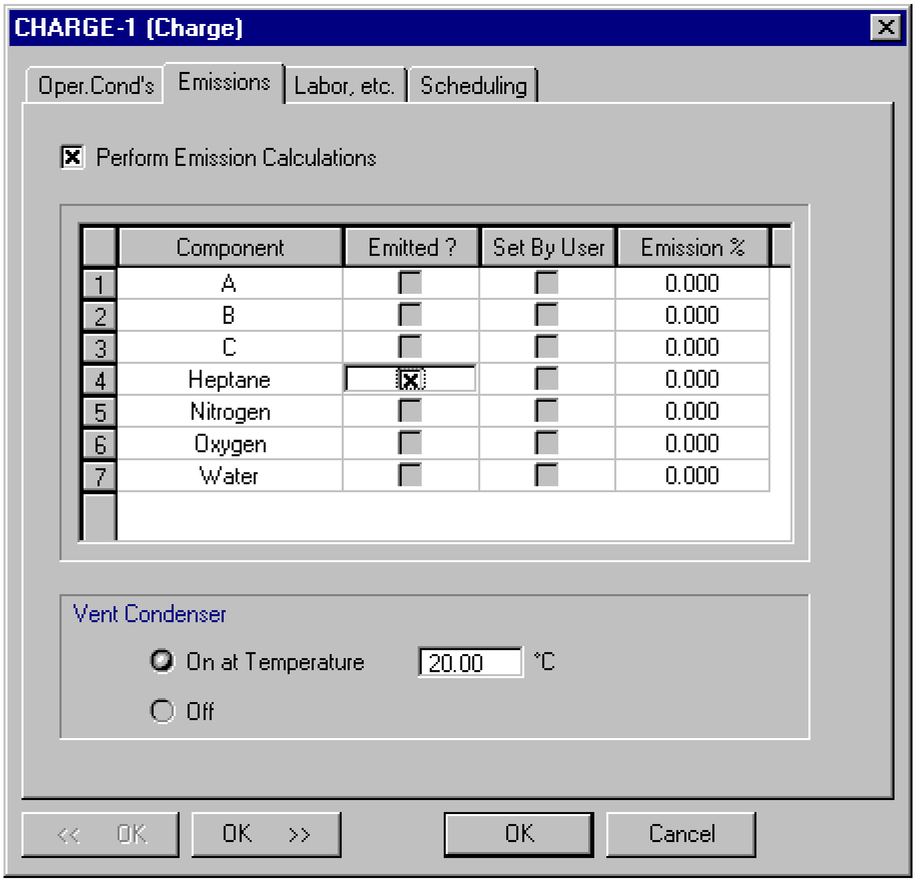


Figure 2.1-q: The Emissions tab for the heptane charge.

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 the same way as before, 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 (**Volumes**, and **Reactions**) are present in the Operation Data dialog (more detailed information on reaction operations can be found in the second example that deals with a Synthetic Pharmaceutical process).

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).

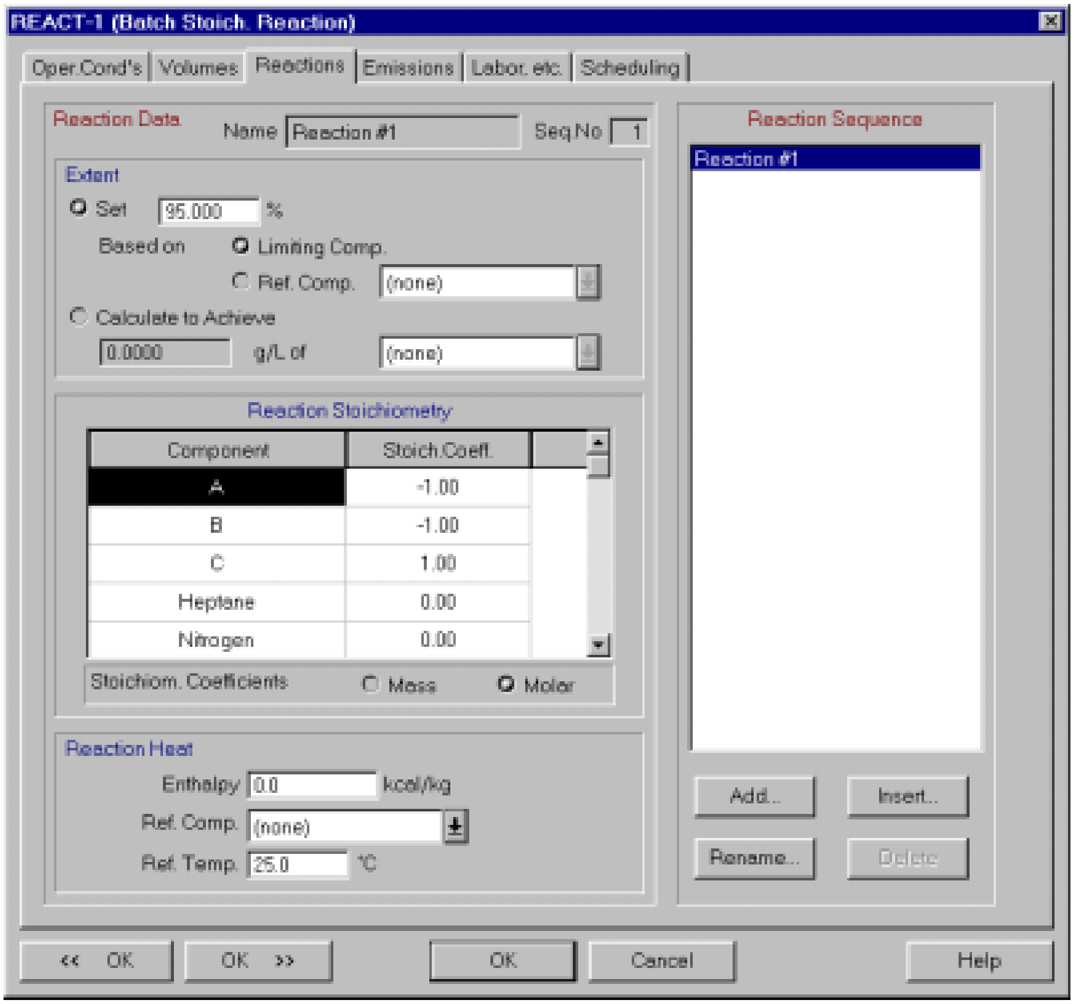


Figure 2.1-r: The Reactions tab.

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 each molecule of product (C):

$$A + B \rightarrow C$$

To enter this, select the molar stoichiometric coefficients option and enter -1, -1, and 1, respectively, for A, B, and C. For more information on specifying reaction coefficients, please see Chapter 2.2. In addition to specifying the stoichiometric coefficients, you will need to specify the extent of reaction. For your 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 menus at the top of the screen to specify which stream line will be used for the transfer operation, and what the destination unit procedure will be (see below). 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). This will ensure that the reactor will still be considered "utilized" during the 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.

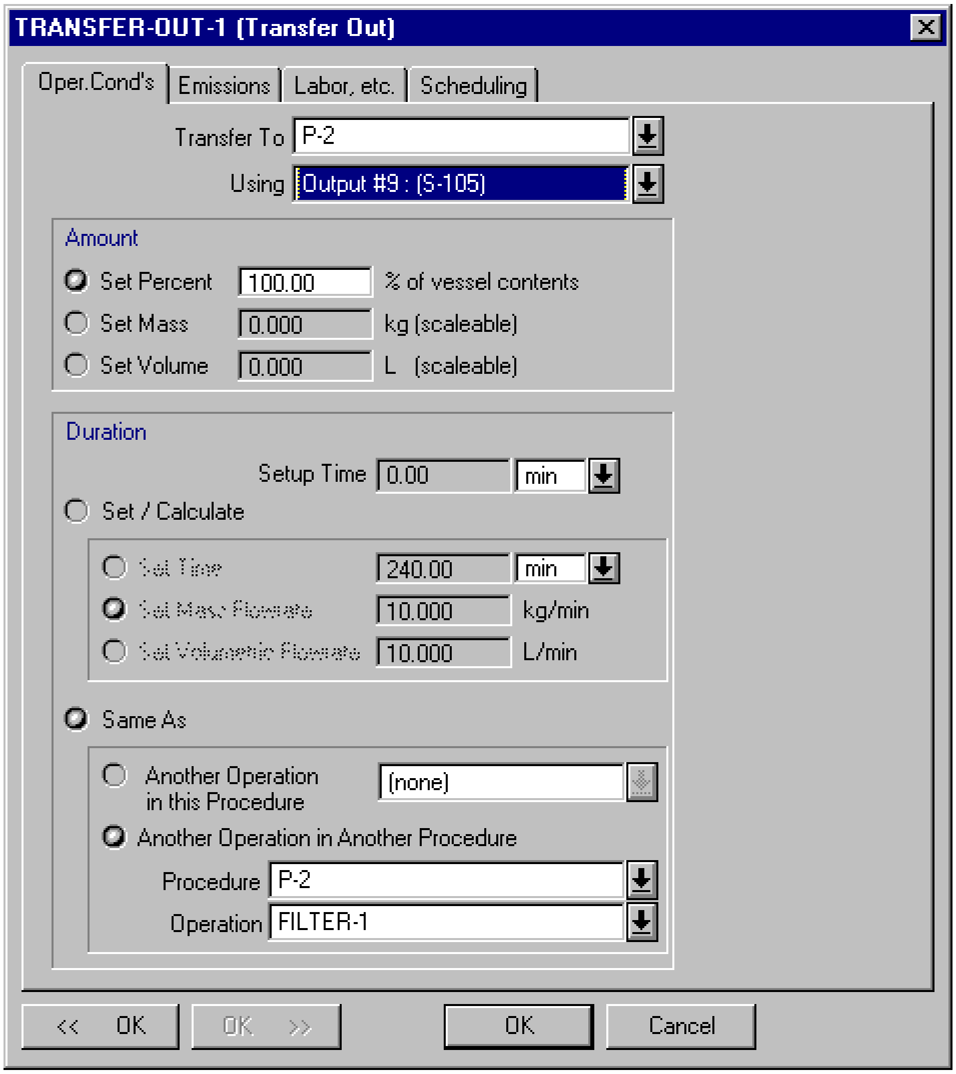


Figure 2.1-s: The Transfer Out operation dialog.

Kinetic Reactions (Optional)

Pro-Designer allows you to specify kinetic reaction parameters and to track the time profile of the reactant and product concentrations. The follow comments describe this process. *You may wish to skip this portion and return to it after having completed the remainder of this section.*

To try out the kinetic reactions feature and select the reactor vessel and add a kinetic reaction operation *before* the existing reaction operation. Next, edit the operation for the new reaction operation (right-click **Operation Data**). The reaction tab on operation dialog allows you to fill in the stoichiometry but *not* the extent of reaction. Instead, there is a **Kinetic Data…** button that brings up the following dialog.

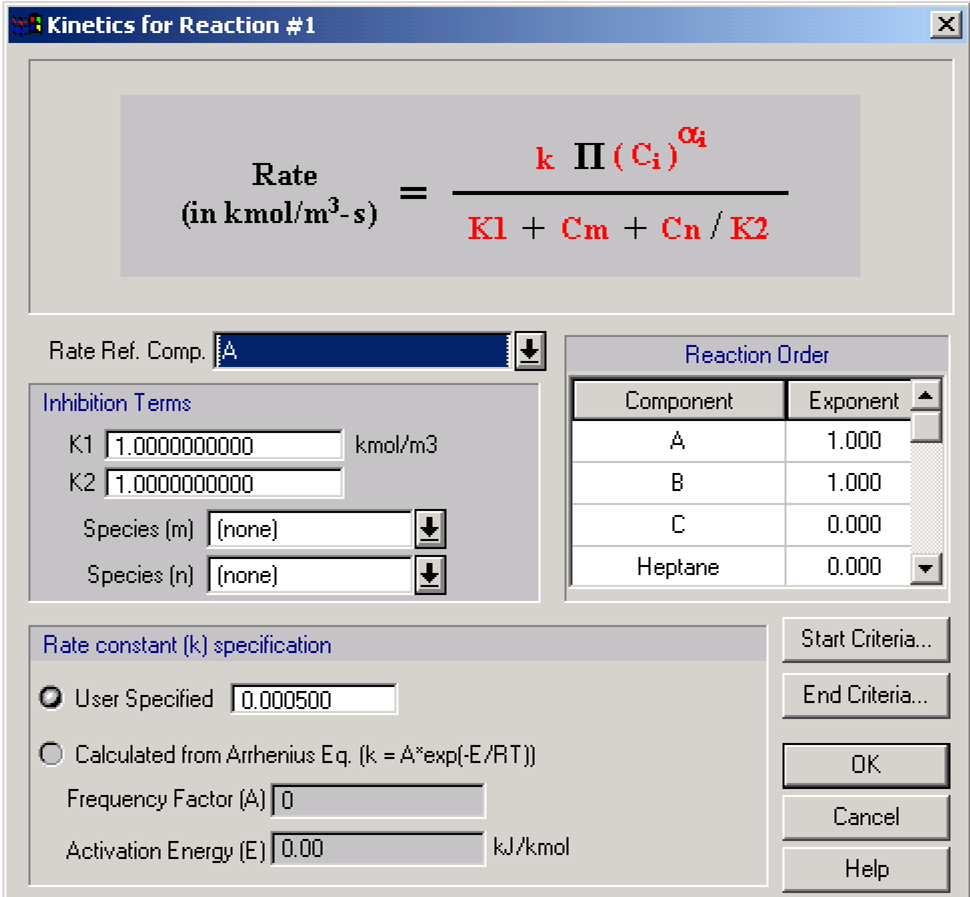


Figure 2.1-t Kinetics dialog of a kinetic reaction operation.

This dialog allows you to enter the kinetic data. In this case you may enter the parameters for the reaction, A + B➔ C. Leave the inhibition terms at their default values and do not specify any inhibition species. Pro-Designer allows for the entry of temperature-dependent rates, but in this case, you should enter a fixed rate constant of 0.0005. Set the exponents for all the species to appear in the rate expression and select OK.

The Profiles tab of a batch kinetic reaction operation that enables the user to specify the variables whose values will be recorded as a function of time.

After solving the material and energy balances click V-101 and select **Dynamic Data Records** ➔ {operation name} ➔ {view data or save data in ASCII or Excel format}. Please note that the "Dynamic Data Records" menu item is present only in procedures that include operations that can generate profiles. Future versions of Pro-Designer will include their own plotting capability and there will be no need to export the data to Excel.

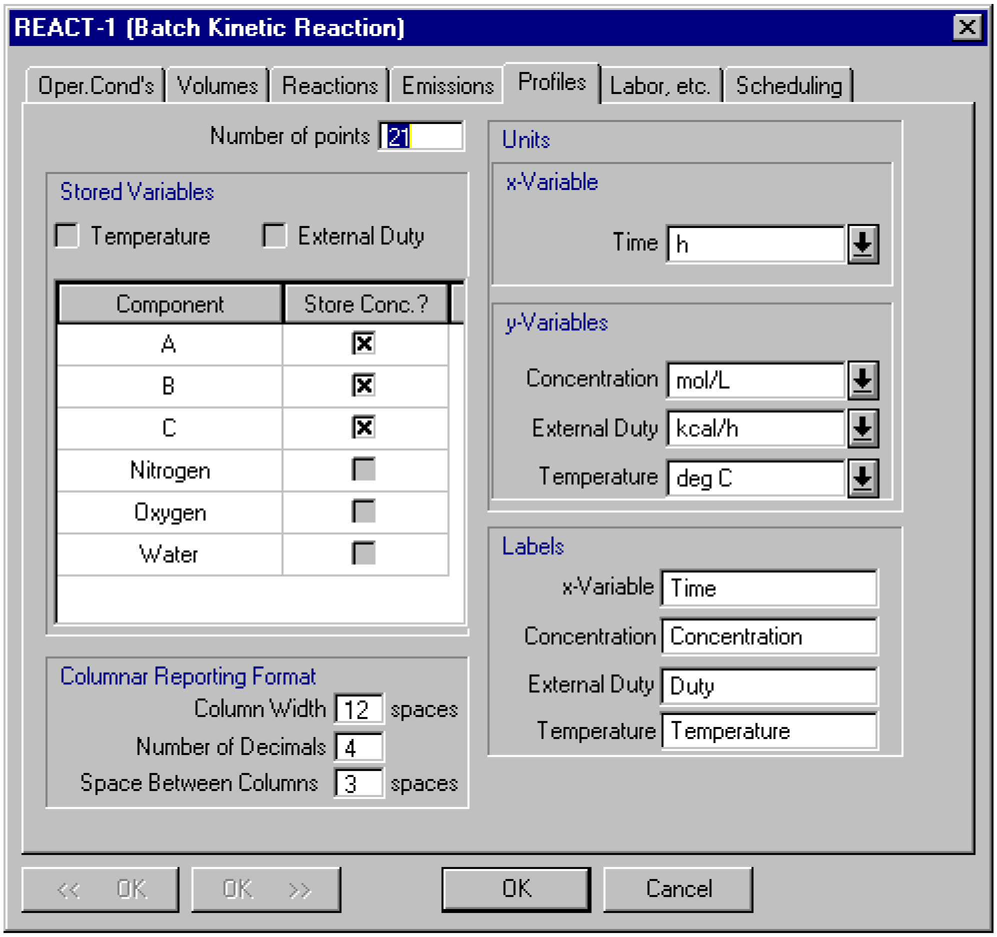


Figure 2.1-u The Profiles tab of a kinetic reaction operation.

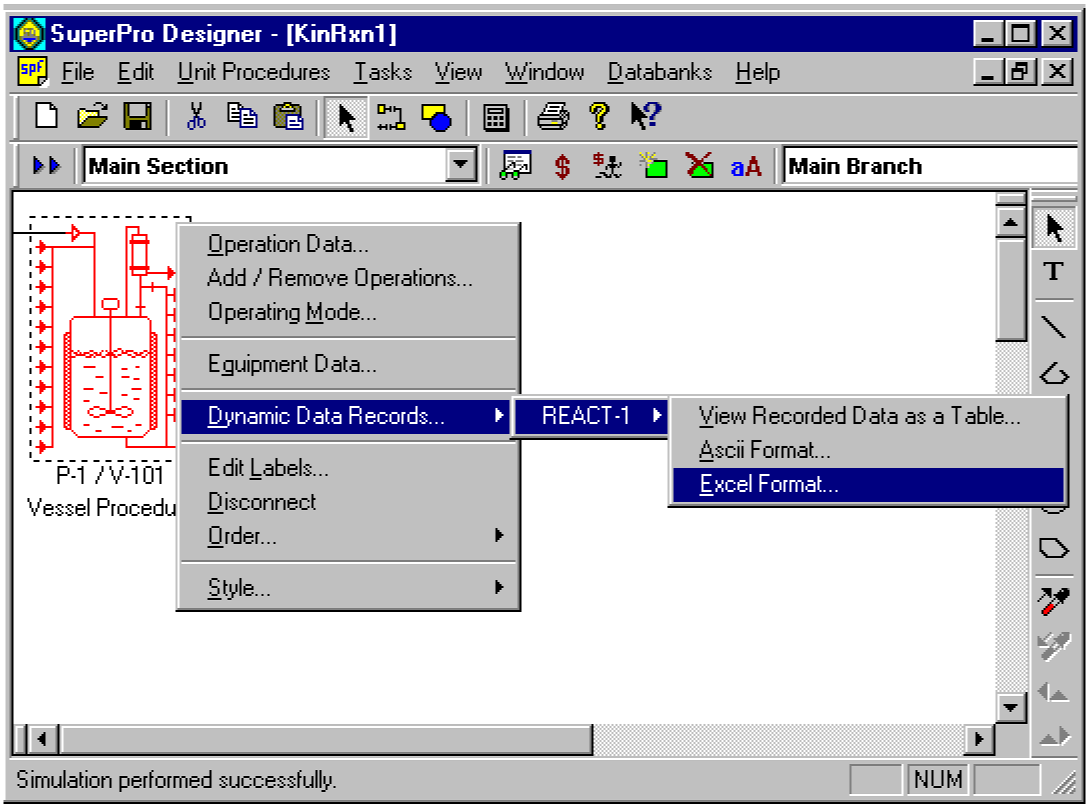


Figure 2.1-v: Generation of Profile data for a batch kinetic reaction.

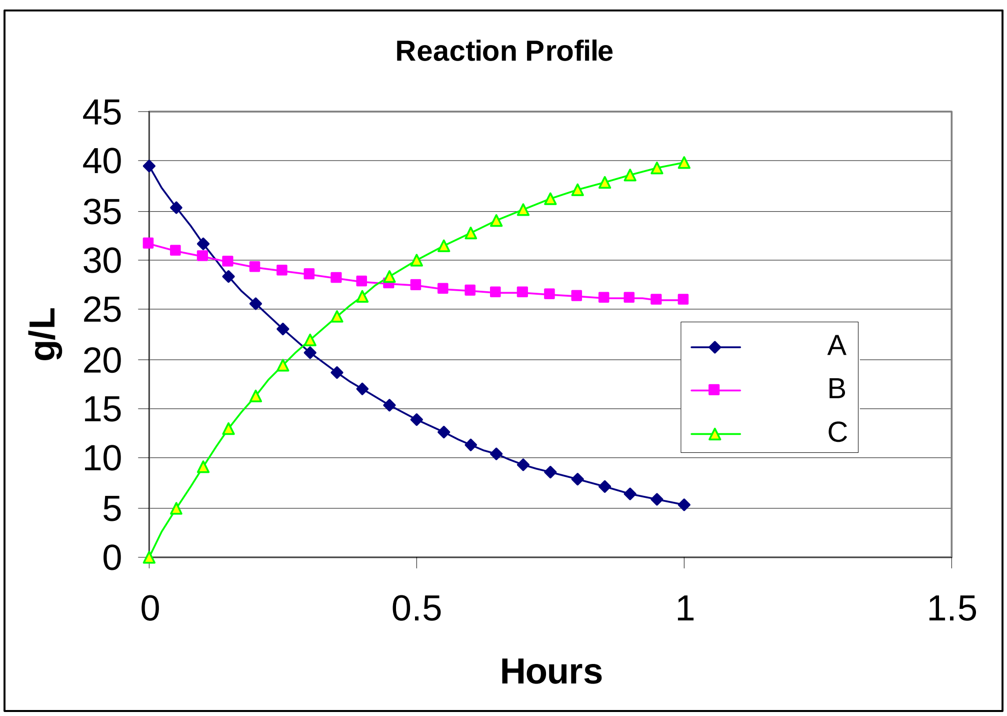


Figure 2.1-w: Reaction Profiles (from Excel)

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 (everything else has 0% removed). 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.

Next, please visit the Scheduling tab of the filtration operation. This tab is common to 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).

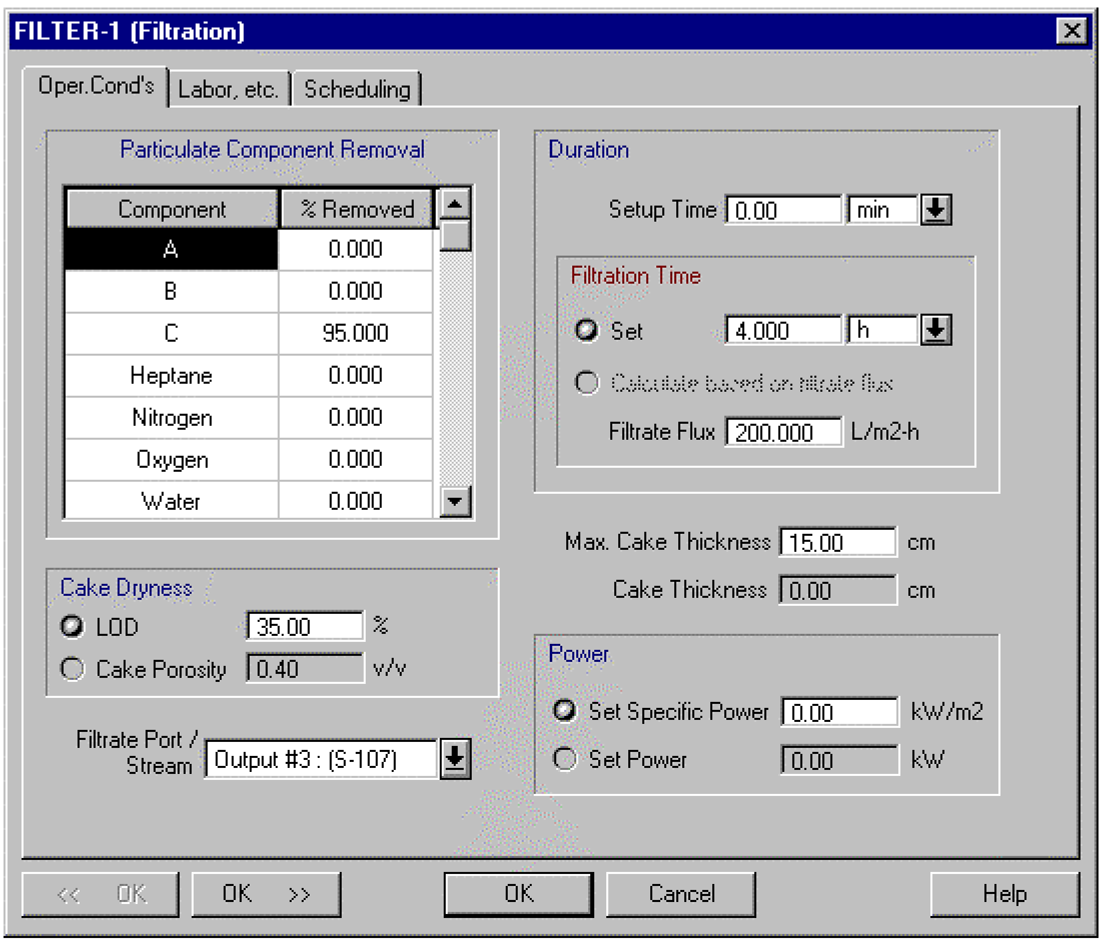


Figure 2.1-x: The Filtration operation dialog.

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 **Edit Composition** button and select Heptane. You will also need to enter a value for the amount of Heptane used (although the program will override this value later during simulation). 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**.

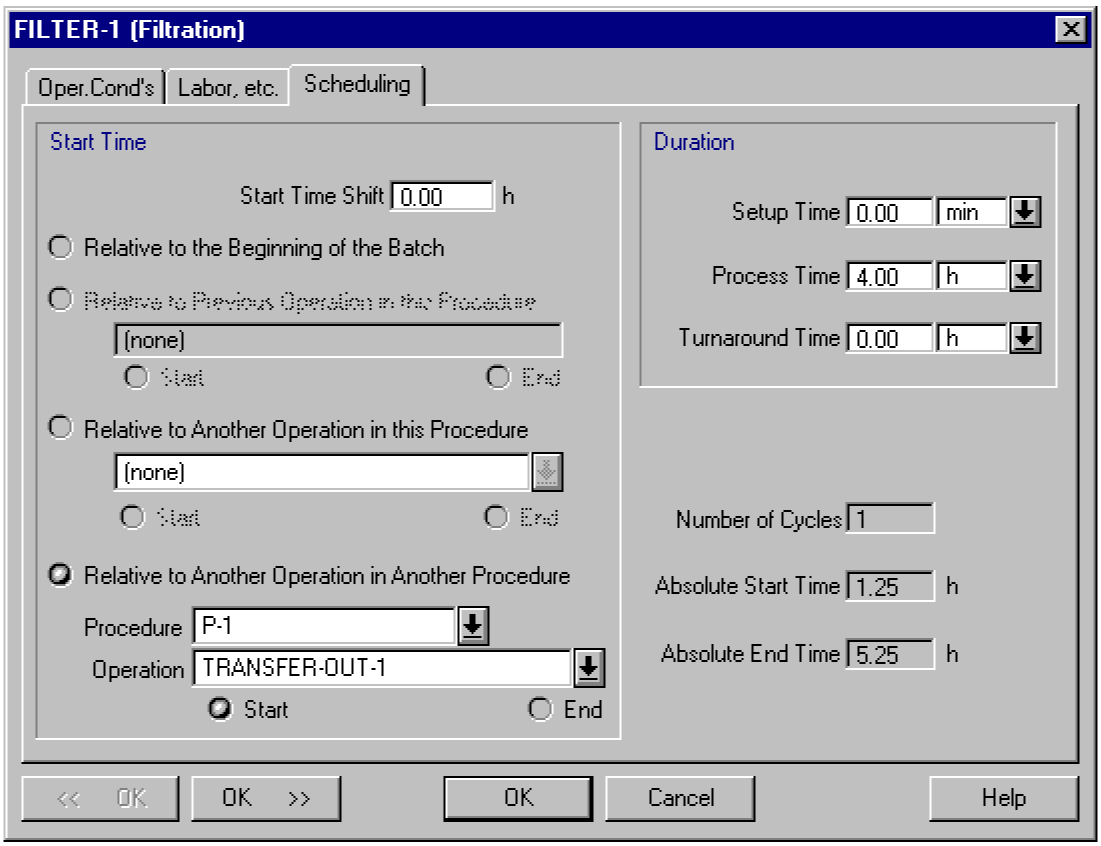


Figure 2.1-y: The Scheduling tab of the filtration operation.

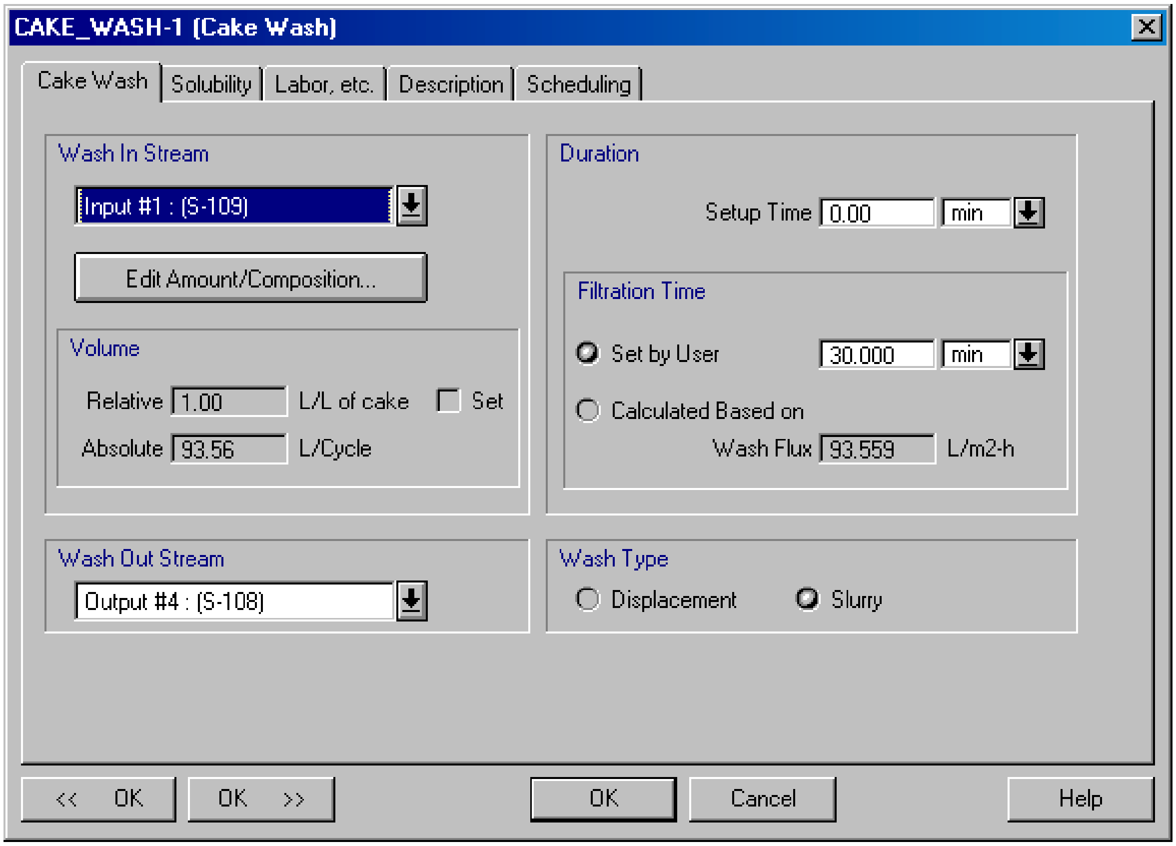


Figure 2.1-z: The Cake Wash dialog.

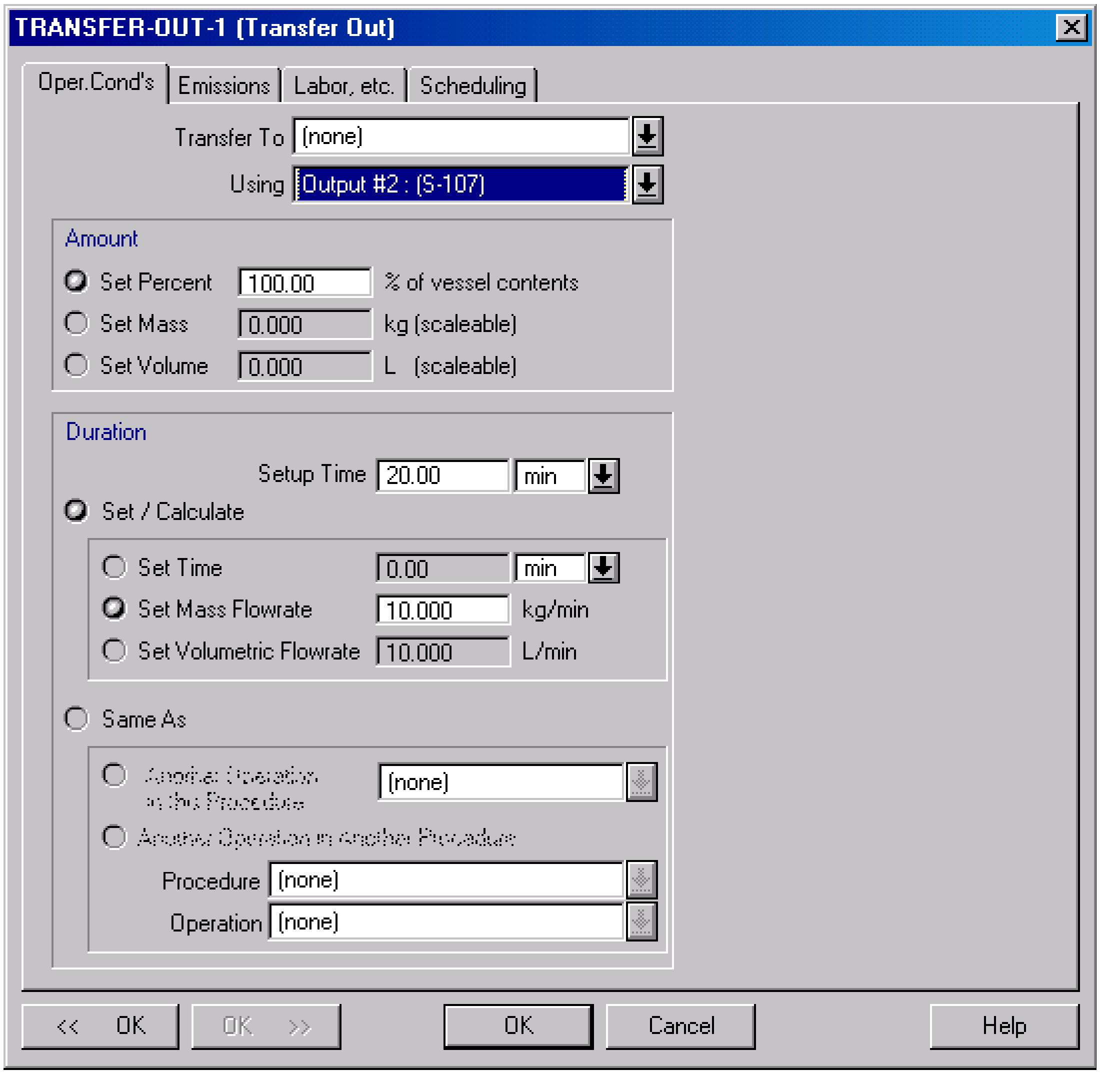


Figure 2.1-aa: The Transfer Out dialog.

You have now finished initializing the operations and streams for this example flowsheet. Use the **File: Save All** 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:

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 by selecting the **Tasks: Generate Stream Report (SR)...** option from the main menu. The resulting report can be viewed by selecting the **View: Stream Report** option of 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 the Stream 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 **Edit: Flowsheet Options: Preferences: Stream Report Options**. In order to access this dialog, be sure that the flowsheet window is not maximized and that no equipment is selected.
5. To see the calculated equipment sizes, right-click on a unit procedure icon and choose the **Equipment Data…** option. Through this tab, you can provide information for equipment sizing, selection, and purchase cost estimation (the cost estimation features will be explained in greater detail later in this chapter). 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 volume 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 1.46 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**, 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 2 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).

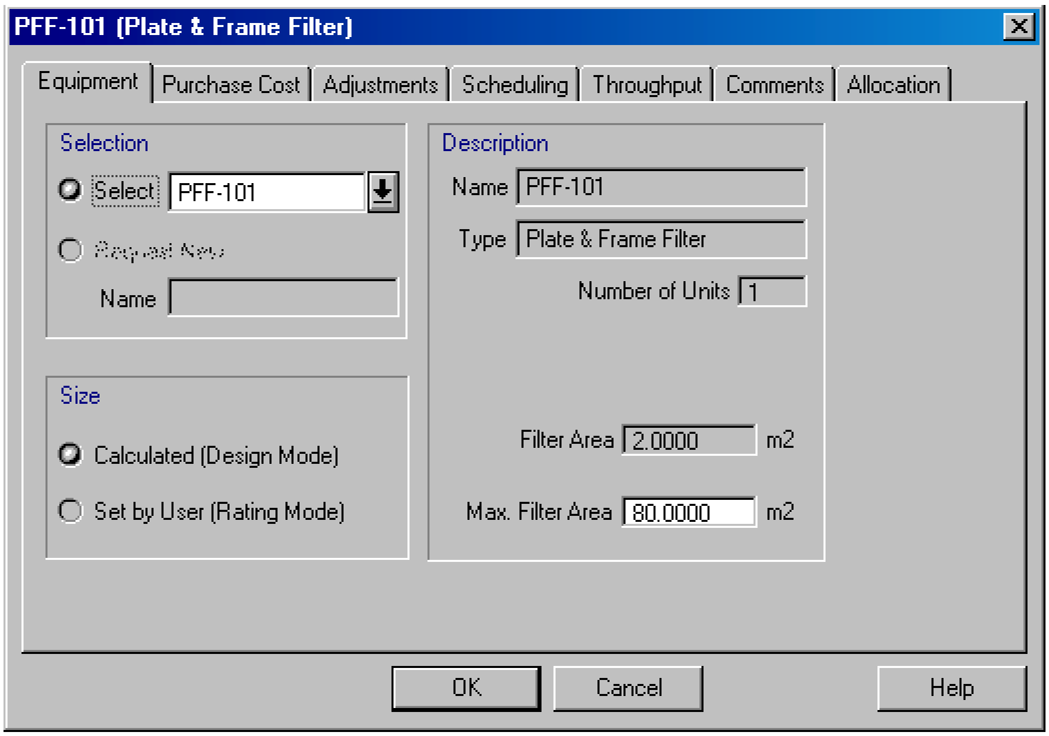


Figure 2.1-bb: The Equipment Data tab of the Plate & Frame Filter.

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, 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.

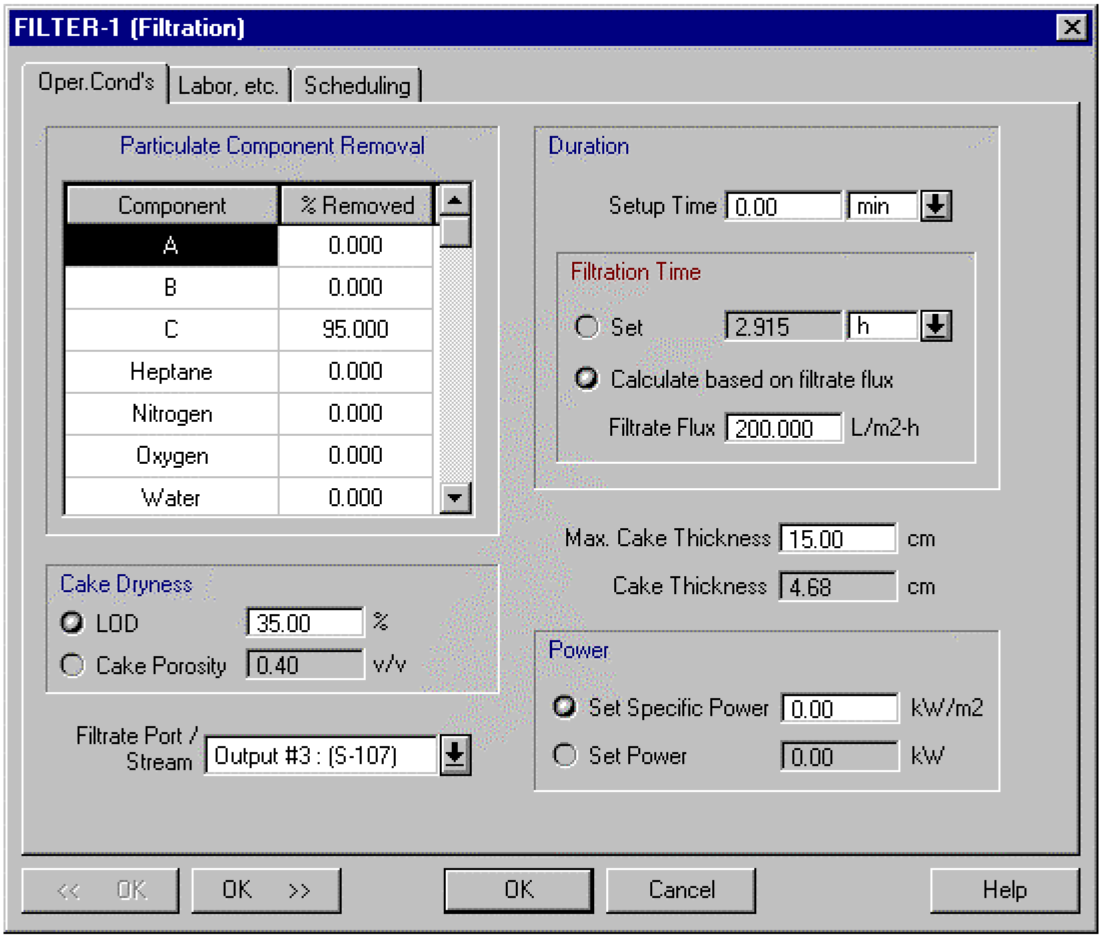


Figure 2.1-cc: Dialog of the Filtration Operation (when the Equipment is in Rating Mode).

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

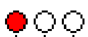
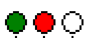
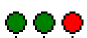
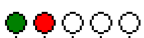
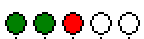
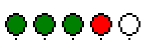
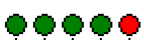
   has been successfully simulated already

   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/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.
Effective Batch Time: The time between batch starts. Sometimes called the recipe or plant cycle time.
Minimum Effective Batch Time: The minimum time between batch starts based on the time (scheduling) bottleneck.
Effective Batch Time Slack: The difference between the actual and minimum effective batch times.

If you have specified the entire plant's mode of operation as batch, 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 effective batch time, or

g3. the effective batch 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 plant 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 for an entire plant, select **Tasks: Recipe Scheduling Information...** (see Figure 2.1-dd below).

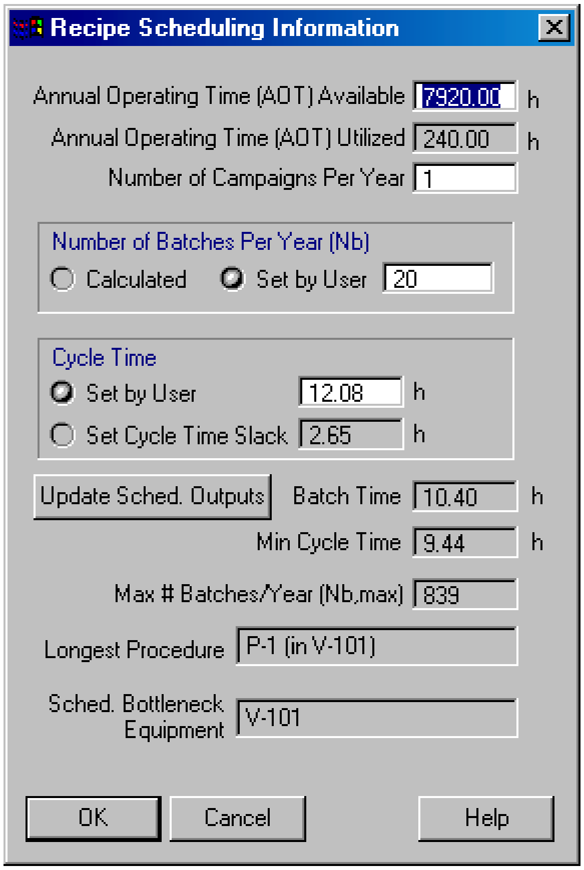


Figure 2.1-dd: Specifying the scheduling information for a batch flowsheet

For your example process, please change the "Set # Batches/Year" field 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 effective plant batch time (as calculated from all the procedures).

3. Calculate the plant's batch time, the plant's effective batch time, the plant's minimum effective plant 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 & SIP skids) Equipment Utilization 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.

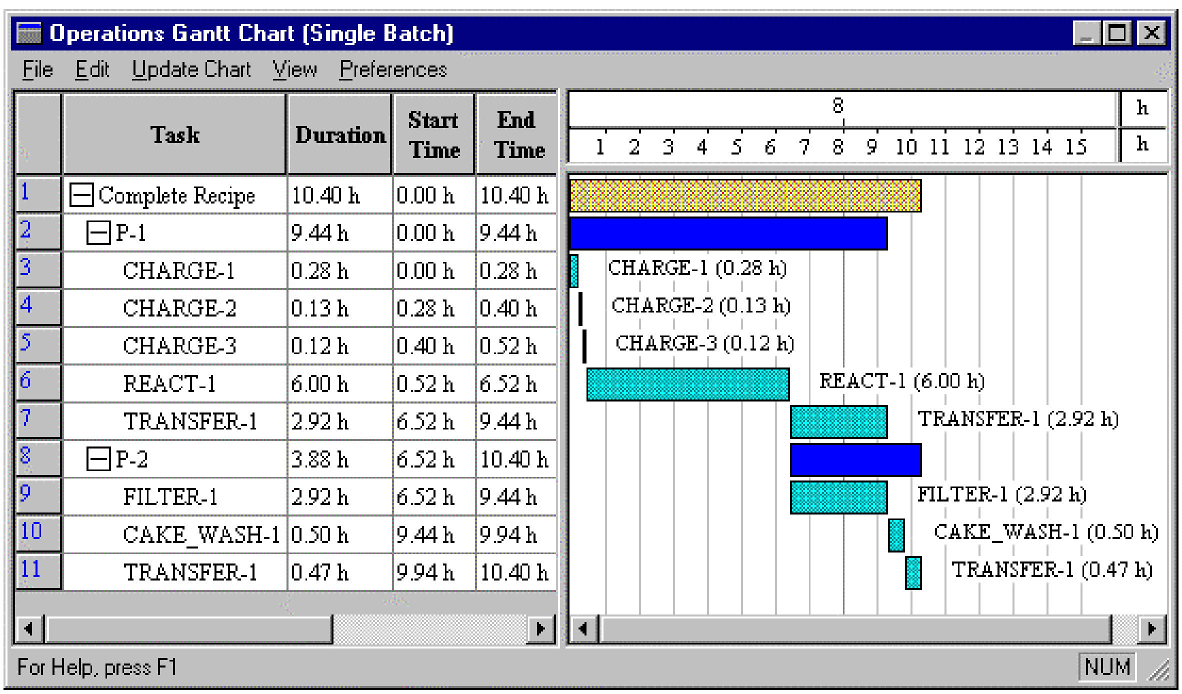


Figure 2.1-ee: The Operations Gantt Chart.

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 plant (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: Main Equipment (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. Effective Plant Batch Time). The actual time between consecutive batches (also known as Effective Plant Batch Time) is 12 hours.

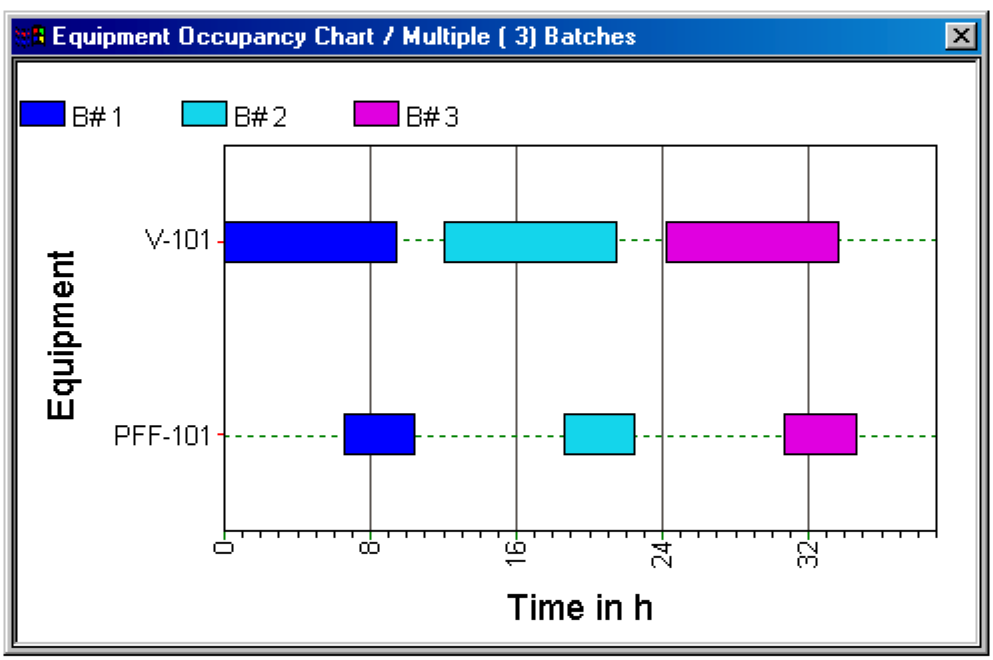


Figure 2.1-ff: Equipment Occupancy Chart (three consecutive batches).

Pro-Designer also generates utilization charts for auxiliary equipment, such as clean-in-place (CIP) and steam-in-place (SIP) skids.

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.

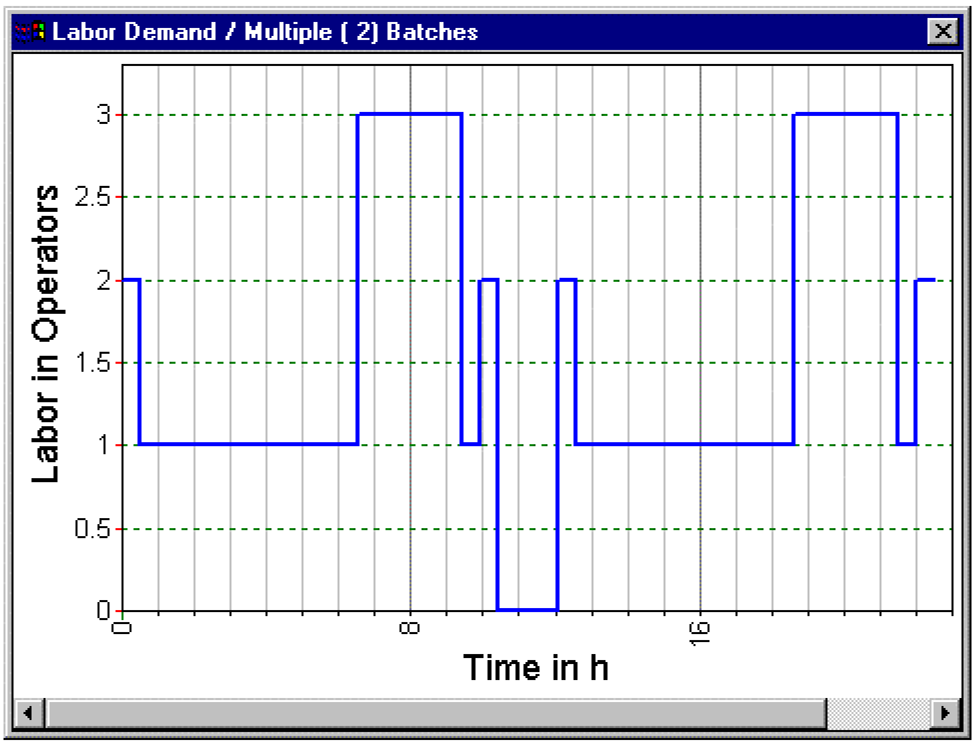


Figure 2.1-gg: The Labor Resource Tracking Chart for the example process

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.

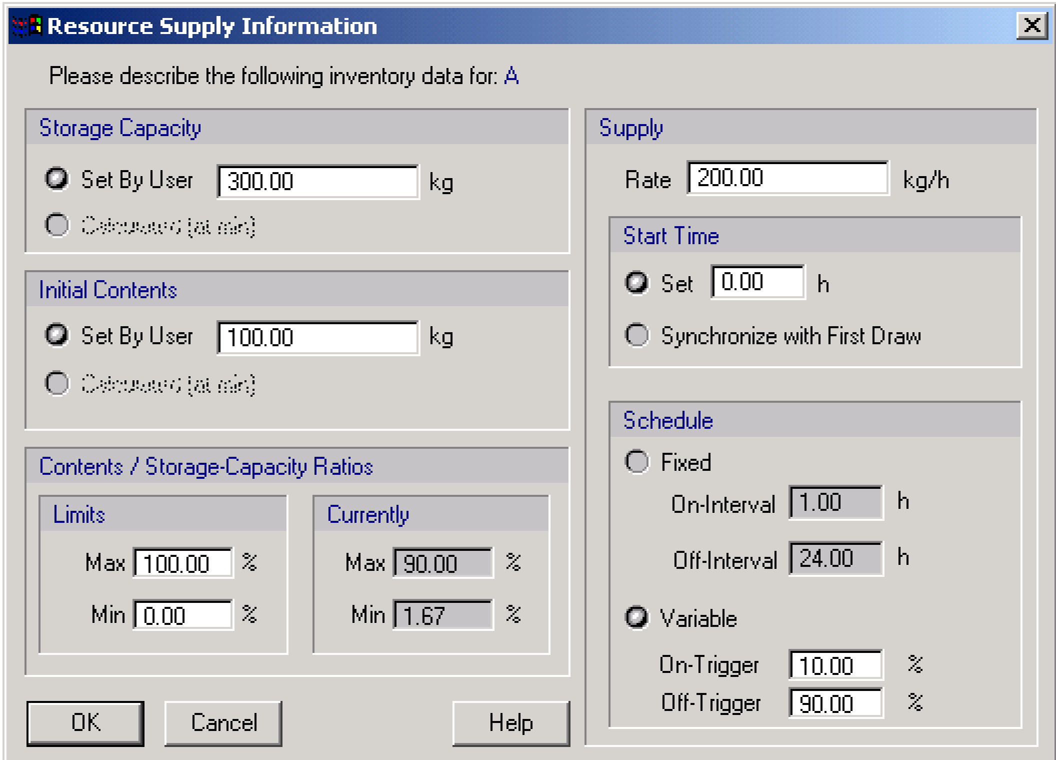


Figure 2.1-hh: The Ingredient Resource Supply Dialog

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.

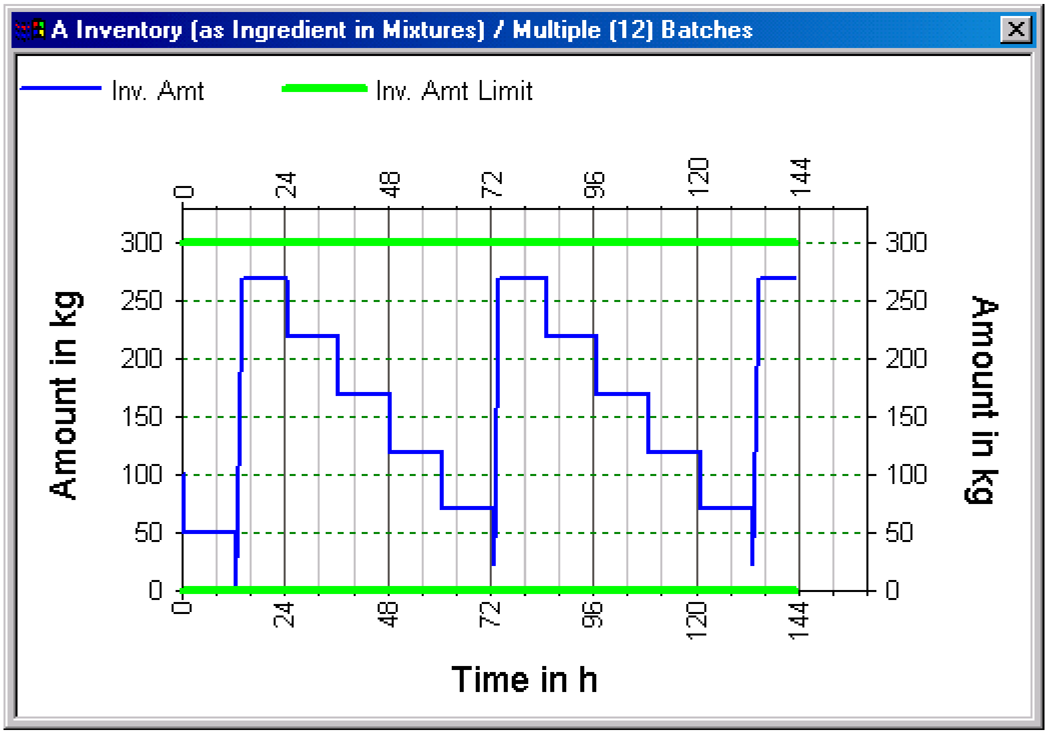


Figure 2.1-ii: The Inventory Profile of Component A

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 product/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. Solve the model and select **View: Throughput Analysis Charts: Utilization**. The utilization chart below will appear.

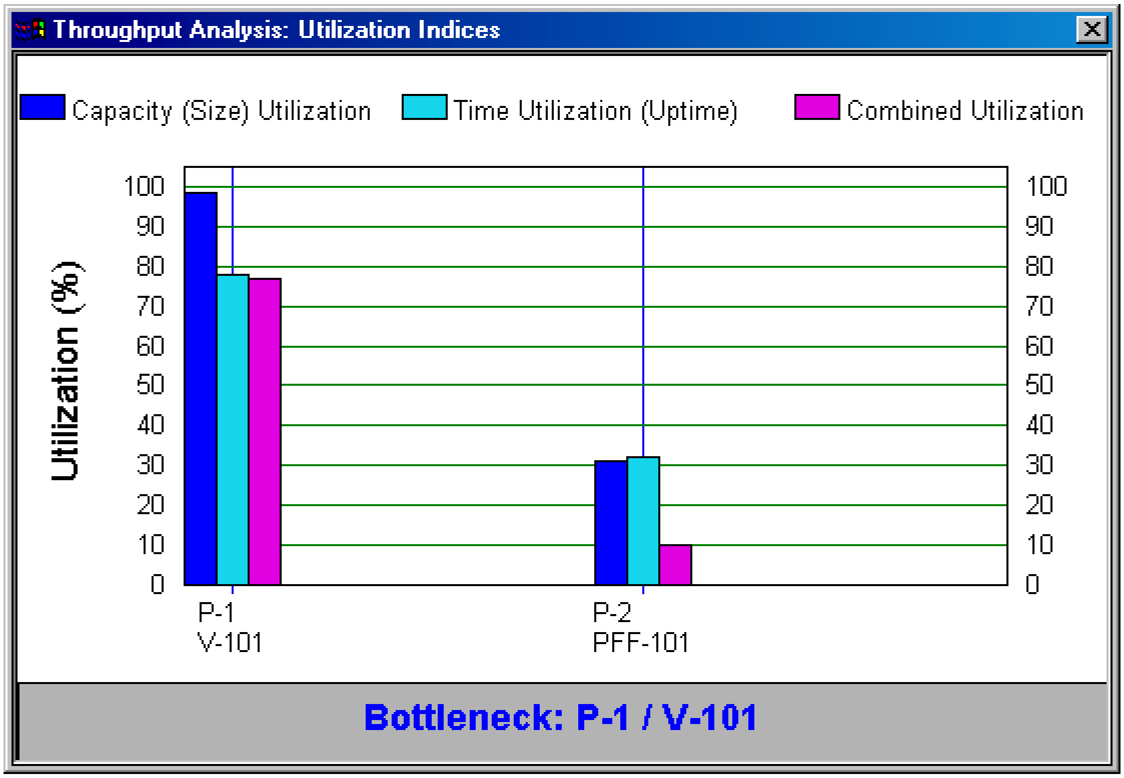


Figure 2.1-jj: Equipment Capacity/Time Utilization Chart

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. In this case the equipment is at capacity, which is not surprising because the model calculated the minimum sizes in rating mode. Also the time utilization is somewhat low because some slack time was introduced.

Select **View: Throughput Analysis Charts: Potential** to view the throughput potential chart below.

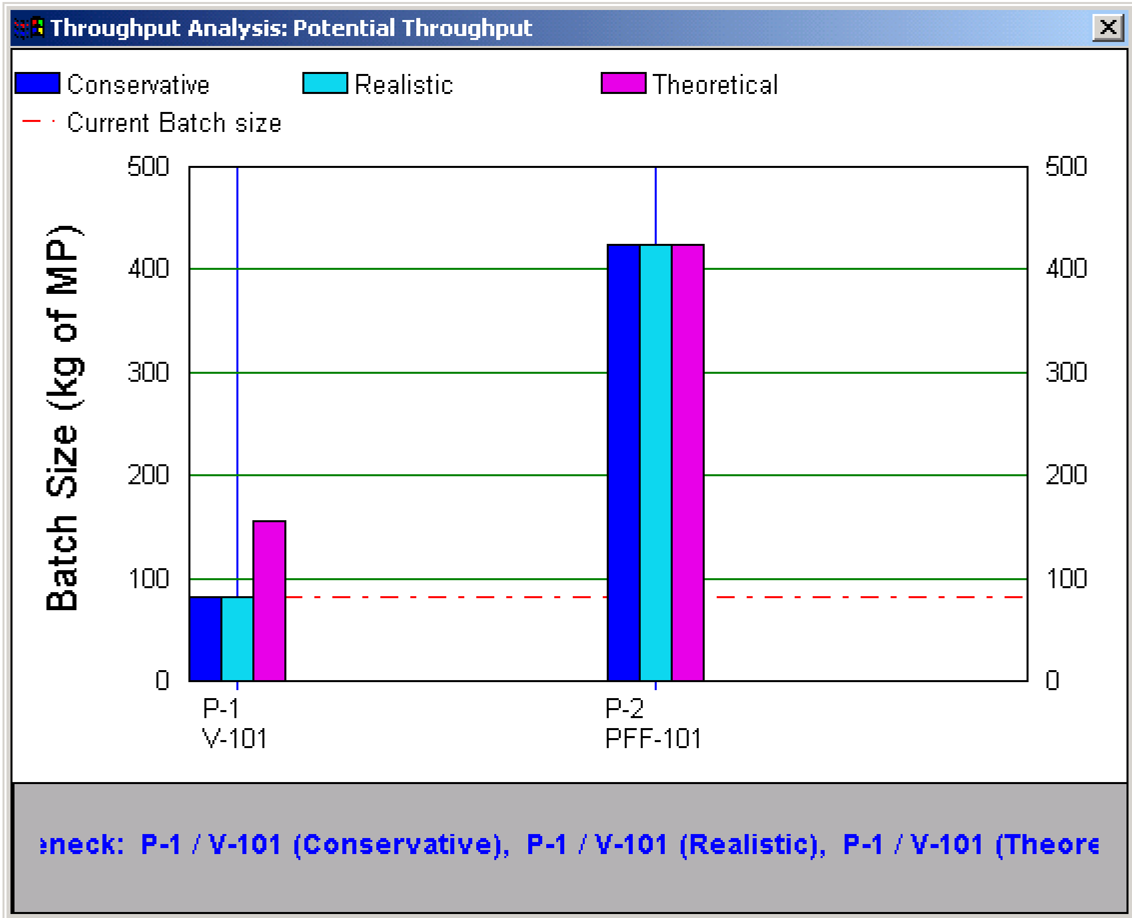


Figure 2.1-kk: Throughput Potential Chart.

This chart shows the potential and actual 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 two 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: Revenue, Raw Material and Waste Streams...** 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, liquid 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 your 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 $200/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).

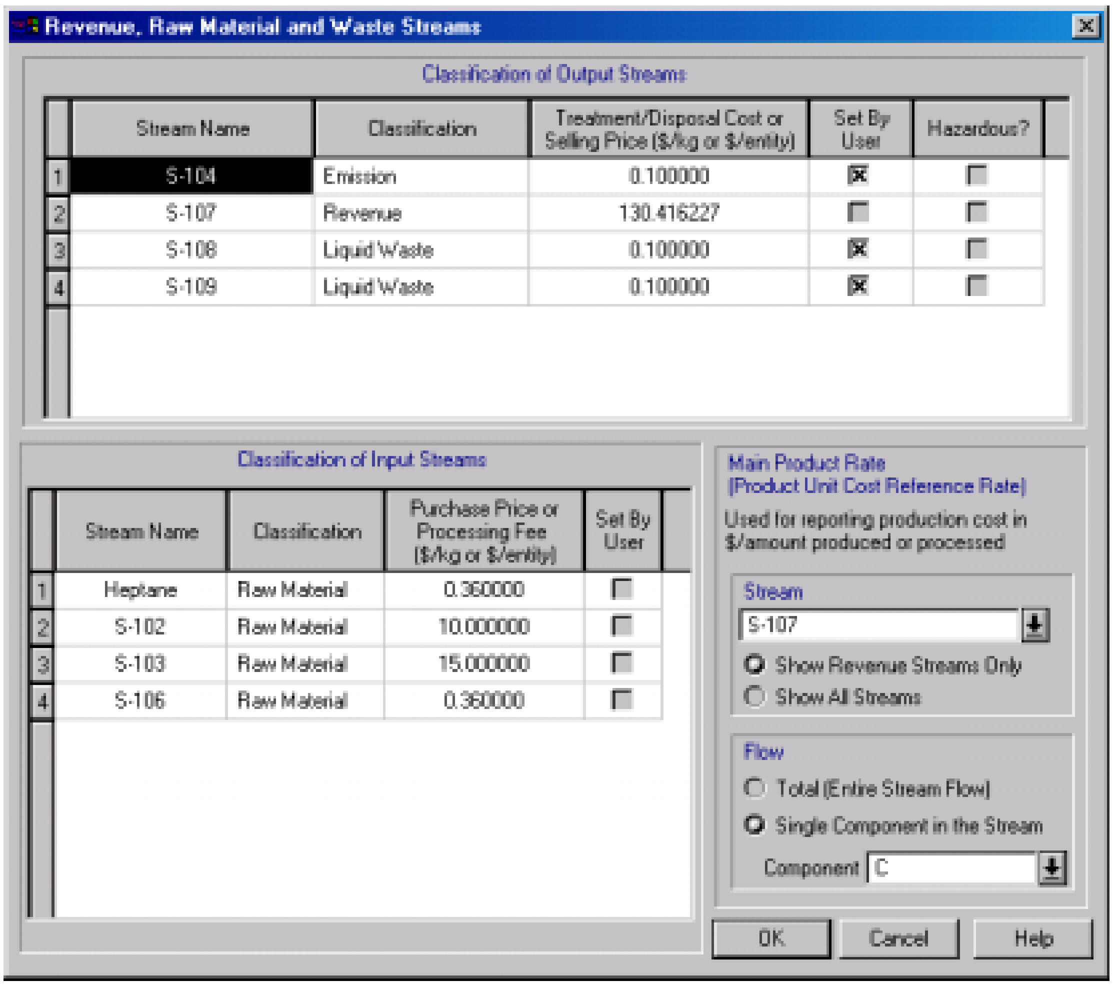


Figure 2.1-ll: The Revenue, Raw Material and Waste Stream dialog box

Note: Classification of a stream as a solid, liquid 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. Variables that affect cost of Consumables (e.g., resin replacement for chromatography columns) are also 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 and Maintenance Costs

These factors are used to estimate the installation and maintenance costs for each piece of equipment as a fraction of their purchase 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.

Usage and Availability Rates

This factor is used to estimate in a lumped way the equipment-dependent operating cost. Values are provided in $/hr of actual use or availability to a project.

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.

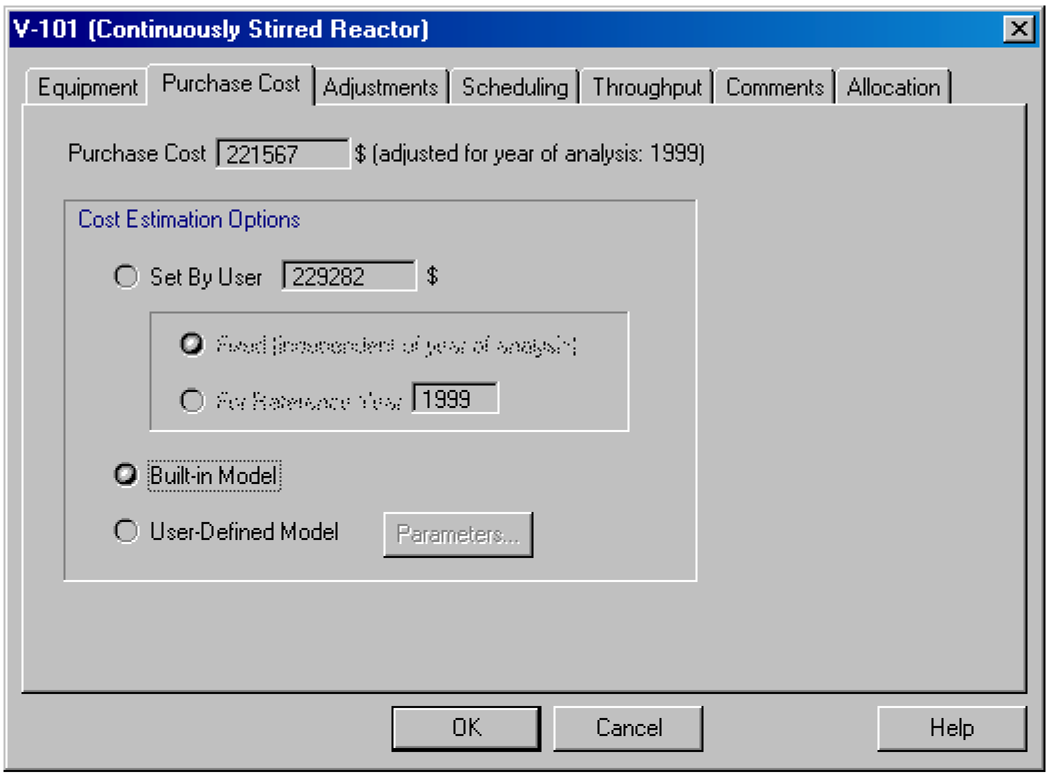


Figure 2.1-mm: The Purchase Cost tab of the Equipment Data dialog box

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.

b) Additional information on cost factors at the process step and equipment levels can be found in Chapters 5 and 8.

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 could also be accessed by right-clicking on a blank area of the flowsheet and selecting **Section (section name): Capital Cost Adjustments**.

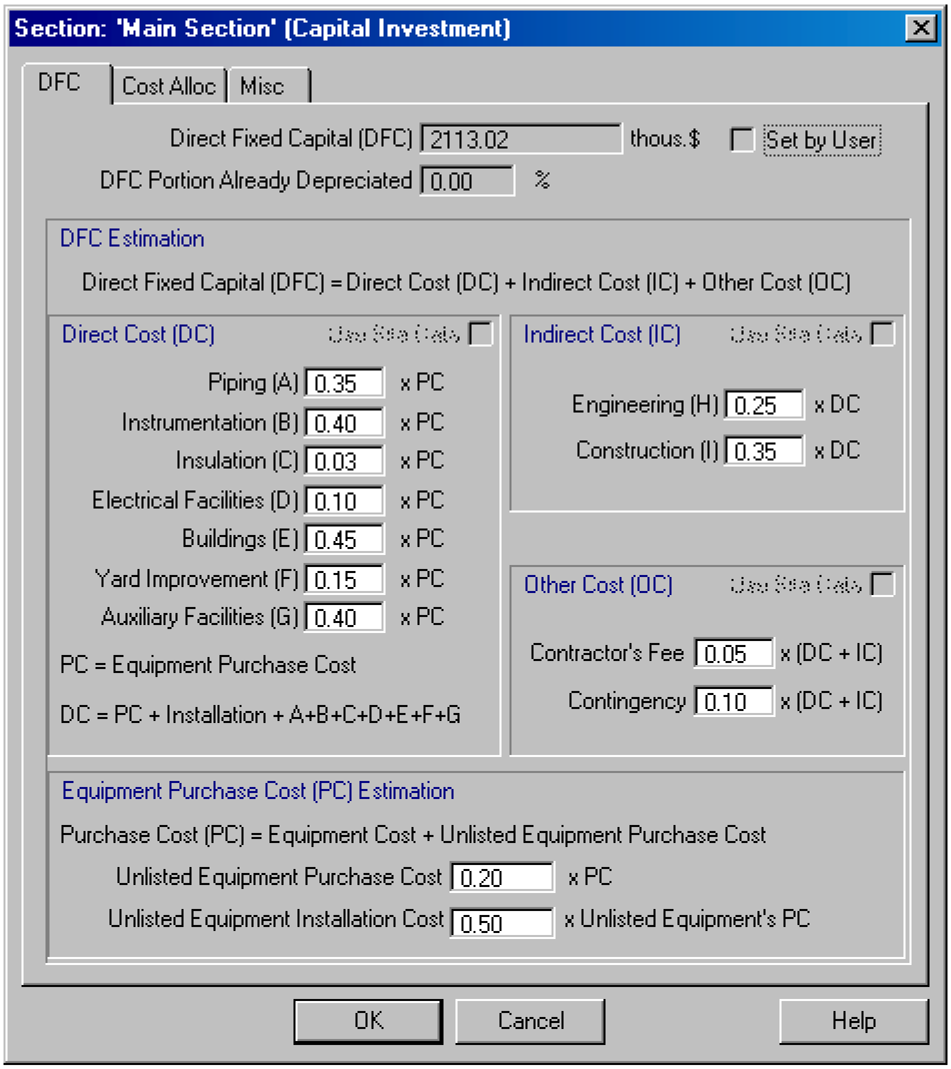


Figure 2.1-nn: The dialog box for Capital Cost Adjustments.

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.

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.

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.

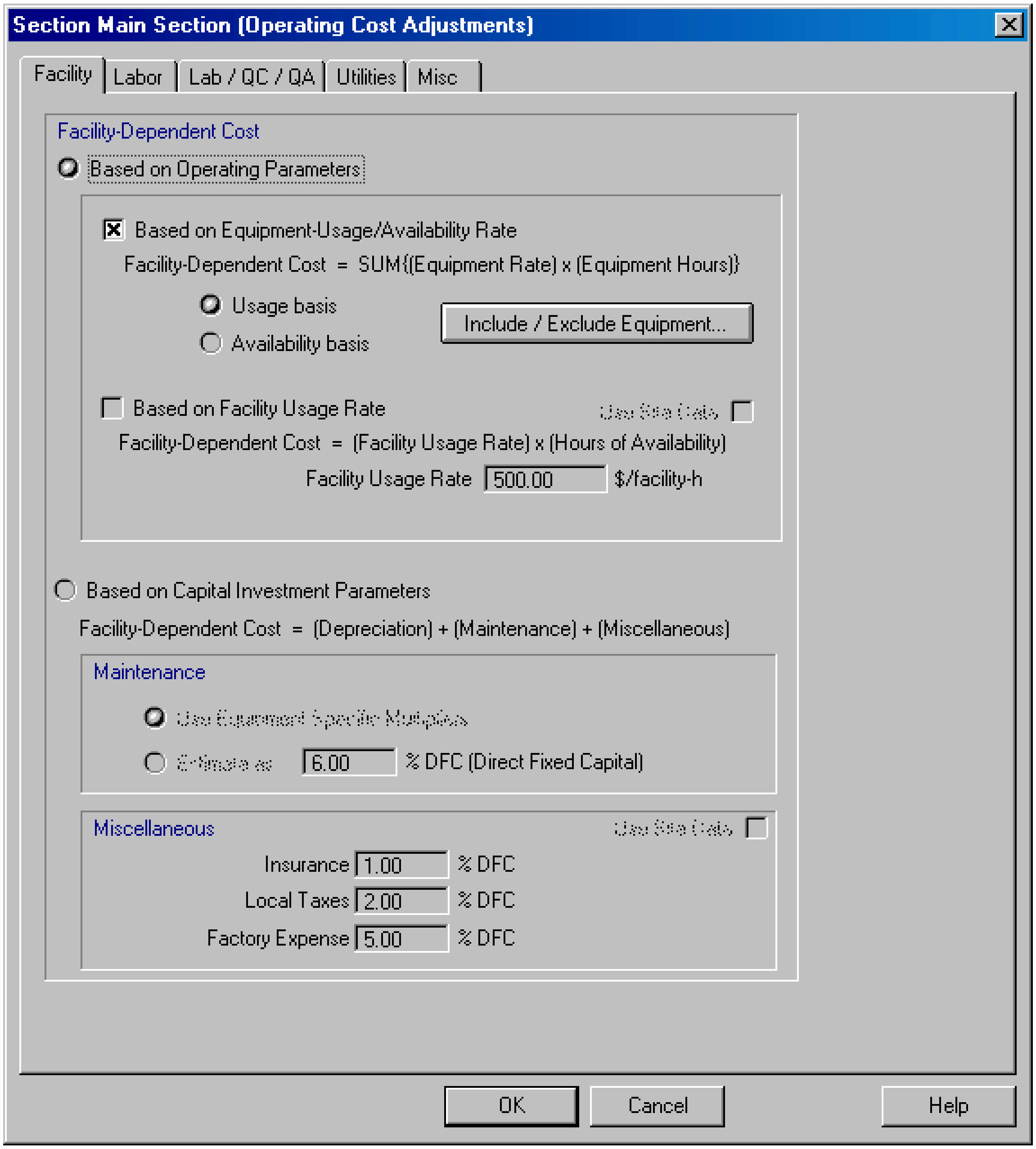


Figure 2.1-oo: The dialog box for Operating Cost Adjustments.

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 Equipment, 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.

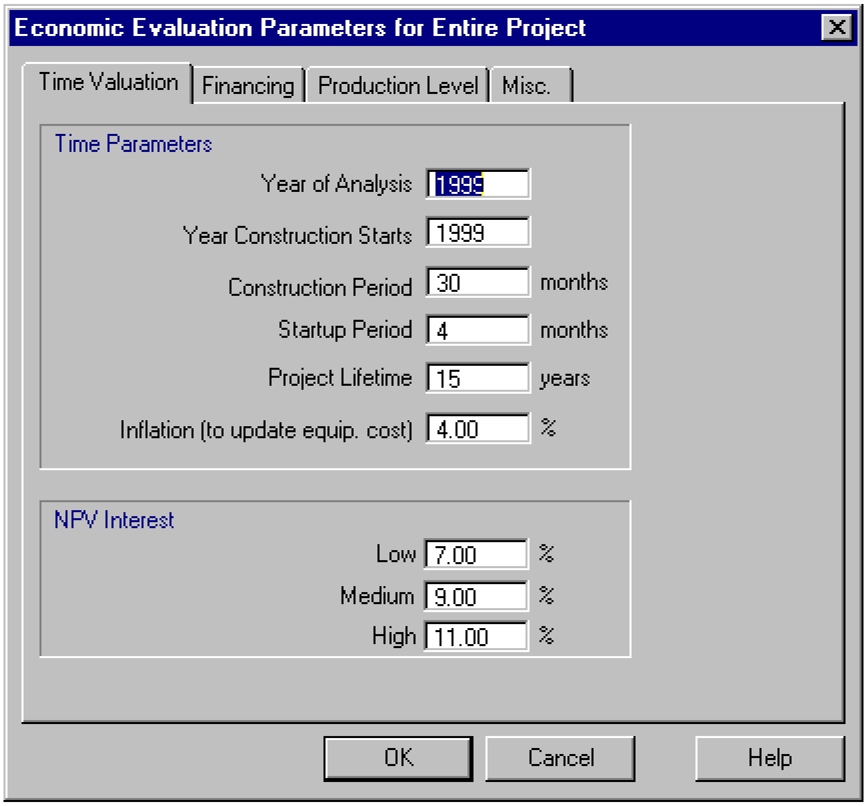


Figure 2.1-pp: Adjusting the economic evaluation parameters at the flowsheet level.

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**. Depending on your interest, you may then do the following:

1. View the equipment purchase cost for each process step by right-clicking the equipment icon, and then 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.
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 this report, select **Tasks: Generate Economic Evaluation Report**. To view it, select **View: Economic Evaluation Report**. Like the stream report, the EER is a text file which may be read by a variety of text editors and word processors. The same report (like any other report) can also be generated in spreadsheet format by selecting **File: Export Reports to Excel.** 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, a profitability analysis and cash flow analysis, loan information, and breakdowns of the capital outlay and loan payments. You can use the EER to make informed decisions about where to focus resources in the optimization of your process. It can also be used to perform realistic comparisons between various process scenarios (e.g. “what-if” scenarios and sensitivity analyses). 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.

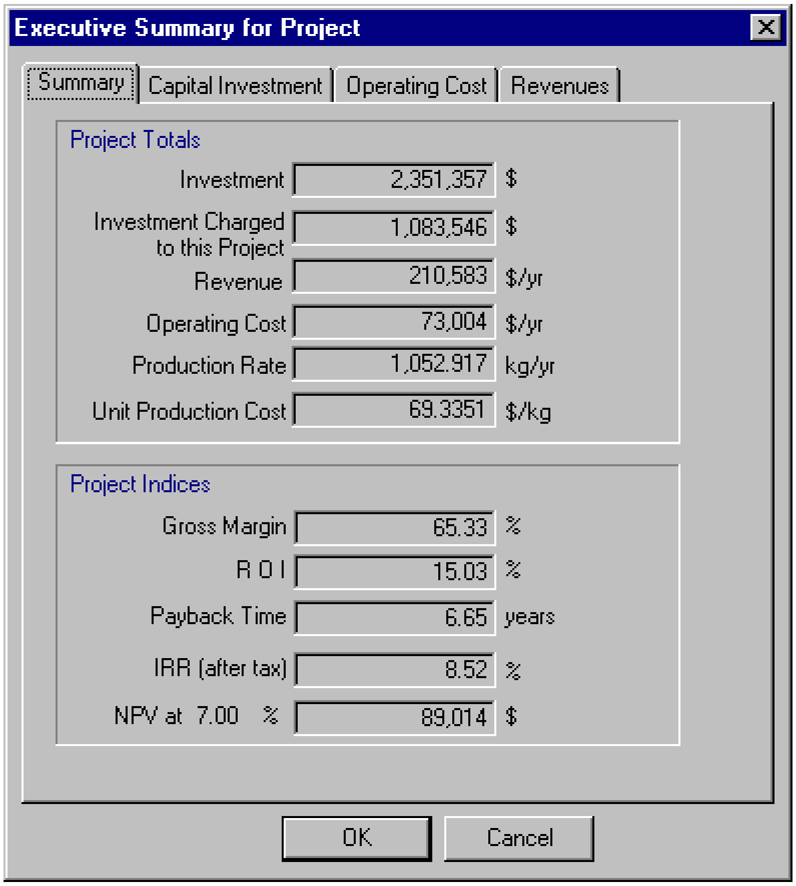


Figure 2.1-qq: The executive summary for the example flowsheet.

2.2.12 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 design cases involving highly non-linear models) they may fail to converge. In these cases, you may fine-tune the convergence characteristics for your 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.

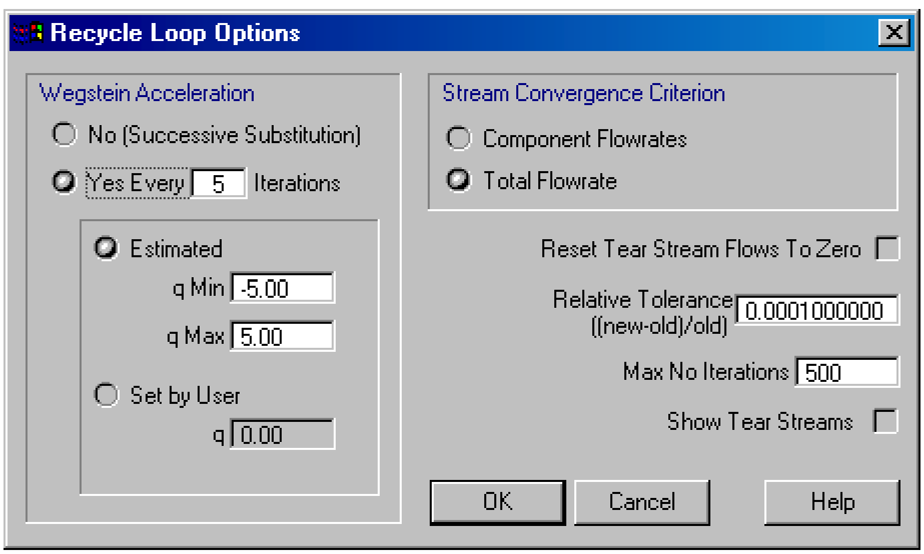


Figure 2.1-rr: Adjusting the convergence parameters for design cases with recycle loops.

GO TO TOP LEVEL CONTENTS