CHEMCAD DYNAMIC COLUMN CALCULATION

User's Guide

Distillation

Continuous
And
Batch
Technologies

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CC-DCOLUMN Version 5.4

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INTRODUCTION

CC-DCOLUMN is an engineering software tool designed to simulate the behavior of distillation columns and their associated equipment.

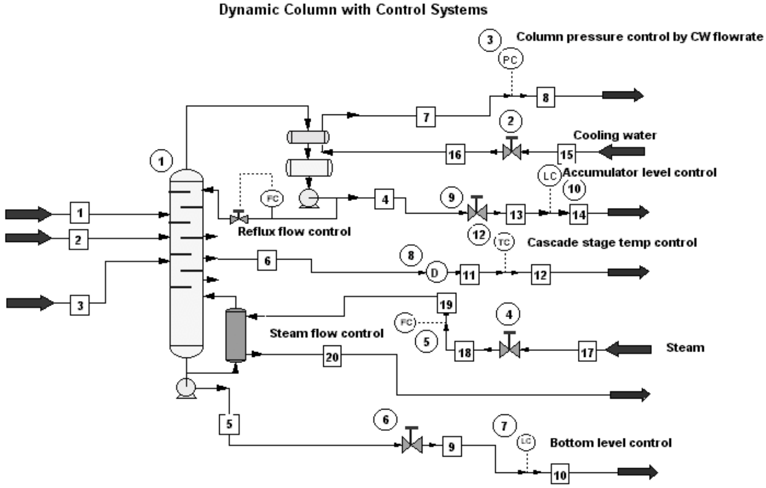
CC-DCOLUMN allows the user to link a distillation column into a DYNAMIC flowhseet. Using CC-DCOLUMN and CC-STEADY STATE lets the user consider varying degrees of holdup in their column.

CC-DCOLUMN provides the tools necessary to evaluate the thermodynamics, equipment and schemes for these processes. This includes:

- A database of physical properties for the 2000 most commonly used chemicals.
- Estimation and regression facilities for those chemicals not in the database.
- Thermodynamic models for the phase equilibrium of a wide range of mixtures ranging from ideal systems to polar and electrolyte systems to polymers.
- PID control system models for controlling temperature, pressure, flowrates, levels and purities in any unit of the process.
- Safety relief simulation.

A typical application is depicted below:

Dynamic Column with Control Systems



CC-DCOLUMN is designed to be used at all levels and stages of distillation process design and analysis. It can be extremely useful to:

- Quantify the requirements of operability, control loop tuning, changes in throughput or ambient conditions, safety demands, etc.
- Perform detailed simulations, which include the equipment and control aspects of the process

- Simulate the effects of disturbances, startups, and shutdowns on key process variables.
- Perform simulations, which are independent from control requirements.
- Validate control schemes.

Many, many variations are possible.

THE CHEMCAD SUITE AND CC-DCOLUMN

CC-DCOLUMN is a module within the CHEMCAD system. As such, it uses all the features which are fundamental to the system. These include:

- The flowsheet drawing features.
- The data input facilities.
- The CHEMCAD physical properties database.
- All thermodynamic options and data available in the CHEMCAD Suite.
- Output facilities such as viewing, plotting, and reporting.
- Regression facilities for physical properties, phase equilibrium, and electrolytes.
- Equipment sizing tools.
- Safety relief design and evaluation.
- Units operations that are common in both steady-state and dynamic simulations. These include calculator, component separator, controller, divider, Excel UnitOp, fired heater, flash vessel, heat exchanger, LLV flash, mixer, node, phase generator, pump, stream reference, valve.
- Sensitivity analysis.
- VBA and OPC connectivity.
- The on-line Help System.

These features and how to use them are described in detail in the CC-STEADY STATE User's Guide and the On-line Help System to which the user gets referred. Those descriptions will not be repeated in this guide.

MAIN FEATURES OF CC-DCOLUMN

The use of and technical details of the main features of CC-DCOLUMN are described in this user guide. These include:

- The dynamic model of SCDS distillation UnitOp.
- The dynamic model of TPLS distillation UnitOp.
- The dynamic model of TOWR distillation UnitOp.

- The dynamic vessel.
- Miscellaneous dynamic UnitOps –RAMP, Time Delay, Task, Time Switch.
- The dynamics menu.
- The dynamics tool bar.

INSTALLATION

By default CC-DCOLUMN is always installed with the CHEMCAD Suite. If the any program of the CHEMCAD Suite has been installed there is not any special procedure to install CC-DCOLUMN because it is completely integrated with the CHEMCAD Suite and does not run in a separate interface. The use of CC-DCOLUMN only depends on the user's license. Please refer to the installation section of the CC-STEADY STATE Users Guide.

SETTING UP A DYNAMIC SIMULATION: AN OVERVIEW

Many of the steps listed below are the same in a dynamic simulation as in a steady state simulation (CC-STEADY STATE).

The steps for setting up a dynamic flowsheet are:

1. Start a new job
2. Select engineering units
3. Turn on the dynamics mode
4. Draw the flowsheet
5. Select components
6. Select thermodynamics options
7. Specify feed streams and initial stream conditions
8. Specify UnitOps
9. Run the simulation
10. Review the results with RESULTS and PLOT
11. Re-run the simulation or extend the run from the current simulation time
12. Generate reports

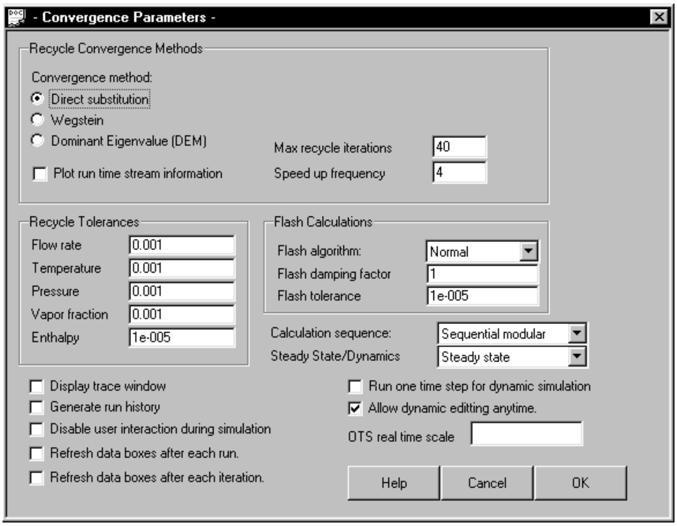
Most steps and are described in detail in the CC-STEADY STATE User's Guide and in the On-line Help System to which the user gets referred. Those descriptions will not be repeated in this guide.

TURNING ON THE DYNAMIC MODE

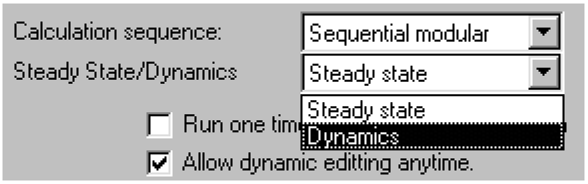
This is done on the **Convergence** dialog box under the **Run** command on the main menu bar.

Procedure:

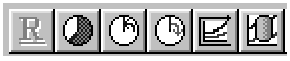
Click the **Run** command on the main menu bar. Click on the **Convergence** option at the top of the menu The following screen will appear:



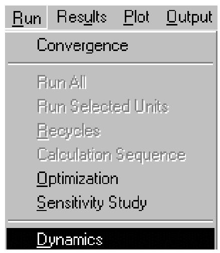
Select the **Steady State/Dynamics** combo box. Scroll down and select **Dynamics** as shown in the picture below.

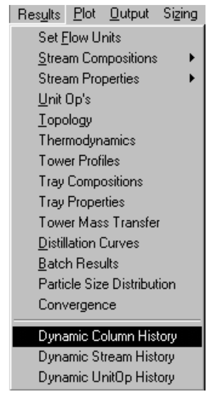


Click **OK** to save the changes. As a result the steady-state Run button will be turned off and the dynamic buttons on the toolbar will be turned on. They will be colored and no longer shaded (see picture below).



Also some dynamics commands will be activated such as the **Dynamics** command on the **Run** menu and the **dynamic results** commands on the **Results** menu (see pictures below). The Dynamics command on the Run menu will allow the user





THE DYNAMICS MENU

The DYNAMICS MENU provides the commands for:

1. Running the dynamics simulation
2. Managing the data associated with the runs
3. Recording and displaying the desired results

CC-DCOLUMN maintains several sets of flowsheet data files in order to manage all of the situations and manipulations the user may choose to execute. These files fall into the following categories:

1. Time Zero files:

These files contain the initial state information; that is, all the streams and equipment specifications at time equals zero. Whenever the user runs from time zero, CC-DCOLUMN copies all the specified data into a series of files called TIMEO.XXX, where XXX stands for a series of file extensions. That way, the user may always return to the initial state if desired.

The contents of the #TIMEO files, and therefore of the initial state, cannot be modified unless the user first restores the initial state (using the command provided for this purpose) and then edits the data. Unless this is done, access to initial state data will be blocked by the program.

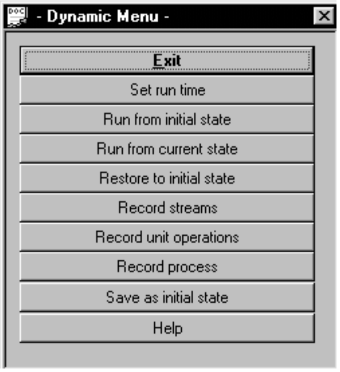
2. Current State files:

These files contain all the system data at the end of the last simulation unless the user has restored the initial state. Then they contain the initial state.

3. Recorded files:

These files contain the answers; that is, the time history of the simulation. Batch reactor variables are saved automatically. All other variables are saved only if the user specifically requests it.

The dynamics menu has the following options:



Exit:

Exit dynamics menu without executing simulator.

Set Run Time:

This option brings up a screen which allows you to set the overall duration of the run (" Overall Run-Time") and the time increment between successive time slices ("System Timestep"). The duration can be specified as a specific time or as an event.

Run from initial state:

This option resets the flowsheet to the case #TIMEO (the initial conditions) and begins the dynamic simulation.

Run from current state:

Runs the flowsheet from the current conditions.

Restore to initial state:

Copies the flowsheet conditions from the case #TIMEO files to the current state files.

Record Streams:

This option enables the user to specify which streams are to be saved, i.e., have their time histories saved. These streams can then be printed in a report or plotted in a graph using other options in the dynamics menu. This option also allows the user to select which stream variables are to be plotted during runtime.

Record unit operations:

This option enables the user to select which unit operations are to be saved, i.e., to have their time histories saved. These UnitOps can then be printed in a report or plotted in a graph using other options in the dynamics menu. This option also allows the user to select which UnitOp variable is to be plotted during runtime.

Record process:

This option enables you to specify specific times that you want every variable in the process recorded. These recorded results are than available for plotting and printing.

Save as initial state:

This option enables the user to make the current parameters of the dynamic simulation become the new initial state.

Help:

This option opens the help facility of the dynamics menu.

These commands are described below.

SET RUN TIME

This command is used to set the stop criteria of the dynamics run and to specify the time step size (how often the flowsheet equations are integrated). These items must be specified for the calculation to proceed. Clicking this option will cause the following **Set Simulation Run Time dialog box** to be displayed. Please make note of the following:

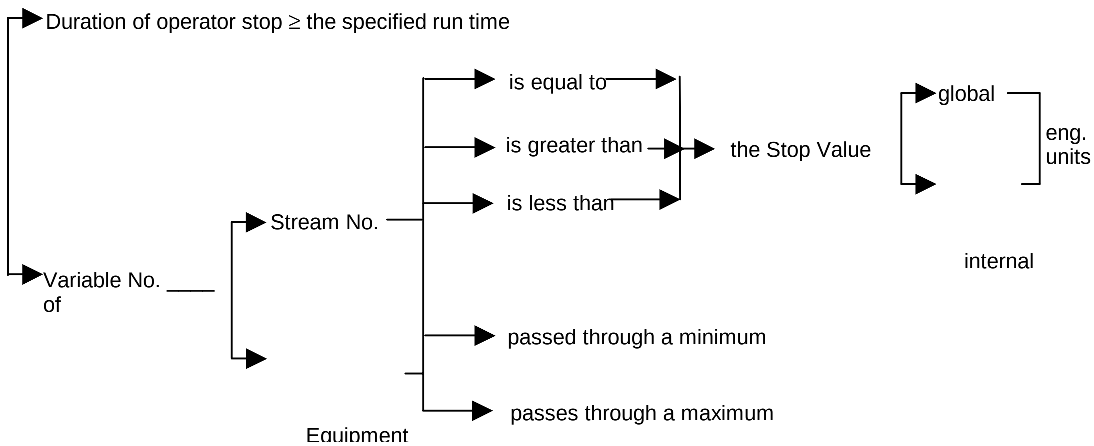
1. More than one operating step can be specified. If a run is made from time zero (i.e., the initial state), all specified operating steps will be run. If the simulation is being run from the current state, then only those operating steps beyond the current time will be run.

   Operating steps can be added at any time, so this feature provides a facility for extending the dynamic simulation indefinitely.

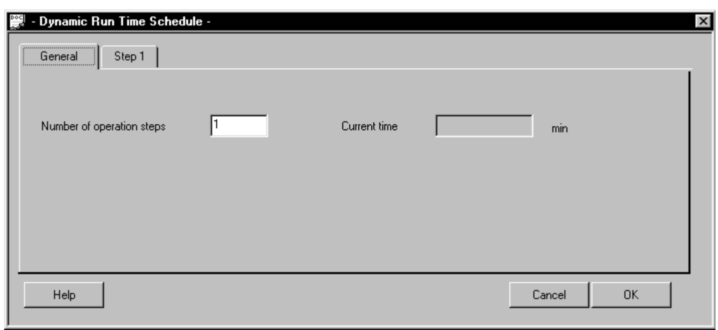
2. The time step size is specified in the **Step size** field.

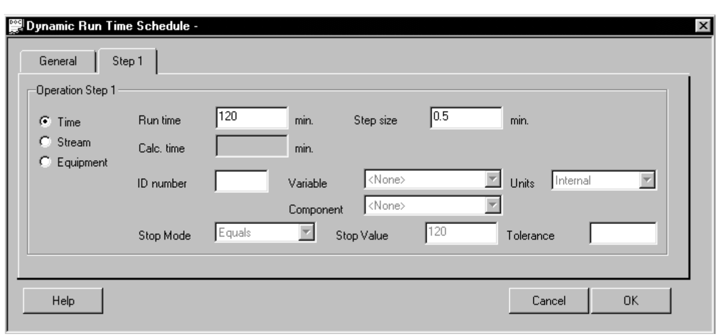
3. Operating step run time limits can be specified as fixed times or as events. These stopping events can be when a UnitOp or Stream variable is equal to, greater than, less than, limited from below or limited from above by a specified value.

The following diagram can summarize the stop criteria:



The Dynamic Run Time Schedule dialog box has two pages that look like this:





GENERAL INPUT

Number of operating steps:

The number of operating steps to be simulated must be entered in this field. Otherwise, the program will only run the first step. Up to ten operating steps can be specified. For each operating step a stop criteria can be specified.

Current Time:

Displays the current simulated time. That is, the time at the end of the last simulated operating step.

Step X:

For each operating step a dialog box displaying the following fields will be provided.

Stop When:

This field identifies the type of stop criteria to be used for this operating stop. Options are:

- Time – stop when the specified run time has been reached.
- Stream – stop when a specified stream variable has met the stop criteria
- Equipment – stop when a specified equipment or UnitOp variable has met the stop criteria.

Run Time:

If the stop criteria are to be time, the duration of the operating step must be entered in this field (in minutes).

Step Size:

The step size determines the frequency of integration during the simulation. Step size is specified in minutes of simulated time. For example, if the operating step is to calculate 100 minutes of simulated time, and the step size is 2 minutes, the program will integrate the flowsheet equations 50 times during the simulation.

The step size selected will have an impact on the accuracy of the results and the speed of the calculation. Smaller time steps will produce smaller errors, but will require more time to make the run.

Step size can be different for every operating step if desired.

ID Number:

If the **Stop When** selection is "Stream" or "Equipment", the ID number of the relevant stream or equipment must be entered in this field.

Variable Number:

If the **Stop When** selection is "Stream" or "Equipment", the number of the relevant stream or equipment variable must be entered in this field. Variable numbers are listed in the on-line help.

Variable Unit:

If the stop criteria are to be based upon a stream or equipment variable, then it is advisable to identify the type of variable which has been selected. Variable Type identifies the engineering units to be applied to the variable. If the variable type is identified, the program will apply the global flowsheet engineering units to the **Stop Value**. If the Variable type is not identified, then the program will apply internal engineering units to the **Stop Value**.

For example, if the stop criteria is to be based upon the temperature of stream 5, and the global flowsheet units for temperature is degrees Celsius, then the "Temperature" option should be selected in the **Variable Unit** field. This will tell the program that the **Stop Value** has units of degrees Celsius. If 'Temperature" is not selected, the program will assume the **Stop Value** is specified in degrees Rankine (CC-DCOLUMN's internal units for temperature).

Component:

If a component purity or flowrate criteria is chosen, identify the relevant component from the list.

Stop Mode:

The stop mode is the numerical operator, which is used to compare the current value of the stopping variable to the stop value. When:

{Current value of stopping variable} <u>operator</u> {Stop Value} <u>is true</u>

then the operating step is over.

The following operators are available:

- **Equal to (=):** This operator will end the operating step when the current value of the stopping variable is within a specified tolerance of the stop value.
- **Greater than (>):** This operator will end the operating step when the current value of the stopping variable exceeds the stop value.
- **Less than (<):** This operator will end the operating step when the current value of the stopping variable is below the stop value.
- **Minimum:** This operator will end the operating step when the value of the stopping variable passes through a minimum.
- **Maximum:** This operator will end the operating step when the value of the stopping variable passes through a maximum.

Stop Value:

This is the numerical value of the stopping criteria. If "Stream" or "Equipment" was selected in the **Stop When** field, the stop value must be specified. If "Time" was selected in the **Stop When** field, the stop value field is not used.

Stop Tolerance:

This is the acceptable tolerance to be used when the "equal to" **Stop Mode** is used.

Calculated Run Time:

If "Stream" or "Equipment" was selected in the **Stop When** field, the program will calculate the time it took to complete the operating step. That value will be displayed in this field. Units are always minutes.

RUN FROM TIME ZERO

Selecting this option will cause the program to return to the initial conditions and rerun the entire simulation. All results from previous simulations will be discarded.

RUN FROM CURRENT STATE

Selecting this option will continue the simulation from the current state, i.e., from the last calculated result. In order to use this option, an operating step beyond the current state must be scheduled on the **Set runtime** option above.

RESTORE TO INITIAL STATE

This option will restore the initial conditions specified. All previous calculations will be discarded. It is necessary to exercise this option in order to change certain flowsheet variables. Once a simulation has taken place, CC-DCOLUMN will not allow you to change any variables, which might produce thermodynamic inconsistencies, if the simulation is continued. Therefore, the restore command is necessary to enable changes to these variables.

RECORD STREAMS AND RECORD UNIT OPERATIONS

Unless otherwise specified the user, CC-DCOLUMN will only record the histories of batch reactors and dynamic columns. For all other UnitOp and streams only the initial and final variable values are recorded. If desired, to view, plot, or report the historical results of these other UnitOps and streams, then you must instruct the program to do so using the **Record Streams** and **Record Unit Operations** menu options. Each options calls a dialog box in which you can list the streams and/or UnitOps that you wish recorded. Selections can be typed in or chosen with the mouse. Once an item is selected, then all of the variables associated with that item are recorded.

RECORD PROCESS

This dialog box is used to identify times (simulated) when the entire process is to be recorded. Recording the entire process means that every variable in the process will be written to disk. It can be a slow process.

SAVE AS INITIAL STATE

Selecting this option will cause the program to set the current conditions of the dynamic run as the new initial condition. All parameters from the previous initial state will be discarded and it will not be possible to recover data for the previous state. The user will be prompted and asked for a confirmation. If the user

HELP

This button will open the help facility of the dynamics menu.

REVIEWING DYNAMIC RESULTS

Dynamic results can be obtained on the **Results** menu. The user should select one of three general dynamic options at the bottom of the Results command: **Dynamic Column History**, **Dynamic Stream History** and **Dynamic UnitOp History**.

Please notice the following points when viewing dynamic results.

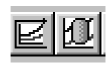
1. Clicking on the **Results** command on the menu bar will cause the **Results** menu to open. This menu contains a set of options for reviewing program output.
2. The answers for dynamic vessels can be reviewed using the **Dynamic UnitOp History** option.
3. Dynamic column results are reviewed using the **Dynamic Column History** option.
4. The answers for other dynamic unit operations are reviewed using the **Dynamic UnitOp History** command.
5. Stream histories are obtained using the **Dynamic Stream History** option.
6. The Unit Operations option can be used to produce a display of the input for a dynamic UnitOp. Certain calculated values, such as final temperature, final level, etc., will also be displayed.
7. The Streams option will display properties and composition of any stream at end of the simulation.
8. A UnitOp and stream histories can be obtained only for recorded UnitOps and streams.

PLOTTING DYNAMIC RESULTS

To plot a recorded variable there are two options. The user can use the dynamic plot commands on the **Plot** menu or he/she can use the dynamic results buttons on the tool bar.

Stream histories and UnitOp histories are plotted using the Batch Reactor/DVSL History, Dynamic Column History, Dynamic Stream History, and UnitOp History options on the Plot menu. With the exception of batch reactors and dynamic columns, **you must indicate to the program that a given stream or UnitOp is to be recorded before the simulation is run**, otherwise the data will not be available to plot.

Dynamic plot results can be obtained by selecting one of the dynamic options at the bottom of the **Plot** menu or by clicking on the Dynamic Plots buttons on the menu bar (see pictures below):



DYNAMIC COLUMN HISTORY

After running a Dynamic Column, you may plot several of the recorded values using this option. Once you click this option or the, you are asked to select the dynamic column on your flowsheet. Once you click **OK**, you will see the following dialog box:

Variable to be plotted

Define the variable to be plotted on the y-axis. Select one from the pull-down list.

Object to be plotted

Select one of the following. This field may not be needed if the variable specified above does not require a location (e.g., Reflux Ratio).

- Distillate
- Bottom
- Stage

Stage Information

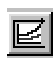
If a plot for one of the stages in the column is desired, specify the following:

- Stage No. – Enter the stage number for which the properties will be plotted.
- Phase – Indicate whether you are plotting data for the liquid or vapor phase.
- Time Unit / Frequency

Time Unit

Specify what time unit you want to use for the x-axis and the frequency you want plotted (hr, min, sec).

Plot Frequency
This is the number of time steps between plotting results. If the simulation integration time step is one minute and the plot frequency is five, the results will be plotted every five (simulated) minutes.



Y-axis min/max values

CC-DCOLUMN allows tuning up the range for the plot of a recorded variable. Specify a minimum and maximum for the y-axis of your plot

Components to be plotted

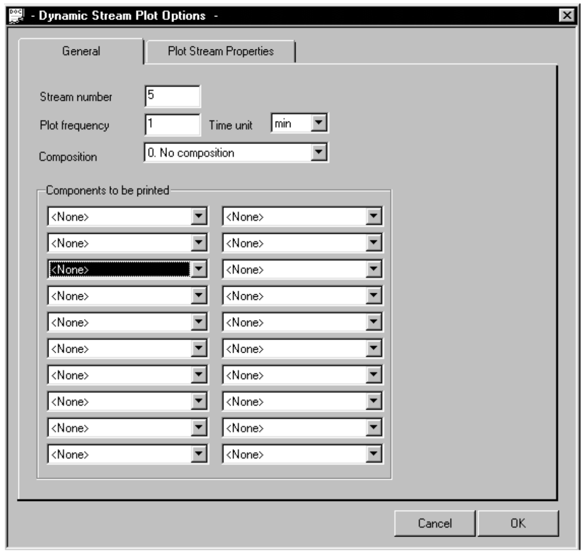
You may plot up to ten components by selecting them in this section.. If the plot you select is any related to flow or concentration (i.e. mole/mass/mass frac/ etc) you may want to select the component(s) to be plotted. Select components from the pull-down list.

DYNAMIC STREAM HISTORY

After running a dynamic flowsheet, you can plot stream variables versus time, if you have specified that a stream be recorded in the Dynamics Menu.

To plot a dynamic recorded variable go to the **Plot** menu and select the **Dynamic Stream History** option. You may also click on the **Dynamic Stream History button on** the menu bar:

Selecting this option will open the following dialog box:



Stream number

Define the stream number to be plotted. You must have specified that this stream be recorded.

Plot Frequency/Time Unit

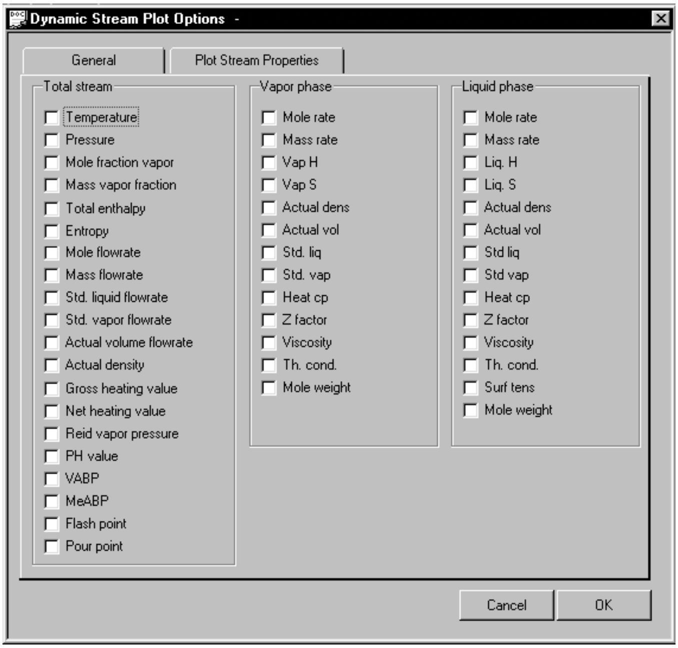
Specify the frequency and time for the stream variables to be plotted.

Composition / Components

Specify whether or not you desire a composition/time plot and the units you desire (i.e. mole/mass/mass frac/ etc). Also specify which components are to be plotted.

Stream Variables

Click on the **Plot Stream Properties** tab. The following screen will appear:



Specify which stream variables to plot by using the check boxes next to the variable names. Click **OK** to save the changes and open the stream property plot CC-DCOLUMN will create.

DYNAMIC COLUMN MODELS

OVERVIEW

CC-DCOLUMN provides three different dynamic distillation models. Figure 1 provides a pictorial summary of the dynamic columns available:

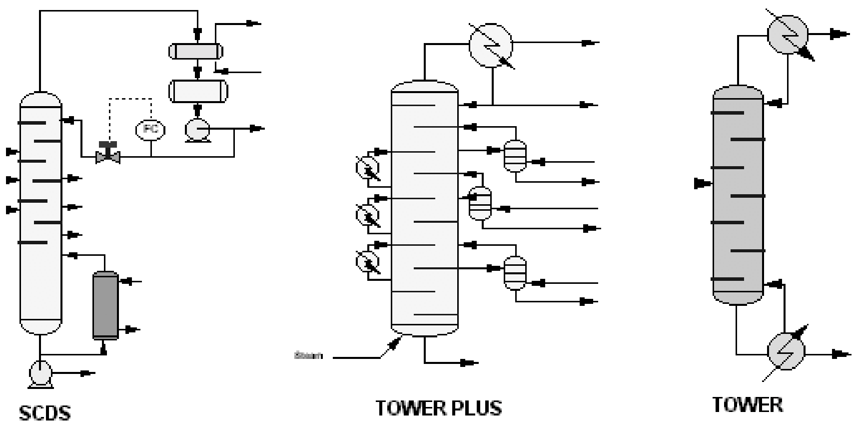


Figure 1

These models can be used in simple simulations without control system (assuming a perfect control scheme) or in more complex studies with control systems.

The dynamic models of SCDS, TPLS and TOWR are extensions of their steady state models. Therefore it is assumed the user is already familiar with the specification, topology, convergence of these models common to CC-STEADY STATE. In this section we will discuss the dynamic features and specifications of the SDCS, TPLS and TOWR models. The SCDS distillation UnitOp can also perform dynamic calculations with the mass transfer models.

DYNAMIC COLUMNS INPUT

After inputting or editing of the steady-state specifications, a dynamic column requires the completion of the following dialog boxes:

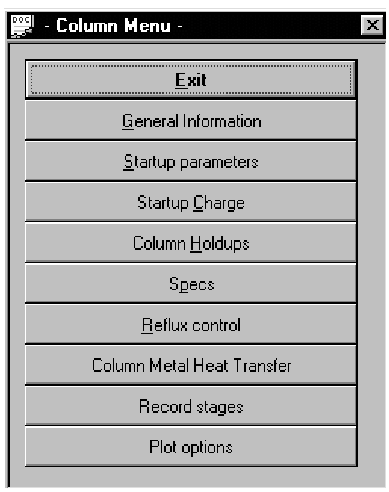
- The **General Information** dialog box
- The **Startup Parameters** dialog box
- The **Startup Charges** dialog box

- The **Column Holdups** dialog box
- The **Specs** dialog box
- The **Reflux control** dialog box
- The **Column Metal Heat Transfer** dialog box
- The **Record stages** dialog box
- The **Plot Options** dialog box

It is not necessary that all of these dialog boxes be completed for every problem. Obviously you do not need to complete the **Startup Charge** dialog box if you are simulating a process from steady-state condition. CC-DCOLUMN will not permit access to those dialog boxes that are not relevant to the current simulation. CC-DCOLUMN "access decisions" are made based upon specifications made in the **General Information** dialog box.

THE DYNAMIC COLUMN MENU

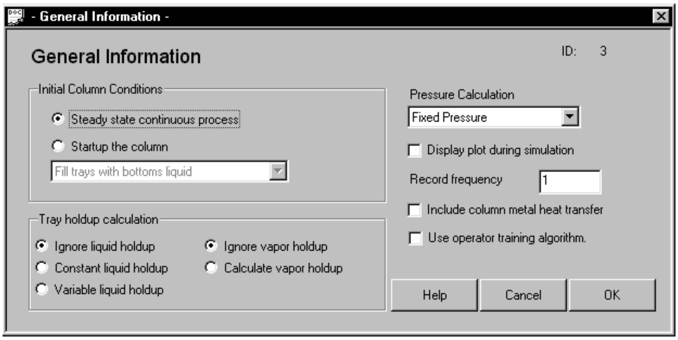
All of the above listed items are accessed through the Dynamic Column Menu, which appears whenever you finish editing the steady-state specifications of SCDS, TPLS, TOWR and the dynamic mode of CC-DCOLUMN is turned on. To access a dialog box, you simply click on the appropriate Dynamic Column Menu item. When the dialog box is closed, you will return to this menu.



A field description of the input for each of these dialog boxes is provided below:

THE GENERAL INFORMATION DIALOG BOX

The **General Information** dialog box is used to specify whether the simulation begins at startup or steady state condition; if startup is to be wet or dry; and what type of holdup and pressure calculations are to be performed.



Initial Column Conditions

Specify if the simulation is to begin from steady state or from startup conditions. If it is to begin from startup, the user must also identify whether it is to be a dry or wet startup.

If the simulation is to begin from a steady state condition, a steady state simulation must be run before the dynamic simulation is executed (a license of CC-STEADY STATE is required). The program will take the existing steady state results (and specifications) as starting point for the dynamic simulation.

If the simulation is to begin from startup conditions, then some initial liquid must be defined on the Startup Charge dialog box. This is true for both dry and wet startup. In both cases, this liquid is the initial charge in the bottom of the column. For wet startups the composition, temperature, and pressure of the starting liquid on the trays is assumed to be the same as the charge in the bottom. The amounts are determined from the holdups.

Tray holdup calculation

These fields are used to define how vapor and liquid holdups are to be determined during the simulation. Vapor holdups can only be calculated calculation if variable holdup is selected for the liquid phase. The default is to ignore the holdups in both phases.

Liquid holdup can be constant, variable, or ignored (assumed to be zero). Variable holdup may be ignored or calculated.

Constant Liquid Holdup

The user must specify the amounts of the holdups if constant holdup is selected. This is done on the Column Holdups dialog box. These amounts can be specified in mass, mole, or volume units and can be different on every stage if desired.

Variable Liquid Holdup

The program calculates variable holdups. This calculation is a function of tray (or packing) type and geometry. Therefore, this information must be specified for the calculation to proceed. These specifications are made under the Column Holdups option of the Dynamic Column menu.

Vapor Holdups

Vapor holdups can be included in the calculation (if variable liquid holdups was selected) or ignored (assumed to be zero). If they are included, they are always assumed to be constant volume. The volume is determined from the column geometry.

Pressure Calculation

The column pressure can be fixed by the user or calculated by the program. If it is to be calculated by the program, then variable liquid holdups must be selected above, and the column geometry must be specified. Column geometry is specified using the **Column Holdups** option of the **Dynamic Column Menu**.

The pressure calculation matches the fluid volumes to the column geometry and includes the tray (or packing) pressure drop. The program calculates tray and packing pressure drops.

Display plot during simulation

To plot results of the simulation on the screen during the simulation, place a check mark in this box. The data to be displayed is chosen in the Plot Options dialog.

Record frequency

This is the number of time steps between saving of the results. If the simulation integration time step is one minute and the record frequency is five, the results will be saved every five (simulated) minutes.

Include Column Metal Heat Transfer

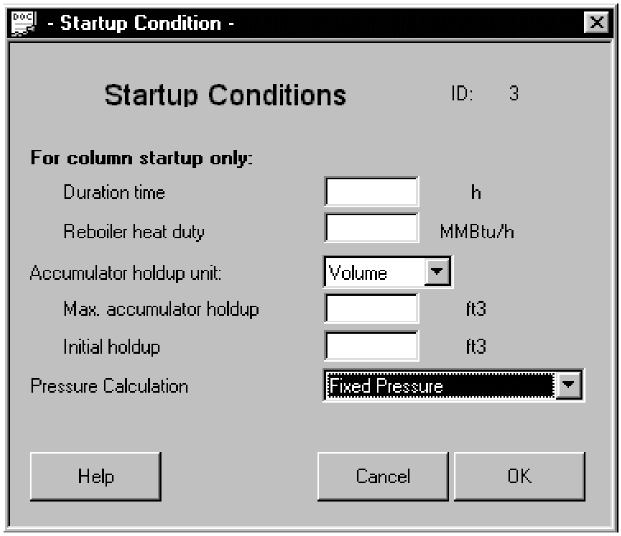
It is possible to include in CC-DCOLUMN's calculations ambient heat losses/gains. If the simulation will take heat transfer into account, then check this option. If you do so, the **Metal Heat Transfer** dialog box will be available on the **Dynamic Column Menu**.

Use Operator Training Algorithm

CC-DCOLUMN as a powerful and flexible dynamic simulation tool can work as an engineering engine for operating training systems such as CC-OTS. This option allows OTS systems to interact with CC-DCOLUMN.

THE STARTUP PARAMETERS DIALOG BOX

The **Startup Conditions** dialog box is used to specify startup time and conditions. Obviously this dialog box is used only when a startup is to be simulated.



The specifications made on this dialog box apply only to the startup period. All fields on this screen are required.

Duration Time

Define the duration of the startup period here.

Reboiler heat duty

During the startup time, the reboiler duty will be fixed at the value provided in the Reboiler heat duty field. If you want to vary this value during startup, you can use the RAMP Controller UnitOp to schedule it.

Accumulator Holdups

The user must also specify the initial and maximum condenser accumulator holdups during startup.

Accumulator holdup unit

Choose the base units for the condenser accumulator holdup specification. Options are mass of holdup, moles of holdup, volume of holdup, or liquid level in the condenser accumulator.

Maximum and Initial holdup

Accumulator liquid will start at the Initial holdup value and rise to the Max accumulator holdup value.

Between these two values there will be no reflux to the column. Once the maximum holdup value has been reached, the reflux to the column is any amount in excess of the maximum holdup. This is the total reflux simulation.

Pressure Calculation

Pressure during the startup period can be fixed or variable. Variable pressure is calculated by CC-DCOLUMN and requires specification of the column geometry.

This specification is independent from whether the pressure is fixed or calculated during the simulation (as per the **General Information** dialog). You may have the pressure calculated during the startup portion of you simulation and fixed at a specified value for the remainder of the simulation. The reverse is also possible. There is no restriction on the combination of methods for the startup pressure calculation and the initial conditions pressure calculation.

STARTUP CHARGE

The column startup charge dialog has the same structure and format as a CC-STEADY STATE stream dialog box. Only the flow units are amounts instead of rates. This dialog box also follows the same input conventions as a stream dialog box, therefore:

1. The composition must always be specified. If it is specified as component amounts, then the total amount is determined by CC-DCOLUMN as the sum of the component amounts. If the composition is specified as component fractions (mole, mass, or volume), then the total amount must be user specified.
2. If the specified component fractions do not sum to one CC-DCOLUMN will normalize them.
3. Two (but only two) of the thermodynamic properties, temperature, vapor pressure and pressure; must be specified by the user. Any combination is acceptable. From these two (plus the composition) the program will initialize the charge (i.e., calculate the third plus enthalpy).
4. A user specified vapor fraction of one (1.0) is taken to mean the dew point. A user specified vapor fraction of zero (0.0) is taken to mean the bubble point.
5. Enthalpy cannot be user specified.

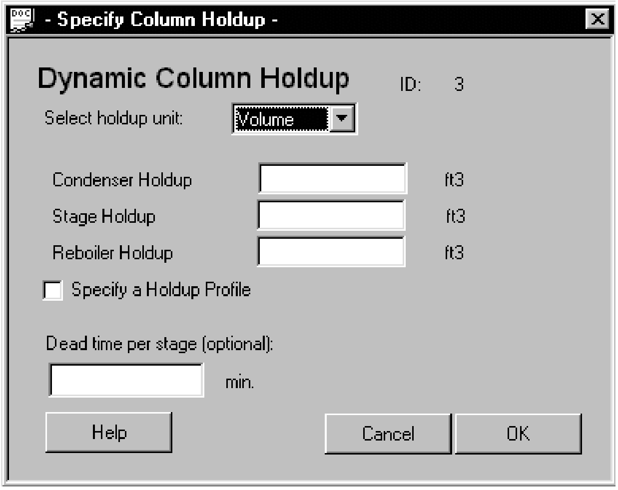
Please refer to the CC-STEADY STATE User's Guide for a detailed description of how to complete stream dialog boxes.

THE COLUMN HOLDUPS DIALOG BOX

The **Column Holdups** dialog box will be only available if the **Constant liquid holdup or Variable liquid hold up** option was selected in the **General Information** dialog box. If one of these options was selected, then the **Column Holdups** dialog box must be completed.

If variable liquid holdups are to be used, the column layout must be specified. This is done using a set of dialog boxes constructed for this purpose. Exactly which dialog boxes appear depends on what device is selected for mass transfer; i.e., valve trays, bubble cap trays, or sieve trays. These dialog boxes appear when you close the Specify Column Holdup dialog box. Entries in the Specify Column Holdup dialog box are unnecessary. Just close this dialog box. The program will prompt you through the rest of the input.

Variable liquid holdup can only be used for simulating trayed columns. Packed columns are assumed to have constant liquid holdup.



Select holdup unit

Holdup units can be in mass, mole, or volume units. Selections are made by opening the list in the: field and then clicking on the desired option.

Condenser holdup

Condenser holdup is the total amount of liquid in the condenser and its' accumulator.

Stage holdup

Stage holdup is the total amount of liquid on each stage. The number of stages is specified by the user on the column's main specifications dialog. The total stage holdup is this number of stages times the stage holdup value input here.

Reboiler holdup

Reboiler holdup is the amount of liquid in the bottom of the column plus the liquid in the reboiler plus the liquid in the reboiler accumulator vessel (if any).

Specify a Holdup Profile

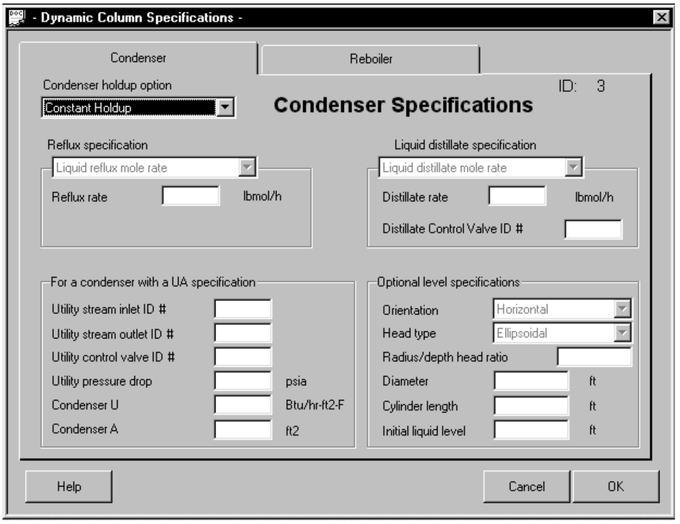
Stage holdups can be specified stage-by-stage if desired. To do this place a check mark in the **Specify a Holdup Profile** field. When this dialog box is closed, the **Stage Holdup** dialog box will open. On this dialog box specify the key stage numbers and holdup values. Holdups for omitted stages are determined by linear interpolation between those stages provided.

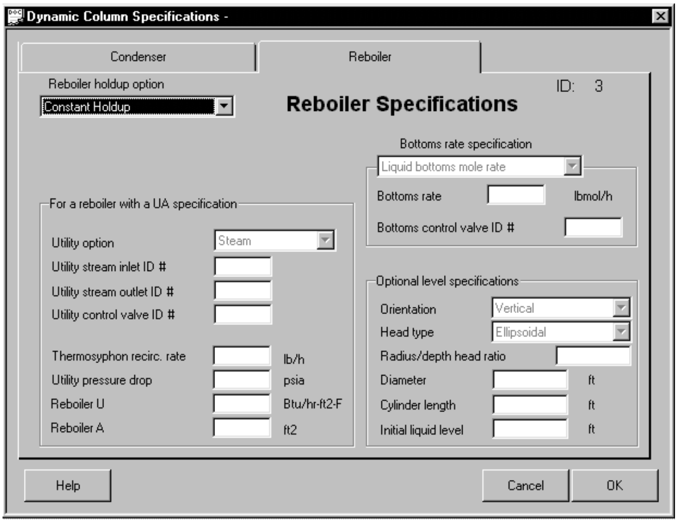
Dead Time per stage (optional)

This option allows the user to directly specify additional stage dead time. The user specifies the duration of the time delay which the stages experience.

THE DYNAMIC COLUMN SPECIFICATIONS DIALOG BOX

The dynamic column specifications dialog box has two pages, which appear below:





CONDENSER INPUT

Condenser holdup option

Condenser holdup can be variable even if stage holdup is constant. **Variable condenser holdup** is treated as if all the condenser liquid is kept in a vessel. The dimensions of this vessel are specified in the **Optional level specifications** fields shown at the bottom right of the dialog box. If variable holdup is selected, these fields must be completed.

If condenser holdup is constant, then the condenser is assumed to operate in accordance with the column condenser spec. For instance, if;

a. A distillate purity specification is made on the Specifications page of the dynamic Distillation Column (SCDS, TPLS, TOWR) dialog box, and

b. Constant condenser holdup is specified on the Condenser page of the **Dynamic Column Specifications** dialog box, and

c. The reflux flowrate is not specified in the Reflux rate field of the **Dynamic Column Specifications** dialog box, then

d. During the dynamic simulation, the program will hold the distillate purity constant at the value specified in item a. above. The reflux flowrate will be adjusted at each time step to maintain this purity.

The above, of course, holds true for any condenser specification made in the column dialog box.

Reflux specification

For variable condenser holdup, the reflux rate must be either fixed or controlled. That is, the user must either specify a fixed reflux flowrate or set up a control system to adjust it dynamically.

A fixed reflux flowrate can be specified in mass, mole, or volume units. The selection is made from the list in the Reflux specification field. The numerical value of the reflux flowrate is given in the Reflux rate field.

The reflux control can be by either an internal control system or an external control system. An internal system is one which is specified and calculated within the SCDS UnitOp. An external control system is one that is specified and calculated outside the SCDS UnitOp using the PID Controller and the Control Valve UnitOp modules. If the control system is internal, the Reflux Control dialog box must be completed. If the control system is to be external, the ID number of the reflux control valve must be entered in the Reflux control valve ID # field of the current dialog box.

Liquid distillate specification

For constant condenser holdup, the liquid distillate is calculated by the program according to the specifications made for the condenser operation (see above Condenser holdup option…). Therefore, these liquid distillate specification fields are not filled in.

For variable condenser holdup, the flow rate of liquid distillates must be either fixed or controlled. That is, the user must either specify a fixed flowrate or set up a control system to adjust it dynamically.

A fixed distillate flowrate can be specified in mass, mole, or volume units. The selection is made from the list in the Liquid distillate specification field. The numerical value of the reflux flowrate is given in the Distillate rate field.

Distillate control is always done using an external control system. The control system is specified and calculated outside the dynamic column UnitOp using the PID Controller and the Control Valve UnitOp modules. Therefore, the ID number of the liquid distillate control valve must be entered in the Distillate Control Valve ID # field of the current dialog box.

For a condenser with a UA specification

If a condenser control system is being used, the user has the option of simulating the condenser operations using UA specifications and a utility control system. Those specifications are made in this set of fields.

The utility stream inlet and outlet ID numbers and the **utility stream control valve ID number** must be specified. The program uses these to determine the utility flowrate and properties.

The **utility pressure drop** specification is optional. If entered the utility outlet pressure will be set to its inlet pressure minus this value.

The **condenser U** is the overall heat transfer coefficient. It must be specified by the user.

The **condenser A** is the heat transfer surface. It also must be specified by the user.

Optional level specifications

If variable condenser holdup is to used, these fields must be entered. Variable condenser holdup is treated as if all the condenser liquid is kept in a vessel. The dimensions of this vessel are specified in the **Optional level specifications** fields.

These specifications only describe the vessel dimensions. Obviously therefore, they only make sense when used in conjunction with a level control system.

Orientation – The vessel may be horizontal or vertical. Obviously, this specification will impact when the accumulated condenser liquid overflows its level specification.

Head type – Vessel heads can be ellipsoidal, hemispherical, bumped, or flat. This too will affect when the level specification is exceeded.

Radius/depth head ratio – The head ratio will determine the amount of liquid held by the vessel head. This will influence the vessel liquid level. If this field is left blank, the program will use default values.

Diameter – This is the inside diameter of the vessel.

Cylinder length – This is the tangent to tangent length of the vessel.

Initial liquid level – This is the liquid level at the start of the simulation.

REBOILER INPUT

Reboiler holdup can be variable even if stage holdup is constant. Variable reboiler holdup is treated as if all the liquid is kept in a vessel. If effect this is so, since the bulk of the "reboiler accumulator" liquid is held in the bottom of the column vessel. The dimensions to be used to calculate reboiler holdup are specified in the Optional level specifications fields shown at the bottom right of this dialog box page. If variable hold up is selected, these fields must be completed.

If reboiler holdup is constant, then the reboiler is assumed to operate in accordance with the column reboiler spec. For instance, if;

a. A bottoms purity specification is made on the Specifications page of the Distillation Column dialog box, and

b. Constant reboiler holdup is specified on the Reboiler page of the Column Specifications dialog box, and

c. The bottoms flowrate is not specified in the Bottoms rate field of the Column Specifications dialog box, then

d. During the dynamic simulation, the program will hold the bottoms purity constant at the value specified in item a. above. The bottoms flowrate will be adjusted at each time step to maintain this purity.

The above, of course, holds true for any condenser specification made in the SCDS, TPLS or TOWR dialog box.

Bottoms rate specification

For variable reboiler holdup, the bottoms rate must be either fixed or controlled. That is, the user must either specify a fixed bottoms flowrate or set up a control system to adjust it dynamically.

A fixed bottoms flowrate can be specified in mass, mole, or volume units. The selection is made from the list in the Bottoms rate specification field. The numerical value of the bottoms flowrate is given in the Bottoms rate field.

Bottoms flowrate control is always done using an external control system. The control system is specified and calculated outside the dynamic column UnitOp using the PID Controller and the Control Valve UnitOp modules. Therefore, the ID number of the bottoms control valve must be entered in the Bottoms Control Valve ID # field of the current dialog box.

For a reboiler with a UA specification

If a reboiler control system is being used, the user has the option of simulating the reboiler operations using UA specifications and a utility control system. Those specifications are made in this set of fields.

The **utility stream inlet and outlet ID** numbers and the **utility stream control valve ID** number must be specified. The program uses these to determine the utility flowrate and properties.

If a thermosyphon reboiler is to be simulated, the recirculation rate must be specified in the **Thermosyphon Recirculation Rate** field.

The **utility pressure drop** specification is optional. If entered the utility outlet pressure will be set to its inlet pressure minus this value.

The **reboiler U** is the overall heat transfer coefficient. It must be specified by the user.

The **reboiler A** is the heat transfer surface. It also must be specified by the user.

Optional level specifications

If variable reboiler holdup is to used, these fields must be entered. Variable reboiler holdup is treated as if all the reboiler liquid is kept in a vessel. The dimensions of this vessel are specified in the **Optional level specifications** fields.

These specifications only describe the vessel dimensions. Obviously therefore, they only make sense when used in conjunction with a level control system.

Orientation – The vessel may be horizontal or vertical. Obviously, this specification will impact when the accumulated condenser liquid overflows its level specification.

Head type – Vessel heads can be ellipsoidal, hemispherical, bumped, or flat. This too will affect when the level specification is exceeded.

Radius/depth head ratio – The head ratio will determine the amount of liquid held by the vessel head. This will influence the vessel liquid level. If this field is left blank, the program will use default values.

Diameter – This is the inside diameter of the vessel.

Cylinder length – This is the tangent to tangent length of the vessel.

Initial liquid level – This is the liquid level at the start of the simulation.

THE REFLUX CONTROL DIALOG BOX

This page is used to describe the Reflux control valve. The input is similar to that for the Control Valve unit operation (CVAL) and is described below.

The control valve calculates the flowrate through the valve based on the input signal it receives from a controller. The module can handle compressible and incompressible flow as well as critical and sub-critical flow. The control valve calculates the following variables at each time step:

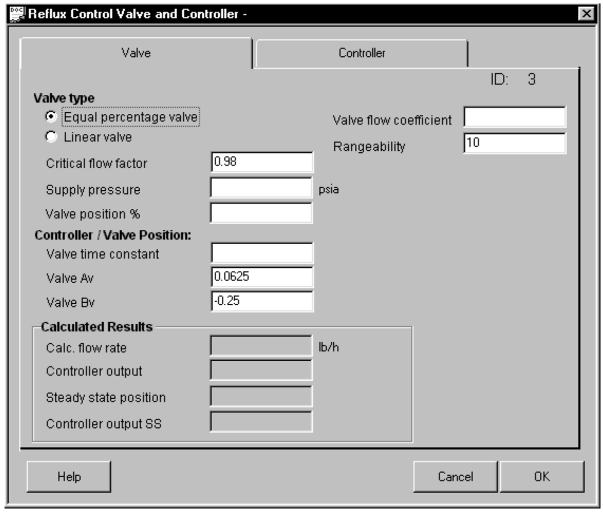
1. The valve position.
2. The flow through the valve.

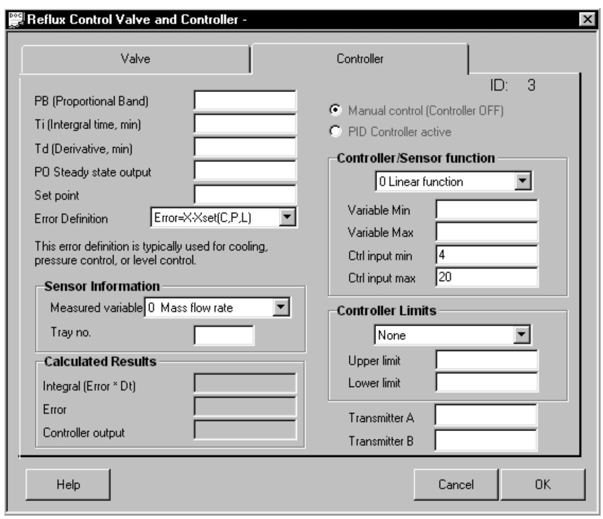
The flowrate of the inlet and outlet streams will be reset to the control valve calculated flow.

The Reflux Control dialog box will be only available if following specifications were made:

1. The **Variable Holdup** option was selected on the **Condenser Specifications** page of the Dynamic **Column Specifications** dialog box**.**
2. The **By Control Valve** option was selected for the Reflux specifications on the **Condenser Specifications** page of the Dynamic **Column Specifications** dialog box**.**

The **Reflux control** dialog box has two pages, which appear below:


Reflux Control Valve and Controller -
Valve
Controller
ID: 3
Valve type
Equal percentage valve
Linear valve
Valve flow coefficient
Rangeability
10
Critical flow factor
0.98
Supply pressure
psia
Valve position %
Controller / Valve Position:
Valve time constant
Valve Av
0.0625
Valve Bv
-0.25
Calculated Results
Calc. flow rate
lb/h
Controller output
Steady state position
Controller output SS
Help
Cancel
OK


Reflux Control Valve and Controller -
Valve
Controller
ID: 3
PB (Proportional Band)
Ti (Intergral time, min)
Td (Derivative, min)
PO Steady state output
Set point
Error Definition
Error=X-Xset(C,P,L)
This error definition is typically used for cooling, pressure control, or level control.
Sensor Information
Measured variable
0 Mass flow rate
Tray no.
Calculated Results
Integral (Error * Dt)
Error
Controller output
Manual control (Controller OFF)
PID Controller active
Controller/Sensor function
0 Linear function
Variable Min
Variable Max
Ctrl input min
4
Ctrl input max
20
Controller Limits
None
Upper limit
Lower limit
Transmitter A
Transmitter B
Help
Cancel
OK

VALVE INPUT

Valve type

Choose from either linear or equal percentage valves.

Linear valves relate the actual valve flow to the capacity valve flow by the following relation:

$$\text{Actual Flow} = \frac{U}{100}\left(1 - \frac{1}{R}\right)(\text{Valve Capacity})$$

Equal percentage valves relate actual flow to capacity valve flow as follows:

$$\text{Actual Flow} = R^{\left(\frac{U}{100} - 1\right)}(\text{Valve Capacity})$$

Valve flow coefficient

This is the valve Cv. This field must be entered. If you do not know a good value for Cv, use the valve sizing option under the **Sizing** menu. This option will calculate a good value for this field.

The definition of the flow coefficient is defined as follows:

$$C_V = Q\left(\frac{SG_f}{\Delta P_s}\right)^{0.5}$$

Rangeability

Rangeability is the ratio of the maximum to minimum controllable flow. This value is most important for equal percentage valves because the relationship of R to U is non-linear. The default is 10.

Critical Flow Factor

The critical flow factor, C_f, is used to determine if the flow through the valve is above or below critical velocity. If flow is subcritical, the valve position determines the flow. If critical flow conditions exist, then flow is calculated as follows:

Non-compressible critical flow:

$$Q = \frac{C_V \cdot C_f}{\sqrt{\frac{SG_f}{\Delta P_s}}}$$

$$\Delta P_s = P_1 - \left[0.96 - 0.28\left(\frac{P_V}{P_c}\right)^{0.5}\right]P_V$$ Compressible Critical Flow:

$$Q = \frac{834 \cdot C_f \cdot P_1}{\sqrt{SG_f \cdot T}}$$

where

Q	=	Flow, US gpm for liquids; SCFH for gases
C_v	=	Valve flow coefficient
C_f	=	Critical flow factor
P_1	=	Inlet pressure in psia
P_c	=	Critical pressure of the fluid
SG_f	=	Specific gravity of fluid; liquids referred to water at standard conditions; gases referred to air at standard conditions
T	=	Flow temperature, *R*

Valve time constant

The time constant, Tv, is used in the time position calculation below:

$$T_V\left(\frac{dU}{dt}\right) + U = A_V \cdot P + B_V$$

Tv must be positive; therefore, the term $T_v\left(\frac{dU}{dt}\right)$ tends to slow down the valve response to the controller signal. The larger the value of this term, the more it slows down the response.

Valve Av

This is the Av term in the control valve position equation above. In the default condition, the controller output is assumed to be between 4 and 20 milliamps and the term $T_v\left(\frac{dU}{dt}\right) = 0(zero)$ Since at the minimum position, the valve is closed and u = 0 and at the maximum position, the valve is fully open and u = l, then,

0	=	Av * 4 + Bv
1	=	Av * 20 + Bv

therefore

Av	=	0.0625
Bv	=	0.25

These are the program default values for Av and Bv.

CALCULATED RESULTS

Calc. flow rate

The value displayed in this field is the current instantaneous flowrate through the valve.

Controller output

This is the value currently being received from the controller.

Steady state position

This is the steady state valve position determined from the steady state controller output, Po.

Controller output SS

This is the output signal from the controller at steady state. CC-DCOLUMN calculates this at the initial valve position, assumed to be closed.

CONTROLLER INPUT

The PID Controller continuously measures a user-specified variable and, based upon the specified setpoint for that variable, sends a controller output signal (in milliamps) to the control valve. The controller can include proportional, derivative, and/or integral action in its signal computation. Cascade controllers are permitted. The user may specify the control loop and controller limits if so desired. Also, the controller time step may be set to a smaller value than the flowsheet integration time step.

PB (proportional band)

The proportional band (PB) helps determine the speed of the controller output signal according to the following equation:

$$P_{out} = P + I + D + P_0$$

where

P_{out} = Controller output signal in milliamps

$$P = \frac{100}{PB} \cdot \text{error} = \text{proportional action}$$

$$I = \frac{100}{PB} \cdot \left(\frac{1}{T_i}\right) \cdot \int (\text{error})\, dt = \text{integral action}$$

$$D = \frac{100}{PB} \cdot T_d \cdot \frac{d(\text{error})}{dt} = \text{derivative action}$$

and

P_0 = Controller signal at steady state

PB = Proportional band

T_i = Integral time constant in minutes

T_d = Derivative time constant in minutes

error = Current controller input - the controller input at steady state

Ti (integral time, min)

This is the integral time constant defined above in the proportional band explanation. The smaller Ti is, the faster the controller will respond. Ti must be 0 or positive. If T = 0 or Ti > 1010, no integral action will be taken.

Integral control removes the offset produced by proportional control alone. Decreasing Ti gives a faster controller response but introduces a tendency to overshoot the setpoint producing oscillations.

Td (derivative, min)

Td is the derivative time constant in minutes. Derivative control anticipates the convergence on the setpoint so that any overshooting on oscillation is minimized. Derivative control is not frequently used because sensor signal noise makes measurement of the derivative difficult.

Po (steady state output)

Po is the value of the controller signal (in milliamps) at the steady state. If this field is left blank, Po will be calculated by the program based upon the initial state of the process.

The steady state output term allows the controller to function linearly on either side of the setpoint. Setting Uss = 100% will fully open the control valve as soon as the controller is activated, whereas Uss = 0 starts the system with the valve closed and the controller will open the valve slowly in response to the error signal.

Errors Definition

At the user's option, the error may be defined in one of two ways:

1. Error = X - X set
2. Error = X set - X

where X = Controller input (in milliamps) at the current value of the measured variable.

X set = Controller input (in milliamps) at the setpoint value of the measured variable.

Equation (1) above should be used when the function being controlled is for cooling, pressure control, or level control.

Equation (2) above should be used when the function being controlled is for heating or flowrate control.

These are guidelines. The general rule is as follows. The user should select the error function, which ensures that the control variable will move toward the setpoint if an error exists. For instance, if the service being controlled is steam flowrate to the jacket and the setpoint is the reactor main temperature, the function "Error = X set - X" should be selected. This is true because when the reactor main temperature is below the setpoint, the error will be positive and the steam valve will open. If in the same situation, Error = X - X set was chosen, the error would be negative and the steam valve would close, thus moving away from our target - not closer to it.

Setpoint

Enter the setpoint for the controller. This input is required, and the value must be non-zero.

SENSOR INFORMATION

Measured Variable

The measured variable is the variable we are trying to control. For instance, it we want to control the mass flowrate of the reflux at 10,000 lbs. per hour, then the measured variable is mass flowrate and the set point is 10,000 lbs. per hour.

The available options are:

- mass flow rate of the reflux
- molar flow rate of the reflux
- volume flow rate of the liquid reflux
- accumulator liquid level
- temperature of a specified tray

Tray No.

If the measured variable is the temperature of a specified tray, then the tray (stage) number must be entered in this field.

Controller/Sensor Function:

The functional relationship between the controller input and the output from the sensor is as follows:

Cin = Ac + Bc * X + Cc * X2

Cin = Controller input in milliamps

X = Value of the measured variable in the user specified engineering units

The coefficients Ac , Bc, Cc are calculated by the program using the function type and variables shown below Controller/sensor function:

The user may specify whether the sensor function is linear or quadratic. The default is linear. The quadratic form should be selected if the measured variable is flowrate. Otherwise, linear can be used.

The user must specify the minimum and maximum values of the measured variable.

The minimum and maximum sensor output values may be specified by the user if desired. The default values are 4 and 20 milliamps, respectively.

Control limit

Indicate whether the controller limits specified are relative to the setpoint or to the limits. If no limits are specified, "None" should be specified here.

Upper limit and Lower limit

The upper and lower limits put "dead bands" in the controller response. For instance, if the setpoint = 200°F and the lower limit is 195°F, the cooling water controller will shut the control valve off once the temperature falls below 195°F.

Transmitter A and Transmitter B

These fields allow the user to input the parameters for the optional model to simulate the transmitter error in PIDC. The controller input from the sensor is modeled as:

$$C = A * S + B$$

where

S is the signal from the sensor

A and B are the parameters input by the user. The default values are A = 1 and B = 0

C is the signal received by the controller

CALCULATED RESULTS

Measured Variable

Integral:

If integral action is specified (I.e., if Ti is specified), the integral contribution to the controller output function will be shown here.

Error

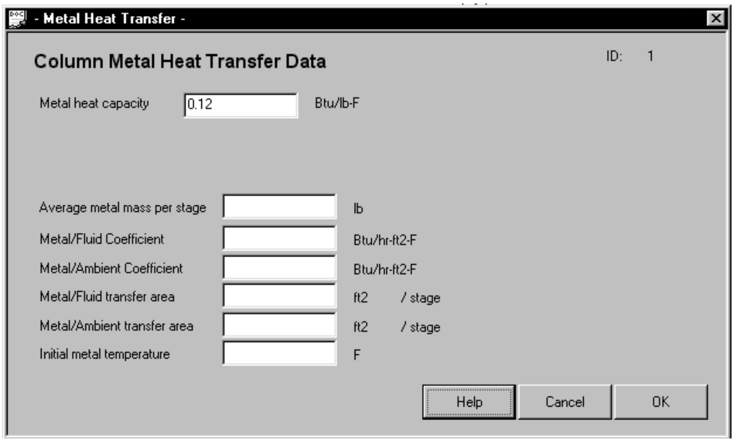
The last computed error is displayed here.

Controller output

This is the last output signal from the controller.

THE COLUMN METAL HEAT TRANSFER DIALOG BOX

The **Column Metal Heat Transfer** dialog box will be only available if the **include column metal heat transfer** option on the General Information dialog box was checked. All items of this dialog box must be completed. The **Column Metal Heat Transfer** dialog box is shown below:



Metal Heat Capacity – Input the metal heat capacity in this field.

Average metal mass per stage – Input the average metal mass per stage.

Metal/Ambient Coefficient – Input the heat transfer coefficient between metal and the ambient.

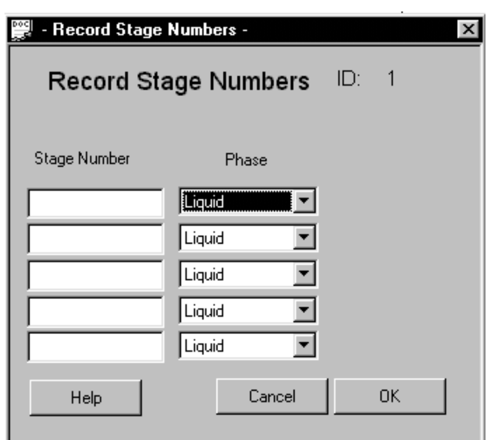
Metal/Fluid Coefficient – Input the heat transfer coefficient between metal and the fluid.

Metal/Ambient transfer area – Input the heat transfer area per stage between metal and the fluid.

Initial metal temperature – Input the initial metal temperature.

THE RECORD STAGES DIALOG BOX

CC-DCOLUMN does not save all of the results from a dynamic column simulation. The data for time histories are simply too voluminous for this. The user must identify which output is to be saved. For stage results this is done with the **Record Stages** dialog box.



The stage number and the phase must be specified. CC-DCOLUMN numbers stages from the top down with the condenser (if present) being stage number one and the reboiler (if present) being the last stage. Only five stage can be saved (recorded).

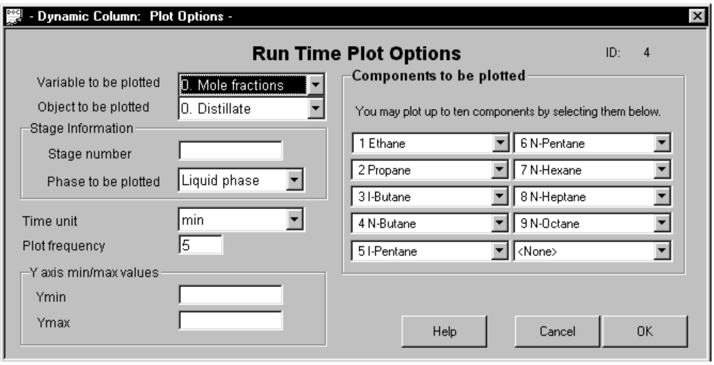
A stage must be recorded before it can be plotted or printed out.

Recorded stage information includes:

- Composition.
- Flow rates.
- Temperature.
- Pressure.

THE PLOT OPTIONS DIALOG BOX

The **Dynamic Column Plot** dialog box is shown below:



Variable to be plotted

Define the variable to be plotted on the y-axis. Select one from the pull-down list.

Object to be plotted

Select one of the following. This field may not be needed if the variable specified above does not require a location (e.g., Reflux Ratio).

- Distillate
- Bottom
- Stage

Stage Information

If a plot for one of the stages in the column is desired, specify the following:

- Stage No. – Enter the stage number for which the properties will be plotted.
- Phase – Indicate whether you are plotting data for the liquid or vapor phase.
- Time Unit / Frequency

Time Unit

Specify what time unit you want to use for the x-axis and the frequency you want plotted (hr, min, sec).

Plot Frequency

This is the number of time steps between plotting results. If the simulation integration time step is one minute and the plot frequency is five, the results will be plotted every five (simulated) minutes.

Y-axis min/max values

CC-DCOLUMN allows tuning up the range for the plot of a recorded variable. Specify a minimum and maximum for the y-axis of your plot

Components to be plotted

You may plot up to ten components by selecting them in this section.. If the plot you select is any related to flow or concentration (i.e. mole/mass/mass frac/ etc) you may want to select the component(s) to be plotted. Select components from the pull-down list.

THE PID CONTROLLER/CONTROL VALVE MODEL

Because the PID Controller and the valve(s) it controls (Control Valve) always work together, they have been described together in this one section. This makes the overall logic of the control system easier to understand. If it were not for the need to model cascade control/ systems (where master controllers control slave controllers), the PID Controller UnitOp and the Control Valve UnitOp could be combined into a single module.

The standard control system (not cascade) consists of three conceptual parts; The sensor, the PID Controller, and the Control Valve (and its actuator).

The actions of this system are:

1. The sensor monitors or measures the set point variable and converts its measurement into an electrical (milliamp) signal, which it transmits to the PID controller.
2. The PID Controller uses this signal to compute an error. The error is the difference between the set point milliamp equivalent and the electrical signal coming from the sensor. The PID Controller then uses this error to generate a controller signal, also in milliamps, which controls the valve.
3. The control valve actuator uses the controller signal to open and close the valve. The amount of the valve movement is a function of the amplitude of the PID control signal. As the valve opens and closes, the flow rate through it changes.

Computationally, this system proceeds as follows:

1. Determine the actual value of the set point variable. For instance, determine the reactor temperature in degrees F.
2. Calculate the sensor function (signal) in milliamps.
3. Calculate the error from the set point and the sensor signal.
4. Using the error compute the PID Controller output (signal) in milliamps.
5. Using the PID Controller signal, calculate the new valve position (present open or shut).
6. Based on the valve position, calculate the flow through the valve.

This is a how CC-ReACS models a PID Control system.

This process must be repeated many times per time step to accurately represent the action of real systems.

The details of these steps are described below.

DETERMINE THE MEASURED VALUES OF THE SET POINT VARIABLE

Set point variables are the quantities that you want to hold at a specified value through manipulation of the control system. They are what you want to control. For instance, if you want to keep the reactor pressure as close to a desired value as possible by adjusting its vapor draw rate, the reactor pressure is your set point variable. The program calculates the current value of a set point variable.

CC-DCOLUMN will allow almost any parameter in the flowsheet to be a set point variable. The user identifies this variable and specifies its set point value when he/she enters the input for the PID Controller UnitOp. During the simulation, its current value is continuously read.

CALCULATE THE SENSOR OUTPUT SIGNAL

The sensor output function is:

$$S = A + B \cdot X + C \cdot X^2$$

where

S is the sensor output signal in milliamps. A, B, C are coefficients of the function, x is the current value of the measured (set point) variable in flowsheet engineering units.

The coefficients A, B, and C are calculated by the program from the maximum and minimum input and output of the sensor. This calculation is made below:

1. The user must specify the following items:
   a. Whether the sensor function is linear or quadratic.
   b. The maximum and minimum sensor output signal (in milliamps). Default values are 20 and 4 milliamps.

c. The values of the measured variable at the sensor maximum and minimum output signal. Described in another way:

- The "maximum" value of the measured variable generates the maximum sensor output signal. If the measured variable rises above this "maximum", the sensor output remains at the same upper boundary value.

- The "minimum" value of the measured variable generates the minimum sensor output signal. If the measured variable falls below this "minimum", the sensor output remains at the same lower boundary value.

2. If the sensor function is to be linear, the coefficients A and B are determined from the specified maximums and minimums.

3. If the sensor function is to be quadratic, then the coefficients B and C are computed from the specified maximums and minimum.

THE PID CONTROL FUNCTION

The PID control function is:

$$P_{out} = P + I + D + P_0$$

where

P_{out} = Controller output signal in milliamps

$$P = \frac{100}{PB} \cdot \text{error} = \text{proportional action}$$

$$I = \frac{100}{PB} \cdot \left(\frac{1}{T_i}\right) \cdot \int (\text{error})\,dt = \text{integral action}$$

$$D = \frac{100}{PB} \cdot T_d \cdot \frac{d(\text{error})}{dt} = \text{derivative action}$$

and

P_0 = Controller signal at steady state

PB = Proportional band

T_i = Integral time constant in minutes

T_d = Derivative time constant in minutes

error = Current controller input - the controller input at steady state

At the user's option, the error may be defined in one of two ways:

Error = X - Xset

or

Error = Xset - X

where

X = Controller input (in milliamps) at the current value of the measured variable.

Xset = Controller input (in milliamps) at the set point value of the measured variable.

Equation (1) above should be used when the function being controlled is for cooling, pressure control or level control.

Equation (2) above should be used when the function being controlled is for heating or flow rate control.

These are guidelines. The general rule is as follows. The user should select the error function which ensures that the control variable will move toward the set point if an error exists.

P_0 is the value of the controller signal (in milliamps) at the steady state. If this field is left blank, P_0 will be calculated by the program based upon the initial state of the process.

The steady state output term allows the controller to function linearly on either side of the set point. Setting $P_0 = 0$ starts the system with the valve closed and the controller will open the valve slowly in response to the error signal.

THE VALVE POSITION EQUATION

The valve position is determined using the following equation:

$$T_V \left(\frac{dU}{dt}\right) + U = A_V \cdot P + B_V$$

where

T_v = The valve time constant (default = 0)

U = The valve position (in fractions)

P = The PID Controller output signal in milliamps

A_v, B_v = The valve constants (Defaults are $A_v = 0.0625$ and $B_v = -0.25$)

The user specifies T_v. The default is $T_v = 0$.

The program uses the following information to calculate A_v and B_v:

- The value of T_v
- The value of the PID controller signal when the valve is completely closed (the "minimum" PID Controller signal)
- The value of the PID Controller signal when the valve is fully opens (the "maximum" PID Control signal).

For example, typical maximum and minimum PID Control signals are 20 milliamps (valve fully open) and 4 milliamps (valve fully closed) respectively. If T_v is zero (the default condition), then:

At $U = 1.0_g$ $1.0 = A_v \cdot (20) + B_v$

At $U = 0.0_g$ $0.0 = A_v \cdot (4) + B_v$

$A_v = 0.0625$ and $B_v = -0.25$

These are the defaults.

If, however, $P_{max} = 110$, $P_{min} = 10$ and we keep $T_v = 0$, then:

At $U = 1.0,$ $1.0 = A_v \cdot (110) + B_v$

At $U = 0.0,$ $0.0 = A_v \cdot (10) + B_v$

$A_v = 0.01$ and $B_v = -0.10$

THE CONTROL VALVE FLOWRATE CALCULATION

The valve position is related to the valve flow rate by the following equations:

For Subcritical Non-Compressible Flow:

$$\text{Linear Valves : Flow} = 500 \cdot \frac{U}{100} \cdot \left[1 - \frac{1}{R}\right] \cdot C_v \cdot SG_f \cdot \Delta P$$

$$\text{Equal Percentage Valves : Flow} = 500 \cdot R^{\left(\frac{U}{100} - 1\right)} \cdot C_v \cdot SG_f \cdot \Delta P$$

where

R	=	Rangeability (ratio of maximum to minimum controllable flow)
C_v	=	Valve flow coefficient
SG_f	=	Specific gravity of flowing fluid
ΔP	=	Pressure drop across the valve

For Subcritical Compressible Flow:

$$\text{Linear Valves : Flow} = 3.22 \cdot \frac{U}{100} \cdot \left[1 - \frac{1}{R}\right] \cdot C_v \cdot \left(\Delta P \left(P_1 + P_2\right) SG_f\right)^{0.5}$$

$$\text{Equal Percentage Valves : Flow} = 3.22 \cdot R^{\left(\frac{U}{100} - 1\right)} \cdot C_v \cdot \left(\Delta P \left(P_1 + P_2\right) SG_f\right)^{0.5}$$

where

P_1 and P_2 = Upstream and downstream pressure, respectively

For Critical Non-Compressible Flow:

$$\text{Flow} = 500 \cdot C_v \cdot C_f \left(\frac{SG_f}{\Delta P_s} \right)^{0.5}$$

where

C_f = Critical flow factor, usually supplied by the user; default = 0.98

$$\Delta P_s = P_1 - \left[0.96 - 0.28 \left(\frac{P_v}{P_c} \right)^{0.5} \right] P_v$$

P_v = Vapor pressure of liquid at flowing temperature

P_c = Thermodynamic critical pressure of fluid

For Critical Compressible Flow:

$$\text{Flow} = 2.8 \cdot C_v \cdot C_f \cdot P_l \cdot SG_f^{0.5}$$

The above describes the typical set up for a PID Control system in CC-DCOLUMN. There are certain important variations and expressions of the PID control system, which should be noted:

1. Cascade Control Systems

   In a cascade control system, the valve is controlled by a slave controller which is in turn controlled by a master controller. In this setup, there are two set point variables, one for each controller. The master controller influences the behavior of the slave by changing its set point value. This changes the magnitude (and sometimes the sign) of the error. This effect "cascades" to the control valve.

   This system is illustrated in the figure below:

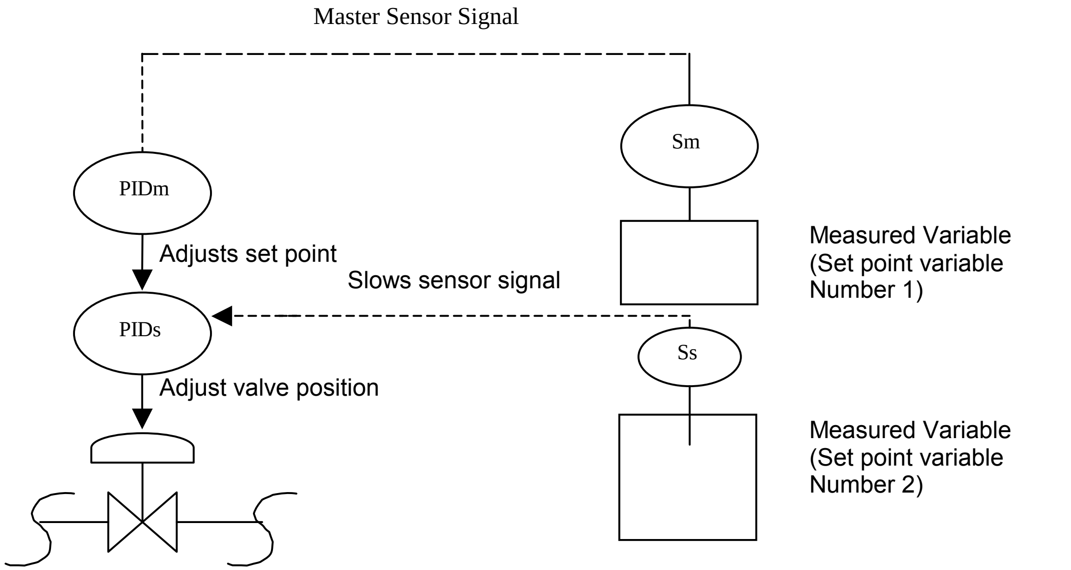


Figure 1
Cascade Control System

The sequence is:

a. The master sensor, Sm, reads the current value of measured variable number one (the "master" measured variable) and generate a signal to the master PID Controller, PIDm.

b. The master controller uses this signal to compute the error and a controller output signal. This signal will be in milliamps and will be between the maximum and minimum allowable controller output signals.

c. The slave controller, PIDs, will use the signal from PIDm to determine what its new set point should be. This is done by interpolating:

$$\frac{P - Pmin}{Pmax - Pmin} = \frac{S - Smin}{Smax - Smin}$$

where

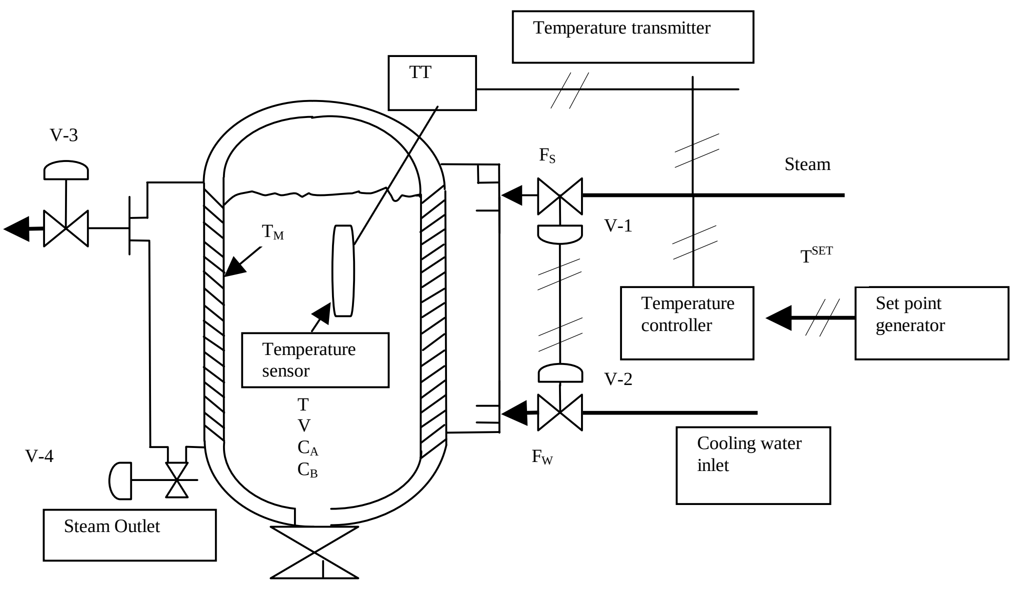
P	=	The current signal from PIDm
Pmax	=	*The maximum signal from PIDm*
Pmin	=	The minimum signal from PIDm
S	=	The new set point value of measured variable No. 2
Sma	=	The maximum set point value of measured variable No. 2
Smin	=	The minimum set point value of measured variable No. 2

d. The slave controller then generates a new PID controller signal to the control valve.

e. The control valve adjusts its position and therefore the flow through the valve.

2. Split Range Controllers

Split range controllers are PID Controllers that control two valves over two mutually exclusive ranges. To illustrate, consider the following batch reactor and its control system.



Steam is initially fed into the jacket to heat up the system to temperatures at which the consecutive reactions begin. Then cooling water must be used in the jacket to remove the exothermic heats of the reactions.

The output signal of the temperature controller goes to two split-ranged valves, a steam and a water valve. The valves will be adjusted so that the stream valve is wide open when the controller output signal, P, equals 20 milliamps and is closed at P = 12 milliamps (i.e., half the full range of the controller output). The water valve will be closed at P = 12 milliamps and wide open at P = 4 milliamps. The reason for hooking up the valves in this manner is to have the correct fail-safe action in the event of an instrument failure. The steam valve will be set to fail closed and the cooling water valve will be set to fail open.

In CC-DCOLUMN, split range control systems are set up in the following way:

a. Identify the two valves to be controlled by the PID controller in the PID Controller dialog box (for input). Now both control valves will receive the controller output signal.

b. Select the valve coefficients, A_v and B_v, so that the valve open mutually exclusive ranges.

Continuing the above example, we would proceed as follows:

i. Specify the steam control valve, V-1, and the cooling water control valve, V-2, as the two valves to be controlled by the PID Controller, TC-1. This done on the **PID Controller dialog box**.

ii. Compute A_v and B_v for the steam valve:

- At P = 20 milliamps, the valve is 100% open.
- At P = 12 milliamps, the valve is 0% open.

where

P is the PID Controller output signal thus, using the valve equation:

$$1.0 = 20\,A_v + B_v$$

$$0.0 = 12\,A_v + B_v$$

solving these equations we get $A_v = 0.125$ and $B_v = -1.5$.

iii. Compute A_v and B_v for the cooling water valve:

- At P = 12 milliamps, the valve is 0% open
- At P = 4 milliamps, the valve is 100% open

then

$$0.0 = 12\,A_v + B_v$$

$$1.0 = 4\,A_v + B_v$$

solving

$$A_v = -0.125 \text{ and } B_v = 1.5$$

3. Enter these A_v and B_v values in the appropriate input fields for the two valves. This done in the Control Valve dialog boxes.
4. Complete the remaining input for the PID Controller and the Control Valves in the usual manner.
5. Controller Limits

Specified limits can be placed on the PID Controller output if so desired. These limits create "dead bands". Dead bands are regions where the controller instructs the valve not to take action even though controller output signal would indicate otherwise.

If absolute ranges are used, then they may need to be reset if the operating set point is changed.

CONTROL VALVE DIALOG BOX

The control valve calculates the flow rate through the valve based on the output signal it receives from a controller. Each control valve, therefore, must have a designated controller ID as part of its input. The module can handle compressible and incompressible flow as well as critical and sub-critical flow. The control valve calculates the following variables at each time step:

1. The valve position.
2. The flow through the valve.

The flow rate of the inlet and outlet streams will be reset to the control valve calculated flow.

The output from the controller is used by the control valve to determine the valve position, that is, how far open (in percentages) the valve is at any point in time. The valve position, U, is determined as follows:

$$T_V\left(\frac{dU}{dt}\right)+U=A_V\cdot P+B_V$$

where

T_v	=	Valve time constant; default = 0
U	=	Valve position (in fractions); must be between 0 and 1
P	=	Controller output signal in milliampers
A_v, B_v	=	Valve constants; defaults: A_v = 0.0625 and B_v = 0.25

Normally the controller output, P, is between 4 and 20 milliamperes. The valve position, *U*, varies between 0 and 1.

The valve position is related to the valve flow rate by the following equations:

C_f	=	Critical flow factor, usually supplied by the user; default = 0.98

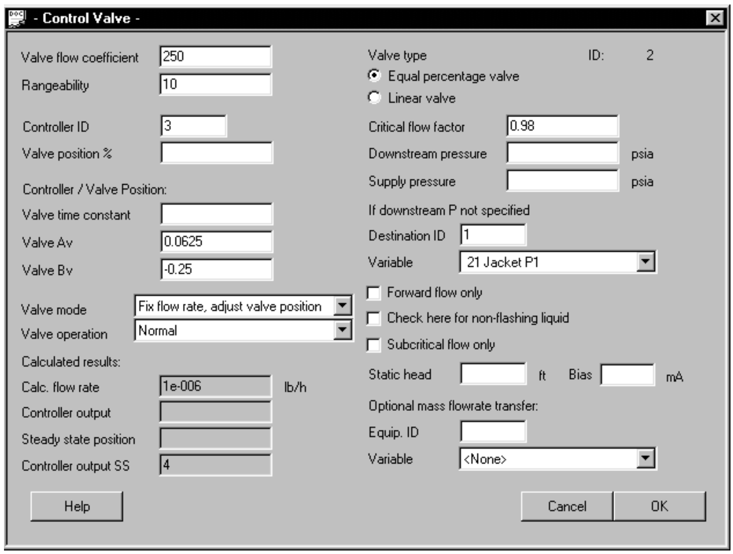
$$\Delta P_S = P_1-\left[0.96-0.28\left(\frac{P_V}{P_C}\right)^{0.5}\right]P_V$$

P_v	=	Vapor pressure of liquid at flowing temperature
P_c	=	Thermodynamic critical pressure of fluid

For Critical Compressible Flow:

$$\text{Flow} = 2.8 \cdot C_v \cdot C_f \cdot P_1 \cdot SG_f^{0.5}$$

PARAMETER DEFINITIONS



Valve Flow Coefficient:
This is the valve C_v. This field must be entered. If you do not know a good value for C_v, use the valve sizing C_v tool. This tool will calculate a good value for this field.

The definition of the flow coefficient is defined as follows:

$$C_v = Q\left(\frac{SG_f}{\Delta P_s}\right)^{0.5}$$

Rangeability:
Rangeability is the ratio of the maximum to minimum controllable flow. This value is most important for equal percentage valves because the relationship of *R* to *U* is non-linear. The default is 10.

Controller ID:
Enter the equipment ID number of the controller (PIDC) which controls this valve. If no controller ID is specified, the program will assume the valve is manual and the valve position will be set to valve position entered in the field below. Therefore, one or the other must be specified.

Valve Position (%):
The valve position ranges from 0 (closed) to 100 (fully open). If the valve is controlled by a controller, the value is determined by the controller signal. If no controller is specified, the valve is assumed to be manual and the user must enter a value here. Units are percentages.

CONTROLLER/VALVE POSITION

Valve Time Constant:
The time constant, T_v, is used in the time position calculation below:

$$T_V\left(\frac{dU}{dt}\right)+U=A_V\cdot P+B_V$$

T_v must be positive; therefore, the term $T_V\left(\frac{dU}{dt}\right)$ tends to slow down the valve response to the controller signal. The larger the value of this term, the more it slows down the response.

Valve A_v and B_v:
These are the A_v and B_v terms in the control valve position equation above. In the default condition, the controller output is assumed to be between 4 and 20 milliamps and the term $T_V\left(\frac{dU}{dt}\right)=0\ \text{(zero)}$. Since at the minimum position, the valve is closed and U = 0 and at the maximum position the valve is fully open and U = l, then the defaults are determined as:

$$0 = A_v * 4 + B_v$$

$$1 = A_v * 20 + B_v$$

therefore

$$A_v = 0.0625$$

$$B_v = 0.25$$

Valve Mode:
The control valve may be manually controlled, i.e., the valve position, instead of being set by a PID controller, may be specifically fixed by the user using any of the following options:

i. Fix the flowrate through the valve and have the program calculate the required valve position. If this option is chosen, the flowrate through the valve is set equal to the inlet stream flowrate.

ii. Fix the valve position, and have CC-DCOLUMN calculate the flow through the valve. If this option is selected, the valve position must be specified in the **Valve Position** field described above.

iii. Fix both the flowrate through the valve and the valve position and have the program calculate the valve outlet pressure. If this option is selected, the fixed flowrate is taken to be the inlet stream flowrate and the valve position must be specified in the **Valve Position** field described above.

Please note the following:

1. These valves may be fixed at a single valve or scheduled using the RAMP Controller.

If both manual control and PID control are set up or "turned on" for a control valve, the PID control is ignored and the manual control valves are the ones used.

Valve Type:
Choose from either linear or equal percentage valves.

Linear valves relate the actual valve flow to the capacity valve flow by the following relation:

$$\text{Actual Flow} = \frac{U}{100}\left(1-\frac{1}{R}\right)(\text{Valve Capacity})$$

Equal percentage valves relate actual flow to capacity valve flow as follows:

$$\text{Actual Flow} = R^{\left(\frac{U}{100}-1\right)}(\text{Valve Capacity})$$

Valve Operation:
This combo box makes it possible to select different options to simulate malfunctions and manually operated valves. Each option allows the user or an operator training system such as CC-OTS to simulate malfunctions and manual operations of CVAL:

Normal: CVAL will operate operate properly and will set the flow rate according to the simulation parameters.

Power failure: CVAL will set flow rate to zero regardless of other simulation parameters.

Manually close: CVAL will set flow rate to zero regardless of other simulation parameters.

Manually open: CVAL will calculate flow rates at 100% open valve position regardless of other simulation parameters such as PID controllers.

Manually set valve position: CVAL will allow the user to input a specified valve position and calculate the flow rate, overriding any other simulation parameter.

Critical Flow Factor:
The critical flow factor, C_f, is used to determine if the flow through the valve is above or below critical velocity. If flow is subcritical, the valve position determines the flow. If critical flow conditions exist, then flow is calculated as follows:

Non-compressible critical flow:

$$Q = \frac{C_v \cdot C_f}{\sqrt{\frac{SG_f}{\Delta P_s}}}$$

$$\Delta P_s = P_1 - \left[0.96 - 0.28 \left(\frac{P_v}{P_c} \right)^{0.5} \right] P_v$$

Compressible Critical Flow:

$$Q = \frac{834 \cdot C_f \cdot P_1}{\sqrt{SG_f \cdot T}}$$

where

Q	=	Flow, US gpm for liquids; SCFH for gases
C_v	=	Valve flow coefficient
C_f	=	Critical flow factor
P_1	=	Inlet pressure in psia
P_c	=	Critical pressure of the fluid
SG_f	=	Specific gravity of fluid; liquids referred to water at standard conditions; gases referred to air at standard conditions
T	=	Flow temperature, R

Downstream Pressure:
The control valve downstream pressure can be specified here. If downstream pressure is not specified, the output pressure of the valve will be determined by the pressure of the downstream unit operation which is specified in the field labeled **Destination ID** or by the jacket pressure (if so specified in the **PID Controller** input.

Supply Pressure:
Enter the control valve supply pressure. If not specified, the pressure of the inlet stream will be used.

IF DOWNSTREAM PRESURE NOT IDENTIFIED

Destination ID:
If the downstream pressure is not specified, the output pressure of the valve will be determined by the pressure of the downstream unit operation specified in this field.

Variable:
If the downstream(s) is going to a batch reactor, it will be necessary to identify which batch reactor pressure (jacket, coil, or process) is to be used. This is done in the **Variable** field. Click on the field to display a list of options. Select the appropriate pressure from this list.

Forward flow only Option: Flow in a piping network can go forward or backward. Checking this option will ensure the flow will go forward .In case backward flow is detected the flow rate will be set to zero.

Non-flashing liquid option:
The flow through the valve can be compressible or non-compressible. If the flow is compressible, select the **Vapor or two-phase flow** option. If the flow is non-compressible, select the **Non-flash liquid** option.

Subcritical flow only Option:
The flow through the valve can reach critical conditions. Piping network might not converge if CVAL is choked. Turning on this option will let the flowsheet converge and warn the user about the critical conditions in CVAL.

Static head:
If an elevation change is to be included in the flow calculation, enter this value in this field. The elevation change will affect the available pressure drop across the valve, and therefore it will affect the flow rate as well.

Bias option:
The actual input of the CVAL will set the output signal from the PID Controller + Bias

OPTIONAL MASS FLOWRATE TRANSFER

These fields can be used to pass the control valve flow rate into another unit operation variable.

Equip ID:
Specify the unit operation ID number of the UnitOp that the flow rate is to be passed to.

Variable:
Specify the variable number of the parameter that the flow rate is to be passed into.

CALCULATED RESULTS

Calc. Flow Rate:
The value displayed in this field is the current instantaneous flow rate through the valve.

Controller Output:
This is the value currently being received from the controller.

Steady State Position:
This is the steady state valve position determined from the steady state controller output, P_0. (See the "PID Controller Field Descriptions".)

Controller Output At Steady State:
This is the output signal from the controller at steady state. CHEMCAD calculates this at the initial valve position, assumed to be closed.

TOPOLOGY

A control valve has one input and up to two outlets. If two outlets are present, the first outlet is vapor and the second outlet is liquid.

PID CONTROLLER DIALOG BOX

The PID Controller continuously measures the user specified variable, and based upon the specified set point for that variable, sends a controller output signal (in milliamps) to the control valve. The controller can include proportional, derivative, and/or integral action in its signal computation. Cascade controllers are permitted. The user may specify the control loop and controller limits if so desired. Also, the controller time step may be set to a smaller value than the flowsheet integration time step.

The controller is actually a sensor and controller, i.e., it measures its own input as well as calculating its output. The controller measures some variables in the flowsheet (generally a batch reactor variable) and from this computes the controller input in milliamps. From this input and the user defined set point, the controller calculates its output, which is subsequently used by the control valve.

The specific logic is as follows:

1. The unit reads the current value of the user identified measured variable.
2. The controller <u>input</u> is calculated using the following expression:

$$C_{in} = A_c + B_c \cdot X + C_c \cdot X^2$$

where

C_{in}	=	Controller input in milliamps
X	=	Current value of the measured variable
A_c, B_c, C_c	=	Coefficients calculated by CC-ReACS

3. The control error (in milliamps) is then calculated as:

Error	=	Cin – Cin @ setpoint; used for cooling, pressure, and level control
Error	=	Cin @ setpoint – Cin; used for flow and heat control

4. From the above error, the controller output is calculated as follows:

$$P_{out} = P + I + D + P_0$$

where P_{out} = Controller output signal in milliamps

$$P = \frac{100}{PB} \cdot \text{error} = \text{proportional action}$$

$$I = \frac{100}{PB} \cdot \left(\frac{1}{T_i}\right) \cdot \int (\text{error})\, dt = \text{integral action}$$

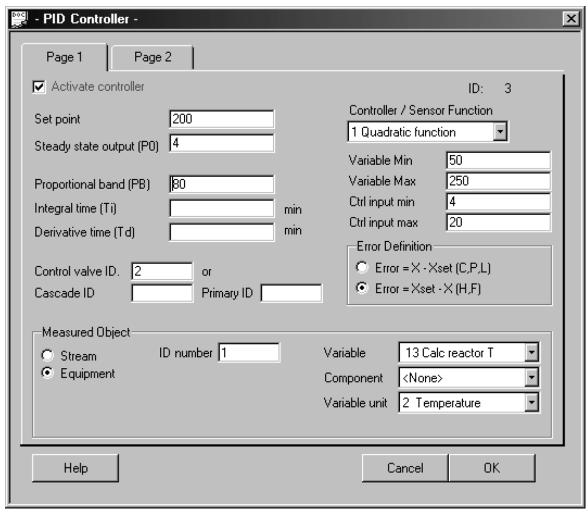
$$D = \frac{100}{PB} \cdot T_d \cdot \frac{d(\text{error})}{dt} = \text{derivative action}$$

$$P_0 = \text{controller signal at steady state}$$

and

PB	=	Proportional band
T_i	=	Integral time constant in minutes
T_d	=	Derivative time constant in minutes
error	=	Current controller input - the controller input at steady state

PARAMETER DEFINITIONS PAGE ONE



Activate Controller:
This choice box turns the control on and off while the simulation is running.

Set Point:
The value of the set point of measured variable is entered in this field. The engineering units for this entry are taken from the flowsheet global engineering units and are displayed to the right of the field.

Steady State Output (P_O):
P_0 is the value of the controller signal (in milliamps) at the steady state. If this field is left blank, P_0 will be calculated by the program based upon the initial state of the process.

The steady state output term allows the controller to function linearly on either side of the set point. Setting P_0 = 0 starts the system with the valve closed and the controller will open the valve slowly in response to the error signal.

Proportional Band (PB):
The proportional band (*PB*) helps determine the speed of the controller output signal according to the above controller output equation.

Increasing *PB* will decrease the sensitivity of the controller and give a slower response. *PB* must be positive.

Proportional action alone is normally insufficient to control a process.

Integral Time (T_i):
This is the integral time constant defined above in the controller output equation. The smaller T_i is, the faster the controller will respond. T_i must be 0 or positive. If T_i = 0 or T_i > 1010, no integral action will be taken.

Integral control removes the offset produced by proportional control alone. Decreasing T_i gives a faster controller response but introduces a tendency to overshoot the set point producing oscillations.

Derivative Time (T_d):
T_d is the derivative time constant in minutes. Derivative control anticipates the convergence on the setpoint so that any overshooting on oscillation is minimized. Derivative control is not frequently used because sensor signal noise makes measurement of the derivative difficult.

Control Valve ID:
The PID Controller must know which control valve or which cascade controller it is controlling. If this controller is controlling a control valve, enter the UnitOp ID of the control valve in this field.

Cascade ID:
If this controller is controlling another controller in a cascade control scheme, enter the UnitOp ID number of the slave controller in this field.

Primary ID:
If this controller is the slave to another controller in a cascade control scheme, enter the UnitOp ID number of the master controller, which is controlling this controller in this field.

CONTROLLER/SENSOR FUNCTION

The functional relationship between the controller input and the output from the sensor is as follows:

$$C_{in} = A_c + B_c \cdot X + C_c \cdot X^2$$

C_{in} = Controller input in milliamps

X = Value of the measured variable in the user specified engineering units

The coefficients A_c , B_c, C_c are calculated by the program using the function type and variables shown below. If the sensor function is to be linear, then A_c and B_c are calculated. If the sensor function is to be quadratic, then B_c and C_c are calculated.

Controller/Sensor Function:
The user may specify whether the sensor function is linear or quadratic. The default is linear. The quadratic form should be selected if the measured variable is flow rate. Otherwise, linear can be used.

Variable Min and Variable Max:
The user may specify the minimum and maximum sensor output values if desired. The default values are 4 and 20 milliamps, respectively.

Ctrl Input Min and Ctrl Input Max:
The user must specify the minimum and maximum values of the measured variable. This is done in these two fields. The program will then determine the coefficients for the above sensor equation.

Error Definition:
At the user's option, the error may be defined in one of two ways:

Error = X - Xset

Error = Xset - X

where

X = Controller input (in milliamps) at the current value of the measured variable.

Xset = Controller input (in milliamps) at the set point value of the measured variable.

Equation (1) above should be used when the function being controlled is for cooling, pressure control, or level control.

Equation (2) above should be used when the function being controlled is for heating or flow rate control.

These are guidelines. The general rule is as follows. The user should select the error function which ensures that the control variable will move toward the set point if an error exists. For instance, if the service being controlled is steam flow rate to the jacket and the set point is the reactor temperature, the function *Error = Xset - X* should be selected. This is true because when the reactor temperature is below the set point, the error will be positive and the steam valve will open. If in the same situation, *Error = X - Xset* was chosen, the error would be negative and the steam valve would close, thus moving away from our target, not closer to it.

MEASURED OBJECT

The measured object is the set point variable. The set point is the condition which must be achieved by the control system. In other words, the measured variable must equal the set point before the controller will stop resetting the control valve.

To let CC-DCOLUMN know which variable is to be measured, the user must do the following:

1. Identify whether the variable is contained in a stream or unit operation.
2. Identify which stream or unit operation is involved. This is the UnitOp or Stream ID.
3. Specify the variable or parameter of the stream or unit operation.
4. Specify the type of engineering units the variable uses.
5. Specify which component the measured variable applies to (if applicable).

The procedure is as follows:

1. Identify whether the variable is a stream or a unit operation variable by clicking the appropriate circle at the field labeled "Stream" or "Equipment".
2. In the "Measured Object ID" field, enter either the stream number or the equipment number in which the measured variable is located.

3. In the “Variable” field select the variable from the list provided by:
    - Clicking on the field to open the list;
    - Scrolling to the desired selection;
    - Clicking on the desired selection.
4. Specify the type of engineering units to be used by making the appropriate selection in the “Variable unit” field. Do this by:
    - Clicking on the field to open the list;
    - Scrolling to the desired selection;
    - Clicking on the desired selection.
5. If the measured variable is a selection which requires component identification, such as “mole fraction or “reaction rate”, you must identify the relevant component in the “Comp” field. The procedure is:
    - Click on the field to open the component list;
    - Scroll to the relevant components;
    - Click on the component to select it.

Stream or Equipment:
The user must identify if the measured variable is a stream variable or an equipment parameter. This is done be clicking on the appropriate circle in this field.

ID Number:
The user must specify the ID number of the stream or piece of equipment that the measured object is associated with.

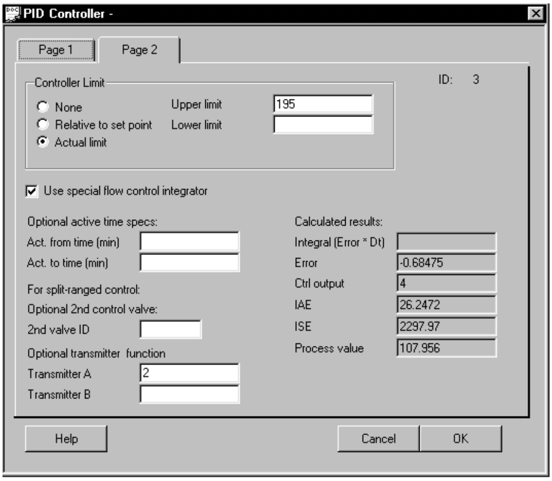
Variable:
Each UnitOp or Stream has a list of variables, which can be used as set point variables. This list is contained in this field and can be displayed by clicking on it. From this list, locate the desired variable and click on it.

Component:
This field contained a list of all the components in the current flowsheet. If a component variable, such as mole fraction or mass flow rate is selected as the “Measured variable” above, then the user must identify which component from this “Measured component” list.

To display the list, click anywhere on the field. Then locate the relevant component by scrolling. To select the component, click on it.

Variable unit:
Use this field to identify the type of engineering units that apply to the measured variable. In other words, if the measured variable is the reactor temperature, selected “2 Temperature” from the list. This will instruct the program to apply the global flowsheet engineering units to the measured variable. Otherwise, internal engineering units will be used.

PARAMETER DEFINITIONS PAGE TWO



Controller Limit:

- O None
- O Relative to set point
- O Actual limit

Specify whether the controller limits specified below are relative to the set point or actual limits. If no limits are specified below, "None" should be specified here.

Upper Limit and Lower Limit:
The upper and lower limits put "dead bands" in the controller response. For instance, if the set point = 200 °F and the lower limit is 195 °F, the cooling water controller will output a minimum signal below 195 °F.

Use special flow control integrator:
This option is used to turn the flow control integrator on and off.

OPTIONAL ACTIVE TIME SPECS

Act. from time (min) and Act. to time (min):
These fields are used to schedule the controller activity; that is to say, to turn it on at one time and off at another. For instance, if the simulation runs for five hours (simulated time), and the controller is only to be active (turned on) between hours two and four, then a value of "120" (minutes) should be entered in the "Act. From time (min)" field and a value of "240" (minutes) should be entered in the "Act. to time (min)" field.

FOR SPLIT RANGE CONTROL

Optional second control valve

2nd valve ID:
Enter the ID number for the second valve in a split range control scheme.

Special control:
This field is used to select the control integration method, which is to be used if the controller is controlling a flow rate.

Optional transmitter function:

These fields allow the user to input the parameters for the optional model to simulate the transmitter error in PIDC. The controller input from the sensor is modeled as:

$$C = A * S + B$$

where

S is the signal from the sensor

A and B are the parameters input by the user. The default values are A = 1 and B = 0

C is the signal received by the controller

CALCULATED RESULTS

Integral (Error * Dt):
If integral action is specified (i.e., if T_i is specified), the integral contribution to the controller output function will be shown here.

Error:
The last computed error is displayed here.

Error	=	X- Xset; or Error = Xset – X
X	=	Current sensor input in milliamps
Xset	=	Sensor input at the set point in milliamps.

Control Output:
The last calculated controller output (P_{out} in milliamps) is displayed here.

IAE:
This field contains the integral average error.

ISE:
This field displays the integral squared error.

THE DYNAMIC VESSEL MODEL

The dynamic vessel unit operations module is a dynamic phase separator and/or accumulator. It is basically a dynamic flash tank with holdups. It is illustrated in figure 2 below.

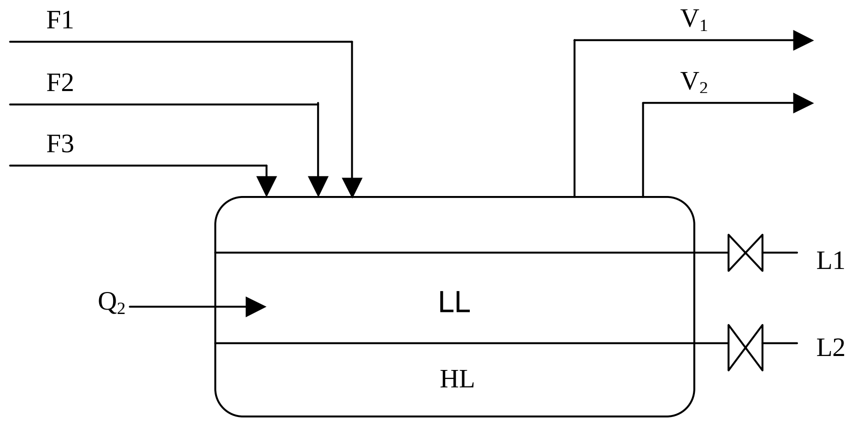


Figure 2

The features and capabilities of the dynamic vessel model are summarized below:

1. It can have up to three feed streams, two vapor outlet streams and two liquid outlet streams.
2. Vapor-liquid and Vapor-liquid-liquid phase calculations are available.
3. Light and heavy liquid phases can be accumulated up to user specified level limits.
4. The vessel operating pressure can be specified or calculated. In other words, pressure can be fixed or dynamic.
5. Four calculation modes are available.
6. The amount of vapor leaving the vessel can be fixed, controlled, or determined by a venting calculation.
7. The amount of liquid exiting the vessel can be a fixed valve or set to the amount of the liquid overflowing a specified liquid level.
8. Multiple vessel geometric can be specified.
9. Safety relief valve performance can be included in the simulation using the DIERS technology.
10. It can be part of a piping network and be solved simultaneously. This includes the static head of the liquid level above the inlet nozzle (for piping networks upstream) and the static head in a liquid outlet stream.

The following major features of the dynamic vessel model are described below:

1. The pressure calculations
2. The calculation modes

3. Maintaining liquid levels by decanting
4. The vapor flow modes
5. DIERS

THE PRESSURE CALCULATIONS

The vessel pressure is calculated by doing a constant volume flash under the current conditions. The program holds the vessel volume constant and varies the vessel pressure until the sum of the vapor and liquid volumes equals the vessel volume. As the conditions change the pressure changes.

The following points should be noted regarding the pressure calculation:

1. If the pressure is to be calculated, the flowrate of the vapor vent or outlet stream must be specified. If it is not, the problem is under specified. However, this specification can be made explicitly by the user by scheduling the vapor flowrate, or it can be made implicitly using a PID Control system. An example of this would be a pressure control system where the vapor flowrate is adjusted to maintain a desired vessel pressure.
2. Specification of an initial charge is optional, but if done can produce certain problems the user needs to be aware of. Frequently, the initial charge specifications will produce volumes that do not match the vessel volume. If the pressure is to be calculated, this can produce unwanted results unless certain conventions are adopted to manage this situation. In CC-ReACS the following conventions are adopted:
    a. If the liquid present exceeds the vessel capacity, an error message is issued and the simulation will not proceed.
    b. If the initial charge is subcooled, then the program will do an adiabatic flash to reset the temperature and pressure to values, which fill the vessel. A warning message will be issued.
    c. If the initial charge is two-phase at the specified temperature and pressure, and the sum of the vapor and liquid volume is not equal to the vessel volume, an error message will be issued. If the user chooses to go ahead with the simulation, then the program proceeds as follows:
        - The vapor and liquid amounts and compositions are determined.
        - The available vapor space is determined by subtracting the liquid volume from the vessel volume.

          $$AVS = RV - LV$$

          where

AVS	=	Available vapor space
RV	=	Vessel volume
LV	=	Liquid volume

        - The "excess" vapor is calculated as:

          $$EV = VV - AVS$$

where

EV	=	Excess vapor
VV	=	Vapor volume of the initial charge

The excess vapor is therefore negative if the initial charge does not fill the vessel.

- The excess vapor is removed from the initial charge so that the vapor space, *AVS*. If the excess volume is negative, this means adding enough vapor (of the same composition as the initial vapor) to fill the available vapor space.

THE CALCULATION MODES

The dynamic vessel module requires the user to specify both a thermal mode and a pressure mode for calculation. The available thermal modes are adiabatic, flash with heat duty, flash with UA & utility and isothermal. The pressure mode options are fixed pressure or calculated pressure. The user must specify which option is to be used in both calculation modes for the calculation to proceed. If no specification is made, defaults are assumed.

The Thermal Mode:
Note: The pressure used in the calculations for any of the following thermal modes depends on the pressure calculation mode selected.

The thermal mode options are:

- **Adiabatic –** This mode assumes that no heat passes through the walls of the vessel. At each time step a flash is performed using the inlet stream(s) composition and enthalpy.
- **Flash with heat duty –** This mode assumes a constant, user specified heat duty on the vessel. At each time step a flash is performed using the inlet stream(s) composition and enthalpy plus the specified duty.
- **Flash with UA and Utility –** In this mode you must enter the dynamic vessel U (overall heat transfer coefficient). This area is calculated from the vessel size or may be fixed using the Area field provided. Also, the vapor vent flow rate must also be specified or controlled. The heat duty is calculated using the equation,

  $$Q = U \cdot A \cdot (\Delta\Delta T$$

  The program calculates the temperature, vapor fraction and enthalpy.

  If this mode is used, the dynamic vessel must be set up with a utility stream on the flowsheet. In other words, it must have two inlet streams one of which is the utility stream, and an outlet utility stream must also be provided.

  At each time step a flash is performed using the inlet stream(s) composition and enthalpy plus the computed heat transfer determined from the above equation.
- **Isothermal –** In this mode the temperature is fixed. At each time step a flash is performed using the inlet stream(s) composition and the specified temperature. A required heat duty is computed.

The Pressure Modes:

- **Fixed pressure** – Using this option, the user specifies the vessel operating pressure. This pressure is then the one used in the flashes mentioned above in the thermal modes.

  During fixed pressure simulation if the vapor is in excess of the available vapor space, the excess vapor is vented. If the computed vapor does not fill the available vapor space, the difference is ignored.

- **Calculated pressure** – If the pressure is to be calculated, the flow through the vapor vent must be specified (it may be zero, but it must be specified). The pressure is then varied until the sum of the vapor volume and the liquid volume equals the vessel volume.

MAINTAINING LIQUID LEVELS BY DECANTING

The flow rate of the liquid outlet streams can be determined in a number of ways. One of these is by decanting an liquid in excess of a specified liquid level. Since the dynamic vessel model can handle two liquid phases if requested, it is important to know the decanting model in order to use it correctly.

The model can be summarized in the following way:

If HL> HLL; then HLF = HL – HLL, and

If TL> LLL; then LLF = LL + HLL – LLL

where

HL = The amount of heavy liquid present before decanting

LL = The amount of light liquid present before decanting

TL = The amount of total liquid present before decanting: TL = HL + LL

HLL = The volume of the vessel made available for accumulating heavy liquid

For flat head cylinders this would be:

HLL = $L_h \cdot \pi r^2$

where

L_h = The specified heavy liquid level

π = pi

r = The radius of the vessel

LLL = The volume which must be filled before any decanting of light liquid can occur

For flat head cylinder this would be:

LLL = $L_L \cdot \pi r^2$

where

L_L = The specified light liquid level

The following should be noted:

1. The specified levels are from the bottom of the vessel
2. Liquid levels are calculated:
    a. Using the full inside diameter for vertical vessels and using the full tangent-to-tangent length for horizontal vessels.
    b. Including the volume of the heads.
3. The excess of heavy liquid is decanting before the light liquid. In other words, the amount of heavy liquid to be decanted is subtracted from the total liquid present before determining how much (if any) light liquid is to be decanted.
4. If the heavy liquid level is below the specified level, then the amount of light liquid present must fill this heavy liquid deficit before any decanting of the light liquid can take place.
5. If we let HLF = the heavy liquid decanted and LLF = the light liquid decanted, four decanting situations can occur:
    a. HL> HLL and (LL+ HLL)> LLL, then

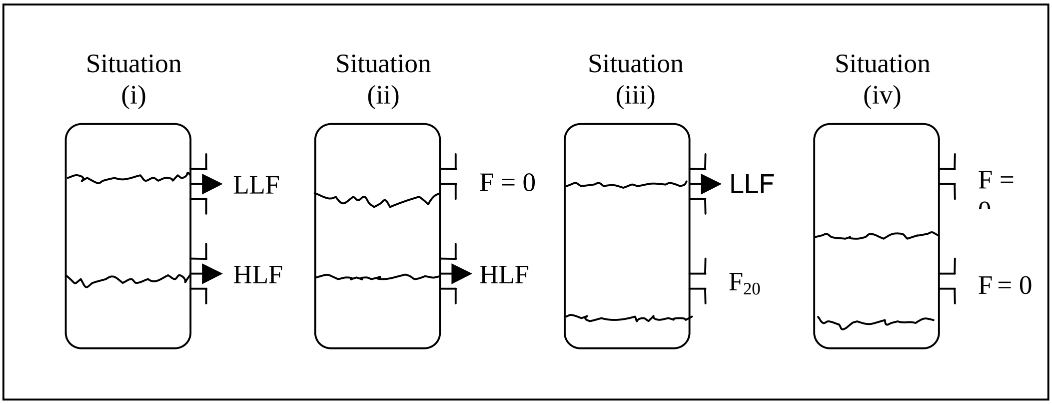
       HLF = HL- HLL and LLF = LL + HLL – LLL
    b. HL> HLL and (LL + HLL) < LLL, then

       HLF = HL – HLL and LLF = o.
    c. HL < HLL and TL > LLL, then

       HLF = 0 and LLF = TL – LLL
    d. HL < HLL and TL< LLL, then

       HLF = 0 and LLF = 0

Their situations are illustrated below:



THE VAPOR FLOW MODELS

The dynamic vessel model requires that a vapor outlet or vent be provided even if it is not used. This means you must draw one on the flowsheet.

In addition, the method for determining the flow through this vent must also be specified. The following options are available:

1. The flow rate can be fixed at a specified valve throughout the simulation.
2. The flowrate can be adjusted by a PID control system.
3. The flowrate can be reset at each time step using a RAMP controller.
4. The flowrate can be calculated using DIERS Technology. This applies to emergency relief situations. The flow through the vapor vent would be that amount that the safety relief valve (or rupture disk) can pass.
5. The flowrate can be set to the amount of vapor generation in excess of the available vapor space. In this mode the pressure must be specified.

The following rules apply:

1. If the pressure is to be dynamically calculated during the simulation, then the vapor flowrate must be specified, set by some form of controller, or determined using DIERS.
2. Flow through the vapor vent can be two-phase if DIERS is used.
3. If the calculation mode is set to the fixed pressure mode, the vapor flow mode is ignored and DIERS cannot be used.

DIERS CALCULATIONS

The CHEMCAD DIERS model is explained in detail in the on-line help system. No effort is made to repeat that information here. The following points, however, are specific to CC-DCOLUMN and CC-ReACS and should be noted.

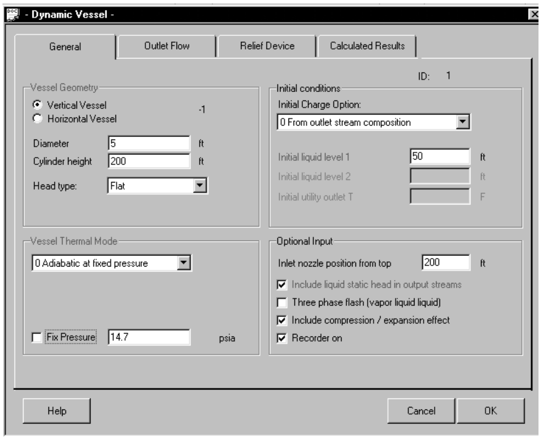
1. Only the DIERS rating calculations can be performed in CC-DCOLUMN and CC-ReACS. In other words, the size of the relief valve and/or rupture disk must be specified. CC-DCOLUMN and CC-ReACS will then calculate the amount and composition, and vapor quality of the material, which passes through the vent. This material is then removed form the heat and material balance.
2. Only the vent pressure is determined dynamically. The valve (disk) backpressure must be specified by the user and is fixed throughout the simulation.
3. If a fire model is selected for the DIERS calculation, then the fire heat input is in addition to any other specified heat input.
4. DIERS cannot be used if the calculation mode is fixed pressure or isothermal.

THE DYNAMIC VESSEL DIALOG BOX

The **Dynamic Vessel** enables the user to model vessel holdups in a dynamic fashion. Features of the dynamic vessel model include:

- Horizontal or vertical vessels
- Ellipsoidal, F & D, Flat, or hemispherical
- Fixed pressure or calculated pressure modes
- Isothermal or non-isothermal modes
- Multiple liquid phases
- Level control
- Specified flow options
- DIERS

PARAMETERS DEFINITIONS – PAGE ONE (GENERAL)



GEOMETRY

Enter the diameter and length of the vessel. Length is defined as the tangent-to-tangent cylinder length. The diameter of the vessel is measured at 90 degrees to the long axis.

Vessel Type:
Specify whether the vessel is horizontal or vertical. This is required input. The default is vertical.

Diameter:
Enter the inside diameter of the vessel measured at 90 degrees to the long axis.

Cylinder height:
Enter the cylinder length defined as the distance between the vessel heads.

Vessel Head Type:
Select the vessel head type. Available options are:

- Ellipsoidal (default)

- F & D (flange and dish)
- Flat
- Hemispherical

Head Ratio:
Enter the head ratio defined as:

$$HR = \frac{\text{overall vessel length} - \text{cylinder length}}{\text{vessel diameter}}$$

The head ratio must be between 0.0 and 1.0.

VESSEL THERMAL MODE

Upon selection of the desired thermal mode, additional input fields will open up. These fields will be appropriate to the selected mode and must be filled in for the thermal mode to operate.

The dynamic vessel module requires the user to specify both a thermal mode and a pressure mode for calculation. The available thermal modes are: adiabatic, flash with heat duty, flash with UA and utility and isothermal. The pressure mode options are fixed pressure or calculated pressure. The user must specify which option is to be used in both calculation modes for the calculation to proceed. If no specification is made, defaults are assumed.

Note: The pressure used in the calculations for any of the following thermal modes depends on the pressure calculation mode selected.

The thermal mode options are:

- **Adiabatic** – This mode assumes that no heat passes through the walls of the vessel. At each time step a flash is performed using the inlet stream(s) composition and enthalpy.
- **Flash with heat duty** – This mode assumes a constant, user specified heat duty on the vessel. At each time step a flash is performed using the inlet stream(s) composition and enthalpy plus the specified duty.
- **Flash with UA and Utility** – In this mode you must enter the dynamic vessel U (overall heat transfer coefficient). This area is calculated from the vessel size or may be fixed using the **Area** field provided. Also, the vapor vent flow rate must also be specified or controlled. The heat duty is calculated using the equation,

  $$Q = U \cdot A \cdot (\Delta T)$$

  The program calculates the temperature, pressure, vapor fraction and enthalpy.

  If this mode is used, the dynamic vessel must be set up with a utility stream on the flowsheet. In other words, it must have two inlet streams one of which is the utility stream, and an outlet utility stream must also be provided.

  At each time step a flash is performed using the inlet stream(s) composition and enthalpy plus the computed heat transfer determined from the above equation.

- **Isothermal** – In this mode the temperature is fixed. At each time step a flash is performed using the inlet stream(s) composition and the specified temperature. A required heat duty is computed.

The Pressure Modes:

- **Fixed pressure** – Using this option, the user specifies the vessel operating pressure. This pressure is then the one used in the flashes mentioned above in the thermal modes.

  During fixed pressure simulation if the vapor is in excess of the available vapor space, the excess vapor is vented. If the computed vapor does not fill the available vapor space, the difference is ignored.

- **Calculated pressure –** If the pressure is to be calculated, the flow through the vapor vent must be specified (it may be zero, but it must be specified). The pressure is then varied until the sum of the vapor volume and the liquid volume equals the vessel volume.

  Pressure modes are specified using the **Fix Pressure** box at the left of the dialog box. If this box is left blank, then the program assumes the pressure is to be calculated. If a checkmark is placed in this box (by clicking on it), then an additional input field will open up. The pressure must be specified in this field.

  It is mandatory to use the **Fix Pressure** option when the dynamic vessel is part of a piping network. In such a case, the dynamic vessel is computed as a node with fixed pressure.

INITIAL CONDITIONS

Initial Charge Options

- **From outlet Stream Composition:** Default mode. Specify an initial liquid level. Specify composition of an attached outlet stream on the flowsheet. During the first time step the vessel will be filled with material based on the composition of the outlet stream. The program assumes that the vessel is well mixed and that the outlet at time zero represents the overall composition of material in the vessel.
- **Specify composition & liquid level**: This mode activates an initial charge dialog when the user presses OK. Specify the overall composition of the initial charge. CC-DCOLUMN will adjust the total flowrate to reach the specified liquid level, based on the specified overall composition. Specify an initial liquid level.
- **Specify mass, calculate liquid level**: This mode activates an initial charge dialog when the user presses OK. Specify the composition of the initial charge. Specify a total flow, which represents the total material for the initial charge. During the first time step the program will calculate the liquid level.

Initial Liquid level 1: Specify the initial liquid level in the vessel. If there are two liquid phases this is the liqht phase. For use with initial charge mode 0 from outlet stream and 1 specify composition & liquid level of charge. Default is zero.

Initial liquid level 2: If there are two liquid phases this is the heavy phase. Specify the level of the second liquid phase (if present). Default is zero.

Initial utility outlet Temperature: If a utility stream is connected (for vessel mode 2 Flash with UA & Utility) specify the outlet temperature of the utility. The default initial utility stream outlet temperature is the utility stream inlet temperature with the assumption that the heat transfer is from latent heat.

OPTIONAL INPUTS

Inlet nozzle position from top:
Default is 0 (inlet at top of vessel). Specify vertical location for the inlet nozzle. Only if you check the liquid static head is option for this vessel, the height of liquid above the inlet nozzle will exert pressure head on the inlet stream. This is useful if the dynamic vessel is part of an equation-based-network with inlet flowrate based on backpressure from the vessel.

Include static head option:
If the inlet and outlets liquid streams of the vessel are connected to piping networks, checking this option will add the static head of the instantaneous liquid level in the vessel to the specified pressure in the vessel. This feature allows performing more realistic piping network simulations in dynamic mode.

Three phase flash:
Checkmark this field to allow three phase (vapor-liquid- liquid) calculations for the dynamic vessel. A light and heavy liquid level will be calculated. If two liquid outlets are connected, the liquid phases will separate at the outlets. The Global K Value setting (**ThermoPhysical** menu > **K-Values**) for vapor – liquid – liquid must be checked for this setting to apply.

Include Compression/Expansion Effect:
Checkmark this box to include work of compression / expansion in the energy balance for the vessel. This will affect the calculated pressure in the vessel. If checked, a First Law energy balance and the Maxwell relation H=U-PV will be used to calculate the pressure effect based on internal energy change of compression / expansion.

Recorder On:
No time history data for the dynamic vessel will be saved (to disk) unless this option is switched on. If the data is not saved, then it is lost once you leave the **DYNAMICS MENU**. This means it will not be available for plotting and printing.

PARAMETER DEFINITIONS – PAGE TWO (OUTLET FLOW)

Liquid Flow Specifications:

Note that a RAMP controller can change the specified value at specified time(s) for all modes except Control valve. This allows setpoint changes without use of a control valve and controller.

- **Mole Flow Rate:** Specify a molar flow rate for the liquid outlet. Liquid level will be calculated based on remaining liquid.
- **Mass Flow Rate:** Specify a mass flow rate for the liquid outlet. Liquid level will be calculated based on remaining liquid.
- **Actual Volume Flow Rate:** Specify a volumetric flow rate for the liquid outlet. Calculated liquid volume will be used to determine the mass of liquid. Liquid level will be calculated based on remaining liquid.

- **Control Valve or UnitOp:** Specify the control valve (CVAL) UnitOp, which controls the outlet flow. A PID controller can be used with the control valve to model a control system. This mode is particularly useful to model a dynamic column with external reflux drum. You may specify a pump, pipe, or compressor UnitOp if the dynamic vessel if part of a Node network.
- **Constant Level:** Specify a liquid level. During each time step excess liquid will be removed to maintain the specified level. If liquid level is below the specification no liquid will be removed.
- **Constant Mole Holdup:** Specify a liquid holdup in molar units. During each time step excess liquid will be removed to maintain the specified holdup. If holdup is less than the specification no liquid will be removed.
- **Constant Mass Holdup:** Specify a liquid holdup in molar units. During each time step excess liquid will be removed to maintain the specified holdup. If holdup is less than the specification no liquid will be removed.

Vapor Flow Specifications:

If the program is to calculate the vessel pressure and a vapor outlet stream is present, then the flow rate of that stream must be fixed at each time step. In CC-ReACS there are two ways of fixing this flow rate:

1. The user may specify the flow rate as constant throughout the simulation; or
2. The flow rate can be reset at each time step by either a PID or a RAMP controller.

In this "pressure calculated" case, you must specify the following:

1. If the vapor flow rate is to be fixed at a constant value for the entire simulation, then select one of options 0, 1 or 2 for the **Mode** (mole, mass, or volume flow units) and enter the flow specification in the **Flow rate** field. The engineering units will be those set as the flowsheet global engineering units.
2. If the vapor flow rate is to be set by a PID controller, then select the **"Set by control valve"** option as the **Mode** and enter the initial flow value in the **Spec** field (in global units for total flow rate).
3. If the vapor flow rate is to be set by a RAMP controller, then select one of options 0, 1, or 2 for the **Mode**, and enter the initial flow rate in the **Spec** field (using the corresponding global units). Then schedule the vapor flows in the RAMP controller input.

If the total amount of material present in the vessel is less than the specified vapor flow rate, then the pressure calculation will fail and issue an error message, but the simulation will continue.

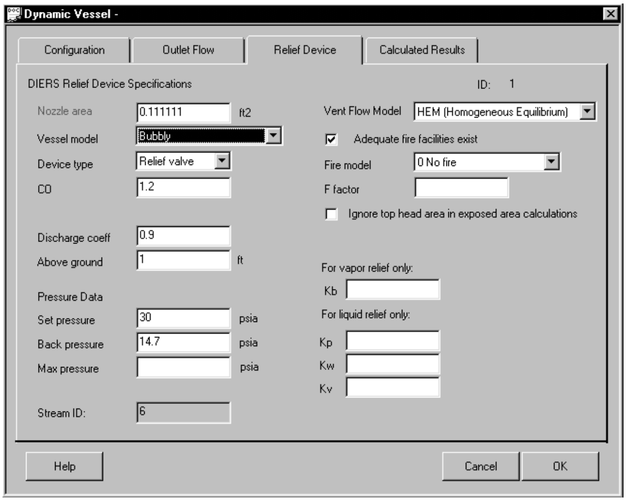
Specify Liquid Levels

Minimum Level:
This optional input will prevent the liquid level from going below a specified mark input by the user. If the level goes below this mark DVSL will stop emptying the vessel until the specified liquid level is reached again. This level is measured from the bottom of the vessel, therefore the default value is zero.

PARAMETER DEFINITIONS – PAGE THREE (RELIEF DEVICE)

DIERS Relief Valve Specifications

The dynamic vessel may be fitted with a relief valve which is simulated by the methods and practices established by the Design Institute for Emergency Relief Systems (DIERS). This description is intended to describe to users how to use the DIERS rating portion of CC-DCOLUMN. It is not intended as a course on relief valve rating. It is assumed that the user is already familiar with relief valve sizing techniques and terms.



Vessel Model:
The fluid characterization of the vessel under relief conditions. Options are as follows:

- Bubbly
- Churn-Turbulent
- Homogenous

The Bubbly vessel model assumes uniform vapor generation in the liquid phase with vapor/liquid disengagement within vessel. The Churn-Turbulent model assumes uniform vapor generation; however, with Churn-Turbulent, there is greater vapor/liquid disengagement. The Homogenous vessel model assumes there is no vapor/liquid disengagement and is useful for viscous fluids or short venting times.

The "Non-boiling height" modification of the Churn-Turbulent vessel model has not been included in this program.

Device Type:
The device type can be a relief valve, a rupture disk, or a relief valve followed by a rupture disk.

C0:
C0 is a data correlation parameter for Bubbly and Churn-Turbulent models. Normal values range from 1.0 to 1.5. Generally speaking, the greater C0, the less likely two-phase venting will occur. Default is 1.2.

Nozzle Area:
The cross sectional area of the relief system nozzle.

Discharge Coefficient:
This is the roughness factor of the relief device. For relief valves, this has a value of 0.975. For rupture discs, this is typically 0.625.

Above Ground:
Please enter the elevation of the vessel above the pad level.

PRESSURE DATA

Set Pressure:
The "lift" or opening pressure of the relief system. Typically this number is within 10% of the maximum design pressure for the vessel.

Back Pressure:
The flare or relief system pressure on the backside of the valve.

Max pressure:
Pressure rating of the vessel.

Vent Flow Model:
The vent flow model may be selected from the following list (see DIERS for full descriptions):

HEM (Homogenous Equilibrium Model)
ERM (Equilibrium Rate Model)
Henry-Fauske HNE
Non_Flashing Liquid
Single Phase Vapor

Adequate fire facilities exist:
This is used in the API 520/521 fire model. Select from options: Adequate fire and drainage facilities exist or adequate fire and drainage facilities do not exist.

Fire Model:
Select one of the following fire models:

0	No Fire
1	API-520/521
2	API-2000
3	OSHA 1910.106
4	NFPA-30

F Factor:
This factor is for adjusting the fire heat load for the environment. A list of standard values is included below:

Environment	F Factor
Bare Vessel	1.0
Insulated Vessel	0.3
Sprinkler System	0.3
Both Insulation and Sprinklers	0.15

Ignore top head in exposed area calculations:
This check box is used to specify whether or not to exclude the area of the top of the vessel for the exposed area calculations.

FOR VAPOR RELIEF ONLY

Kb:
For vapor relief systems, enter the Kb. Kb is defined as the backpressure correction factor for vapor relief.

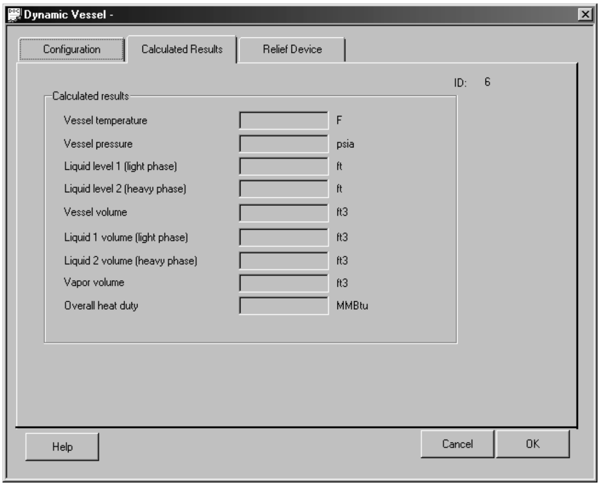
FOR LIQUID RELIEF ONLY

Kp:
For liquid relief systems, this is the capacity correction factor for overpressure.

Kw:
For liquid relief systems, this is the capacity correction factor for backpressure.

Kv:
For liquid relief systems, this is the viscosity correction factor. Kv = 1 for non-viscous fluid.

PARAMETER DEFINITIONS – PAGE FOUR (CALCULATED RESULTS)



Vessel Temperature

Vessel Pressure

Liquid Level 1
This is the liquid level for the light phase liquid. If there is only one phase of liquid, this is the total liquid level.

Liquid Level 2
This is the liquid level for the heavy phase liquid.

Vessel Volume
This is the calculated volume of the vessel.

Liquid1 Volume
This is the liquid volume for the light liquid phase. If there is only one liquid phase, this is the total liquid volume.

Liquid 2 Volume
This is the liquid volume for the heavy liquid phase. If there is only one liquid phase, this is shown as zero.

Vapor Volume
This is the vapor headspace volume.

Overall heat duty
This is the total heat transferred to/from the vessel.

TOPOLOGY

The dynamic vessel may have up to 3 inputs and 3 outlets; the inlets may be in any order. The outlets are listed with the vapor outlet first, followed by the heavy liquid outlet, and then the light liquid outlet. In the event there is only a single liquid phase, all liquid flows out the bottom outlet.

OTHER UNIT OPERATIONS

Other unit operations modules of lesser significance are also provided with a CC-DCOLUMN license.

These include:

- The RAMP Controller
- The Time Delay
- The Time Switch
- Commonly used steady state unit operation

Also available from Chemstations, but not included in a CC-DCOLUMN license, is the batch reactor module, CC-ReACS.

THE RAMP CONTROLLER

The Ramp controller unit is used to change various operating parameters with respect to time. In dynamic simulations, the scheduling ramp may be used to simulate operator functions such as opening a valve at time = t.

Each scheduled ramp can only act on a single parameter.

PARAMETER DEFINITIONS

Controller TypeRAMP can control both: inlet streams and UnitOp parameters:

1. **Stream:** This mode causes the RAMP to adjust an inlet stream variable during simulation.
2. **UnitOp:** This mode causes the RAMP to adjust a unit operations parameter during the simulation.

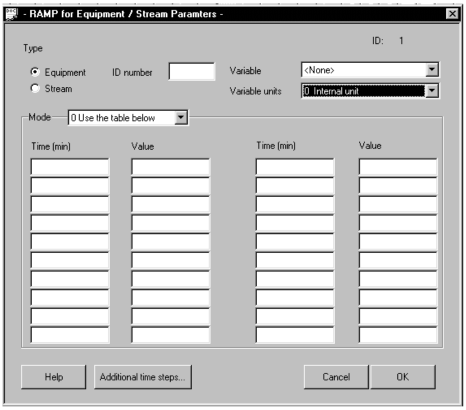
Stream/UnitOp ID:
Enter the ID number for the stream or UnitOp, which has the variable to be reset by the RAMP.

Variable Number:
This field is used to identify the variable, which is to be continuously reset by the RAMP. If this variable is from a dynamic UnitOp or from a stream, a list of the available variables will be displayed and the user may click on the desired item to select it. If the variable is from a steady state UnitOp then you must type in the Variable Number (Variable Numbers can be found in the on-line manual).

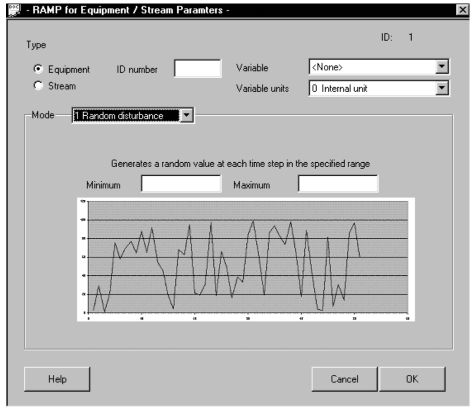
Time (Min) And Value:
This is a spreadsheet style chart of how the value of the parameter changes in time. CC-DCOLUMN automatically interpolates between values to determine the value for each time slice in the dynamic simulation.

Controller Mode
There are three different ways of inputting disturbances. Each one has its own screen.

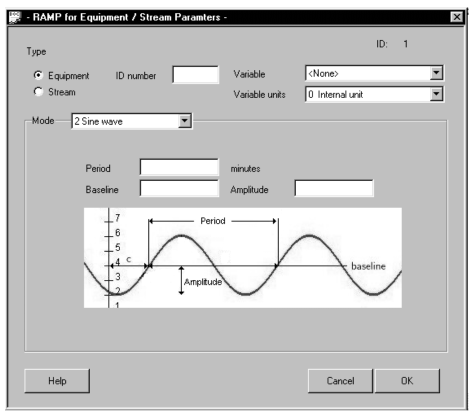
- Use table below: The user can input a table of variable values vs. time directly.



- Random disturbance: The user can input a minimum and maximum value for RAMP to set the variable value randomly.



- Sine wave: The user can input the parameters to simulate a sine wave disturbance.



THE TIME DELAY UNIT OPERATION

The Time Delay unit is used to simulate delays in dynamic simulation, such as pipe delays.

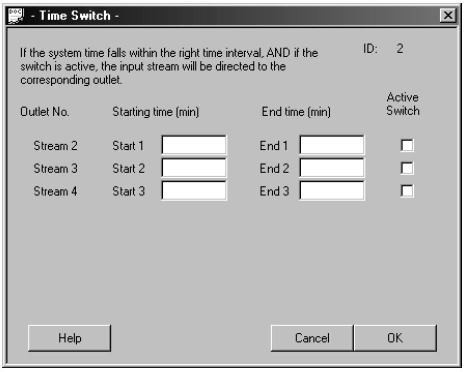
Delay time:
The user specifies the duration of the time delay which the stream experiences.

TOPOLOGY

Time delays have only one inlet and one outlet.

THE TIME SWITCH UNIT OPERATION

The Time Switch UnitOp is a process flow scheduling tool. It provides a time schedule for the direction of these flows.



The dialog box will contain one row of fields for each outlet stream coming form the time switch. This now will enable the user to direct all process input (to the time switch) through the outlet stream during the times specified.

There are four fields for each row. These are:

1. Outlet No.
2. Starting time
3. End time
4. Active switch

These are described below:

Outlet Number: Within the Time Switch, streams are identified by position number. Positions are number from the outside in. In other words, the outlet position located the farthest from the inlet position is position number one. In the above example dialog box, this position is labeled "Stream 1". The outlet position located closest to the inlet position will receive the highest position number. In the above example dialog box, this position is labeled "Stream 3". All other positions are relative to these positions. These statements apply only to the standard Time Switch icon (the icon supplied as part of the CC-ReACS program). The user can create his/her own icon, which follows different valves.

Starting time: This field designates when flow through this outlet will begin. Starting time is specified in minutes from time zero.

End time: This field designates when flow through this outlet is to cease. End time is specified in minutes from time zero.

Active Switch: This field (box) turns the schedule for the outlet on and off. In other words, only if there is a direct mark in this field (box) will flow pass through this unit between the Starting time and the End time.

TOPOLOGY

The Time Switch UnitOp has one inlet and up to eight outlets.

STEADY STATE UNIT OPERATIONS

In addition to the unit operations modules already described, your CC-DCOLUMN license entitles you to use other unit operations modules within the CHEMCAD system. The one restriction on the use of these modules is that they can only be used in dynamic mode. It is easier to identify these UnitOp by listing those that cannot be used under a CC-DCOLUMN license.

All unit operation in the CHEMCAD library is available for use in a CC-DCOLUMN flowsheet (without an additional license) except the following:

1. Steady state UnitOps requiring a CC-STEADY STATE License:
   - SCDS
   - TOWER
   - TOWER-PLUS
   - SHOR (Short Cut distillation)
2. UnitOps requiring a CC-BATCH license:
   - BATCH (the batch distillation column)
3. UnitOps requiring a CC-ReACS License
   - CC-ReACS (the batch reactor module)
4. Features requiring a CC-THERM License:
   - The shell and tube design/rating capability

All other unit operations can be used in dynamic flowsheets. UnitOps commonly used are:

- Mixer
- Divider
- Heat exchanger
- Flash

- Pump
- Compressor
- Tank
- Vessel
- Component separator
- Valve
- Pipe
- Excel UnitOp

> Whenever a steady state unit operation is used in a dynamic flowsheet, the user is making the implicit assumption that the dynamics of that unit operation are very, very fast. Technically, they are assumed to be instantaneous. If this is not a reasonable approximation, consider using the tank and time delay UnitOps to build in some of the dynamic effects of these modules.

DYNAMIC TECHNIQUES

This section is intended to help you with doing dynamic simulation work. Dynamic simulation involves activities much more complex than those encountered in steady state calculations. The user must gather more information about the process under consideration, and knowledge about control systems and instrumentation is advantageous.

Before any complex control system of a technology is installed, a dynamic simulator can be used to analyze the system, to assess its future performance, and to detect possible problems or infeasible schemes. Dynamic simulation can also help during process start-up and in the tuning of the control system.

Dynamic simulation of industrial technologies requires dynamic mathematical models of unit operations as well as a special dynamic "engine" or a solver, and reporting subsystem.

CC-ReACS was the first implemented dynamic module of the CHEMCAD Suite. This engineering software tool was designed to simulate the behavior of batch and semi-batch vessel reactors. CC-ReACS contains all fundamental dynamic units and the solver for general dynamic simulation.

CC-DCOLUMN is a software tool that involves generalized dynamic simulation distillation columns. It can be a powerful tool for studies of batch or semi-batch distillation units, and it can be equally well used for studies of continuous distillation, including complete distillation train of many columns.

The CC-STEADY STATE and CC-DCOLUMN combination is perfect for the design of continuous distillation systems, where CC-STEADY STATE provides theoretical solution of the problem and prepares the initial data for dynamic simulation. Similarly, the combination of CC-BATCH and CC-DCOLUMN is ideal in solving batch and semi-batch distillation systems, as CC-BATCH allows you to understand behavior of the column before control systems are introduced. (CC-BATCH is a CHEMCAD Suite module for batch and semi-batch distillation.)

The mathematical models of CC-DCOLUMN are extensions to the steady state distillation models (SCDS, TPLS, TOWR) by a set of differential equations describing the mass, component and heat balances of a dynamic column. Only the extended dynamic SCDS model can make use of the component mass transfer model as well.

CC-DCOLUMN follows the general philosophy of the CHEMCAD Suite, that is, the program should be easy to use. From this point of view, it can be used as a multipurpose and multifunctional unit operation with a set of built-in process equipment pieces and with a set of built-in control algorithms.

"Easy to use" does not necessarily mean that the program would be successfully operated by users of no experience with dynamic simulation, or those who do not know the special dynamic simulation techniques of the CHEMCAD Suite. This section helps the user to gain this experience.

This section consists of two parts. The first part is a detailed overview of the fundamental techniques of dynamic simulation using the CHEMCAD Suite. The usage of CC-DCOLUMN is discussed in the second part. With continuous and batch distillation examples, we will explain the solution of theoretical and practical problems that can be solved using dynamic simulation.

FUNDAMENTAL TECHNIQUES

THE CONTROL VALVE, CVAL

The control valve (CVAL) calculates the flow rate through the valve. The terms "the control valve" and CVAL are used interchangeably in this manual.

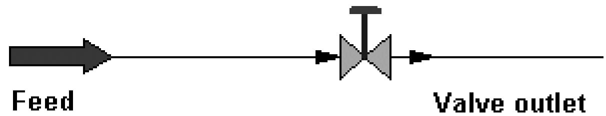
HOW THE CONTROL VALVE MODIFIES THE FLOW RATE

Rule 1.
The Control valve has no volume and has no dynamic property, so the mass flow rate at the outlet is always equal to the mass flow rate at the inlet.

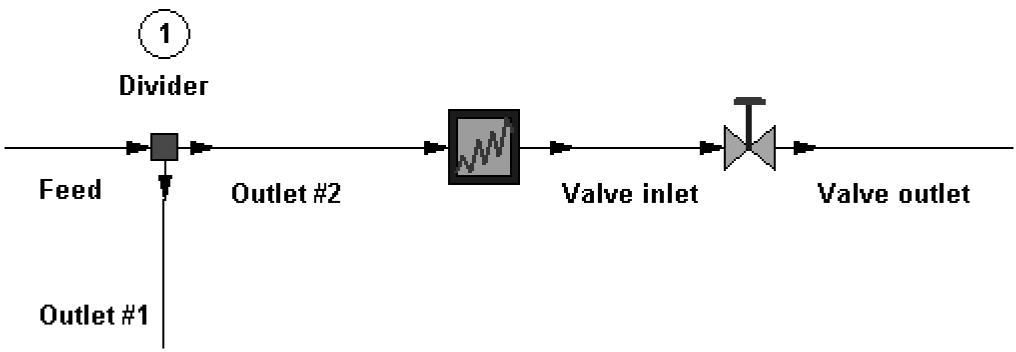
Rule 2.
The user who works with the flowsheet should make use of the calculated flow rate.

Techniques:

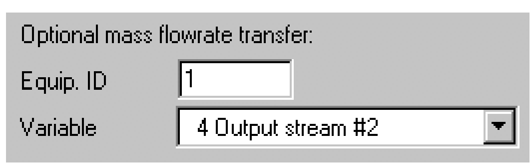
1) Place a control valve at inlet stream of a flowsheet. The control valve should directly follow the feed arrow in the stream. In this case, the flow rate of the inlet and outlet streams will be reset to the flow calculated by the control valve.



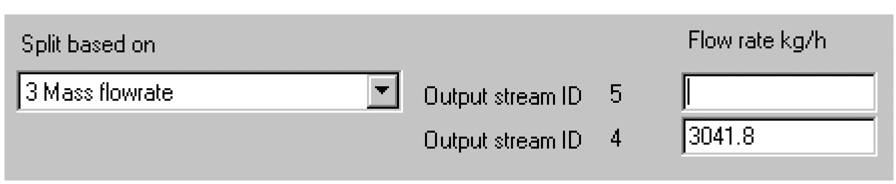
2) Use the "optional mass flow rate transfer" option of CVAL if the source of the inlet stream is a passive unit. A unit is passive if it cannot take over the calculated flow rate from the control valve. Typical passive stream source units are stream divider and stream reference models. The following example shows the technique that uses the stream divider.



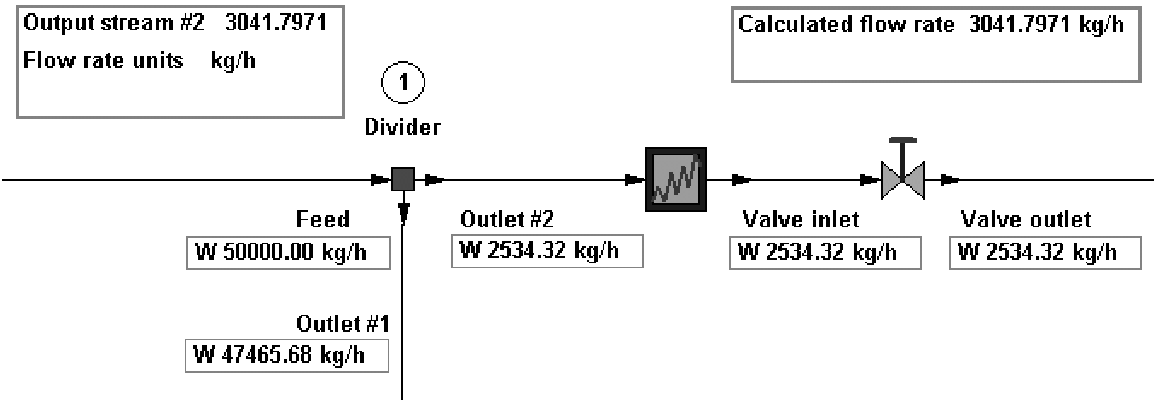
The setting of control valve:



The setting of stream divider:



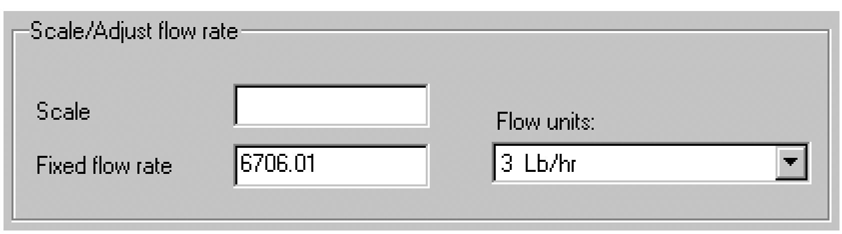
The state of the system at time point (k)



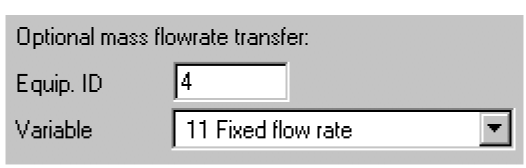
This solution means that at every time point (*k*) the streams – from the source point through the valve - have identical flow rate values as calculated by the control valve at time point (*k-1*). The unit operations have specifications identical to the flow rate calculated by the control valve at time point (*k*) and transferred to the divider unit. (The large difference between stream values calculated at step *k-1* and unit operation specifications set at time *k* results from quick opening of the control valve in this example.)

3) The next technique demonstrates application of the stream reference model.

The settings for stream reference model are:

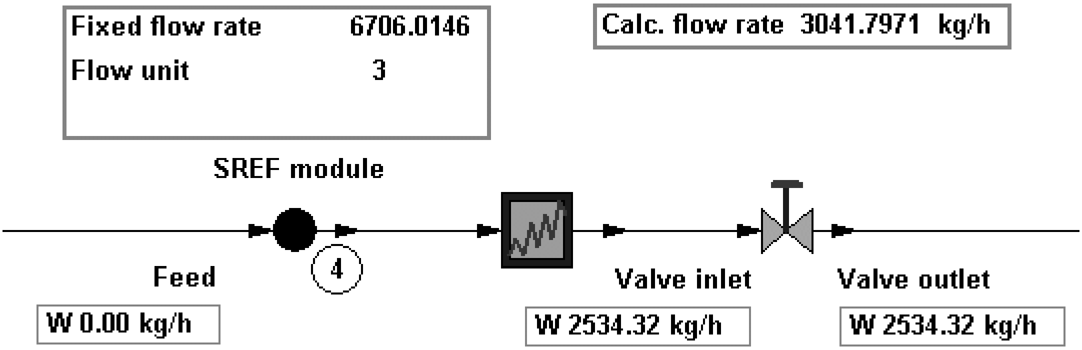


The setting for the control valve is:



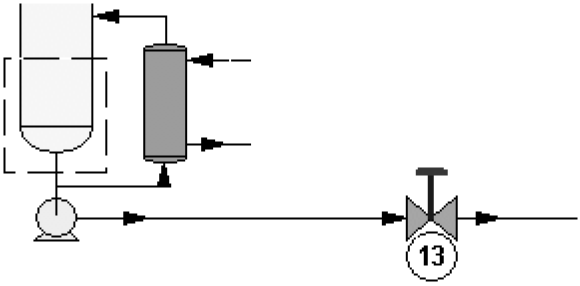
where

Results at time point (*k*) are the following:



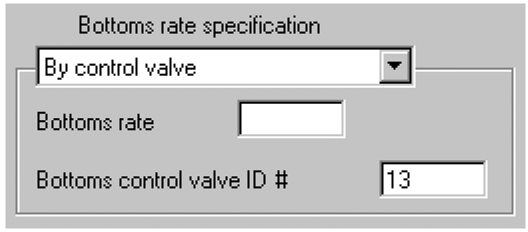
Note: *With the stream reference model, you should consider conversion of engineering units. The actual mass flow rate unit of the example above is kg/h, but the SREF defaults to lb/h. CC-DCOLUMN will copy the internal stored value of mass flow rate = 3041.7971 * 2.20462 = 6706.0146 lb/h from the control valve to the stream reference model. Because of this specific behavior, you should select lb/h as flow unit in stream reference model.*

4) Use the mass flow rate transfer option of active units. A unit is active if it can take over the calculated flow rate from the control valve. Typical active stream source units are the dynamic vessel and the dynamic column models. In this case, you should always specify the ID of the control valve that will calculate the flow rate for the active unit. The next example shows this technique using a dynamic tower model with controlled bottoms flow rate.



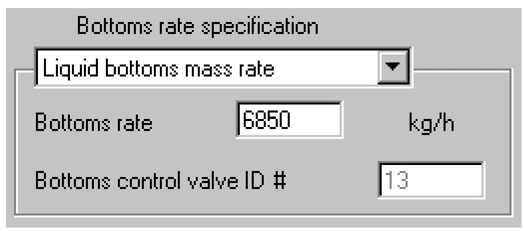
Note: *A horizontal vessel is assumed in the dashed box. This is a part of the dynamic tower model and it is handled by built in algorithms. (Unit ID of column is 10)*

The setting of the "vessel" is:

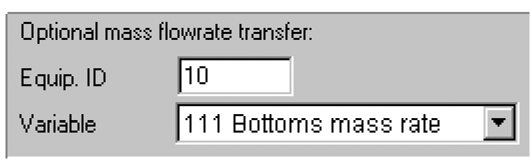


This information is sufficient for the model; the actual value of flow rate will always be transferred from unit 13. In this case, there is no need to specify "flow rate transfer" option in the dialog box of the control valve.

You are allowed, however, to apply the passive unit approach, even if you are working with an active unit. To do that, you would refrain from applying the "By control valve" method of the active unit. The "vessel" specification is now:

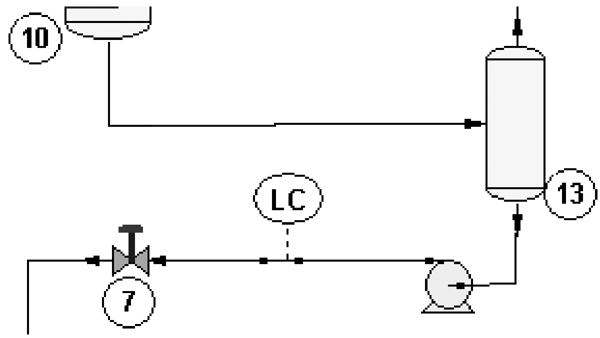


The control valve specification is now:

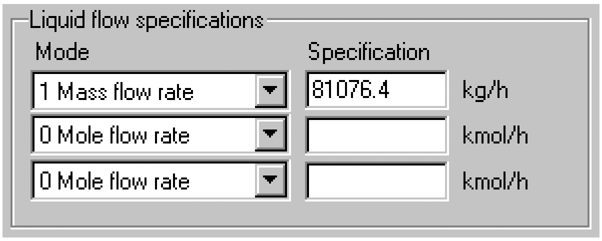


In the example above, you tell CC-DCOLUMN to fix the flow rate of the bottoms stream to some value. Then, you instruct CVAL to copy the calculated flow rate directly to the equipment (unit operation) specification. Both techniques, that is, the active and the passive approach, can be applied interchangeably with active unit operations of CC-DCOLUMN dynamic modules. (Note: The active unit operations are: Dynamic Columns, Batch Reactor, and Dynamic Vessel.)

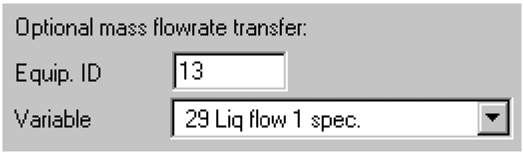
5) The next technique is similar to the previous one. Here we used a separate (discrete) reboiler system: heat exchanger and vessel. In the picture you can see the column bottom and the vessel with a liquid level control loop combined together.



The specification for the vessel is:



and for the control valve it is:



It is usually much simpler to apply the active unit approach because only one specification is needed. The following picture demonstrates this approach for the vessel:

HOW TO MODIFY THE VALVE POSITION

The flow rate through the valve is based on the valve position. The actual value of valve position is stored in the control valve dialog box.

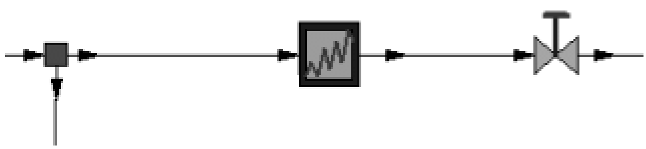
Rule 1.
If a control valve is not related to a controller, then the user should define a method to set the valve position. Note that CC-DCOLUMN always displays a warning message when a controller ID is not defined. From the viewpoint of dynamic simulation, this message can be ignored.

Rule 2.
If the output signal of a PID controller is used to determine the valve position, the control valve must have a designated controller ID as part of its input.

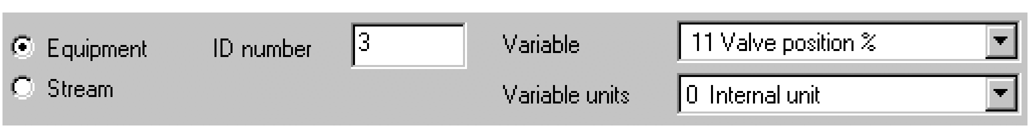
Techniques:

1) The simplest technique is to set a constant valve position as defined by the user before the start of a dynamic simulation. This solution is not very typical, because the user cannot modify the valve position during the simulation.

2) A good and frequently used technique is to define a valve position sequence using RAMP model. You can see below the flowsheet that makes use of this technique, where the Control Valve ID number is 3 and the RAMP ID number is 2:



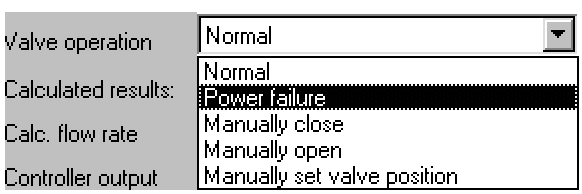
The RAMP specifications are:

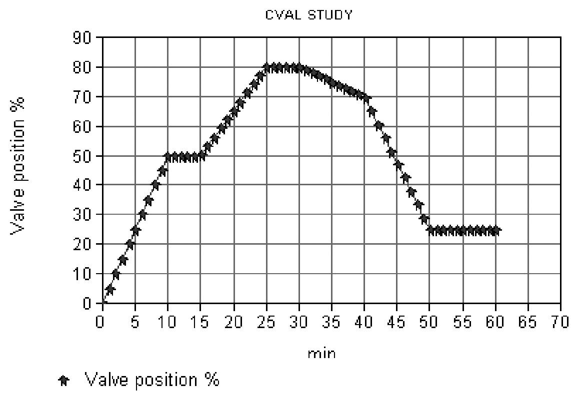


The RAMP schedule is:

Time (min)	Value
	1e-006
10	50
15	50
25	80
30	80
40	70
50	25
60	25

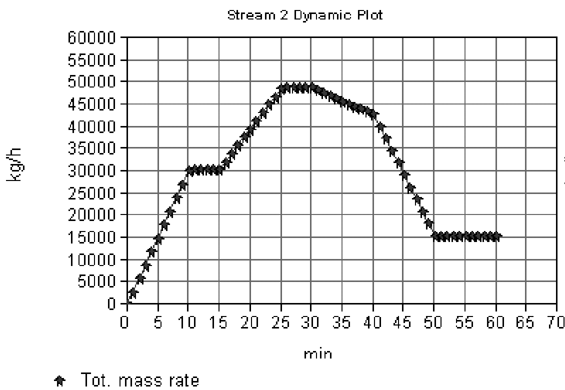
The RAMP model sets the valve position (Parameter ID = 11) of the control valve (Unit ID = 3) by the predefined curve. The time point – value data pairs represent the break points of the continuous curve. CC-DCOLUMN makes a linear interpolation between these points. With a study of batch technologies, we can define special control sequences using 0 % and 100 % valve positions (On / Off or Open / Closed). It is also possible to define special control sequences using the Valve operation option available on the CVAL dialog (see picture below).

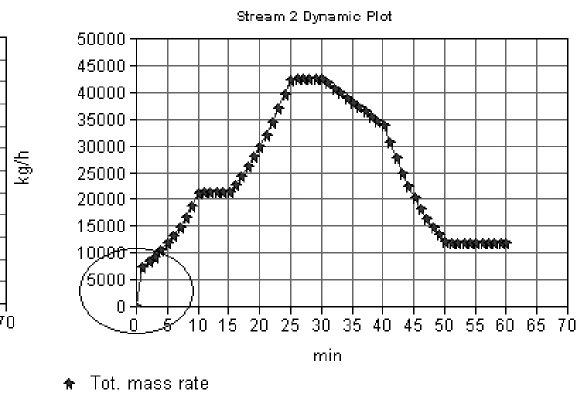




Linear valve

Equal percentage valve





The first picture shows the valve position manipulated by RAMP model. The bottom-left picture shows the actual flow rate for linear valves and the bottom-right one shows it for an equal percentage valves. A circle indicates the critical regime for an equal percentage valve. Detecting this regime, CC-DCOLUMN displays a warning message suggesting, either that the user select a linear valve or to use equal percentage valve of smaller size. From a practical viewpoint, equal percentage valves are recommended for continuous processes and the suggested working range of these valves is in the range of 60% -70% opening. For batch technologies or for valves that would be able to close completely, linear valves should be used, and the maximum flow rate should be matched with the valve for 100% opening.

3) It is possible to use CONT (the steady state controller) model in FF (Feed Forward) mode to set valve position. This enables the program to calculate the desired valve position by a simple algorithm.

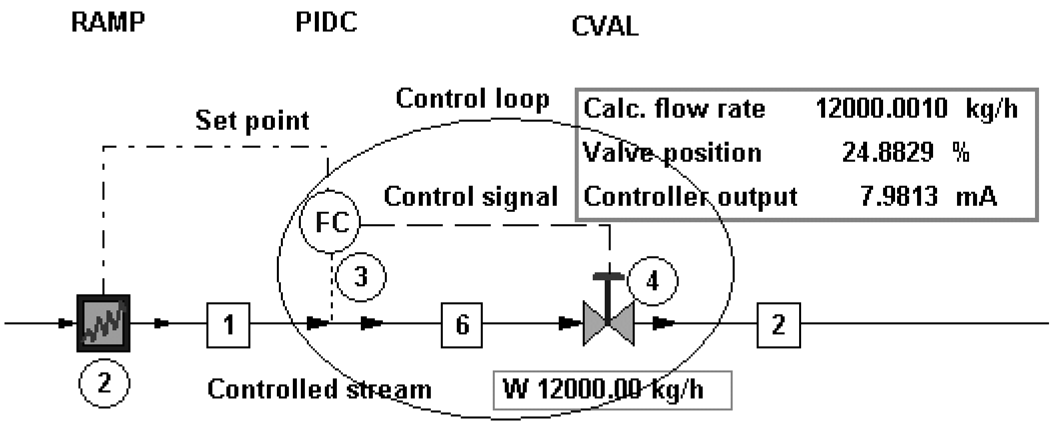
4) Another technique is to directly determine the valve position by a signal from PID controller. The elements found in the next picture form a typical simple control loop. In the technique presented, the RAMP model generates the current values of the set point. Let's study the relationship between the control valve and the PID controller.

CC-DCOLUMN uses cross-linking to define the relationship. In the control valve dialog box, you should define the controller ID number, and in the PID controller dialog box you should specify the ID number of the control valve.

This is a portion of the control valve dialog box:

And this is a portion of the PID controller dialog box:

For instance, the control loop can be organized similar to this one:

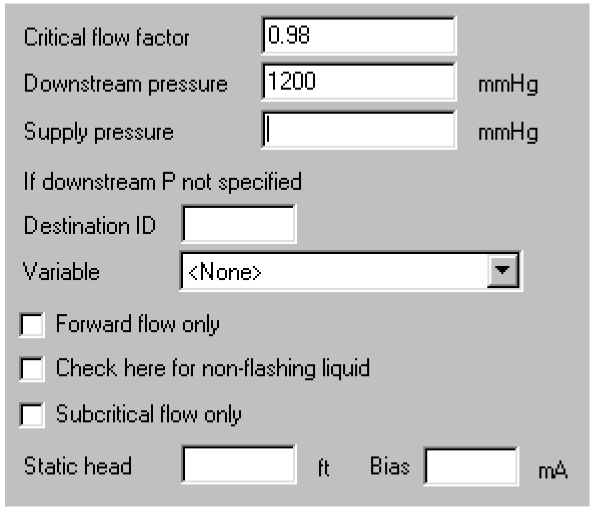


Note:

CC-DCOLUMN uses a signal expressed in milliamperes to transfer information between elements of a control loop. The default range is 4 – 20 mA. The user can modify this by selecting signal expressed in volts, in range of –10 – +10 V for example. In such case, the user should be sure to recalculate the parameters correctly.

The maximum control signal refers to a totally open valve, only in cases where the valve has been defined as NC (Normally Closed). NC valve is the default valve type in CC-DCOLUMN. To redefine a valve as Normally Opened (NO), it is necessary to enter different values for the Av and Bv parameters of the valve. If the 4 –20 mA signal range is used, then these parameters should take values of Av = -0.0625 and Bv = 1.25. In this case, the maximum control signal refers to a totally closed valve.

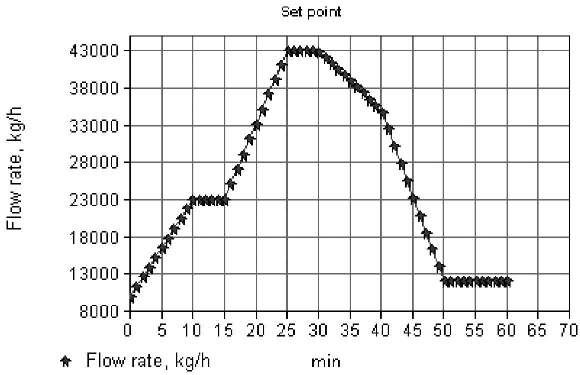
The Control valve has several special parameters. These are:

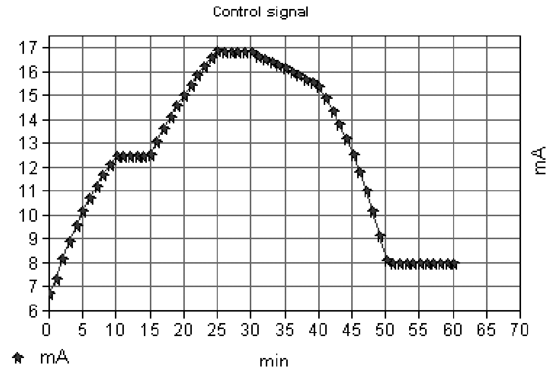


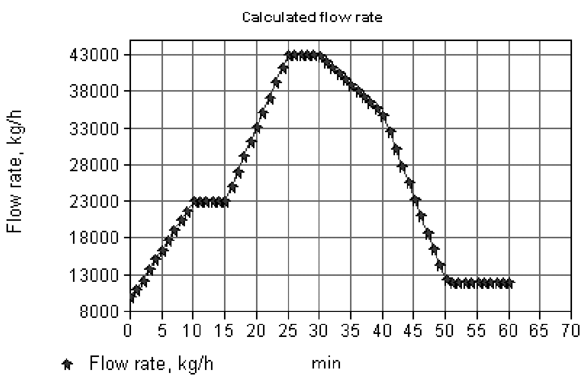
If the downstream is going to pressurized equipment, and the program is to calculate the actual pressure of this unit, use downstream specification (Destination ID). In this case, the downstream pressure specification refers to the **initial value** only. However, in this case it is **required** to specify initial downstream pressure.

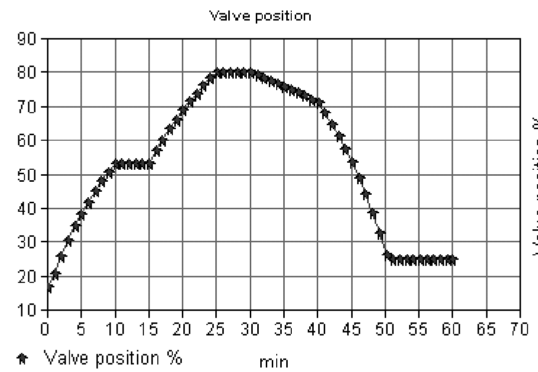
The static head is a similar additive variable, and it can be constant or variable (when modified by a FF controller).

The next picture displays signals taken from the above example loop. It is apparent that an equal percentage NC valve has been used (as the signal grows, then the opening grows; this valve never closes completely.)

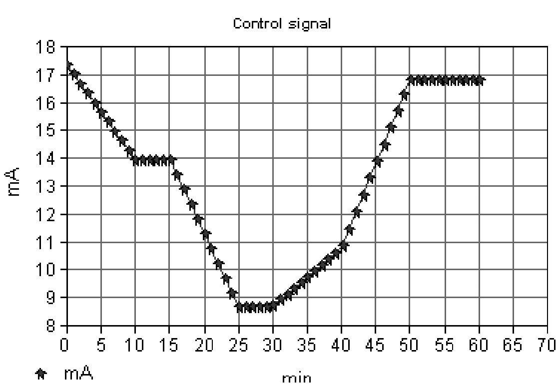


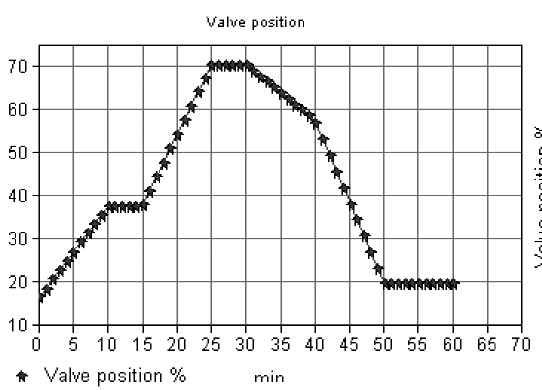






The control signal and valve position for NO linear valve follow:





It must be pointed out that applying a Normally Opened valve requires re-defining the PID controller parameters as well. It will be described in the section "How to specify error function".

SIZING, INITIAL STATE OF CONTROL VALVE, TROUBLESHOOTING

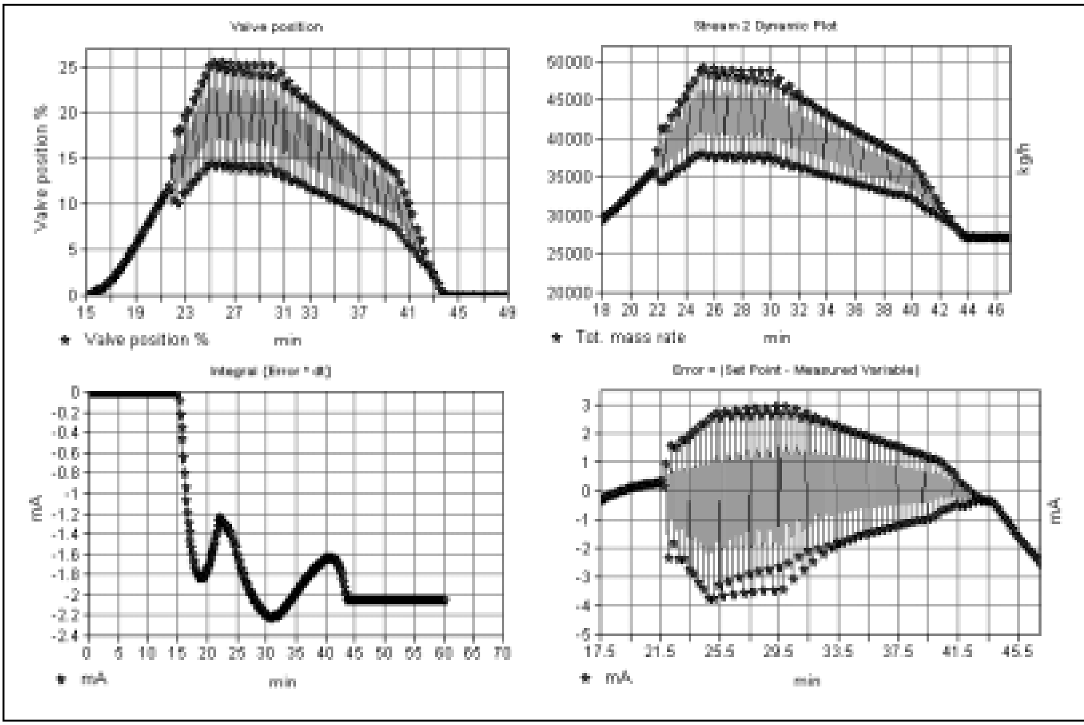
The size of a valve is defined by valve flow coefficient (Cv). This value can be determined from existing valve specifications or it can be defined by the user. CC-DCOLUMN provides the user with a control valve sizing function if the user needs it. The Cv depends on the physical properties of the stream and on the pressure drop of the valve. Recommended steps in CC-DCOLUMN are:

- Switch to steady state simulation mode
- Specify the inlet stream of valve (set the flow rate to the maximum possible value)
- Estimate the pressure drop
- Run the sizing option
- Verify the calculated variables (CC-DCOLUMN writes them into the parameter list of the CVAL automatically)
- Calculate control valve only (that is, "run" it with "selected units" option)
- Verify calculated valve position
- Repeat these steps until you can accept the valve size

> ***Note:*** *The value of Cv = 9 has been set in CC-DCOLUMN. If you are working with very small stream flow rates, then this valve size may be too large. In such a case, follow these rules: For a good range of control, the calculated flow coefficient (Cvc – actual valve flow coefficient ratio) should fall between 0.5 – 0.8. Because the sizing routine gives the Cvc value, then you can estimate the value of Cv, too. You can try finding optimum ranges for linear and equal percentage valves independently. The estimated Cv value should be entered* ***manually*** *into the CVAL dialog box, to replace the standard minimum value of 9.*

At the end of the sizing procedure (and possibly after entering the correct value of Cv by hand) you will want to get the initial state of the valve. Calculating the flowsheet in steady state is then the best way of getting initial parameters for future dynamic simulations.

Troubleshooting: An oversized control valve can be a source of oscillation in a controlled system. The following plots show examples of "valve chattering" caused by using an excessively large valve. The solution here is to decrease the valve size.

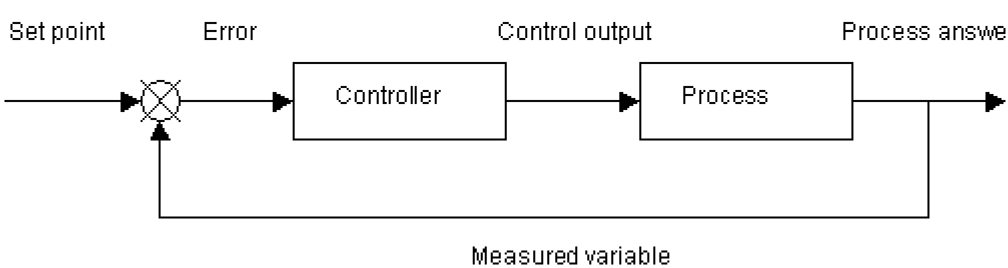


The PID Controller, PIDC

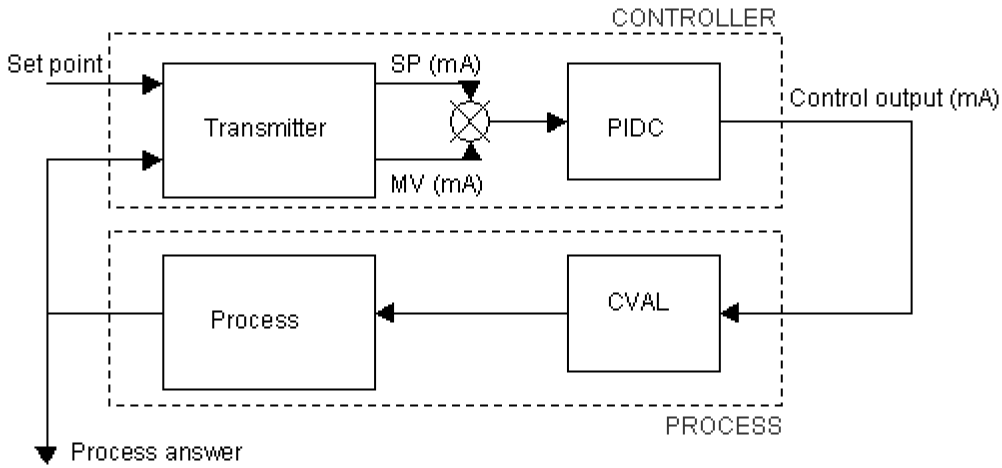
The PID Controller continuously measures the user specified variable, and based upon the specified set point for that variable, sends a controller output signal to a control valve.

WHAT IS A CONTROL LOOP?

A schematic diagram of one possible local control loop is shown below:



The structure of the loop using CC-DCOLUMN models is a little bit different:

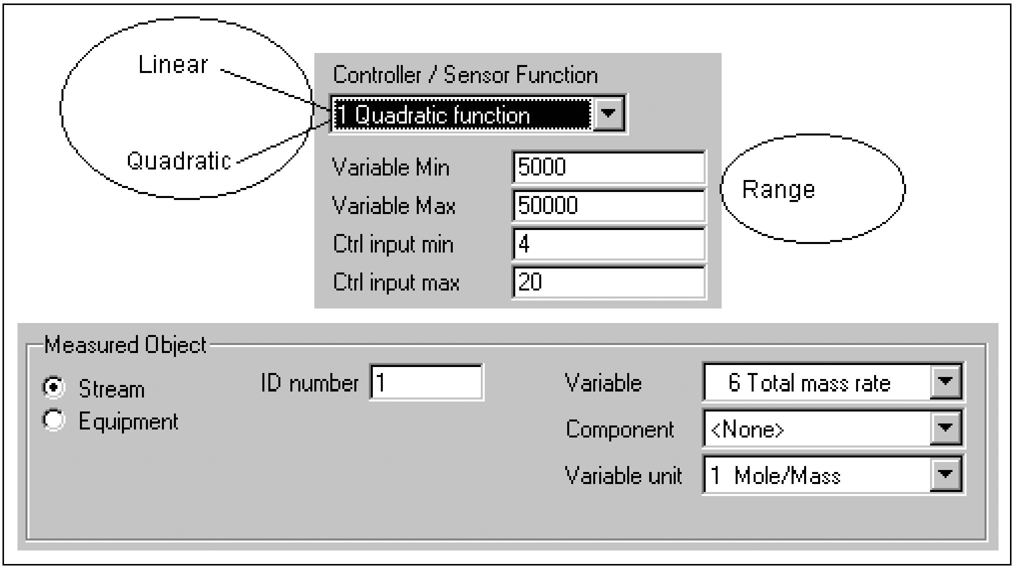


We would like to point out that the transmitter (or sensor) is a part of the CC-DCOLUMN PID controller module and the CC-DCOLUMN control valve is a part of the process. Any change in the setting of these units will require tuning of parameters of the PID algorithm. We have already discussed the control valve settings. The specification of the transmitter is related to the specification of the PID parameters in the PIDC model. From now on we will use the word “transmitter” and not the word “sensor” here, because we will be concentrating on the 4 – 20 mA signal produced by transmitter. The working method of a sensor is not important from this standpoint.

HOW TO SPECIFY A TRANSMITTER

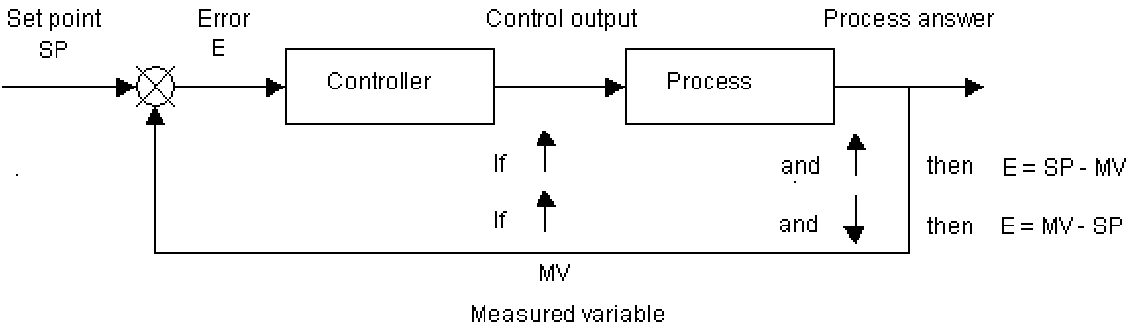
You need to understand how the parameters of a transmitter in the PIDC dialog box should be specified. The measured variable definition and the range of the measured variable are involved. If problems in operation of any control loop occur, then we recommend inspecting the range definition first.

> ***Notes:*** *Any modification of range will influence the sensitivity of the controller, so tuning the PID parameters will be necessary. Apply the quadratic type equation for mass flow rate control, and the linear equation otherwise.*



HOW TO SPECIFY ERROR FUNCTION

The control error is defined as the difference between the current value of the measured variable and the desired value (the set point). The desired value can be either a constant or a time dependant variable. A graphical explanation of the error function is given below:



So, if the measured variable increases and the process response increases, then the error function is defined as the difference between the set point and the measured value (definition 1); If measured value increases and the process response decreases, then the error function is defined as the difference between the measured value and the set point (definition 2).

Note: *The error function is calculated in milliamps (or volts).*

Examples**:**

Assume you are measuring the temperature at the process outlet of a heat exchanger and regulating that temperature by controlling the heating agent flow rate at the utility inlet, and the control output is to close the NC valve causing the measured temperature to decrease (the answer decreases), then you should apply definition (1).

Assume you are regulating the liquid level in a vessel by controlling the liquid outflow from the bottom of the vessel. The control valve is located at the liquid outflow stream, and you measure the liquid level in the vessel. If the NC valve opens (control output increases), then the measured variable (the level as the process answer) decreases. Your error definition should be (2).

Now, you would like to control the level in the vessel, but you prefer to locate the valve at the feed inlet to the vessel; the NC valve opens (control output increases) and the measured variable (the level as the process answer) increases too. You would apply definition (1).

HOW TO SPECIFY PARAMETERS OF PID

You have to keep in mind the working sequence of a controller:

- It reads the measured value and transforms it to mA by the sensor / transmitter function
- It reads the set point value and transforms it to mA by the sensor / transmitter function
- It calculates the error using the error function selected by user

The calculation a PID algorithm means

calculate the P term as:

$$P = \frac{100}{PB} \cdot \text{error}$$

PB is the gain of the process defined by:

$$(\Delta(\text{process\_answer}) / \Delta(\text{control\_output})) \cdot 100$$

calculate the I term as:

$$I = \frac{100}{PB} \cdot \frac{1}{T_I} \cdot \int \text{error} \cdot dt$$

TI is the integral time constant in minutes (the time unit is minutes in the dynamic simulation) calculate the D term as:

$$D = \frac{100}{PB} * Td * \frac{d(error)}{dt}$$

Td is the derivative time constant in minutes.

calculate the control output signal as

$$C_{output} = P + I + D + C^0_{output}$$

C^0_{output} is the output at steady state, calculated at the initialization of the simulation.

-in the equations above P,I,D and the calculated control outputs have mA as the unit of measure

Example: calculations for a P I (proportional, integral) controller:

Control valve is NC, linear, range 4 – 20 mA
Transmitter of measured temperature is linear, range 20 – 80 C : 4 – 20 mA
10 % opening on the control valve decreases the temperature by 1.5 °C
What is the value of PB?

The controller output is 66% at the steady state working point (at the set point for example)
If the current temperature is higher than the set point by 0.1 °C, then

- what is the new control output, and
- what is the new valve position?

Solution:

$$\Delta(control\_output) = (20 – 4) * 10 / 100 = 1.6 \text{ mA}$$

From the equation of transmitter we get

$$\Delta(process\_answer) = 1.5 * (20 – 4) / (80 – 20) = 0.4 \text{ mA}$$

PB = 100 * 0.4 / 1.6 = 25

$$C^0_{output} = (20 – 4) * 66 / 100 = 10.56 \text{ mA}$$

If the current temperature readout is higher than the set point by 0.1 C, then

$$\text{Error} = (MV - SP) = 0.1 * (20 - 4) / (80 - 20) = 0.0267 \text{ mA}$$

The current control output (with simplified I-term calculation) is:

$$C^{0}_{output} = 100 / 25 * 0.0267 + 10.56 = 10.67 \text{ mA}$$

The new valve position is 10.67 * 100 / (20 – 4) = 66.67 %

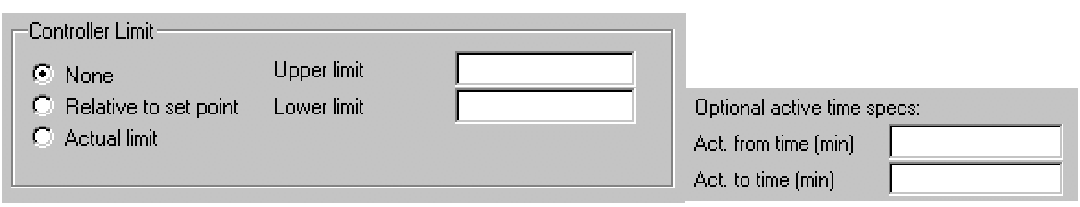
In most situations, it is enough to apply the PI algorithm. The overall rules of PI tuning are:

- Estimate time constant as part of the time (typically, 60% – 65%) needed to move the system from a steady state point to another steady state (in the example above, this is the time for the experiment to reach final temperature after a change of cooling stream)
- If you observe slow response of the control loop then decrease the time constant
- If you experience oscillation during the simulation then increase the time constant

Guidelines for advanced parameter tuning can be found in handbooks for control engineers. It must be pointed out that a simulation performed in steady state can help you find several valuable parameters. It is also important to run steady state simulations to determine the initial state for the dynamic calculations.

SPECIAL PARAMETERS OF THE PIDC MODEL

You can find these parameters in the second tab of the PIDC dialog box. It is important to understand that CC-DCOLUMN PIDC is a model of an analog controller or, in other words, the model models an analog valve actuation. This kind of actuator does not keep the valve at its last position, but eventually moves it to its final position. This final position is fully closed (NC valve) or fully opened (NO valve).



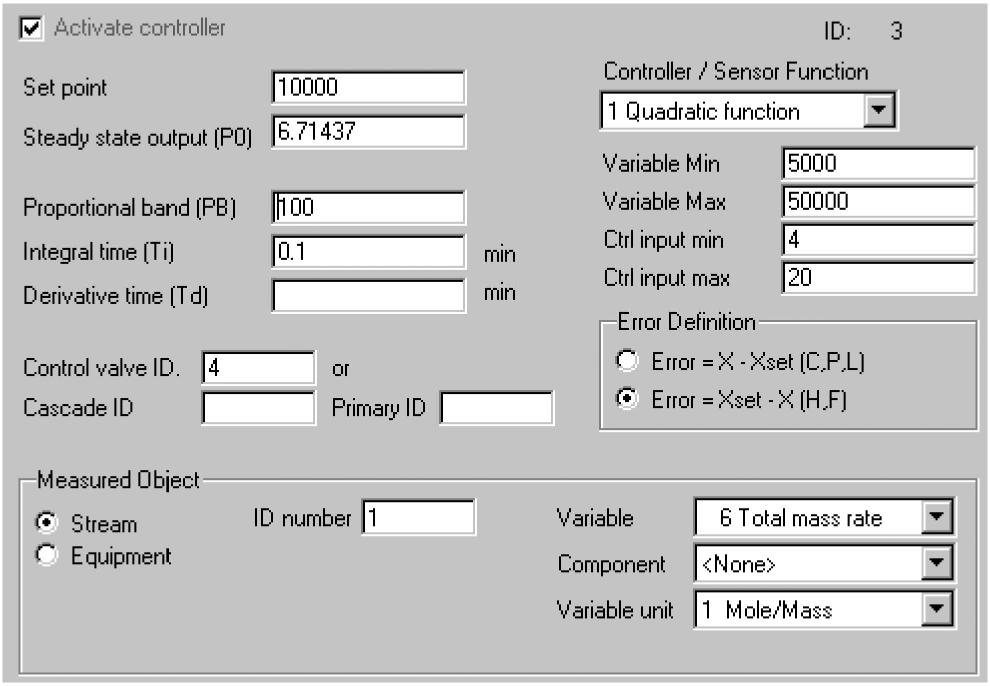
The special options can be used in batch or semi-batch technologies. If a controller goes into the limited area or it is out of active time then its output gets the minimal value and it will close or open very quickly.

This working mode can have a lot of benefits but it can also cause oscillation. The use of these parameters strongly depends on the technology and on the concept of control.

CONTROL STRUCTURES

We have discussed the schematic diagram of an easy control structure. This is the local control loop. The operators of a process control system should define the set point for any local loop. The set point can be constant over a period of time, or the operator can modify it from time to time.

Applying a constant set point in dynamic simulation is easy. It is enough to define the set point value in the dialog box of PID controller model.



WHAT IS THE LOCATION OF THE PID CONTROLLER IN THE FLOWSHEET

The first rule in CC-DCOLUMN is that the PID controller is a unit operation and it should be connected to other unit operations with process streams. The second important rule is that the layout of the control loop should always be carefully analyzed. You have to consider both location of the control valve and the location of the PID controller.

In most cases, you insert the controller and the control valve into an existing flowsheet. Therefore, you need to analyze the flowsheet itself. Check for the following points:

- What are the practical rules of control engineering

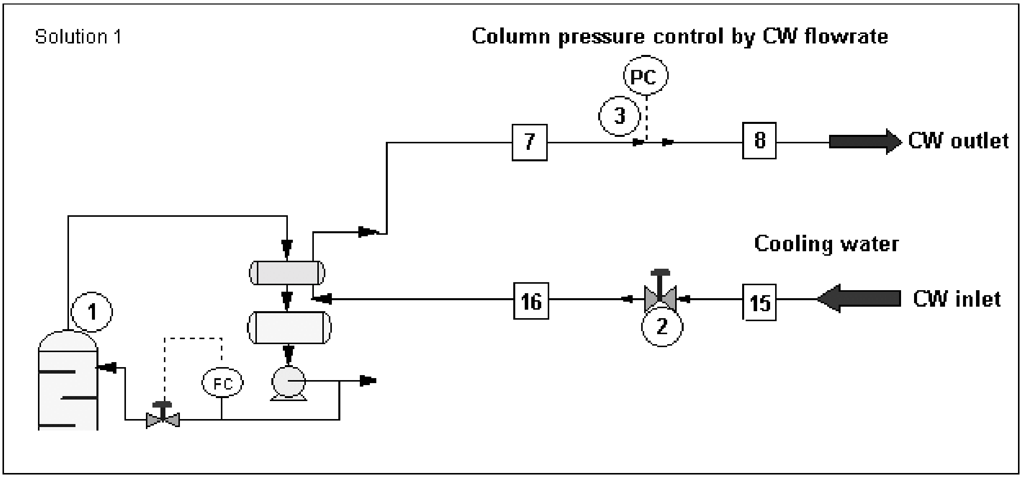
- Where is the measured variable (is it a stream, or is it a unit operation variable)
- Where is the adjusted point (location of control valve in the flowsheet)
- What unit operations are between the adjusted and measured points
- What is the actual and / or possible calculation sequence
- What is the time step of the dynamic simulation

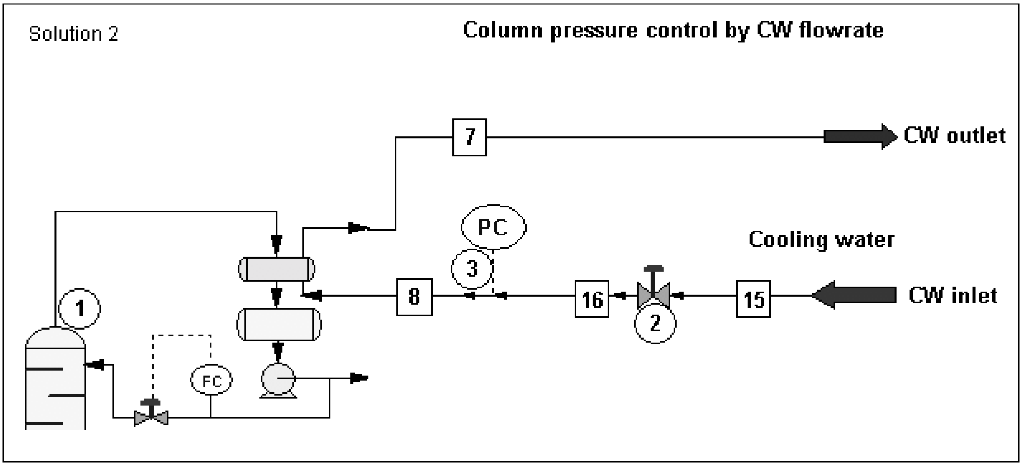
The selection of location is easy if the controlled variable is the flow rate of a process stream. You just insert the controller into the appropriate stream and this stream becomes the inlet stream of the controller. The location of the control valve can be before or after the controller.

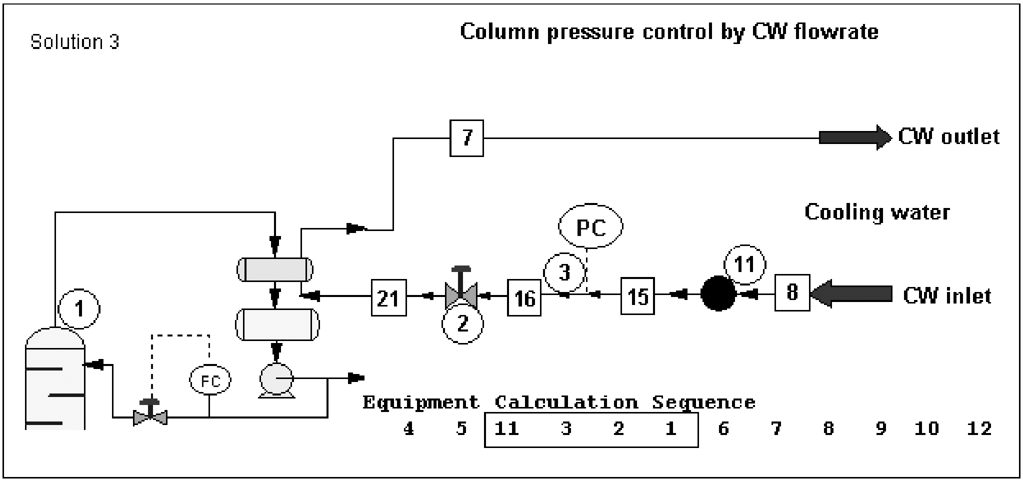
In all other situations, you should take into account that the measured object is defined in the control model. Therefore, you are free to locate the controller anywhere in the flowsheet. For practical reasons, it is the best is to locate controller and control valve together on the same stream. So, under optimal conditions, you would locate the controller at the stream where the control valve has been placed to adjust the process.
The intention of the examples of this manual is to demonstrate good schemes for the control systems of distillation columns. You can follow this logic when you apply more powerful control structures than a local loop.

In the next example you will see three different solutions for the control of column pressure. All of them work:

- The locations of the control elements resemble the classical way of thinking in the first solution.
- The second solution follows the logic described above as “use controller and control valve together in the same stream”.
- In the last solution, we made a little change in the sequence of unit operations, but the solution handles the calculation sequence (unit 1, unit 2, unit 3, …) much better than two preceding solutions.


Solution 1
Column pressure control by CW flowrate
PC
3
7
8
CW outlet
Cooling water
16
2
15
CW inlet
1
FC


Solution 2
Column pressure control by CW flowrate
7
CW outlet
PC
3
Cooling water
8
16
2
15
CW inlet
1
FC



CC-DCOLUMN provides complex control structures as follows:

- Cascade control system
- Set point tracking control system
- Set point control system

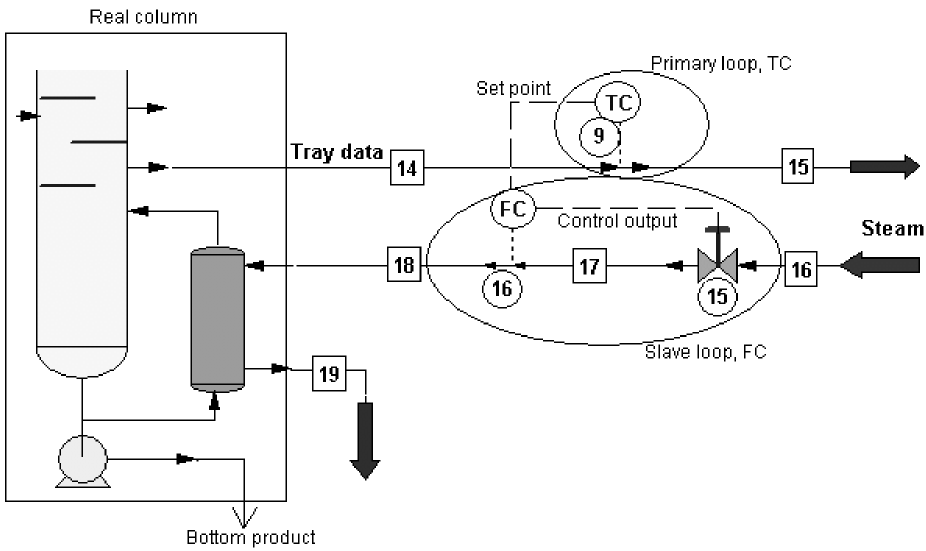
HOW TO USE CASCADE CONTROL SYSTEM

The PIDC model of CC-DCOLUMN includes all parameters needed for a cascade control structure. We will explain the parameters by example of a typical control solution.

The picture below shows a part of a technology. The objective is to maintain the temperature of a tray in the bottom section of a distillation column when the concentration of the feed changes.

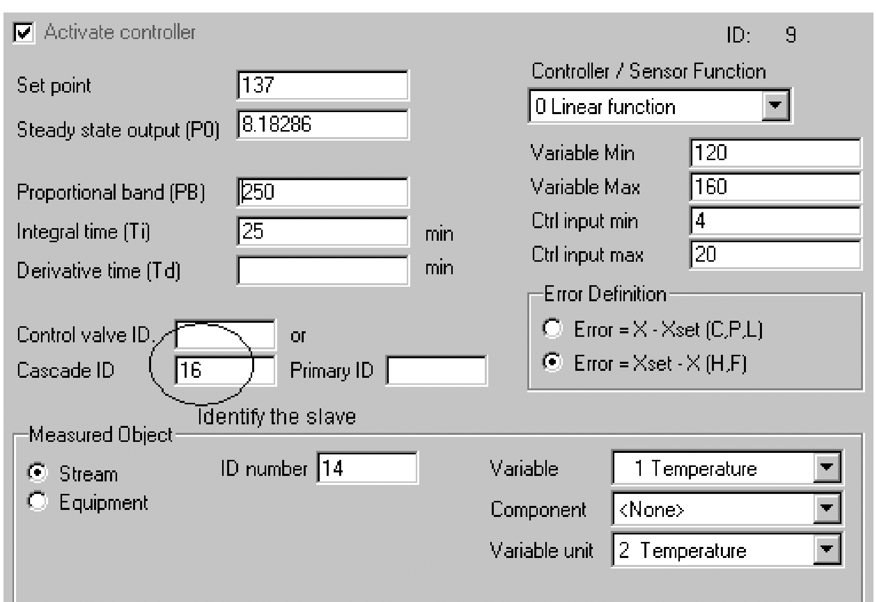
We have defined a pseudo side stream [14]. This stream has nearly zero mass flow rate but it transfers the temperature, pressure and concentration data of the tray to which the stream has been connected. Primary controller [9] has been inserted into this stream. The measured variable is the temperature of the stream, which is equal to the tray temperature.

The adjusted variable is the set point of the slave controller [16]. We then manipulate the steam flow rate of the reboiler [15] by adjusting the slave controller set point.

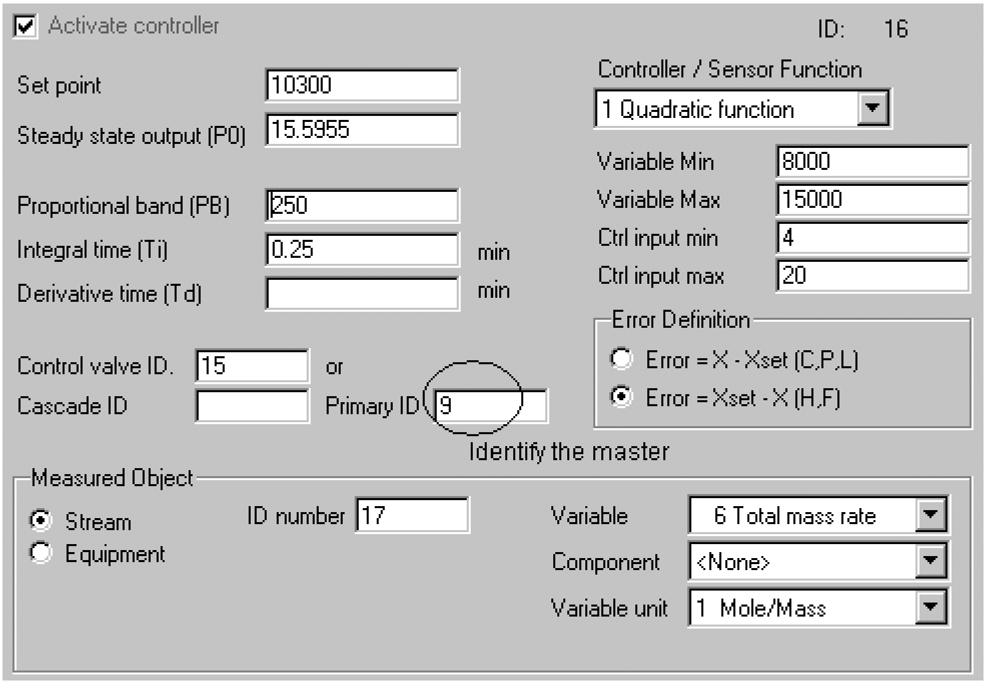


The CC-DCOLUMN dialog box defines the relationships between the units.

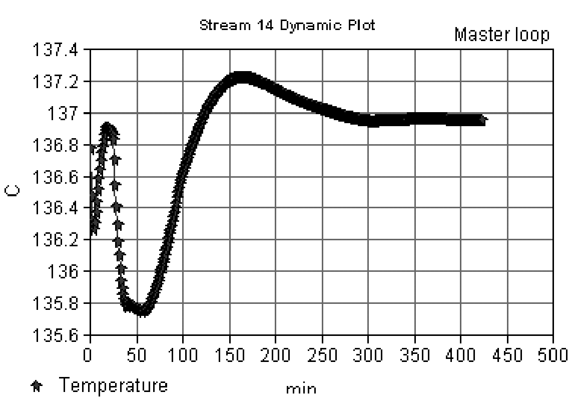
For the primary loop the only special definition is the slave identification:

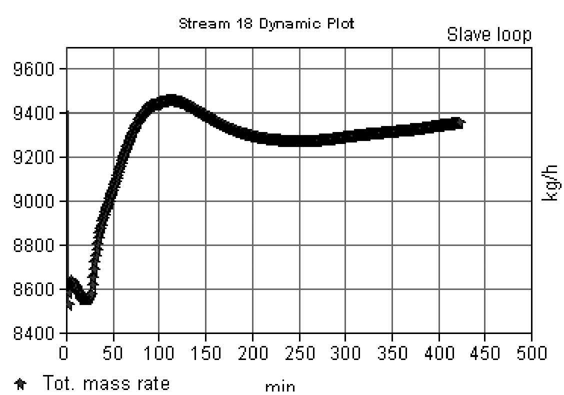


For the slave loop, the only special definition is the master or primary loop identification:



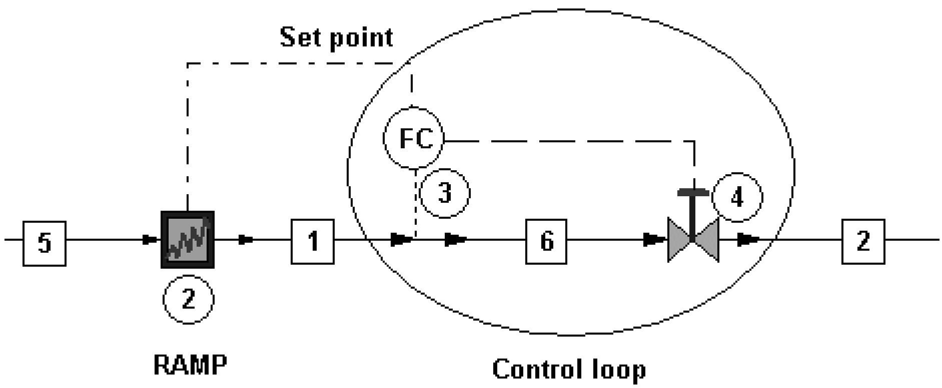
The units mutually communicate with analog signal expressed in milliampers. The actual temperature and mass flow rate profiles can be seen below:



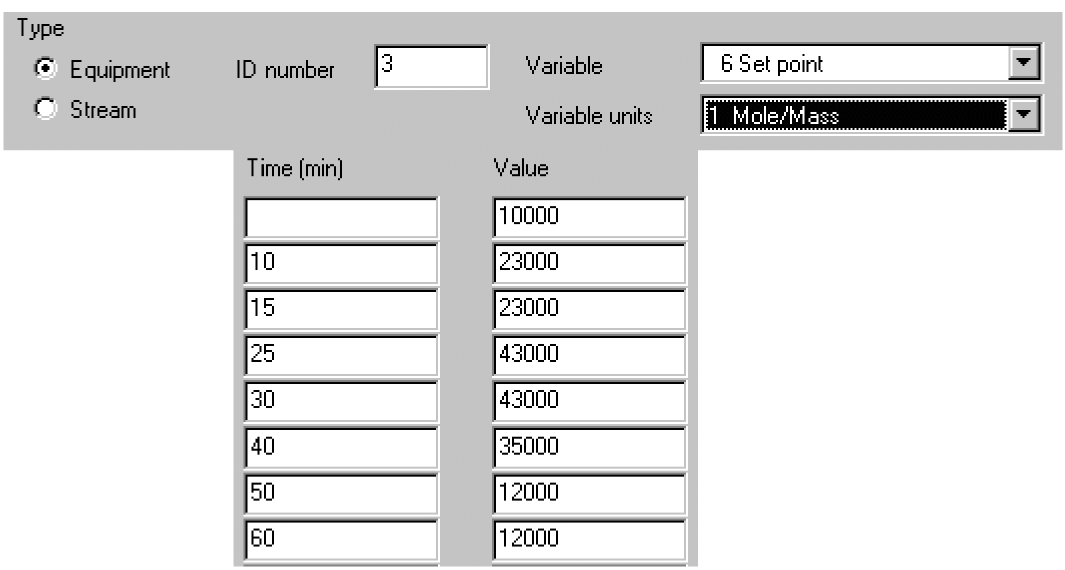


HOW TO DEFINE A SET POINT TRACKING SYSTEM

Using the RAMP model of CC-DCOLUMN, you can define time dependent profiles for any variable in the flowsheet. Therefore, you can use RAMPs for setting any set point. The following simple example demonstrates position setting at the valve:



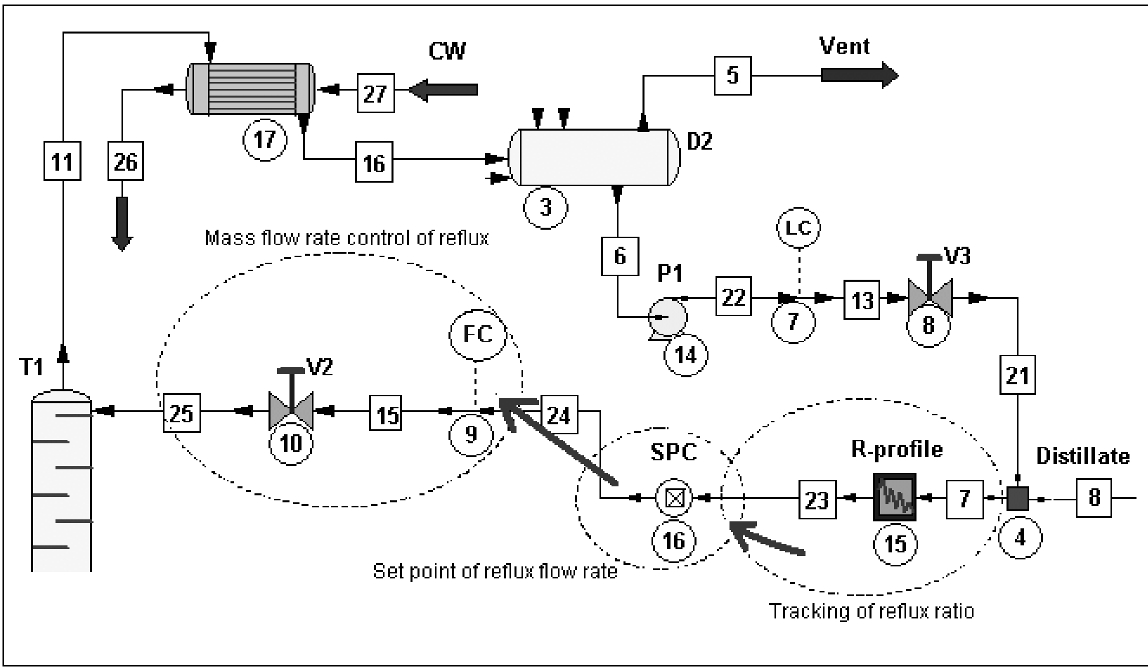
The RAMP model has the following parameters:



HOW TO DEFINE A SET POINT CONTROL SYSTEM

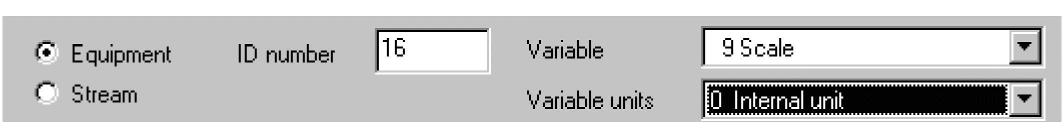
Set point control can be achieved by inserting a new unit into the control structure to calculate the real time set points using on line process data. In the manual, we will demonstrate a simple example only. Advanced users can change the calculator model with Excel unit operation or with special, user-written calculation algorithms.

This example uses a batch technology and we used the set point controller of the local control loop to control the reflux flow rate. Part of the technology follows:



The reflux ratio versus time profile is given. R-profile (RAMP) model keeps track of the profile and passes the actual reflux ratio to the SPC model (Set Point Controller), which produces an actual set point for FC (local flow rate) controller. The red arrows show the direction of information transfer. There is no information conversion to mA and back in this case.

The setting of RAMP follows:



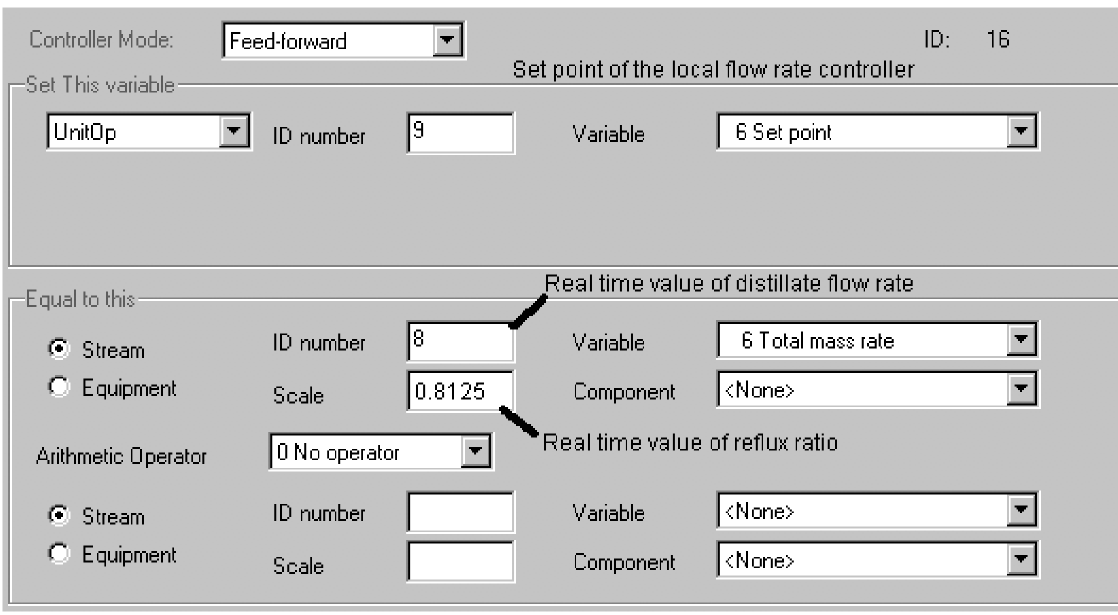
The SPC model calculates the actual reflux flow rate = set point value as desired, according to the equation:

R = Rratio * D {Adjusted variable = Scale factor * Measured variable}

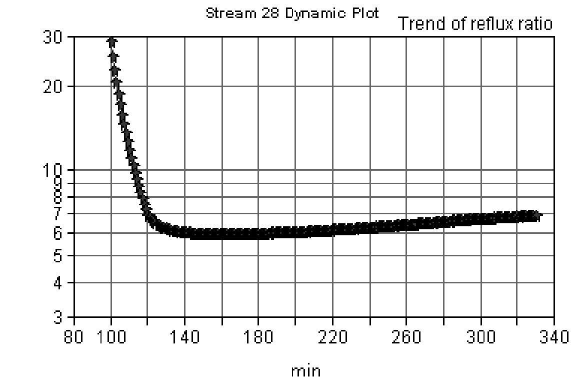
where R and D are reflux and distillate flow rates, respectively.

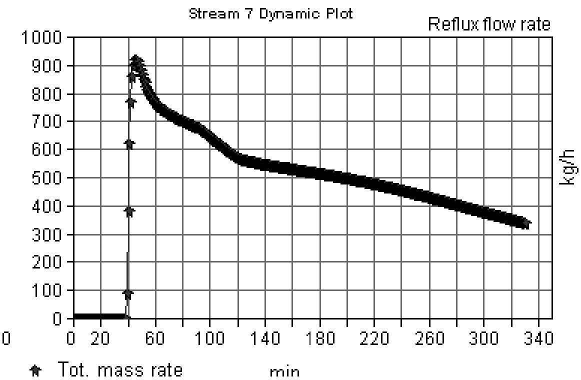
The SPC model reads the real time data of the distillate flow rate; (this is the stream 8), calculates the real time set point and writes this into the parameter table of the FC model. Eventually, FC controller (PIDC) modifies the reflux flow rate. It is also possible to calculate on-line value of reflux ratio – see the trend charts.

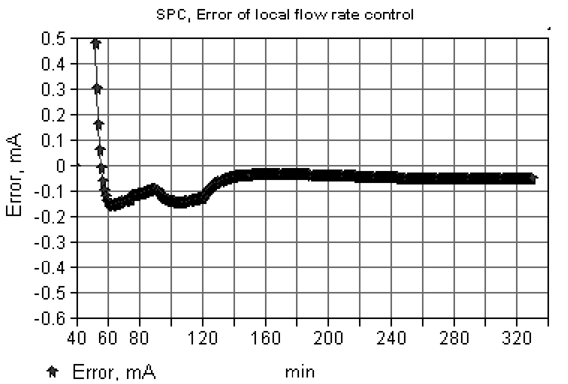
The SPC was modeled using the CC-DCOLUMN CONT (Steady State Controller). The data entered into the dialog box of CONT are:

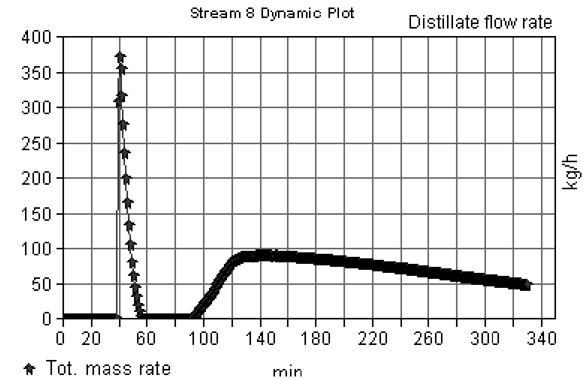


Below are several trend charts demonstrating the response of the control system, which appears to be satisfactory.









Using the error chart, we can calculate the maximum error of the reflux flow control. This is 14 kg/h and the overall difference is 5 kg/h. It is also necessary to point out that the column was under start up conditions for 30 minutes at total reflux, and the actual reflux ratio profile was activated after startup finished.

APPLICATIONS OF STEADY STATE MODELS IN DYNAMIC SIMULATION

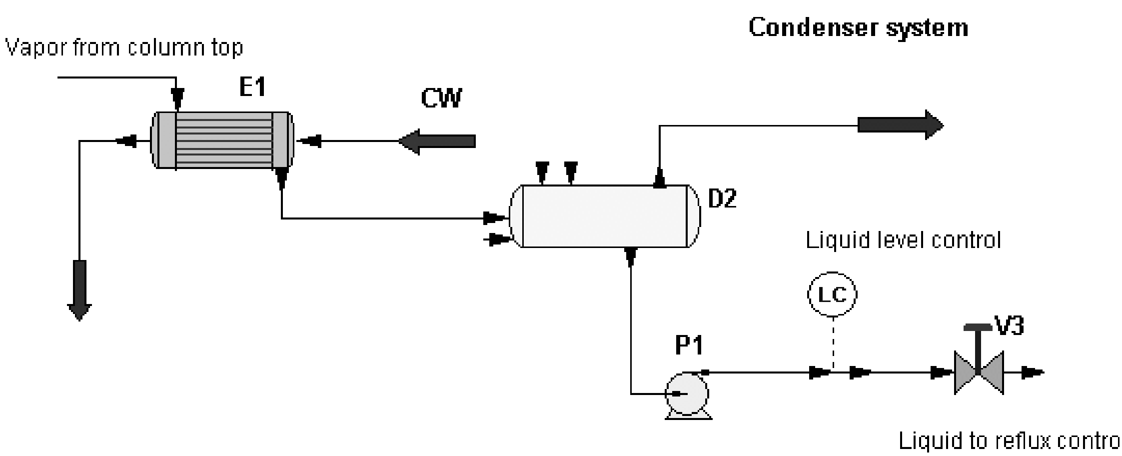
Earlier, we demonstrated that the stream mixer (MIXE) and the stream divider (DIVI) could be applied as steady state unit operations in dynamic mode. Theoretically, these units do not have any volume or dynamic properties. They are simulated with simple mass and heat balance equations. The basis of this philosophy is the fact that the space of the processes of mixing and / or of stream distribution is small. The residence time and time constant of these unit operations are very small compared to the time step of dynamic simulation, which is in turn much smaller than time constant of a distillation tower for example. Therefore, we can neglect the diagnosis of these units. The steady state model of the valve model (VALV) simulates pressure drop only and it is similar to MIXE and DIVI in this respect. You can make similar assumptions for liquid pump (PUMP) or for gas compressor / expander (COMP / EXPN).

In many cases, you can accept the simple assumption described above for heat exchanger (HTXR) and for pipes (PIPE). In such cases, you can neglect the influence of unit's dynamics on the process dynamics because it can be in fact small, or because you can assume that the control of temperature (heat exchanger) is perfect.

> **Fundamental Rule**
>
> Never manipulate intensive variables of a stream directly. Use a one-sided heat exchanger with outlet temperature definition to set a stream temperature. Use one of the VALV, PUMP, COMP or EXPN models to manipulate a stream pressure. Try to use pre-defined streams or separate component streams combined with mixer or component separator model for manipulation of concentration. You can combine these solutions in combination with a RAMP model as well.

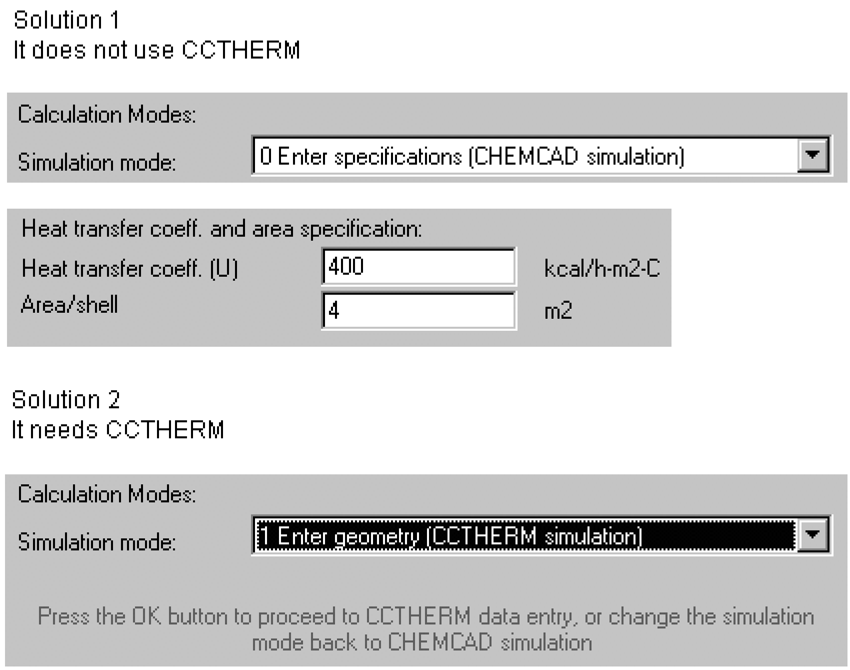
HOW TO USE THE HTXR MODEL

Discussed here is a more complicated system using HTXR as a simple temperature setting device. The example is a separated condenser system for a distillation column. It provides total condensation.



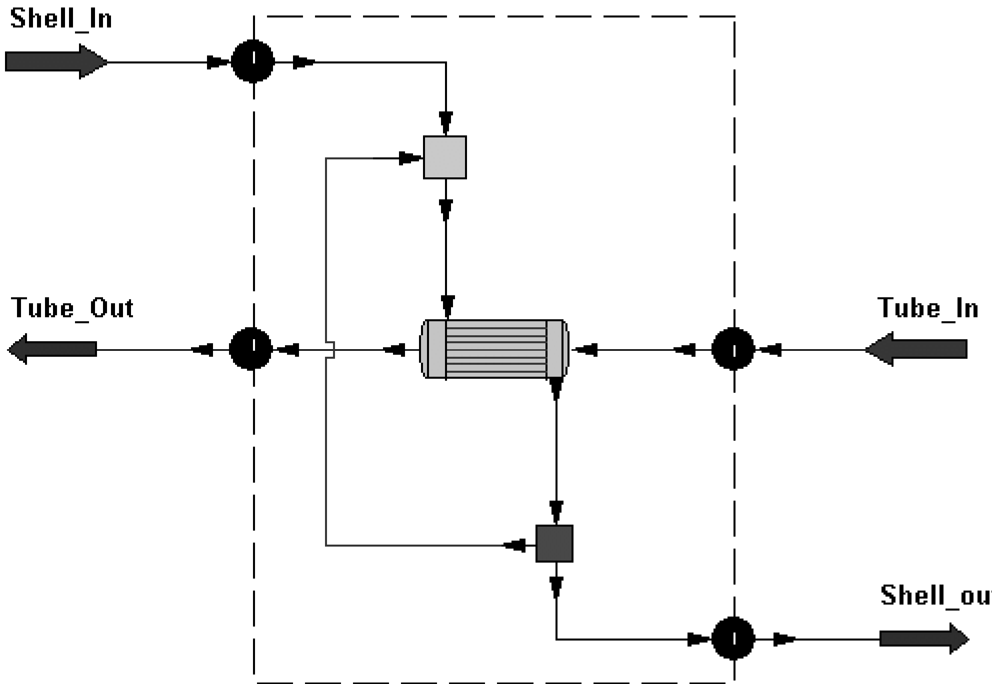
Solution 1.
Specify the heat transfer area and heat transfer coefficient of unit E1. This is a good approach because it means using the rating mode for the heat exchanger but the heat transfer coefficient is kept constant.

Solution 2.
Use the "simulation mode" of CC-THERM to re-calculate the value of the heat transfer coefficient. This is a rating mode also and uses the exchanger geometry to determine the outlet stream conditions.



Both solutions use steady state modules for the heat exchanger.

For advanced use of CC-DCOLUMN, we can present a quasi-dynamic simulation of heat exchanger:

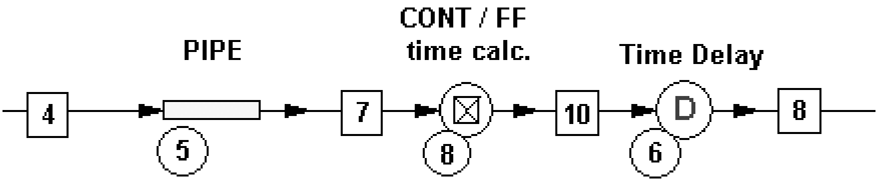


The dashed box covers the dynamic model of the heat exchanger. Each of the stream reference (SREF) unit operations copies its inlet to its outlet using a scale factor. The scale factor is the time step (unit is hours) for the inlet points and reciprocal of time step for the outlet points. The shell side at the start of calculation defines the initial state of the internal recycle stream: flow rate = mass (volume * density), T, P, and concentration have values of stream Shell_In at time zero. This simple model can take into account the dynamic properties of the shell side.

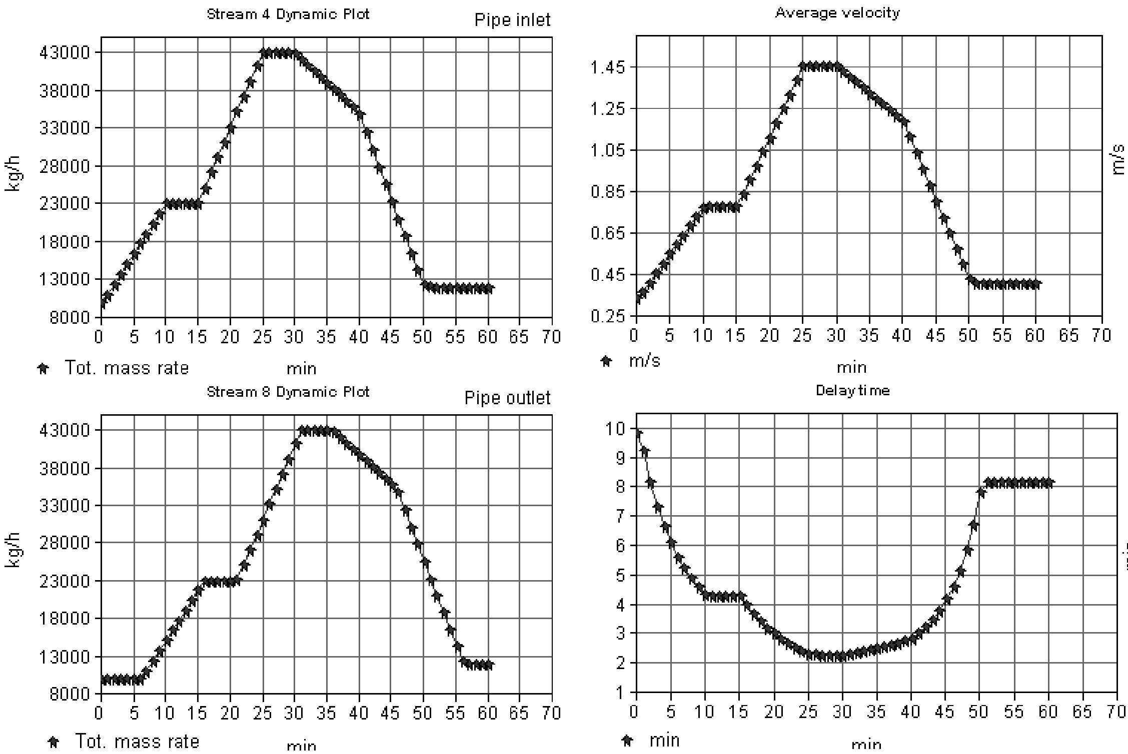
HOW TO USE THE PIPE MODEL

To calculate the piping pressure losses between equipment, you normally use the PIPE model. You can assume that a plug flow model can describe the flow inside a pipe. This assumption results in a well-defined residence time. If you cannot neglect the effect of this time delay, then you can apply the following solution.

Flowsheet

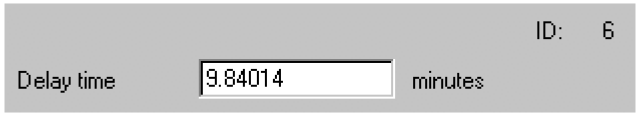


Solution



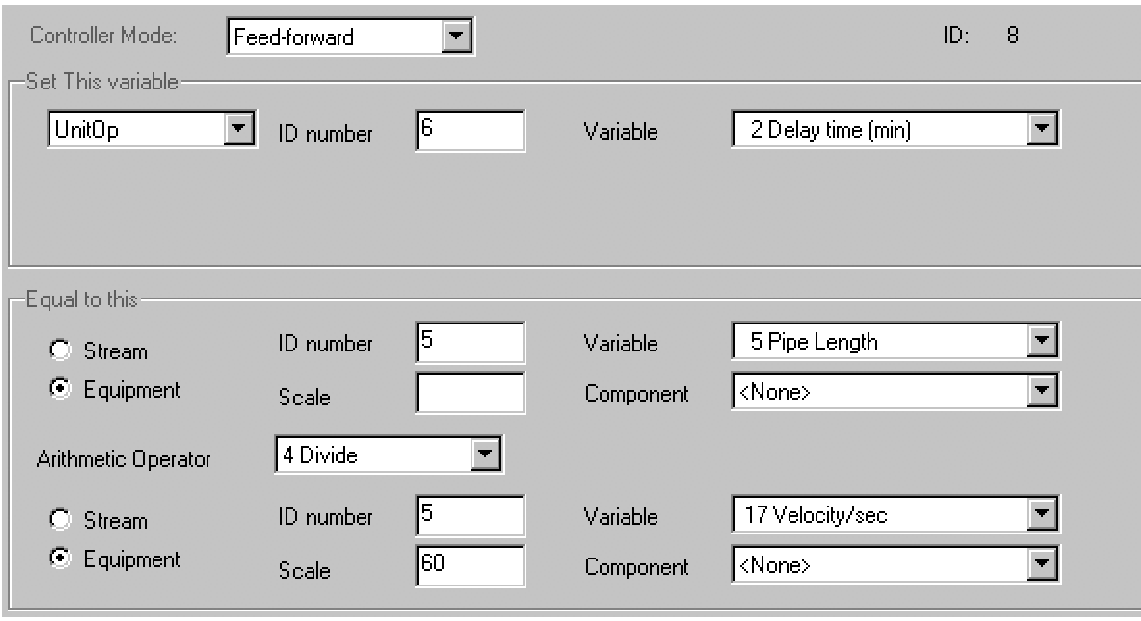
Tables

Time delay (DLAY) unit operation gets calculated data from the control model.



The control model uses the equation as follows:

Time = (Pipe_length) / (Linear _velocity * 60)   [min]



DYNAMIC SIMULATION OF A DISTILLATION COLUMN

The SCDS, TPLS and TOWR distillation models can be used to perform dynamic distillation simulations. They can be used to analyze dynamic responses of distillation columns without any control system around it, or you can use controllers. A wide range analysis, ranging from the very simple to the very complex can be performed. To run the distillation models in dynamics, you need a license for CC-DCOLUMN.

Since the dynamic distillation menu is common to three models available (SCDS, TPLS, TOWR) all examples in this manual will be run using the SCDS distillation model.

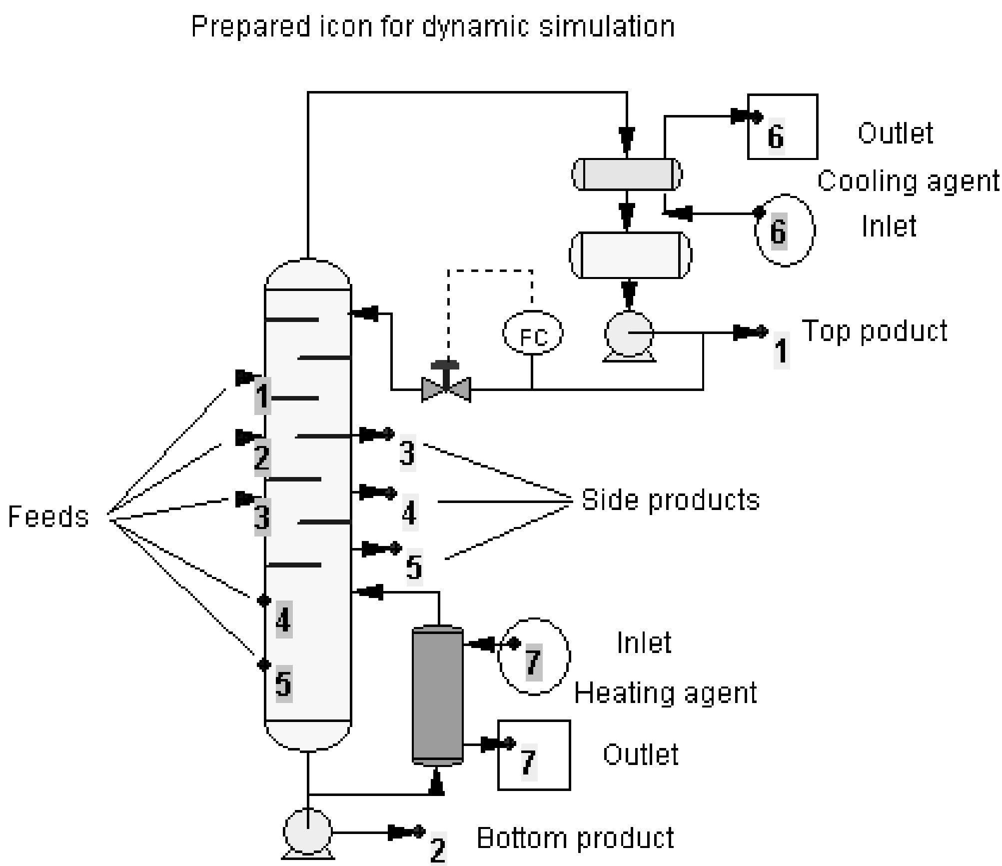
WHICH ICON OF SCDS SHOULD YOU USE IN A DYNAMIC SIMULATION?

The icons of CHEMCAD unit operations include three different things, these are

- the symbol; this is a visualization of the equipment
- the model; this is mathematical algorithm used for the calculation of that equipment
- the link; this makes the connection between the symbol and model; in practical terms, the product of linking is the icon.

According to this concept, you can theoretically use any of CC-DCOLUMN SCDS icons (and their unit operations) in a dynamic simulation. Practically, it is better to select the specialized Dynamic Column SCDS icon if your intention is to connect the distillation unit to other unit operations. This is because, not all icons have enough connection points (inlet / outlet points on the symbol).

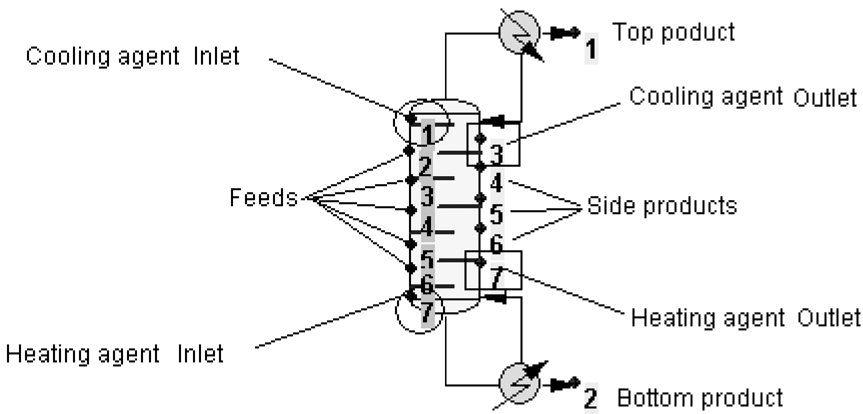
Therefore, the following SCDS icon is recommended:



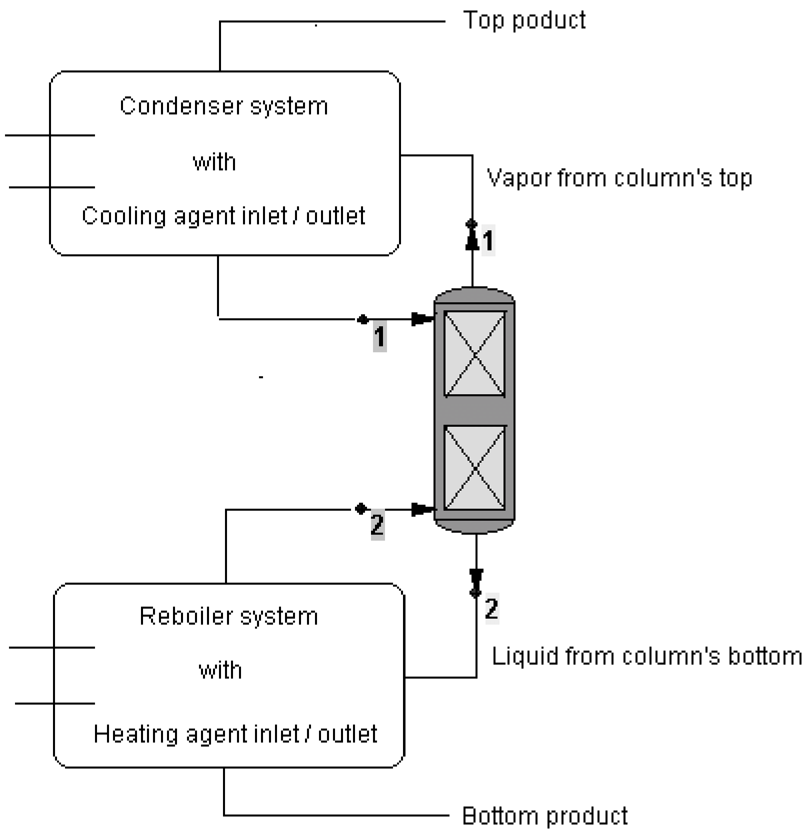
This icon involves built-in control loops and built-in dynamic vessels (both for condenser and / or reboiler systems).

The next icon does not look as attractive, but it can be used as well, as it includes enough connection points.

Use of an overall icon for dynamic simulation



You can simulate systems with separated cooling/heating, too. The next picture shows this concept and a possible solution for a packed batch distillation column.



In special cases you might want to draw your own icon with CHEMCAD's built in symbol editor.

COLUMN DYNAMICS WITHOUT ANY CONTROLLER

Let's start studying techniques of dynamic column calculations with a typical distillation problem. Let's choose a situation where the feed of a well-working column changes. This job is installed together with other examples during the installation of the CHEMCAD Suite. Job name is FEEDCHANGEDCOLM. It contains the starting data and information.

The components and thermodynamic calculation methods follow:

```
COMPONENTS
          ID #          Name

   1         3       Ethane
   2         4       Propane
   3         5       I-Butane
   4         6       N-Butane
   5         7       I-Pentane
   6         8       N-Pentane
   7        10       N-Hexane
   8        11       N-Heptane
   9        12       N-Octane

THERMODYNAMICS

 K-value model     :  SRK
 Enthalpy model    :  SRK
 Liquid density    :  Library
```

The feed changes at the start of the study from Feed_1 to Feed_2 as:

```
-----------------------------------------------
Stream Name                   Feed_1        Feed_2
-----------------------------------------------
Temp  C                      50.0000       50.0000
Pres  bar                    15.0000       15.0000
-----------------------------------------------
Total kg/h                19800.0000    20000.0000
-----------------------------------------------

Component        Kg/hr      Kg/hr
Ethane            1200       1473
Propane           3400     3156.4
I-Butane          4000     3787.7
N-Butane          4100     4839.8
I-Pentane         2500     2314.7
N-Pentane         2000     1893.8
N-Hexane          1300     1262.6
N-Heptane          800      841.7
N-Octane           500      430.3
-----------------------------------------------
```

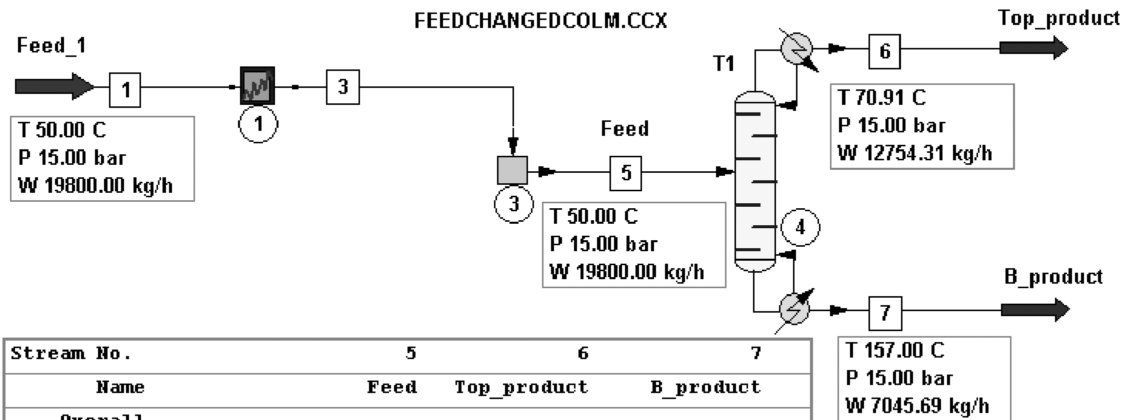
The column is in steady state before the change of feed and it works properly with the following parameters:

No. of stages	30	
1st feed stage	15	
Condenser type	1	Partial condenser
Select condenser mode:	1	Specified by reflux ratio
Condenser spec.	3.0000	Rr = R/D
Reboiler mode temperature	3	Specified by bottom
Reboiler spec.	157.0000	T_bottom, C
Top pressure	15.0000	P_top, bar

You can implement the change of feeds with a simple use of RAMP modules with the following parameters:

		RAMP on Feed_1	RAMP on Feed_2	Remarks
Stream ID		1	2	
Variable No.		6	6	Mass flow rate
Variable unit		1	1	Mole / Mass
	Time (min)	Value (kg/h)	Value (kg/h)	
	0.0	19800.00	1.0000e-06	
	0.001	1.0000e-06	20000.00	
	300.000	1.0000e-06	20000.00	

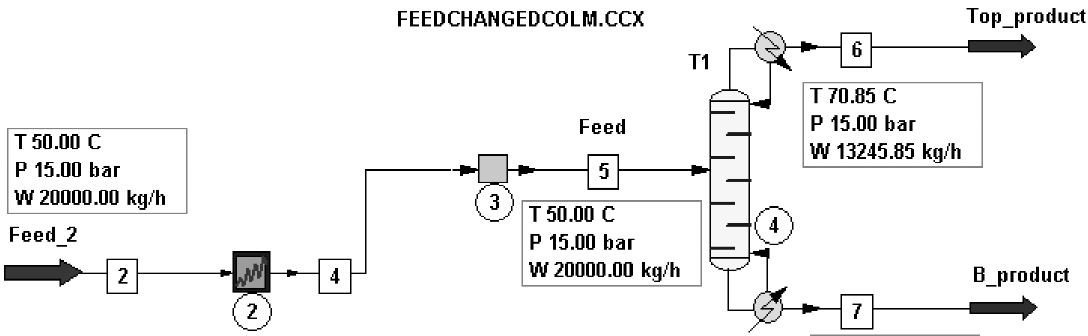
You would calculate the steady state values first. The following picture presents the important data before the change of feed. This is the initial state of the system.



Stream No.	5	6	7
Name	Feed	Top_product	B_product
- - Overall - -			
Mass flow kg/h	19800.0000	12754.3069	7045.6910
Temp C	50.0000	70.9092	157.0000
Pres bar	15.0000	15.0000	15.0000
Enth MJ/h	-49748.	-29079.	-14233.
Actual vol m3/h	40.4790	381.6108	15.1052
Component mass %			
Ethane	6.060605	9.408585	0.000000
Propane	17.171720	26.657665	0.000002
I-Butane	20.202020	31.360367	0.002873
N-Butane	20.707068	32.124320	0.039234
I-Pentane	12.626261	0.431192	34.702116
N-Pentane	10.101009	0.017871	28.353789
N-Hexane	6.565656	0.000000	18.450989
N-Heptane	4.040404	0.000000	11.354457
N-Octane	2.525252	0.000000	7.096534

It is good to know the final state of the column (or, in other words: to know the answer to the question) before you start the dynamic simulation. Which parameters should be used for this calculation? If you keep the original operating parameters, that is, R/D and bottom temperature, then the question is: "what is the capacity of the column? "

This is the answer:



Stream No.	5	6	7
Name	Feed	Top_product	B_product
- - Overall - -			
Mass flow kg/h	20000.0000	13245.8513	6754.1463
Temp C	50.0000	70.8536	157.0000
Pres bar	15.0000	15.0000	15.0000
Enth MJ/h	-50376.	-30209.	-13642.
Actual vol m3/h	41.6694	400.3912	14.5073
Component mass %			
Ethane	7.368420	11.125625	0.000000
Propane	15.789469	23.840620	0.000004
I-Butane	18.947369	28.603441	0.010424
N-Butane	24.210522	36.409566	0.286435
I-Pentane	11.578951	0.019816	34.248072
N-Pentane	9.473687	0.000927	28.051126
N-Hexane	6.315793	0.000000	18.701971
N-Heptane	4.210529	0.000000	12.467980
N-Octane	2.105263	0.000000	6.233986

The new feed contains new component concentrations and produces new product streams. From the standpoint of the required separation, you should check the key components only:

	Before (wt. %)	After (wt. %)
N - Pentane (top)	0.017871	0.000927
I – Butane (bottom)	0.002873	0.010424

The results reflect the change of component concentration in the feed and anticipate enough capacity but still do not necessarily provide an adequate picture of the column operation. The reason is the specified simulation parameters are not for column operations. Operating parameters, R/D and bottom temperature, are typical design parameters for steady state, but more appropriate operating selections for the initial condition of the column would be the real operating parameters, such as heat duty of reboiler and heat duty of condenser.

According to the first steady state calculation these values would be:

Heat duty of condenser	12515.9 MJ/h
Heat duty of reboiler	18942 MJ/h

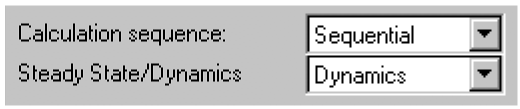
Now, you can repeat the steady state calculation after the feed change keeping operating parameters as given above at constant values.

The main streams are now:

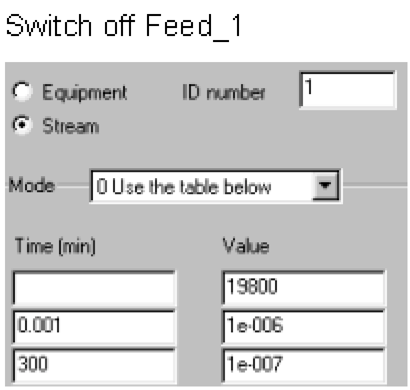
Stream No.	5	6	7
Name	Feed	Top_product	B_product
- - Overall - -			
Mass flow kg/h	20000.0000	13008.1991	6991.7937
Temp C	50.0000	70.3335	153.4132
Pres bar	15.0000	15.0000	15.0000
Enth MJ/h	-50376.	-29717.	-14232.
Actual vol m3/h	41.6694	393.9026	15.3340
Component mass %			
Ethane	7.368420	11.328880	0.000000
Propane	15.789469	24.276155	0.000025
I-Butane	18.947370	29.073516	0.107718
N-Butane	24.210523	35.315049	3.550608
I-Pentane	11.578952	0.005958	33.110449
N-Pentane	9.473686	0.000439	27.098614
N-Hexane	6.315792	0.000000	18.066294
N-Heptane	4.210529	0.000000	12.044196
N-Octane	2.105263	0.000000	6.022095

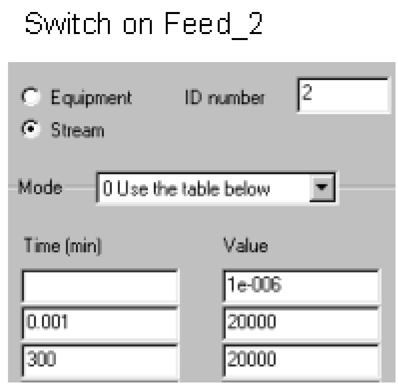
Examining the bottom product, you can see that without any modification the column cannot produce acceptable purity at the bottom anymore; temperature decreased 3.5 C, and the concentration of I-Butane increased to 0.11 w%.

You can study this behavior of the column using the dynamic column model of CC-DCOLUMN. Select this option in the "Run / Convergence" sub-menu.

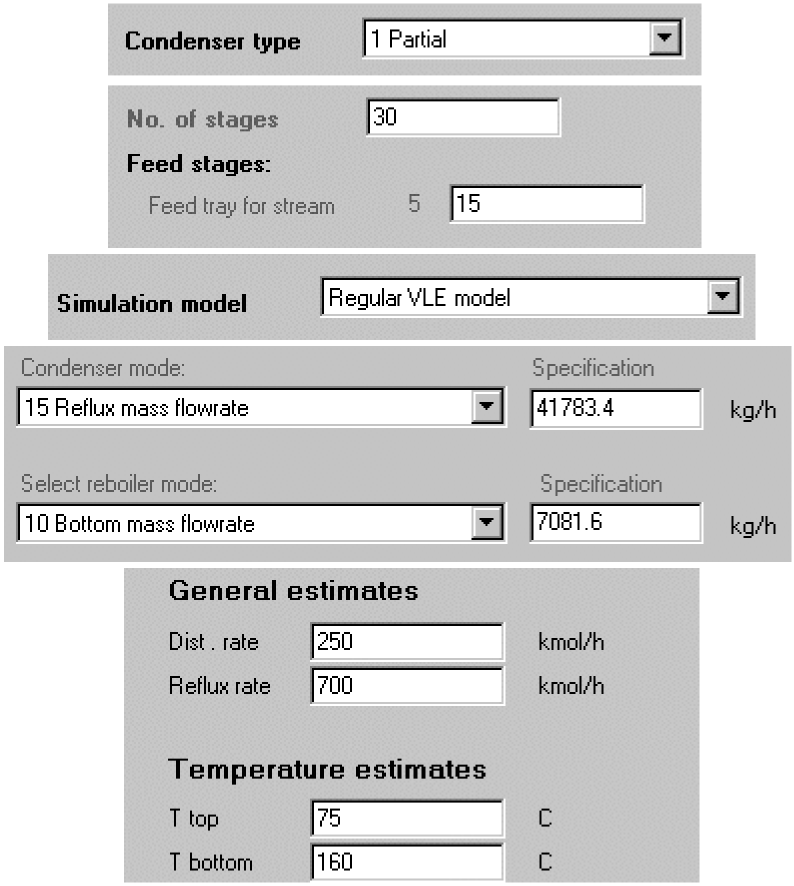


You need to use RAMP modules now:





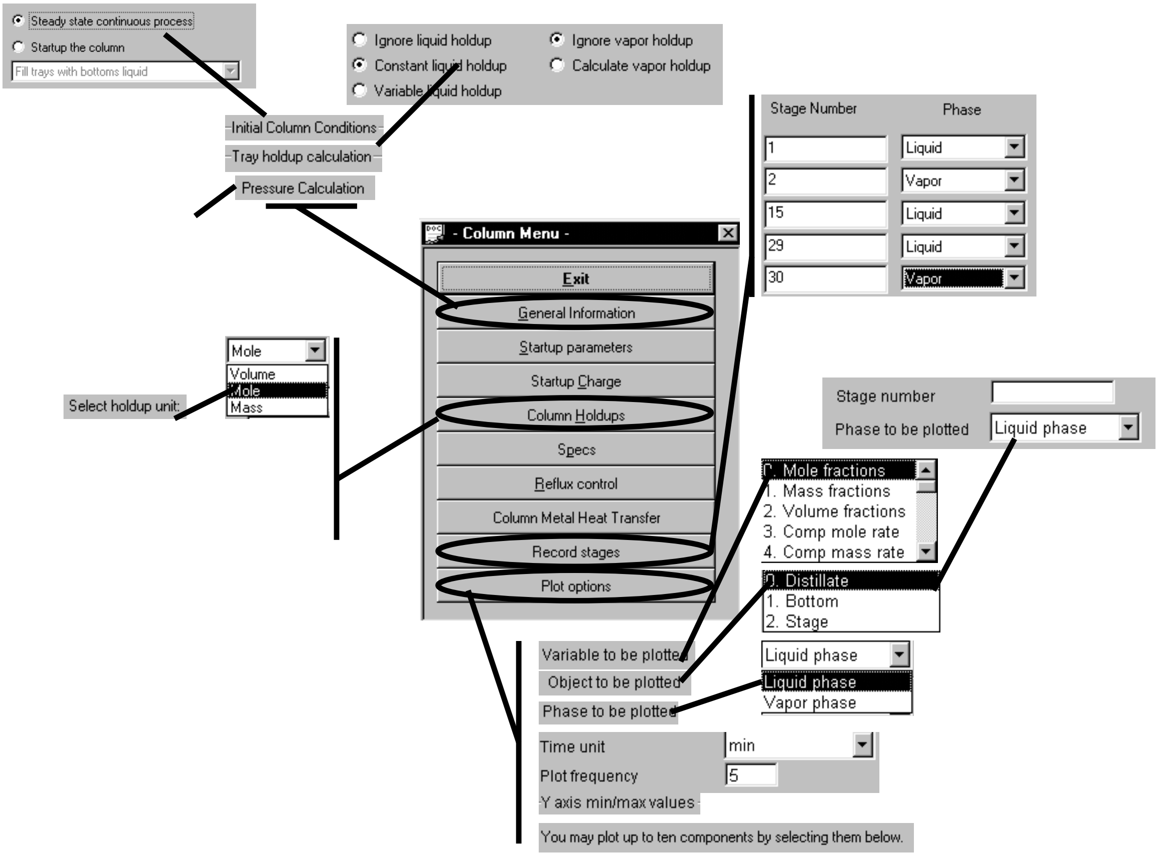
In dynamic simulation, you normally do not want to use the condenser and reboiler specifications in the same way as in steady state. Therefore, we selected bottom mass flow rate and reflux flow rate for the column specs.



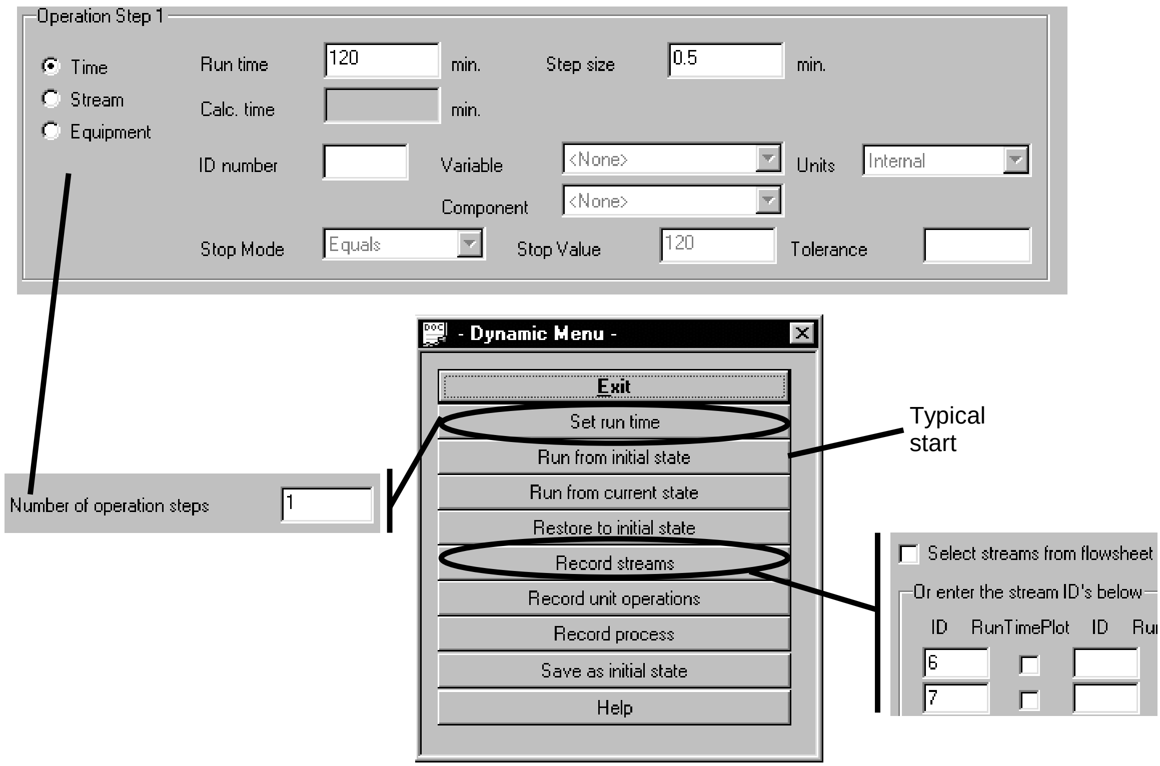
For the first dynamic simulation use *minimal settings*. The meaning of "minimal settings" is:

- Calculate a continuous process starting from steady state for the initial state.
- Ignore the vapor holdup and specify constant liquid holdup in moles; specify all trays the same.
- Do not calculate the condenser and reboiler system separately. Use the overall specifications for distillation column.
- Record data of selected trays only and request on-line plotting of product concentration.

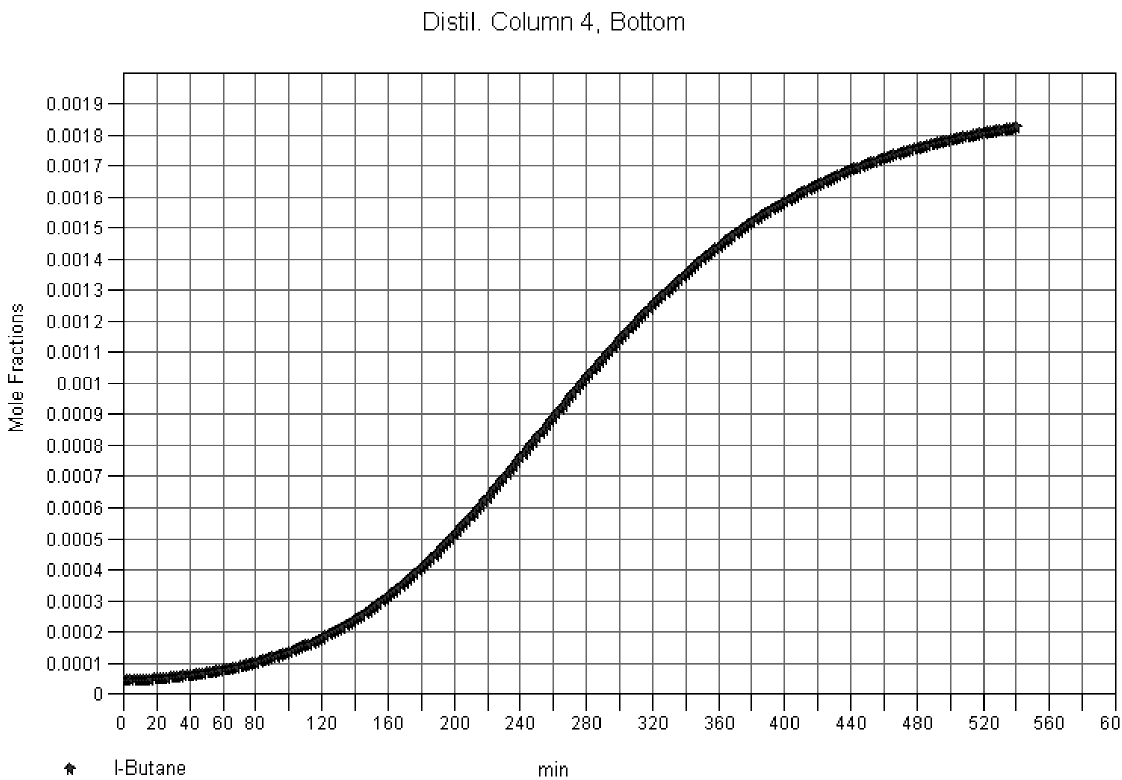
The picture below gives an overview of these settings.



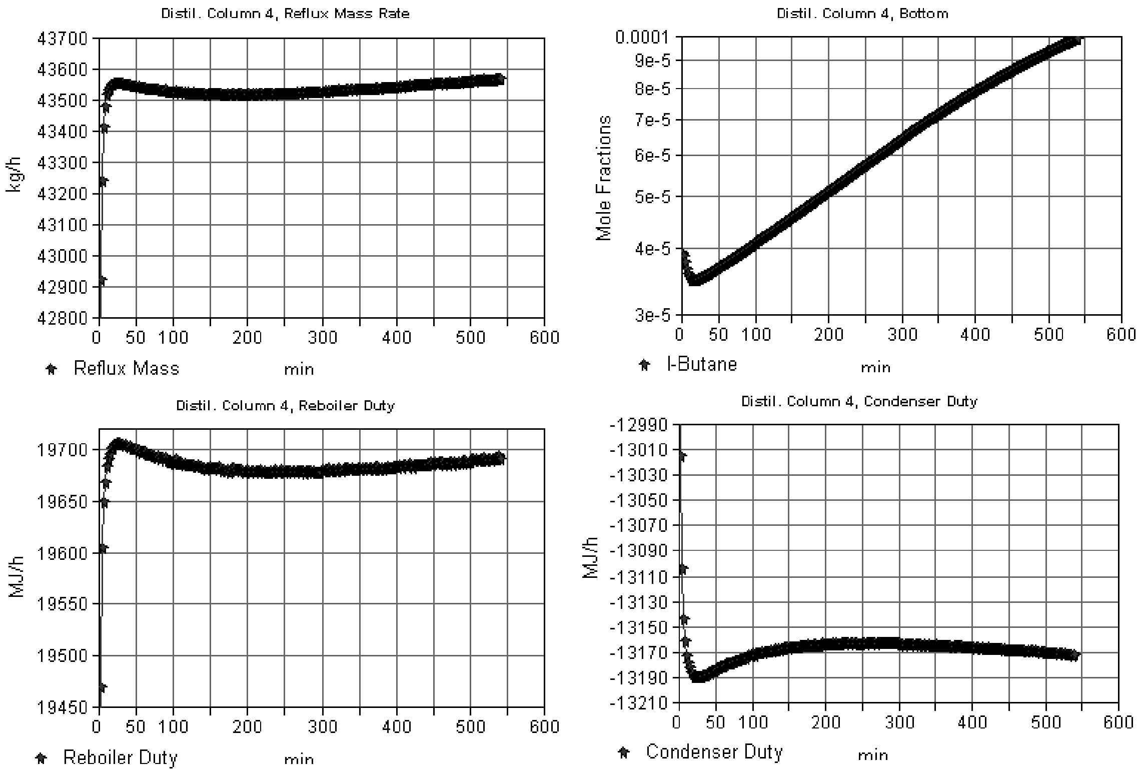
For the dynamic simulation, we should specify the time duration of the simulation and the time step size.



The following plot gives the I-Butane concentration in the bottom product when the bottom and reflux streams are kept constant.

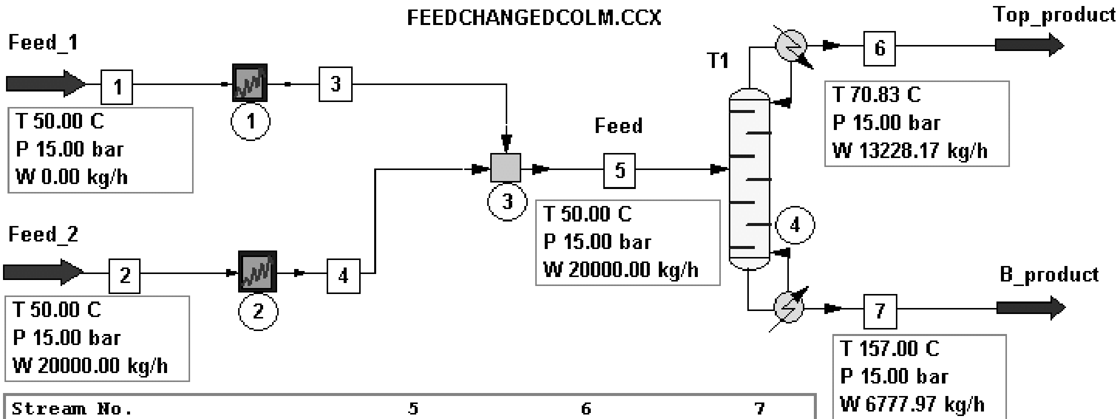


If you return to the original R/D = 3 and T_bottom = 157 °C parameters, and then repeat the dynamic simulation, you will get information about the operating parameters needed for the condenser and reboiler.



According to the chart, you can tell that good compensation of the noise of the feed requires fast response of the condenser and reboiler system, and it will result in rapid changes in the flow rate of the reflux stream. No real control equipment can do this. However, you have been able to determine an appropriate control strategy. It must be pointed out that this strategy produces an overshoot and a slow, asymptotic convergence later.

Let's compare the result of the converged dynamic simulation to the result of the steady state simulation. These can be found below and reflect a good equivalence to the result of steady state simulation (see second material balance of the example above). By running the calculation over a longer simulation period, you would observe smaller differences. Do not expect the results of both types of simulations to be 100% identical.



Stream No.	5	6	7
Name	Feed	Top_product	B_product
- - Overall - -			
Mass flow kg/h	20000.0000	13228.1657	6777.9732
Temp C	50.0000	70.8270	157.0000
Pres bar	15.0000	15.0000	15.0000
Enth MJ/h	-50376.	-30172.	-13692.
Actual vol m3/h	41.6694	399.9170	14.5488
Component mass %			
Ethane	7.368420	11.140431	0.000000
Propane	15.789469	23.870906	0.000003
I-Butane	18.947367	28.616622	0.007322
N-Butane	24.210519	36.339238	0.186775
I-Pentane	11.578950	0.031463	34.499201
N-Pentane	9.473687	0.001347	28.046468
N-Hexane	6.315792	0.000000	18.631923
N-Heptane	4.210529	0.000000	12.419083
N-Octane	2.105263	0.000000	6.209229

In the next step, we extend the dynamic column to represent a more realistic column. The dynamic column model can calculate holdup on each tray if the sizing data is given.

This calculation works for tray-columns only. For packed columns, we suggest entering the holdup profile. In such case, you should estimate the holdups; you can define a different holdup for each segment of the packed column if you like. This approach can be important when you use the mass transfer model for the calculation of the vapor-liquid component transfer and the segment sizes are different.

If you know tray sizes (that is, you are calculating an existing column), then you should enter the available data.

The normal sequence to specify tray sizes is as follows:

- Select the "variable holdup" option in the "Initial Condition" menu
- Open and close the "Column holdups" menu. (There is a hierarchy of specifications and a constant holdup will be overwritten with a holdup profile, the holdup profile will be overwritten with calculated holdup, etc. Therefore, you do not have to delete the "old" specifications. On the other hand, do not forget that the tray holdup calculation does not cover the holdup of condenser and reboiler. You can enter these values in the "Specs = special settings" menu and we will show an example of this later in the manual. For now, let's keep these values as constant.)
- Enter data into the table, which will appear on the screen.

If the work is for the design of a new column, then you should perform tray sizing of the column first, based on the data from the current column calculation. CC-DCOLUMN will display the size data automatically.

For the initial state conditions we get the following size data for sieve trays:

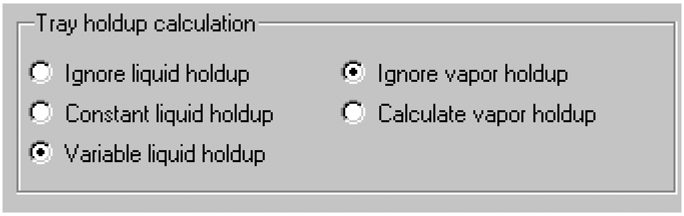
```
Equip.   4   Tray No.   4

  Tray Loadings                        Vapor                Liquid
                                   57933.023 kg/h       45178.718 kg/h
  Density                             36.459 kg/m3        465.603 kg/m3

  Downcomer dimension,             Width  m   Length  m    Area m2
                Side                 0.251      1.535       0.262
                Center               0.262      5.200       0.682
                Off center           0.258      4.633       0.593
  Avg. weir length    m             ................        8.769
  Flow path length    m             ................        0.330
  Flow path width    m              ................        8.836
  Tray area,  m2                    ................        5.309
  Tray active area  m2              ................        2.918
  % flood                           ................       75.490
  Fractional entrainment            ................        0.008
  Aeration factor                   ................        0.685
  Minimum (Weeping) vapor flow  kg/h ...........        49830.489
  Tray press loss,   m              ................        0.069
  Tray press loss, bar              ................        0.003
  Downcomer backup   m              ................        0.139
  Downcomer residence time, sec ................            6.154
  Liquid holdup     m3              ................        0.304
  Liquid holdup     kg              ................      141.508
```

```
Equip.   4   Tray No.  24

Tray Loadings                     Vapor              Liquid
                             82035.384 kg/h      89081.091 kg/h
Density                         43.651 kg/m3       467.739 kg/m3

Downcomer dimension,         Width  m   Length  m    Area m2
               Side            0.314      1.695       0.365
               Center          0.374      5.200       0.972
               Off center      0.367      4.641       0.845
Avg. weir length    m         ................        8.936
Flow path length    m         ................        0.216
Flow path width    m          ................        8.888
Tray area,  m2                ................        5.309
Tray active area  m2          ................        1.919
% flood                       ................       77.725
Fractional entrainment        ................        0.005
Aeration factor               ................        0.612
Minimum (Weeping) vapor flow  kg/h ...........    72773.794
Tray press loss,   m          ................        0.069
Tray press loss, bar          ................        0.003
Downcomer backup   m          ................        0.148
Downcomer residence time, sec ................        4.750
Liquid holdup     m3          ................        0.342
Liquid holdup     kg          ................      160.178
```

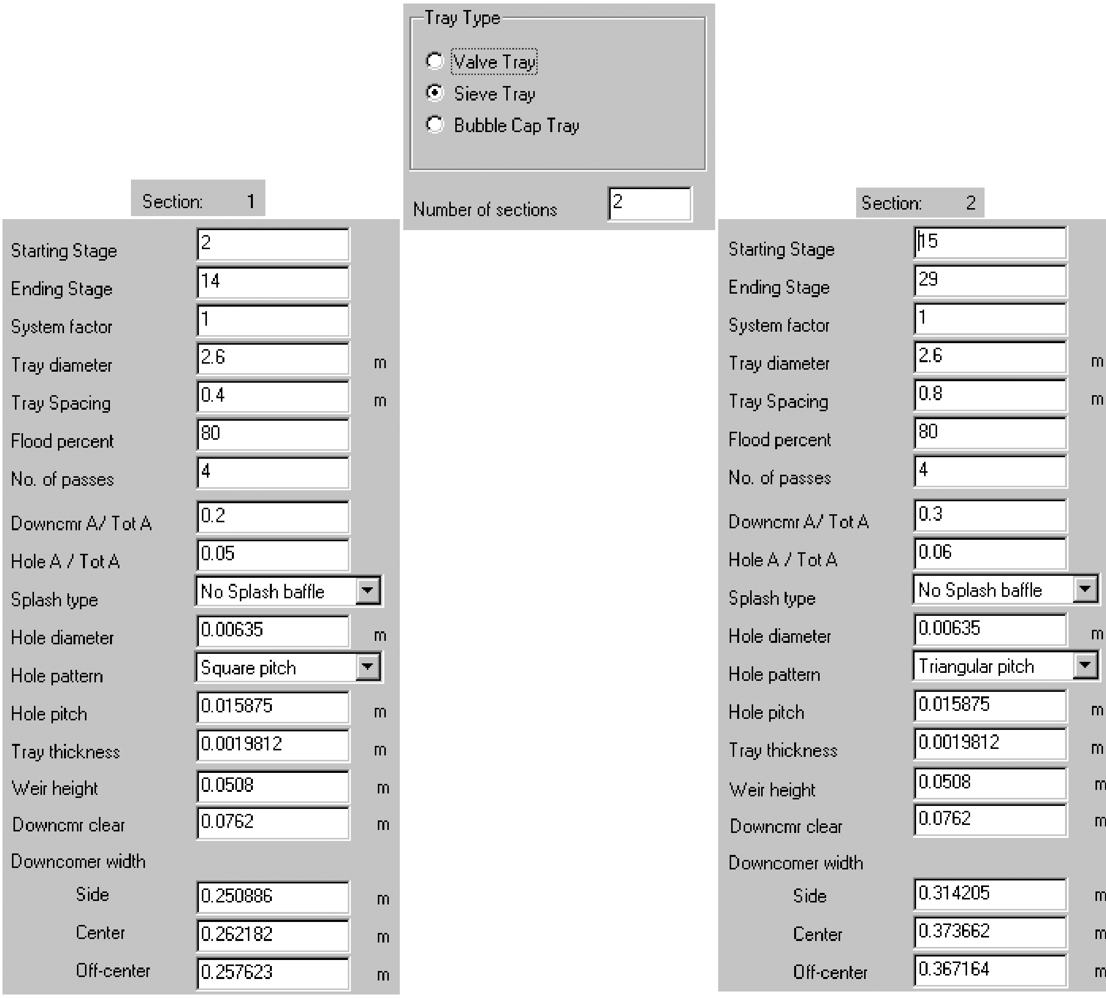
The sizing program calculates the total pressure drop as well:

```
Total column pressure drop =       0.087 bar
```

The new specification in the General Information menu is then:



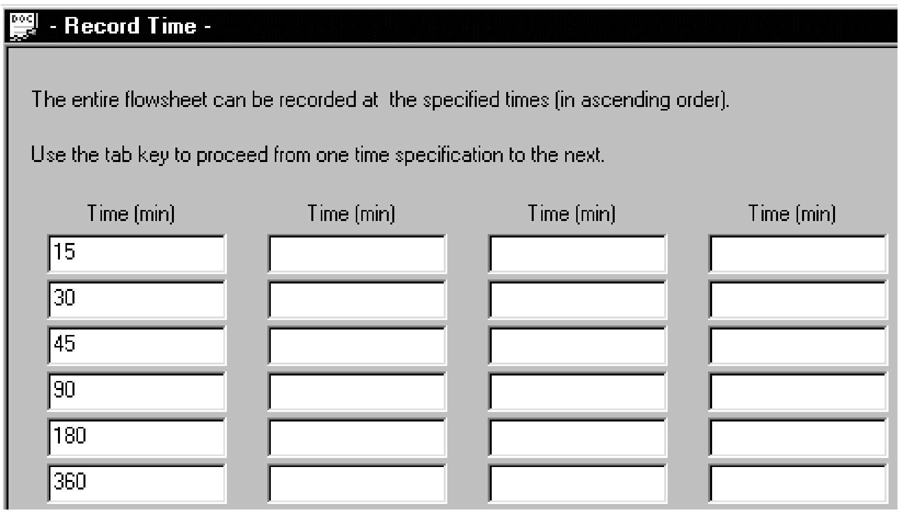
Let's use the following tray specifications:



The pressure drop is constant in the dynamic column calculation. The program does not calculate new pressure drops at each time stop. The "variable pressure" option means a new top pressure is calculated at each time point. The actual pressure of a tray is calculated from the variable top pressure and from the interpolated pressure drop based on the tray position and on the total pressure drop. This calculation can be important for columns equipped with total condenser.

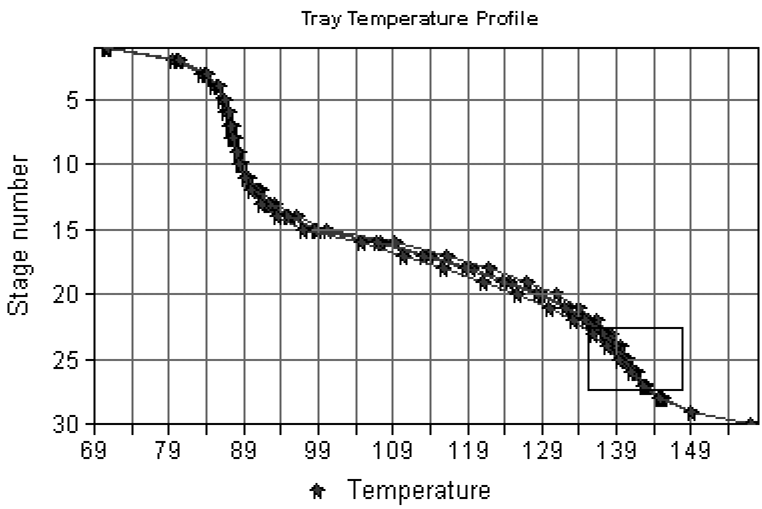
Before you install any control loops around the column, we will make an analysis of the dynamic properties of the column. Several time dependent cases can be recorded during the simulation if the "Record process" option of the "Dynamic menu" is selected.

For example:



CC-DCOLUMN will save a set of case studies automatically according to this table. The case studies will be given names such as: #D15, #D30, … It is possible to examine individual case studies, normally after the simulation.

The plot below presents sample temperature profiles taken from saved case studies. The objective is to understand the sensitivity of the column and to find a "good tray" for the temperature control system. We decided to select a tray from the area enclosed in the box in the picture. The common property of trays from 24 to 26 is in the fact that the temperature profiles show an inflection point here. We have selected tray 24 for measurement and control of temperature for the bottom section of the column.



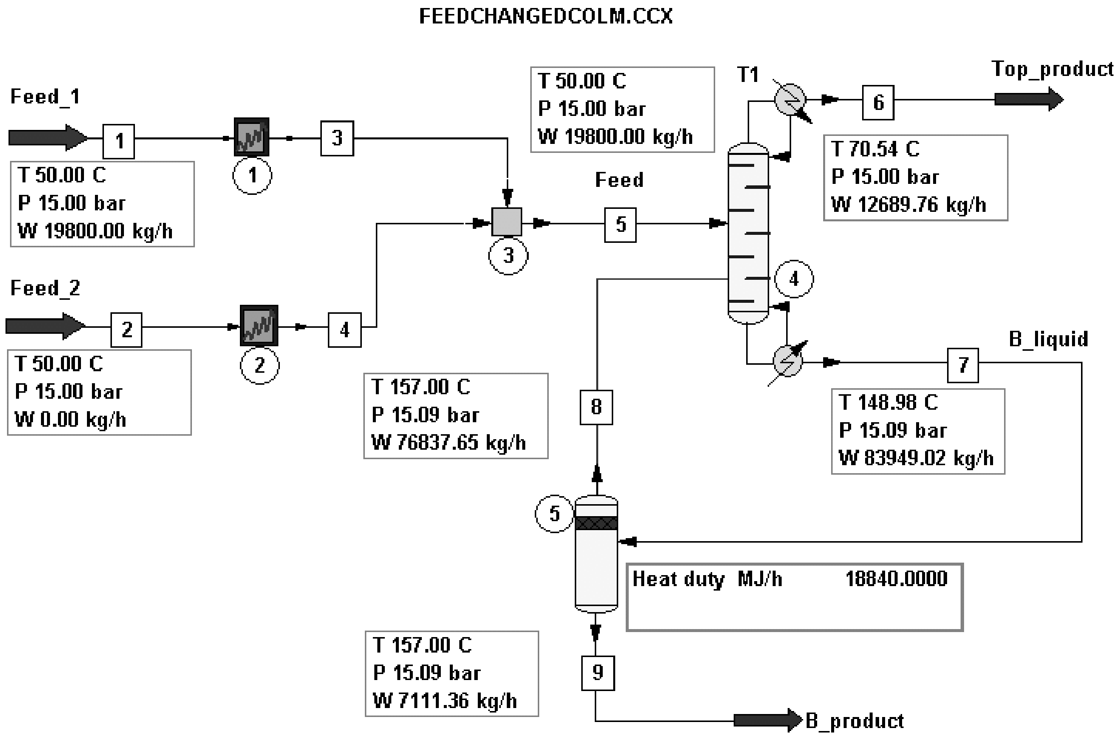
In the control system, we will try to maintain nearly constant temperature of this tray.

HOW TO INSTALL CONTROL LOOPS FOR A COLUMN

Let's explain the sequence of work for the reboiler system of this example.

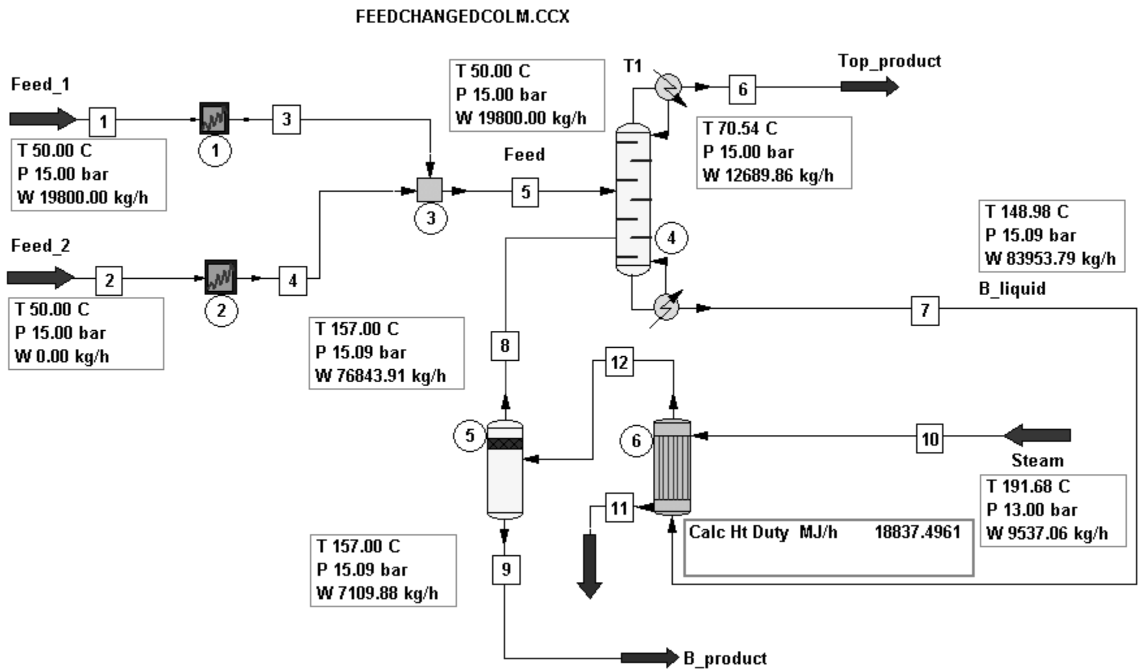
Step 1.

- Switch simulation mode from dynamic to steady state
- Insert a multipurpose flash module into the stream of B_product (bottom product)
- Connect the vapor outlet of flash to the column, this will be the vaporized stream from the reboiler
- The original column outlet is the inlet of flash, this stream is coming from the last tray (segment), its new name is B_liquid
- The liquid outlet of the vessel is the bottom product of the column
- Modify the settings of column: there is no reboiler, so decrease the number of trays by one and specify the new feed on the last tray
- Estimate the B_liquid stream using the result of last calculation (liquid from tray 29)
- Specify flash with temperature (Tb = 157 °C) and pressure (left it blank)
- Use the recycle run option to converge the loop containing unit 5 and unit 8

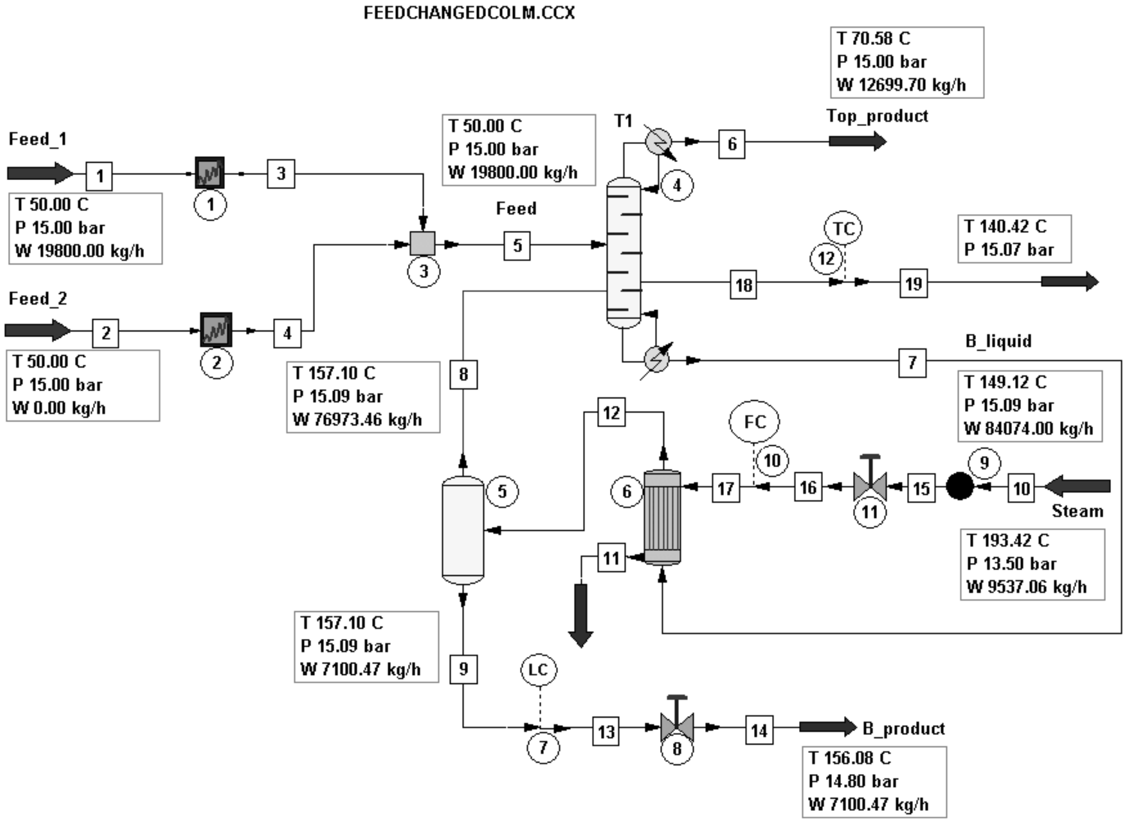


Step 2

- Insert a heat exchanger before flash
- Use steam as utility – heating – agent
- Using several options of overall HTXR module and / or using the CC-THERM module of the CHEMCAD Suite, obtain the size data of the reboiler heat exchanger, finally use rating definitions (area and heat transfer coefficient)
- Delete specification of vessel
- Use the vessel sizing tool for the flash (keep the column diameter for vessel diameter)
- Run the new system and achieve the converged solution


FEEDCHANGEDCOLM.CCX
Feed_1
T 50.00 C
P 15.00 bar
W 19800.00 kg/h
Feed_2
T 50.00 C
P 15.00 bar
W 0.00 kg/h
T 50.00 C
P 15.00 bar
W 19800.00 kg/h
Feed
T1
Top_product
T 70.54 C
P 15.00 bar
W 12689.86 kg/h
T 148.98 C
P 15.09 bar
W 83953.79 kg/h
B_liquid
T 157.00 C
P 15.09 bar
W 76843.91 kg/h
Steam
T 191.68 C
P 13.00 bar
W 9537.06 kg/h
Calc Ht Duty MJ/h 18837.4961
T 157.00 C
P 15.09 bar
W 7109.88 kg/h
B_product

Step 3



This is the result of the steady state process and this is the initial state of the dynamic simulation.

This sequence follows:

- Swap the flash module with dynamic vessel module and specify it using flash size data or by existing equipment data
- Insert a liquid level control loop into the B_product stream, use control valve sizing tool or enter existing data
- Specify the controller
- Run the units in the control loop and check the initial values (transmitter, controller output, valve position, connection or information transfer between the vessel and control valve)
- Repeat these steps and specify the local flow rate control loop of steam

- Use a cascade control system, let the primary loop be a temperature control on the tray 24
- Specify an empty side product stream on tray 24 (column model, mass flow rate =1e-6)
- Run and then verify the cascade control system (define the inlet of TC controller before the calculation; use the data of tray 24; unit numbers for this steady state run are: 12, 9,11,10)
- Use the “Run All” option of steady state simulator and save the result of converged run; this is the initial state of the system, turn the initial flag of column to 1 (reload last result)
- Switch the simulation mode to dynamic

This is a possible result of steps described above:

```
Equip. No.                        5
       Name             Bottom vessel
Pressure  bar                15.0870
Recorder option:                  1       On line recording
Diameter  m                   2.6000      Equal to the column diameter
Cylinder length  m            8.0000      Estimated
Int. liq lev 1  m             3.0000      estimated
Liq flow 1 mode                   3       Control valve (link, vessel is
active)
Liq flow 1 spec.              8.0000            ID

Equip. No.                        6
       Name                  Reboiler     Heat exchanger
U  W/m2-K                    800.0000     Estimated
Area/shell  m2               200.0000     Estimated

Controllers

Equip. No.                        7           10            12
       Name                     LIC          FIC           TIC
PB (Proportional Band)       100.0000     100.0000      100.0000
Ti (Integral time, min)        2.0000       0.5000       15.0000
Set point                      3.0000    9537.0000      140.4000
Error definition                  0            1             1
Control valve ID.                 8           11             0
Measured object                   1 (Unit)     0 (Stream)    0 (Stream)
Measured object ID.               5           16            18
Measured variable                43 (Level )   6 (Flowrate) 1 (Temp)
Variable unit                    18 (Length)   1 (Mass)      2 (Temp)
Cascade ID                        0            0            10
Controller/Sensor Func.           0 (Lin.)     1 (Quadr.)    0 (Lin)
Variable Min                   1.0000    5000.0000      120.0000
Variable Max                   5.0000   15000.0000      160.0000
Ctrl input min                 4.0000       4.0000        4.0000
Ctrl input max                20.0000      20.0000       20.0000
Primary ID                        0           12             0
```

```
Control valves

Equip. No.                        8           11
       Name            Valve-product  Valve-steam
Valve flow coefficient      54.0000     480.0000     Sizing tool
Rangeability                10.0000      10.0000
Critical flow factor         0.9800       0.9800
Downstream pressure bar     14.8000      13.0000     Defined
Controller ID                     7           10
Valve time constant                       0.1000
Valve Av                     0.0625       0.0625     NC valve
Valve Bv                    -0.2500      -0.2500
Equip.  ID                        0            9     Transfer to SREF
Equip. var. no                    0           11     Fixed flow rate
```

The modified column specifications are:

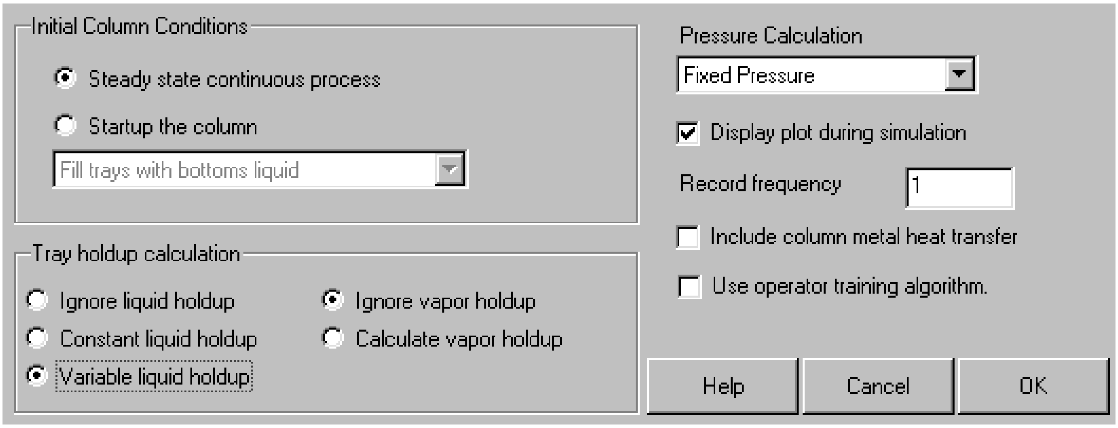
```
Equip. No.                        4
       Name                      T1
No. of stages                    29       1+28
1st feed stage                   15
2nd feed stage                   29
Condenser type                    1            Partial
Select condenser mode:            1            Reflux ratio is specified
Condenser spec.              3.0000            R/D
Side product stage               24
Side product mode                -3            Liquid mass flow rate
Side product spec.      1.0000e-006            Empty stream
Colm press drop  bar         0.0870
Top pressure  bar           15.0000
Iterations                      100
Initial flag                      1
Tray type                         3            Sieve tray
Column diameter  m           2.6000
Tray space  m                0.4000
No of sections                    2
Diameter 2nd sec.  m         2.6000
Section 2 stage no.              15
No of passes (S1)                 4
No of passes (S2)                 4
Weir side width  m           0.2509
Weir center width  m         0.2622
Weir off-center  m           0.2576
Weir side (2)  m             0.3142
Weir center (2)  m           0.3737
```

```
Weir off-center(2)  m        0.3672
Weir height  m               0.0508
Weir height (2)  m           0.0508
System factor                1.0000
```

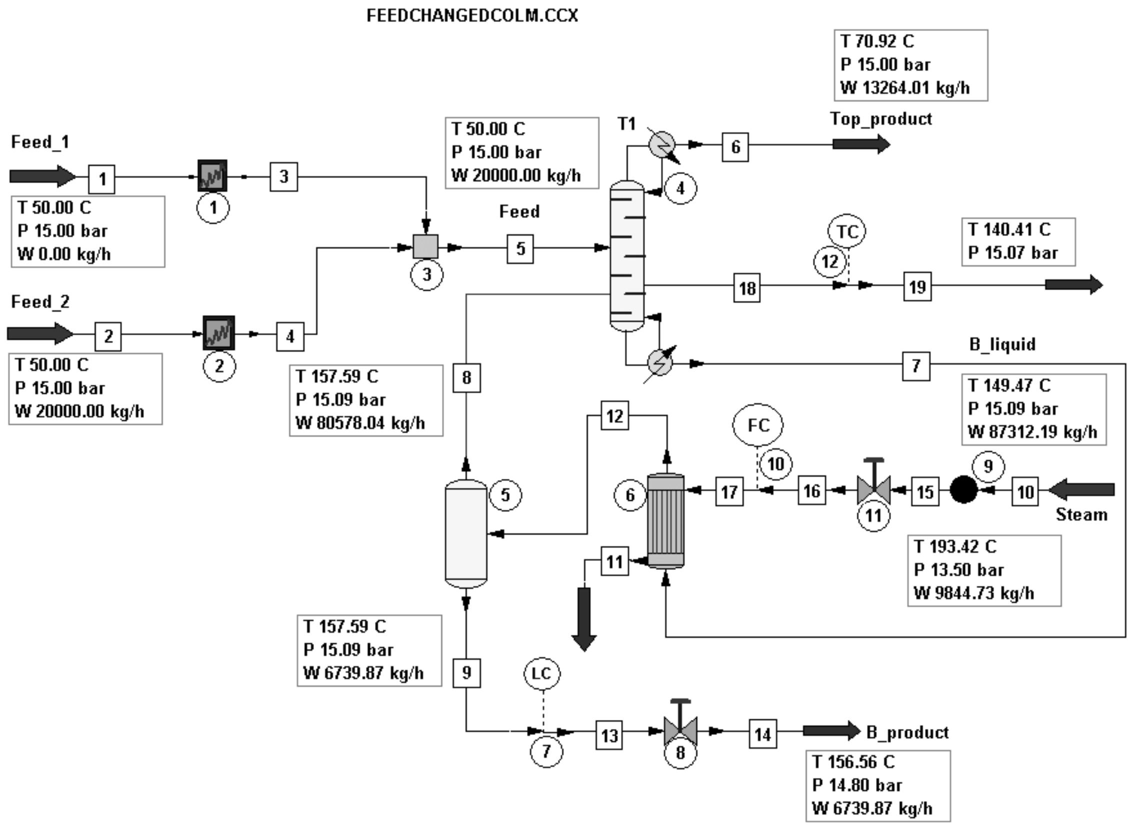
The dynamic parameters of this solution are:

Run time

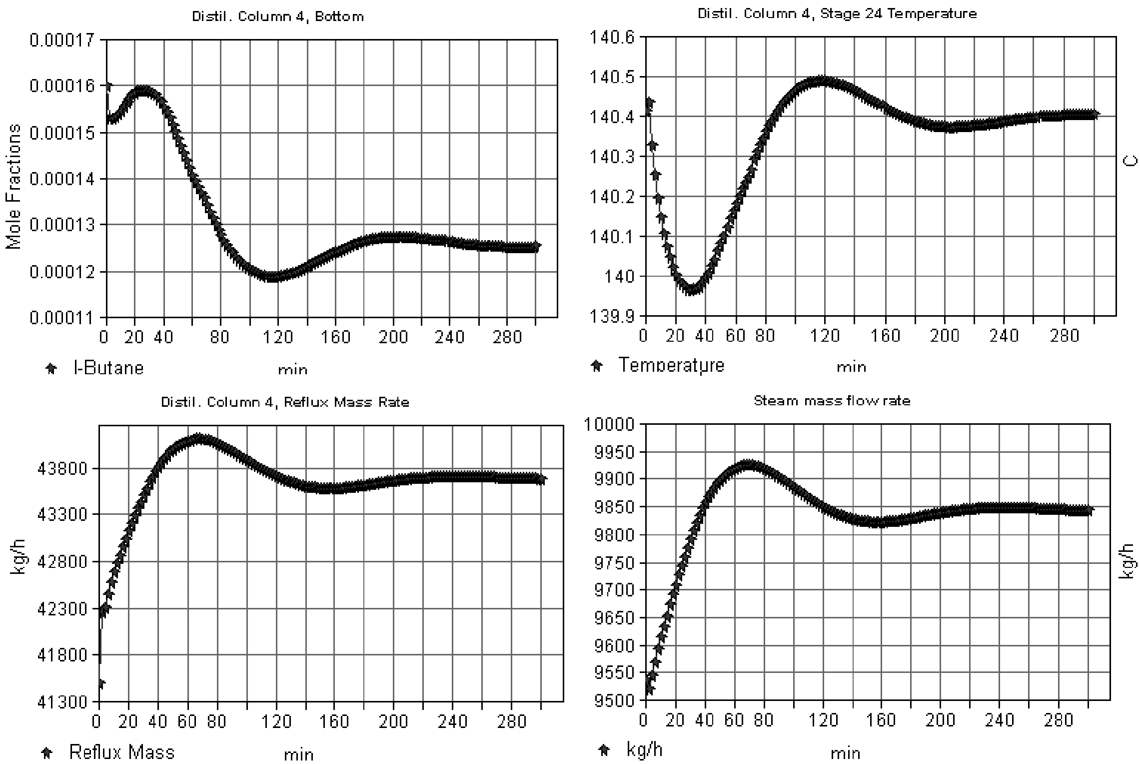
General Information



The result after 300 minutes:



Typical trends:



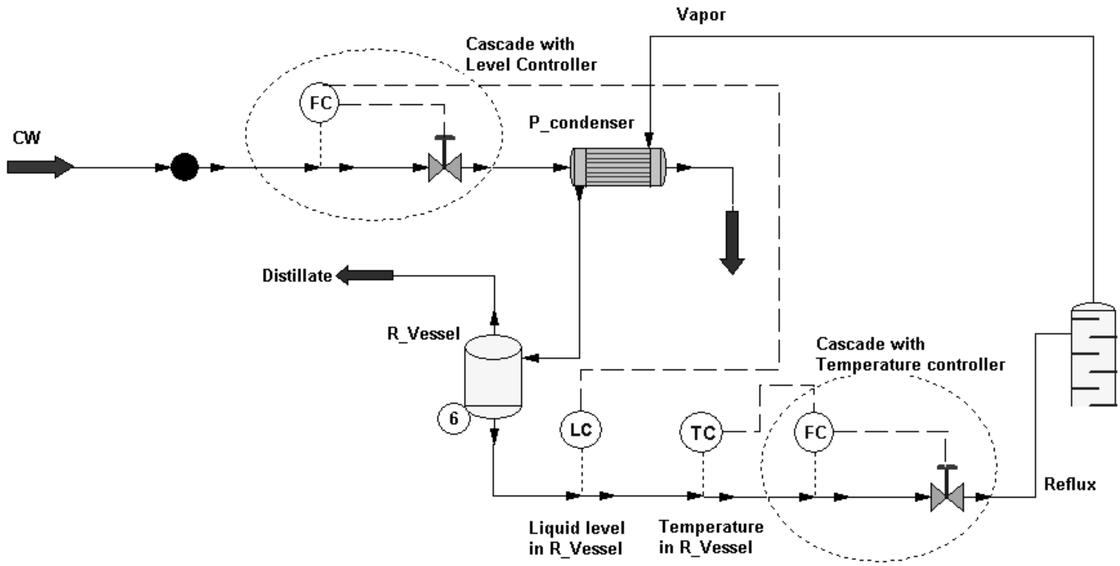
The I-Butane concentration of bottom product is stabilized on a low level of 1250 ppm. The main control variable – temperature of tray 24 – is stabilized at the set point, this is 140.4 °C. The trend of the reflux flow rate and the trend of the steam mass flow rate show a well-controlled and stabilized system.

The Main streams after 300 minutes are:

Stream No.	5	6	14
Name	Feed	Top_product	B_product
- - Overall - -			
Mass flow kg/h	20000.0000	13267.0240	6725.4982
Temp C	50.0000	70.9473	156.7398
Pres bar	15.0000	15.0000	14.0000
Enth MJ/h	-50376.	-30251.	-13562.
Actual vol m3/h	41.6694	400.9909	16.5924
Component mass %			
Ethane	7.368420	11.107228	0.000000
Propane	15.789470	23.798135	0.000002
I-Butane	18.947372	28.546014	0.003855
N-Butane	24.210523	36.446357	0.081836
I-Pentane	11.578953	0.098358	33.931831
N-Pentane	9.473687	0.003906	28.223622
N-Hexane	6.315793	0.000000	18.879268
N-Heptane	4.210529	0.000000	12.578221
N-Octane	2.105263	0.000000	6.301364
Water	0.000000	0.000000	0.000000

Important note: *We suggest you attempt expanding the flowsheet for the condenser system. Use a heat exchanger and a dynamic vessel (isobaric). Use a local flow rate control loop on the cooling water inlet and a primary loop as liquid level control of the reflux vessel. Use a local loop for the flow rate control of reflux and try to combine it with tray temperature controller (cascade) or with any SPC controller. For SPC controller (steady state controller) we recommend the Feed-Forward type algorithm, which can predict the best set point by information of noise.*

Example:



HOW TO USE THE BUILT IN MODELS OF DYNAMIC COLUMN MODULE

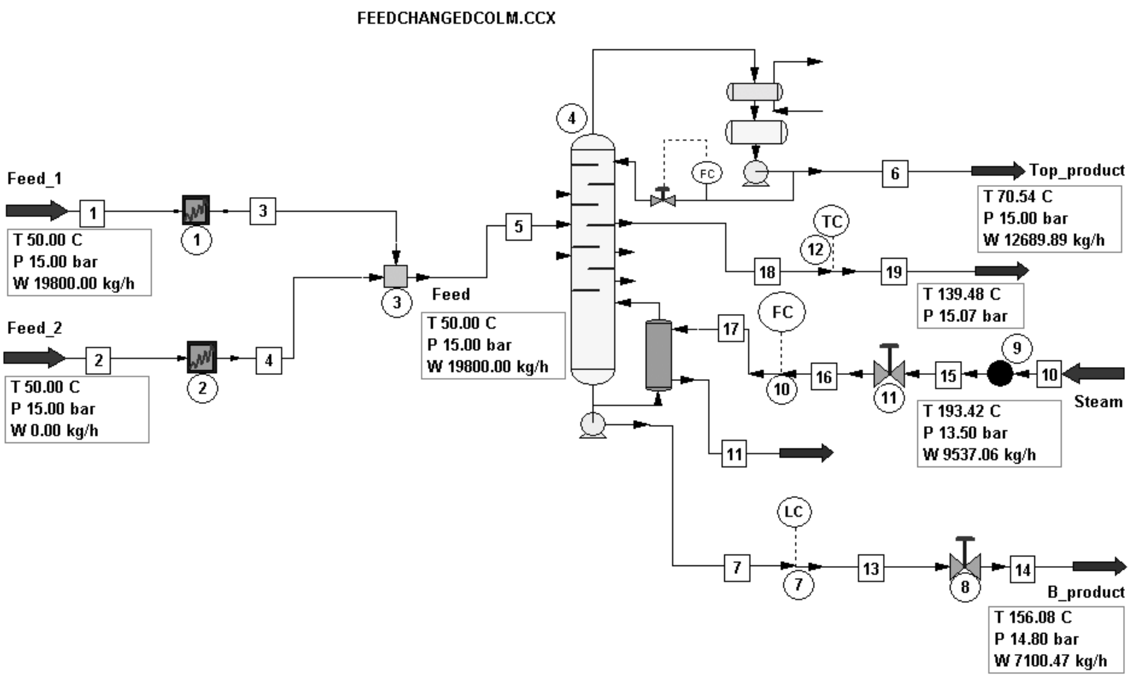
The dynamic column module contains several built-in models. These cover elements of the reboiler and of the condenser system. We will now replace the detailed system described above with the multifunctional capabilities of the dynamic SCDS model.

The sequence of this modification is as follows:

- Switch the simulation mode back to steady state
- Swap the icon of SCDS with the special icon of Dynamic Column SCDS (this change keeps all model parameters while replacing the symbol. (Note: to swap a unit operation with another in the flowsheet editing mode, right click the desired icon, select Swap Unit, and then follow the instructions displayed by CHEMCAD.)
- Remove the vessel and heat exchanger from the flowsheet (try to keep all existing streams and control loops during this work)
- Make use of the vessel and heat exchanger parameters at the dynamic column specification later
- Connect the steam stream to the column icon directly

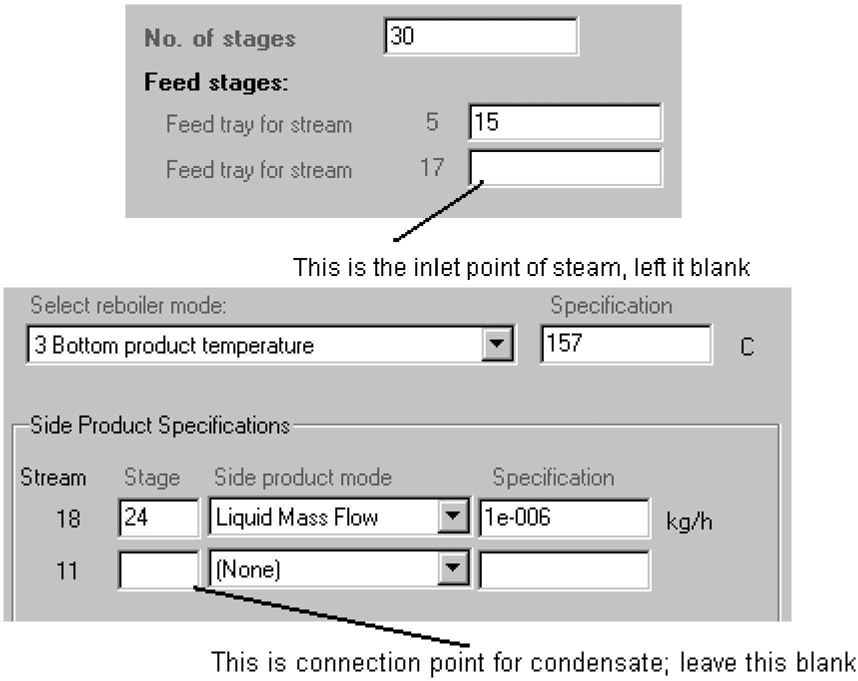
- Modify the inlet stream of the level control loop to become the bottom product of the column. (Most likely, you will need to create temporary streams and unit operations to save existing information; you can also copy the stream information later)
- Calculate all loops separately in steady state and then verify results
- Modify the column parameters: increase the number of trays to the original specification; DO NOT SPECIFY UTILITY STREAMS AS FEED OR SIDE PRODUCT; set the reboiler specification
- Run the whole system and save the converged solution; this is the initial state of the dynamic simulation
- Switch the dynamic simulation mode on

The new flowsheet at initial state looks similar to this one:



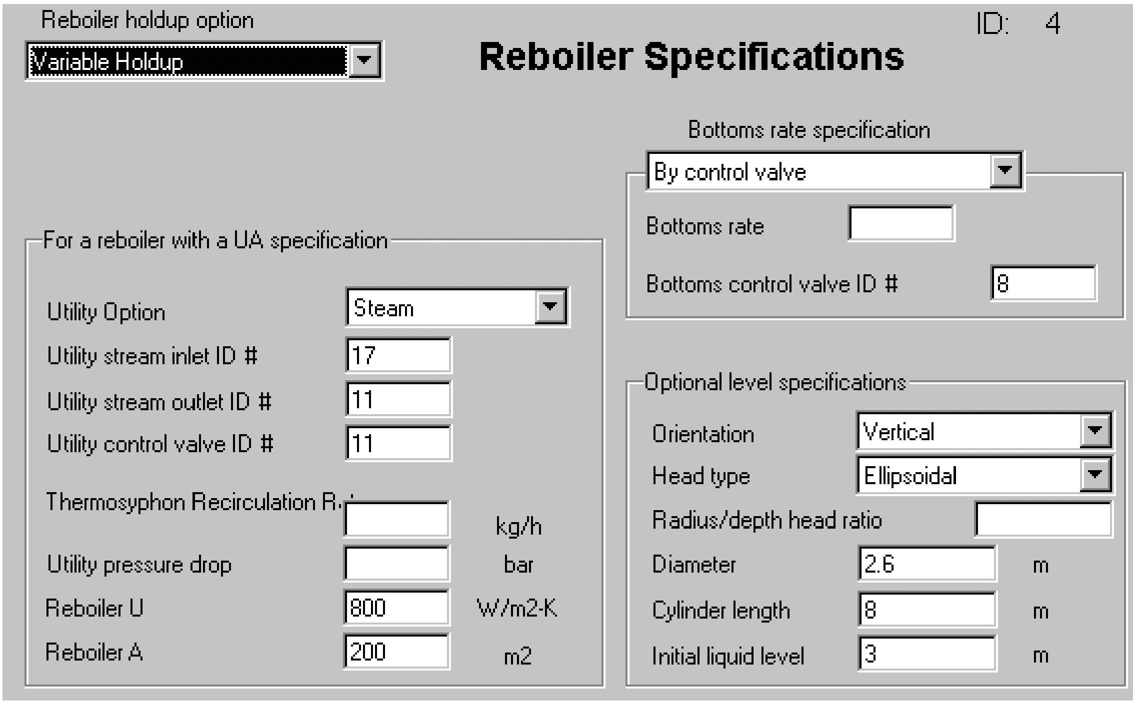
Summary of modifications to the dynamic part follows:

Column specification:

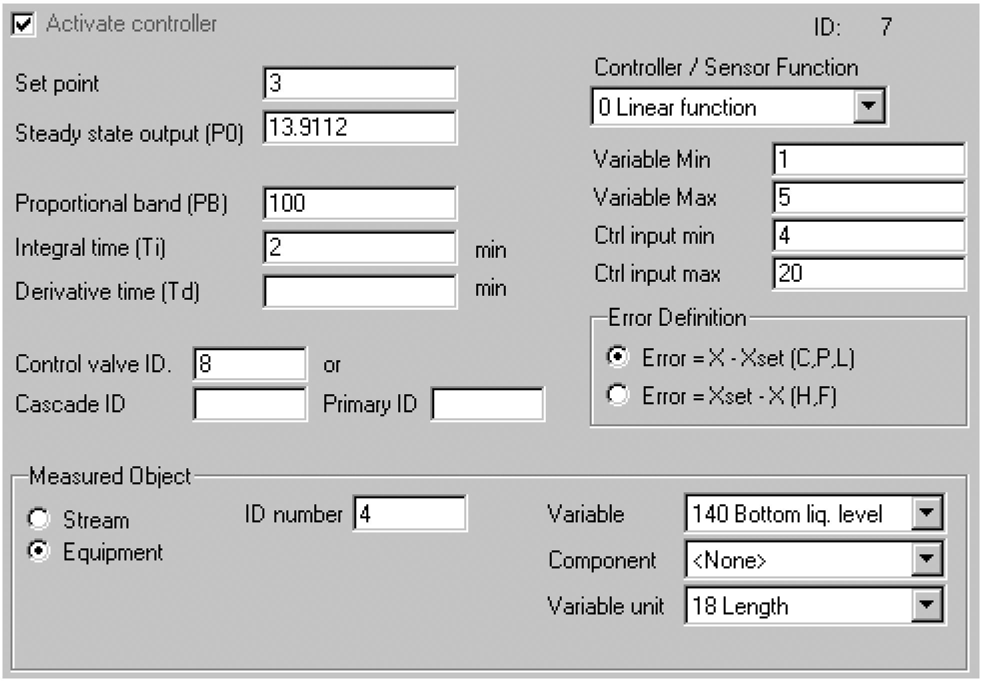


New settings in the dynamic column specification.

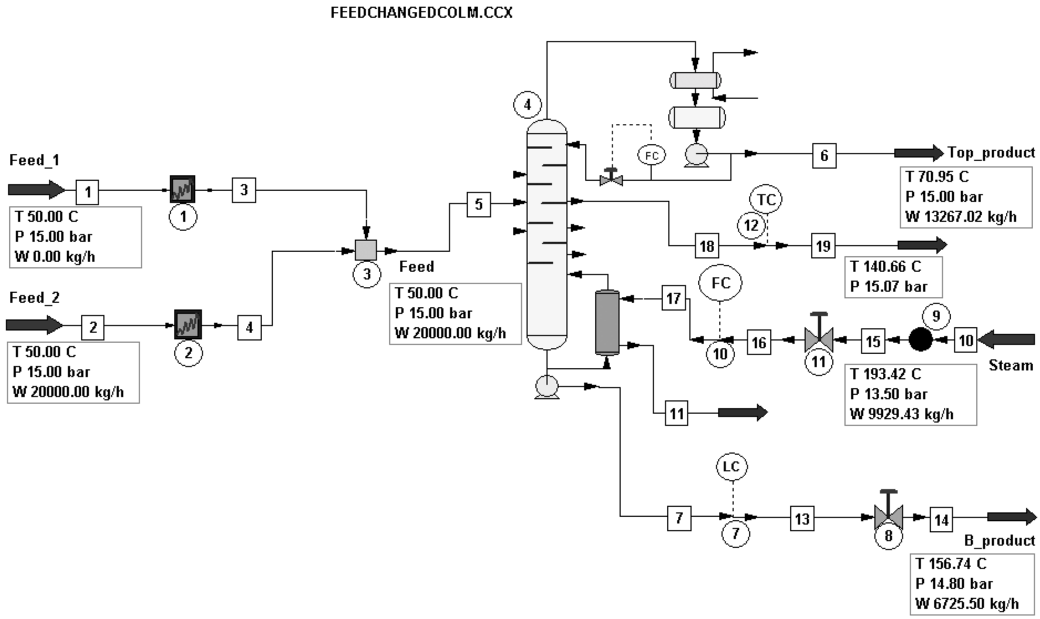
The specification of the reboiler system is as follows:



Change the controller specification (now there is no separate vessel).


Activate controller
ID: 7
Set point
3
Steady state output (P0)
13.9112
Proportional band (PB)
100
Integral time (Ti)
2
min
Derivative time (Td)
min
Control valve ID.
8
or
Cascade ID
Primary ID
Controller / Sensor Function
0 Linear function
Variable Min
1
Variable Max
5
Ctrl input min
4
Ctrl input max
20
Error Definition
Error = X - Xset (C,P,L)
Error = Xset - X (H,F)
Measured Object
Stream
Equipment
ID number
4
Variable
140 Bottom liq. level
Component
<None>
Variable unit
18 Length

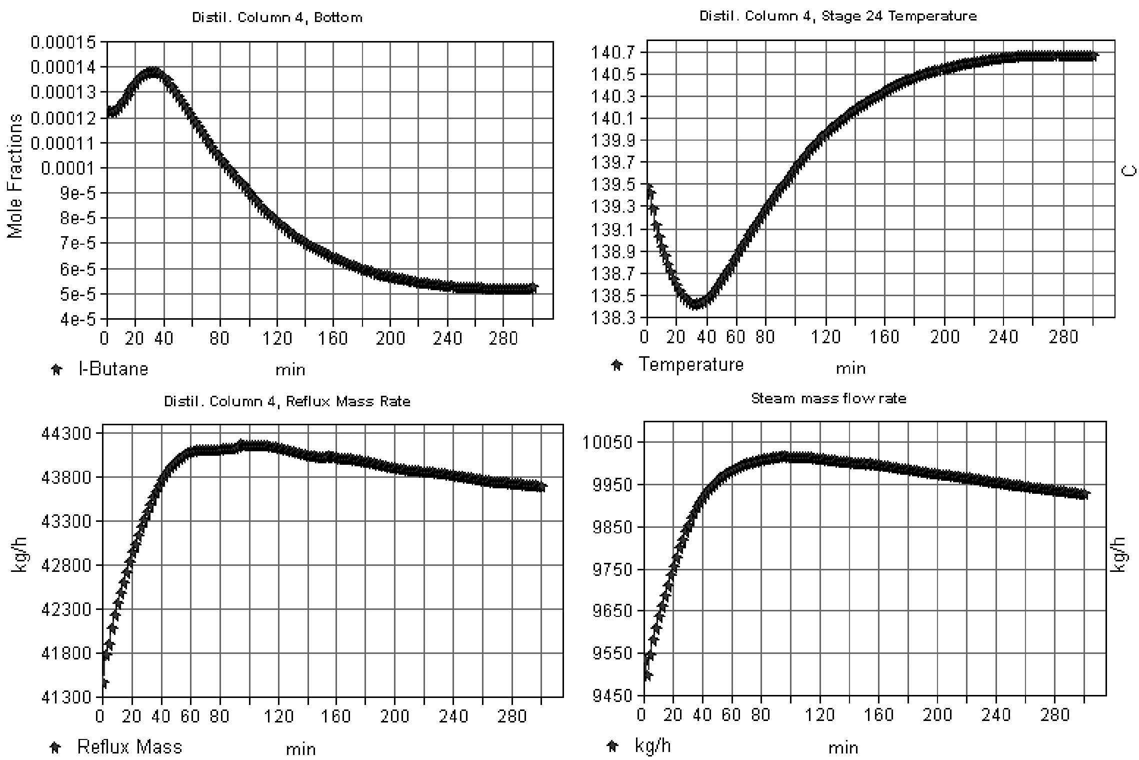
The result after 300 minutes:



The main streams:

Stream No.	5	6	14
Name	Feed	Top_product	B_product
- - Overall - -			
Mass flow kg/h	20000.0000	13267.0240	6725.4982
Temp C	50.0000	70.9473	156.7398
Pres bar	15.0000	15.0000	14.8000
Enth MJ/h	-50376.	-30251.	-13562.
Actual vol m3/h	41.6694	400.9909	16.5924
Component mass %			
Ethane	7.368420	11.107228	0.000000
Propane	15.789470	23.798135	0.000002
I-Butane	18.947372	28.546014	0.003855
N-Butane	24.210523	36.446357	0.081836
I-Pentane	11.578953	0.098358	33.931831
N-Pentane	9.473687	0.003906	28.223632
N-Hexane	6.315793	0.000000	18.079260
N-Heptane	4.210529	0.000000	12.578221
N-Octane	2.105263	0.000000	6.301364
Water	0.000000	0.000000	0.000000

The trends:



This control system also works well. The dynamic properties of the system differ from the first solution; simple copying of original parameters is not sufficient. The same trends would probably be produced if tuning of the parameters of each control loop were performed.

> ***Special Note:*** *This column works with a partial condenser. Do not use the built-in reflux control system for a partial condenser system.*

The next example explains usage of multipurpose dynamic column model for a column equipped with total condenser.

HOW TO USE DYNAMIC COLUMN MODEL FOR CONTROL OF CONDENSER AND REFLUX

The job files for this example are installed automatically during the installation of CHEMCAD. The name of the job is DCOLM_CONT. The installed job is not identical to the example we describe but can be customized for following example.

In this example, the second typical method of dynamic studies is described. This is an analysis of dynamic properties of a closed-loop control system by change of set points. The technology is a continuous process and the study starts from a steady state condition with change of set point.

Our main objective here is to highlight the details of the calculation method for the total condenser system, the reflux flow control and the column pressure control. The same technique for the reboiler system as described in the first detailed example has been applied. The component system and the set of thermodynamic method follow:

```
COMPONENTS
          ID #         Name

   1       117       Methanol
   2       140       Acetone
   3       134       Ethanol
   4        62       Water

THERMODYNAMICS

 K-value model     :  NRTL
                      No corrrection for vapor fugacity
 Enthalpy model    :  Latent Heat
 Liquid density    :  Library
```

Feed streams:

Stream Name	Feed_1	Feed_2	Feed_3
Temp F	150.3300*	160.3300*	130.3300*
Pres mmHg	760.0000*	760.0000*	1250.0000*
Enth Btu/h	-3.6452E+007	-1.4774E+009	-6.2616E+008
Vapor mole fraction	0.00000	0.00000	0.00000
Total lbmol/h	300.0000	12195.0000	6000.0000
Total lb/h	5404.5000	229521.4688	231309.0000
Total std L ft3/hr	86.5857	3742.7737	4613.1787
Total std V scfh	113843.59	4627742.00	2276871.75
Component mass %			
Methanol	0.000000	0.209405	54.024619
Acetone	0.000000	0.759145	37.663904
Ethanol	0.000000	6.021528	5.974995
Water	99.999994	93.009925	2.336485

Utility streams:

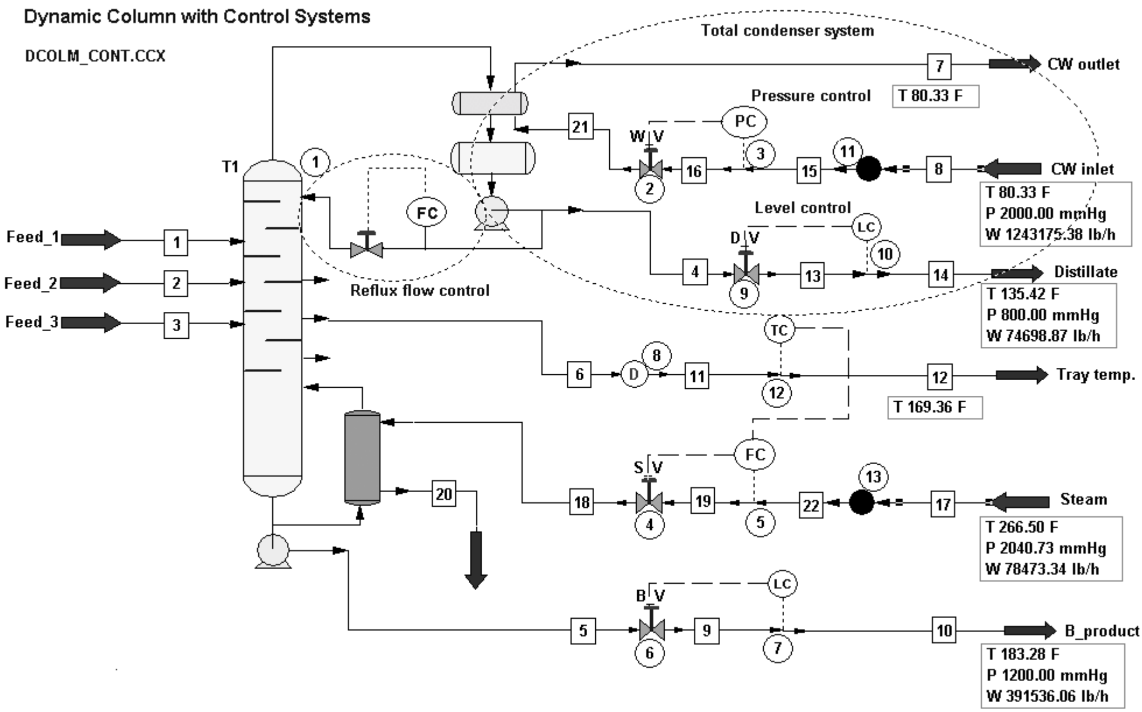
Stream Name	CW inlet	Steam
Temp F	80.3300*	266.5000*
Pres mmHg	2000.0000*	2040.7342
Enth Btu/h	-8.4718E+009	-4.4650E+008
Vapor mole fraction	0.00000	1.0000*

```
Total lbmol/h           69007.7969     4356.0000
Total lb/h            1243175.3750    78473.3359
Total std L ft3/hr      19916.9696     1257.2248
Total std V scfh      26186984.00    1653008.88
Component mass %
Methanol                 0.000000      0.000000
Acetone                  0.000000      0.000000
Ethanol                  0.000000      0.000000
Water                  100.000000    100.000000
```

The steady state calculation reports the converged solution of the column, and this is the initial state of the process. The figures below show the flowsheet and the mass balance. We have marked important parts of the control system in the flowsheet:

- Total condenser system
- Pressure control
- Liquid level control of reflux drum
- Reflux flow rate control

Flowsheet and calculated stream data at initial state.



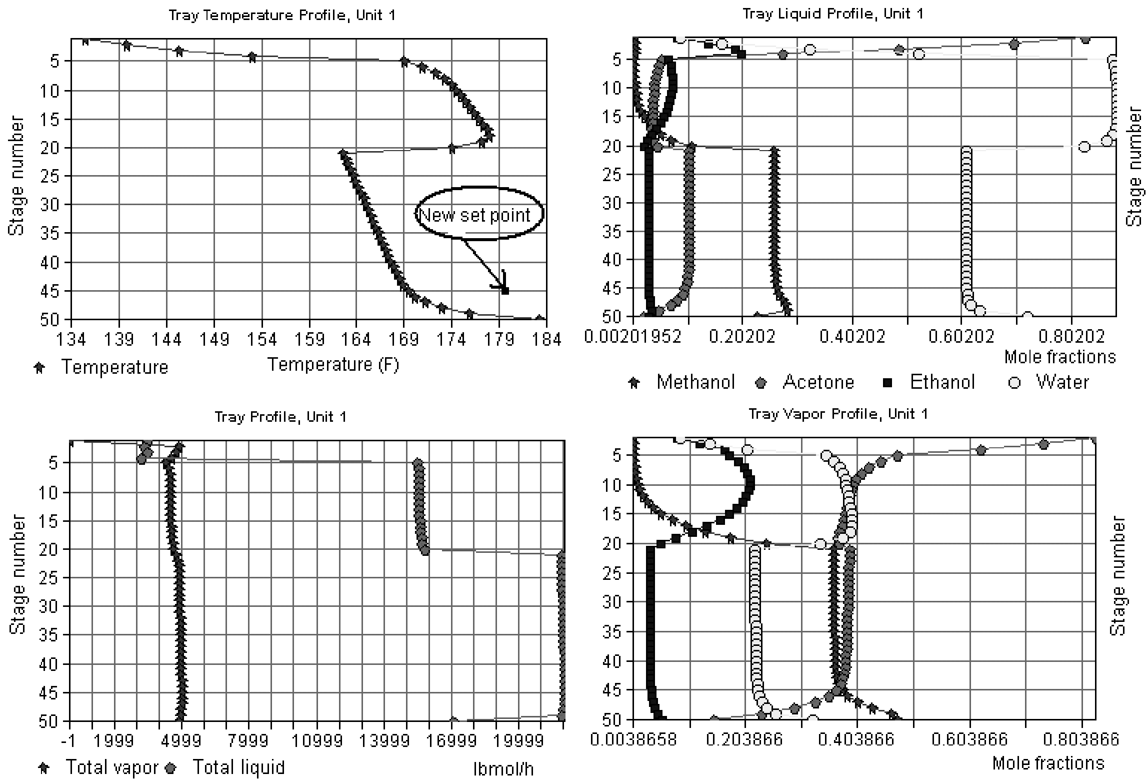
Mass balance at initial state.

Dynamic Column with Control Systems

DCOLM_CONT.CCX

Stream No.	1	2	3	14	10	8	17
Name	Feed_1	Feed_2	Feed_3	Distillate	B_product	CW inlet	Steam
- - Overall - -							
Molar flow lbmol/h	300.0000	12195.0000	6000.0000	1395.0005	17100.0000	69007.7969	4356.0000
Mass flow lb/h	5404.5000	229521.4844	231309.0000	74698.8672	391536.0625	1243175.3750	78473.3359
Temp F	150.3300	160.3300	130.3300	135.4187	183.2754	80.3300	266.5000
Pres mmHg	760.0000	760.0000	1250.0000	800.0000	1200.0000	2000.0000	2040.7342
Vapor mole fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.000
Enth Btu/h	-3.6452E+007	-1.4774E+009	-6.2616E+008	-1.4996E+008	-1.9789E+009	-8.4718E+009	-4.4650E+008
Actual vol ft3/hr	88.3513	3848.7856	4881.7690	1592.7662	7415.0093	19989.1367	844218.2500
Component mass %							
Methanol	0.000000	0.209405	54.024619	0.232895	31.994611	0.000000	0.000000
Acetone	0.000000	0.759145	37.663904	89.833587	5.557016	0.000000	0.000000
Ethanol	0.000000	6.021528	5.974995	7.037702	5.717050	0.000000	0.000000
Water	99.999994	93.009925	2.336485	2.895811	56.731325	100.000000	100.000000

Column profiles at steady state.



In the plot of the column temperature profile, we point to the new set point, which is 10 F above the current temperature. The temperature control loop is the primary loop of the steam flow rate control. For the much faster response of the cascade controllers, we also increased the set point of the flow rate control loop. All other controllers keep the existing set point.

The unit parameters (first part: external controllers and control valves).

Controllers

Equip. No.	7	5	12	
Controller Name	LC-B_level	FC-Steam	TC-Tray_45	
PB (Proportional Band)	200.0000	666.7000	200.0000	
Ti (Integral time, min)	5.0000	0.2500	17.0000	
P0 Steady state output	9.3843	15.2533	7.2400	
Set point	8.0000	***81000.0000***	***180.3300***	***<- NEW SP***
Error definition	0	1	1	
Control valve ID.	6	4	0	

Measured object	1	0	0
Measured object ID.	1 (Unit)	18 (Stream)	11 (Stream)
Measured variable	140 (level)	6 (f-rate)	1 (tempr.)
Variable unit	18 (length)	1 (mass)	2 (tempr.)
State	1	1	1
Cascade ID	0	0	5
Controller/Sensor Func.	0	1	0
Variable Min	6.0000	0.0600	160.3300
Variable Max	10.0000	180000.0000	200.3300
Ctrl input min	4.0000	4.0000	4.0000
Ctrl input max	20.0000	20.0000	20.0000
Primary ID	0	12	0

Controllers

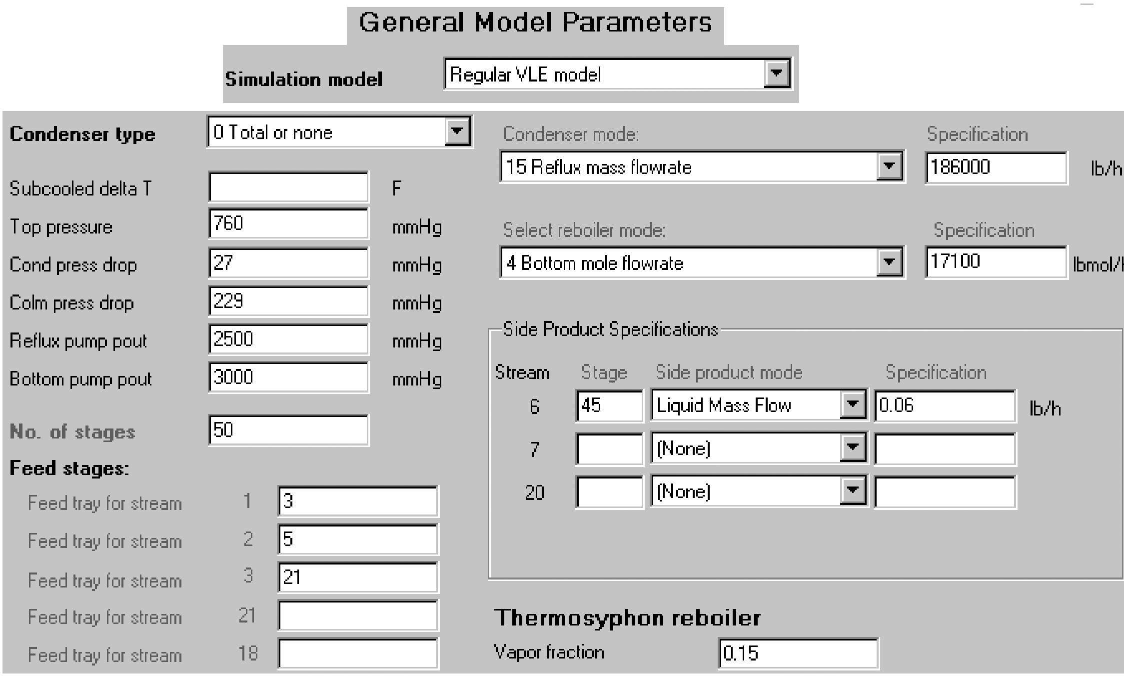
Equip. No.	10	3
Controller Name	LC-C_vessel	PC-Column
PB (Proportional Band)	90.9000	66.7000
Ti (Integral time, min)	3.0000	3.0000
P0 Steady state output	10.3529	11.5918
Set point	3.0000	760.0000
Control valve ID.	9	2
Measured object	1	1
Measured object ID.	1 (Unit)	1 (Unit)
Measured variable	136 (level)	34 (pressure)
Variable unit	18 (length)	4 (pressure)
State	1	1
Variable Min	1.0000e-004	500.0000
Variable Max	10.0000	1000.0000
Ctrl input min	4.0000	4.0000
Ctrl input max	20.0000	20.0000

Control valves

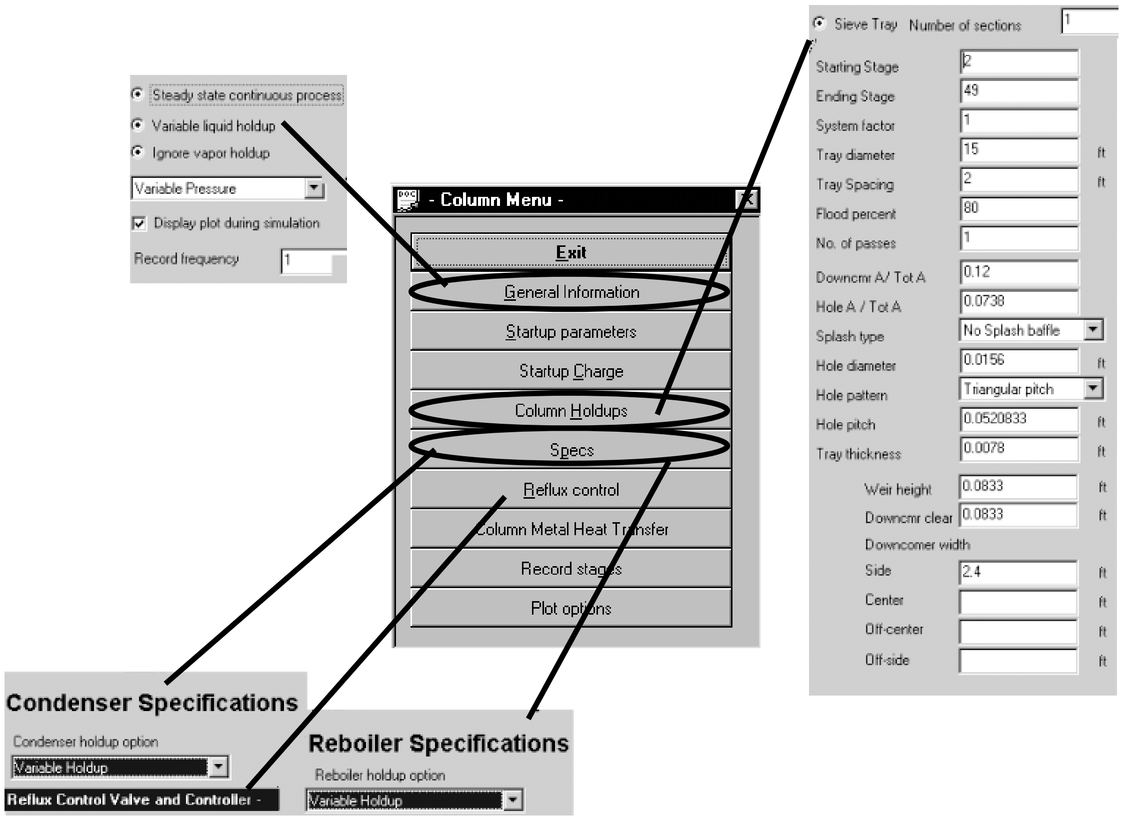
Equip. No.	6	4	9	2
Equip. Name	B_V	S_V	D_V	W_V
Valve flow coefficient	665.0000	2150.0000	120.5000	1720.0000
Rangeability	10.0000	10.0000	10.0000	10.0000
Critical flow factor	0.9800	0.9800	0.9800	0.9800
Downstr. pres.,mmHg	1200.0000	886.0500	800.0000	780.0000
Calc. flow rate lb/h	391536.0625	***78473.3359***	74698.8672	1.2432e+006
		<-actual ->		
Controller ID	7	5	10	3
Valve position %	33.6519	70.3329	39.7056	47.4490
Valve time constant	0.1500	0.2000	0.1500	0.1500
Valve Av	0.0625	0.0625	0.0625	0.0625
Valve Bv	-0.2500	-0.2500	-0.2500	-0.2500
Controller output	9.3843	15.2533	10.3529	11.5918

Steady state position	33.6519	70.3329	39.7056	47.4490
Controller output SS	9.3843	15.2533	10.3529	11.5918
Destination ID	0	1	0	0
Var. No.	0	144	0	0
Phase option	1	0	1	1
Equip. ID	0	13	0	11
Equip. var. no	0	11	0	11

The setting of the dynamic column model (second part: units included into column model).

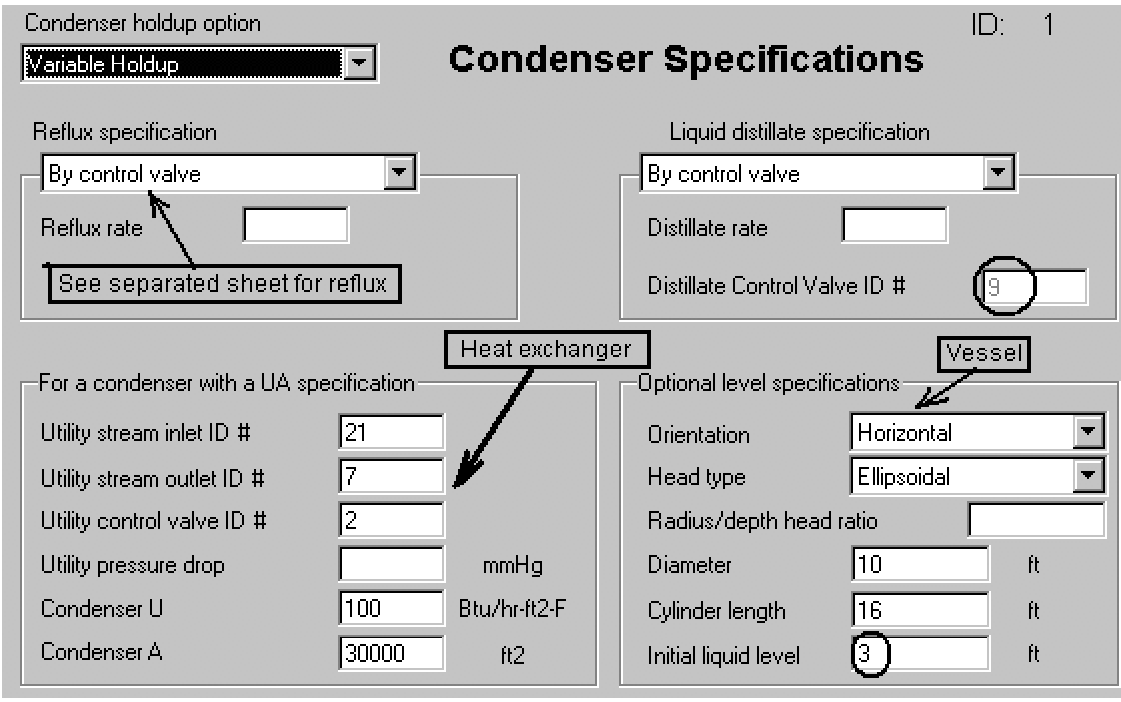


Overview of the dynamic column menu:

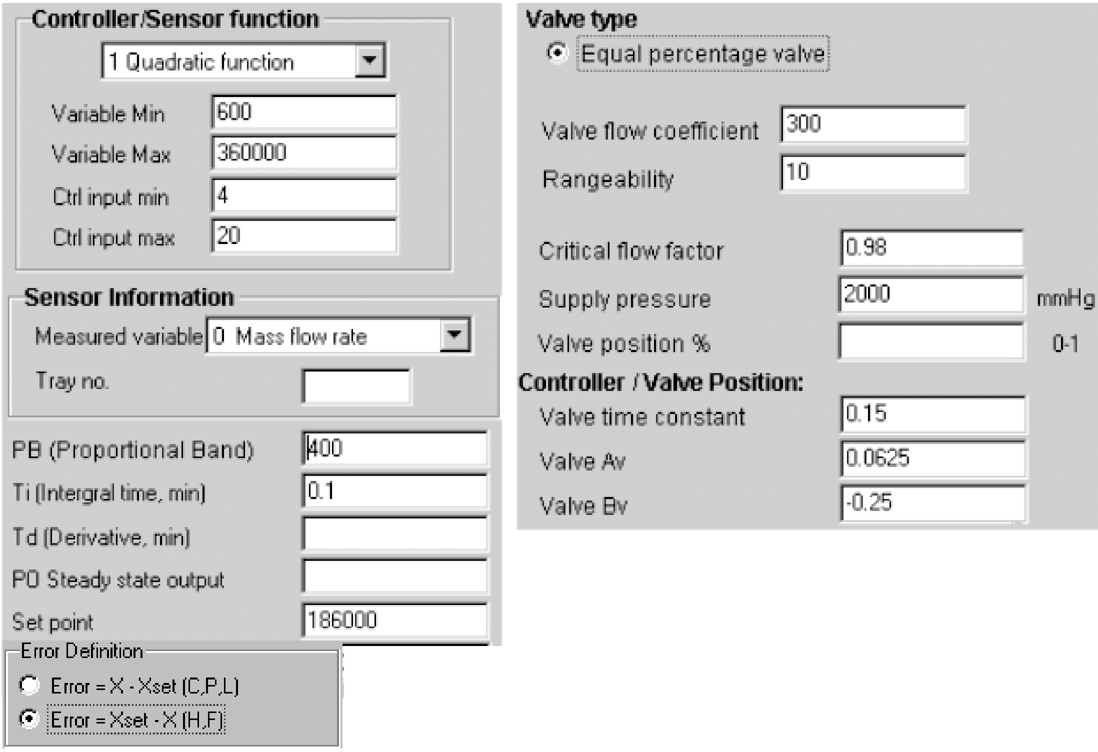


Condenser specification involves a heat exchanger and a dynamic vessel.

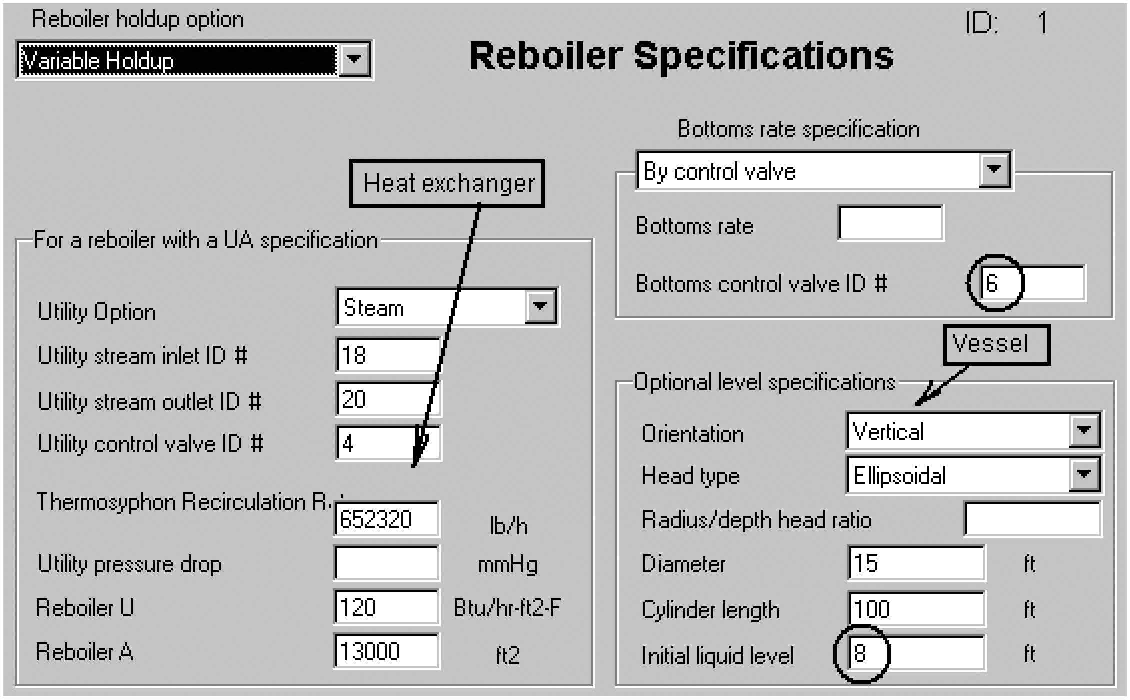
The ID of valve of level controller (active unit in the flow rate transfer) and the initial value of level should be defined here.



Reflux control valve and controller specification (identical with the normal specification).

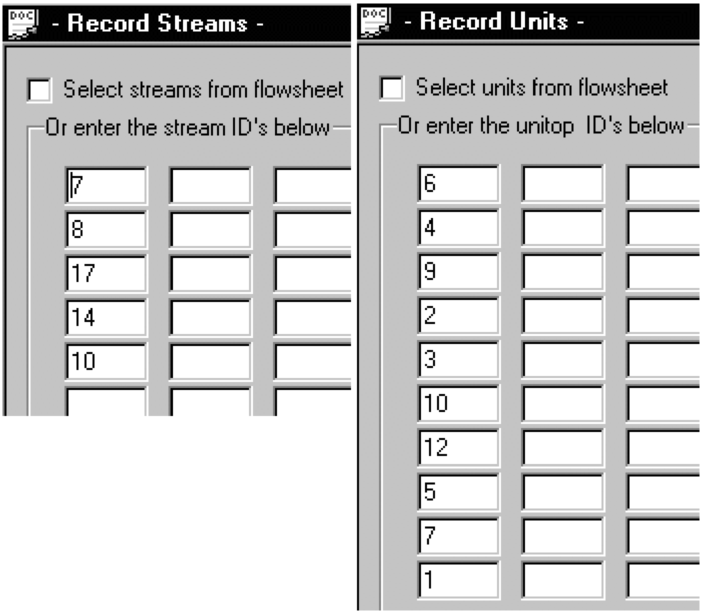

Controller/Sensor function
1 Quadratic function
Variable Min 600
Variable Max 360000
Ctrl input min 4
Ctrl input max 20
Sensor Information
Measured variable 0 Mass flow rate
Tray no.
PB (Proportional Band) 400
Ti (Intergral time, min) 0.1
Td (Derivative, min)
PO Steady state output
Set point 186000
Error Definition
Error = X - Xset (C,P,L)
Error = Xset - X (H,F)
Valve type
Equal percentage valve
Valve flow coefficient 300
Rangeability 10
Critical flow factor 0.98
Supply pressure 2000 mmHg
Valve position % 0-1
Controller / Valve Position:
Valve time constant 0.15
Valve Av 0.0625
Valve Bv -0.25

The reboiler specification involves a heat exchanger and a dynamic vessel. You should define here the ID of the control valve for level controller (active unit in the flow rate transfer) and the initial value of level.

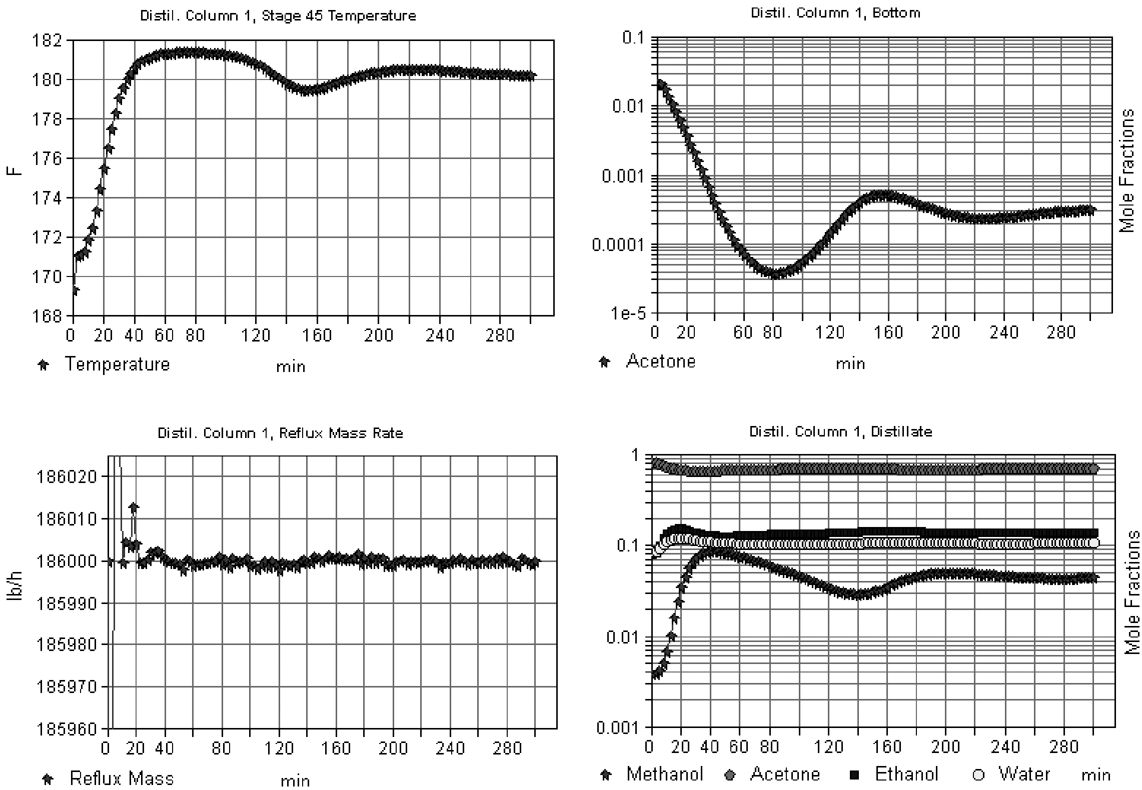


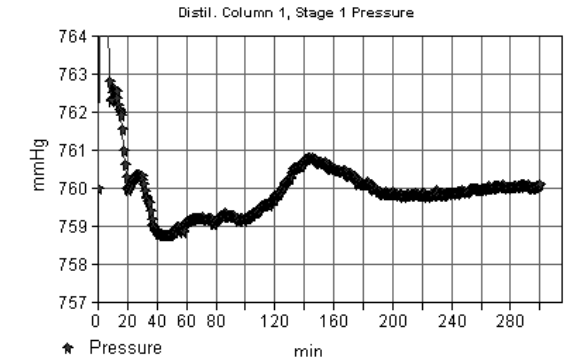
Dynamic run menu:

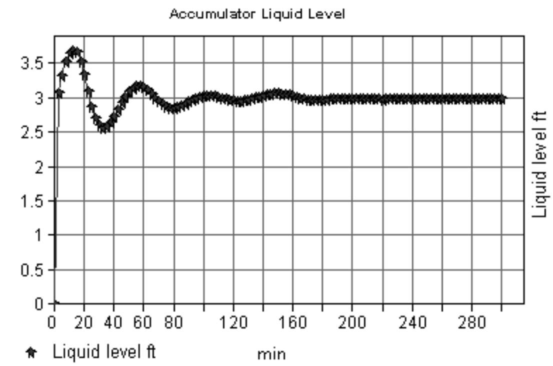
Saved or recorded information:

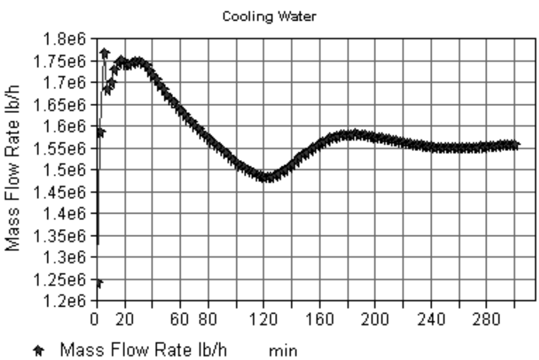


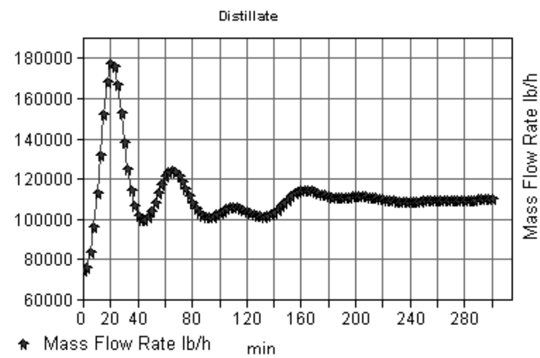
Result after 300 minutes, trends.





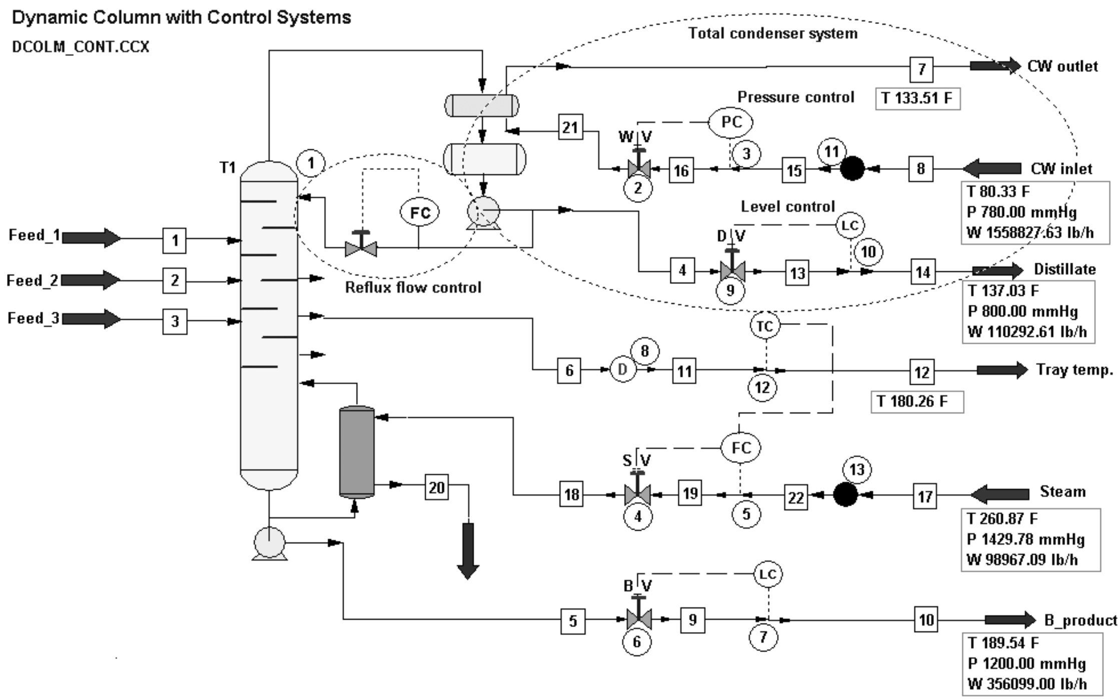






The simulation results indicate a good-working control system. The temperature of tray 45 has been stabilized at the new set point and other controlled variables are at practically steady state values as well. From an operating standpoint, the bottom section of the column works at a higher temperature and we have acetone at a lower concentration in the bottom product, that is, under 0.1 wt %. (The starting value was higher than 5 wt %.)

Flowsheet:



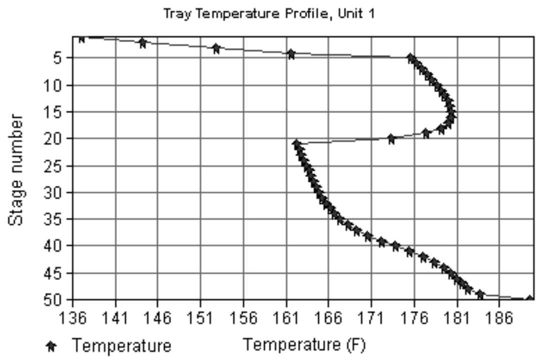
Balance

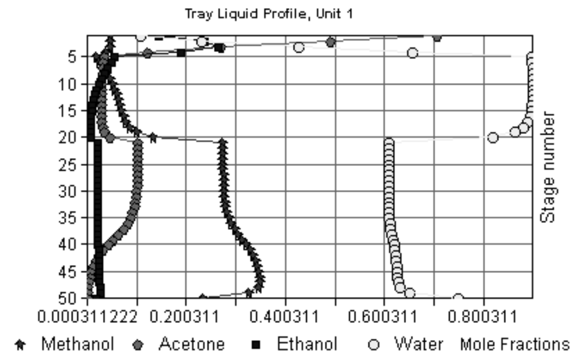
Dynamic Column with Control Systems

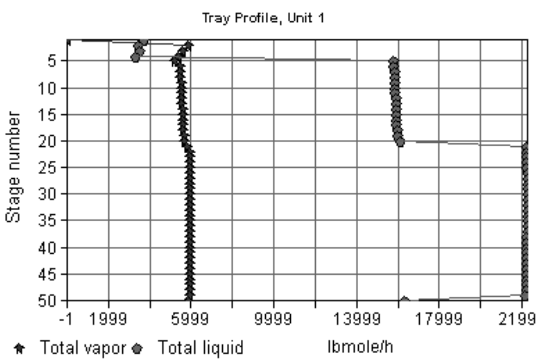
DCOLM_CONT.CCX

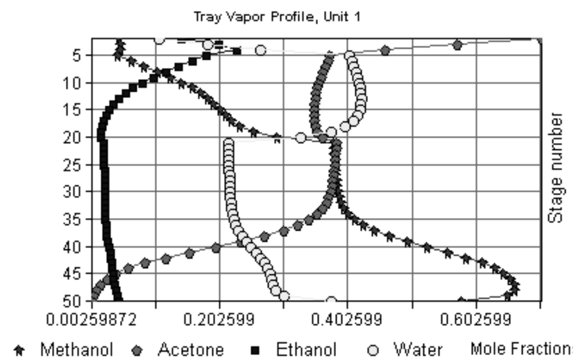
Stream No.	1	2	3	14	10	8	17
Name	Feed_1	Feed_2	Feed_3	Distillate	B_product	CW inlet	Steam
- - Overall - -							
Molar flow lbmol/h	300.0000	12195.0000	6000.0000	2166.8591	16325.7988	86529.4297	5493.5938
Mass flow lb/h	5404.5000	229521.4844	231309.0000	110292.6094	356099.0000	1558827.6250	98967.0859
Temp F	150.3300	160.3300	130.3300	137.0332	189.5399	80.3300	260.8652
Pres mmHg	760.0000	760.0000	1250.0000	800.0000	1200.0000	780.0000	1429.7788
Vapor mole fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.000
Enth Btu/h	-3.6452E+007	-1.4774E+009	-6.2616E+008	-2.3495E+008	-1.8926E+009	-1.0623E+010	-5.6311E+008
Actual vol ft3/hr	88.3513	3848.7856	4881.7690	2347.2515	6660.5732	25064.5391	1516005.7500
Component mass %							
Methanol	0.000000	0.209405	54.024619	2.807423	34.336859	0.000000	0.000000
Acetone	0.000000	0.759145	37.663904	80.511367	0.082871	0.000000	0.000000
Ethanol	0.000000	6.021528	5.974995	12.873179	3.808446	0.000000	0.000000
Water	99.999994	93.009925	2.336485	3.808033	61.771828	100.000000	100.000000

The column profiles after 300 minutes dynamic simulation show significant differences to the initial state in the bottom section of the column.









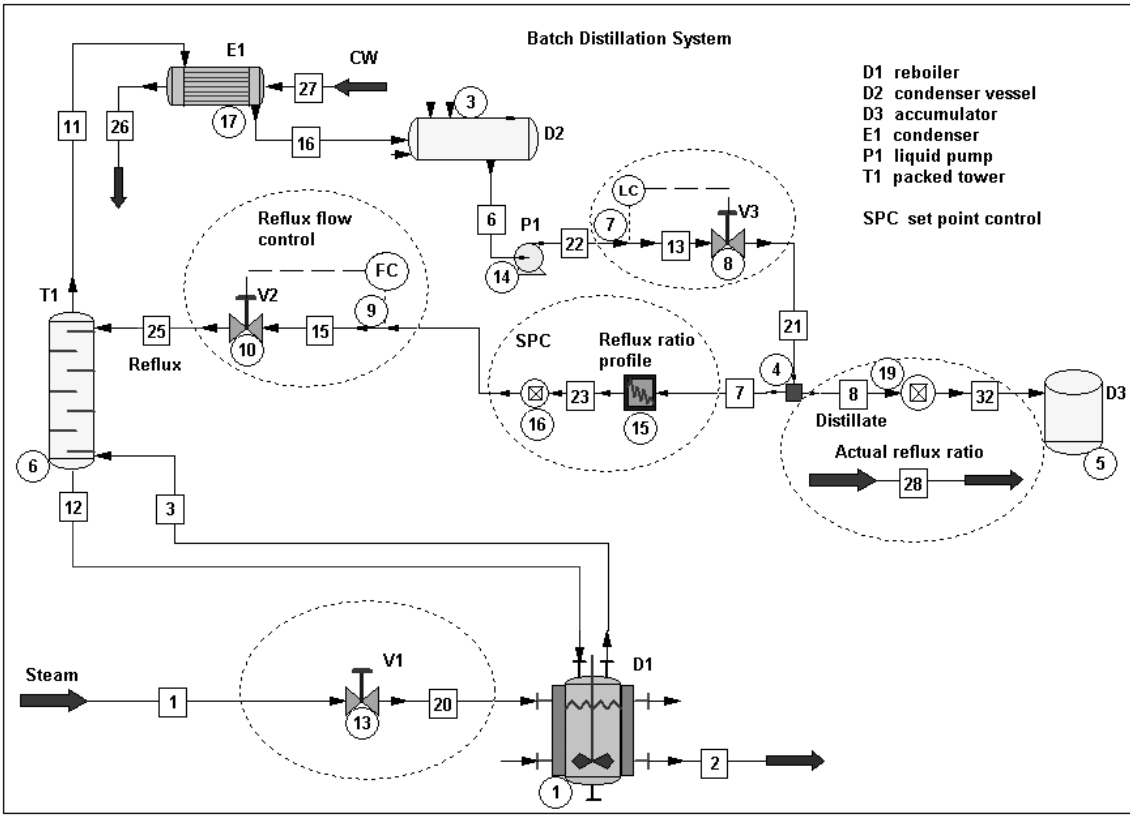
DYNAMIC COLUMN MODEL FOR BATCH DISTILLATION SYSTEMS, STARTUP PROBLEMS

This problem is typical. A component should be recovered from a mixture. This mixture is strongly non-ideal and contains components in very different concentrations. Considering the volume of the raw material and the properties of mixture, it was decided that batch distillation unit would be suitable.

The job was initially studied with the CC-BATCH module to estimate several operating parameters.

Batch distillation technology is not limited to a distillation column but it also involves several auxiliary equipment pieces: heat exchangers for vaporization of liquid mixture and for condensation of vapor; vessels to accumulate the distillation products; pumps and several devices of control system.

A typical configuration of the technology can be seen in the following flowsheet:



The parts of the control system are circled. The T1 column is modeled with CC-DCOLUMN.

Each charge needs same operating steps:

- startup of the system
- continuous regime under controlled parameters
- shutdown of the production

The multifunctional unit of CC-DCOLUMN is able to simulate this technology using built-in models. For practical reasons, we split the system into independent equipment pieces, and we used the SCDS model for the distillation column only. We will explain the analogy between this detailed solution and the universal model description of SCDS later.

The charge is defined by:

```
Stream Name                    Charge
Temp  C                       20.0000
Pres  bar                     10.2000
Enth  kcal               -2.5459E+006
Vapor mole fraction           0.00000
Total kmol                    25.3385
Total kg                    1801.5414
Total std L m3                 2.0000
Component mass %
Methanol                     7.000002
Ethyl Acetate               89.999998
Water                        3.000000
```

The thermodynamical and transport calculation methods selected were the NRTL K-Values with fugacity correction, latent heat for enthalpy, and Lu's method for density.

The list of equipments is:

- D1 jacketed vessel with steam heating, batch reactor model (BREA)
- D2 accumulator to collect the condensed liquid after the condenser (DVSL)
- D3 accumulator to collect the distilled product (DVSL)
- E1 tubular heat exchanger with water cooling, steady state model (HTXR)
- P1 liquid pump, steady state model (PUMP)
- T1 distillation tower with Intalox saddle random packing, SCDS dynamic column model

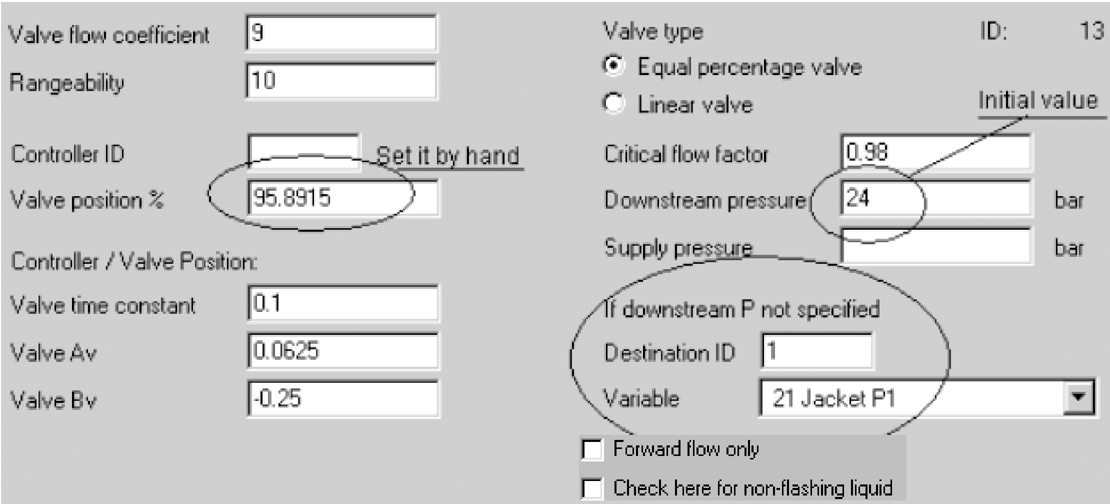
The control system involves

- Reflux flow rate local control loop, V2 (control valve) and FC (PID controller)
- Level local control loop, V3 (control valve) and LC (PID controller)
- V1 control valve for steam inlet.

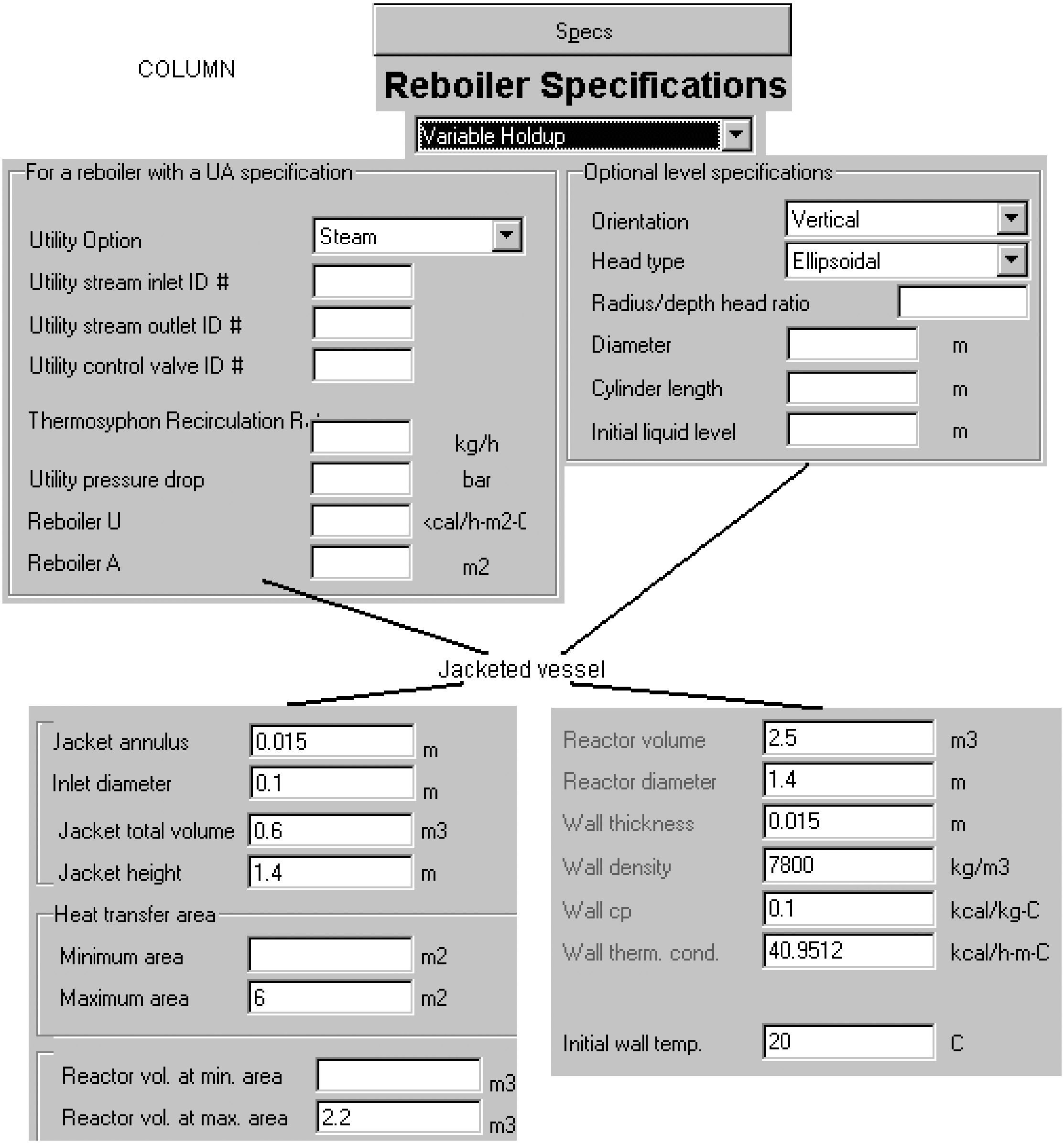
For the set point control (SPC) of the reflux flow rate control loop, a steady state control module (CONT) has been used together with a RAMP module. The RAMP module produces the time dependent reflux ratio. A fuller description of SPC can be found in the section "How to define a set point control system" on page 18.

Notes:

(1) The jacket pressure controls the steam feed flow rate automatically. This mechanism can be defined in this way:



(2) The *reboiler has been defined as discrete unit operation, the batch reactor. The following picture shows analogy between the definition of the built in reboiler of the CC-DCOLUMN model (top), and similar definition of reboiler made of separate batch reactor (bottom):*


Specs
COLUMN
Reboiler Specifications
Variable Holdup
For a reboiler with a UA specification
Utility Option
Steam
Utility stream inlet ID #
Utility stream outlet ID #
Utility control valve ID #
Thermosyphon Recirculation R
kg/h
Utility pressure drop
bar
Reboiler U
kcal/h-m2-C
Reboiler A
m2
Optional level specifications
Orientation
Vertical
Head type
Ellipsoidal
Radius/depth head ratio
Diameter
m
Cylinder length
m
Initial liquid level
m
Jacketed vessel
Jacket annulus
0.015
m
Inlet diameter
0.1
m
Jacket total volume
0.6
m3
Jacket height
1.4
m
Heat transfer area
Minimum area
m2
Maximum area
6
m2
Reactor vol. at min. area
m3
Reactor vol. at max. area
2.2
m3
Reactor volume
2.5
m3
Reactor diameter
1.4
m
Wall thickness
0.015
m
Wall density
7800
kg/m3
Wall cp
0.1
kcal/kg-C
Wall therm. cond.
40.9512
kcal/h-m-C
Initial wall temp.
20
C

(3) There is a similar analogy between built in units of CC-DCOLUMN (such as the accumulator, the condenser, and the reflux control loop), and similar units made of discrete unit operations. A summary of the existing unit operations follows:

Vessels:

Equip. No.	3	5	
Equip. Name	D2	D3	
Pressure bar	10.2000	10.0000	
Recorder option:	1	1	Record history
Diameter m	0.6000	1.4000	
Cylinder length m	1.8000	2.0000	
Head type:	3	3	
Int. liq lev 1 m	1.0000e-010	1.0000e-010	Empty vessels at start
Liq flow 1 mode	***3***	0	
Liq flow 1 spec.	***8.0000***		***Controlled by CVAL 8***

Control Valves:

Equip. No.	10	8	
Equip. Name	V2	V3	
Valve flow coefficient	9.0000	9.0000	
Rangeability	10.0000	10.0000	
Valve type	1	1	
Critical flow factor	0.9800	0.9800	
Downstream pressure, bar	10.2000	10.4000	
Controller ID	9	7	
Valve time constant	0.1000		
Valve Av	0.0625	0.0625	
Valve Bv	-0.2500	-0.2500	
Phase option	1	1	
Equip. ID	***4***	0	***Flow rate transfer***
Equip. var. no	***3***	0	

PID Controllers:

Equip. No.	9	7	
Equip. Name	FC	LC	
PB (Proportional Band)	125.0000	25.0000	
Ti (Integral time, min)	0.5000	5.0000	
P0 Steady state output	4.0000	4.0000	
Set point	***1.0000e-006***	0.9000	***Controlled by SPC***
Error definition	1	0	
Control valve ID.	10	8	
Measured object	0	1	
Measured object ID.	7	3	
Measured variable	6	43	
Variable unit	1	18	
State	1	1	

```
Controller/Sensor Func.         1            0
Variable Min           1.0000e-006  1.0000e-006
Variable Max              1500.0000       2.0000
Ctrl input min               4.0000       4.0000
Ctrl input max              20.0000      20.0000
```

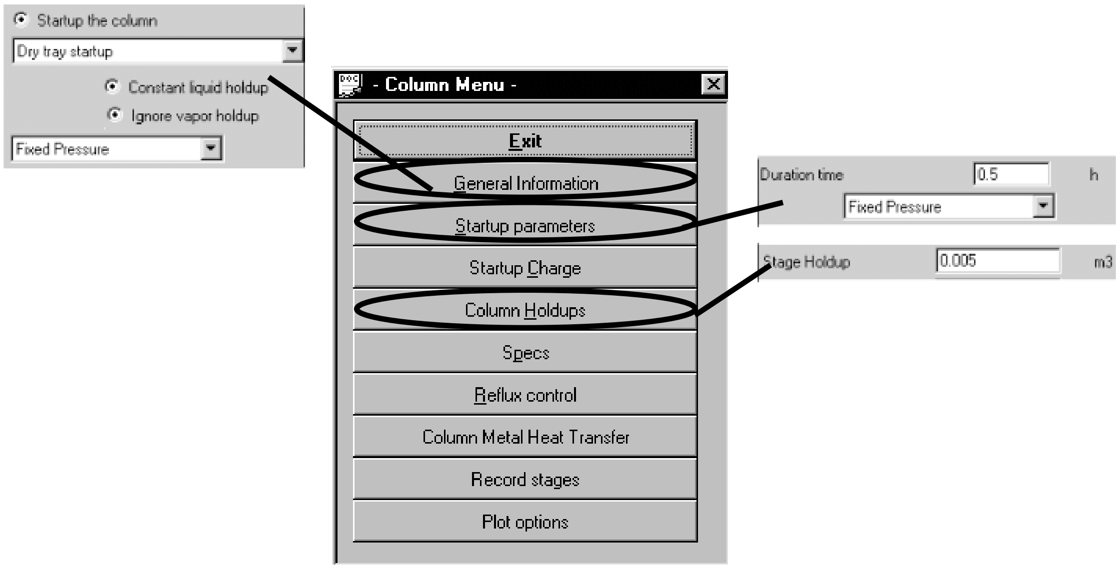
Heat Exchanger:

```
Equip. No.                    17
Equip. Name                   E1
U  kcal/h-m2-C          400.0000
Area/shell  m2            4.0000
```

Elements of SPC calculation:

```
RAMP
Equip. No.                    15
Equip. Name            R-profile
Equip/Stream ID               16      CONT module
Varaible No.                   9      Scale
                           0.999      time & value
              90.0         0.999
             120.0         0.8500
             300.0         0.8500


CONT
Equip. No.                    16
Equip. Name                   SPC
Mode                           1      FF
Equip. no. adjusted            9      Reflux controller
Variable No.                   6      Set point
 Measured variables:
Number                        21      Liquid stream from condenser
Variable                       6      Mass flow rate
Scale                     1.0000      Defined by RAMP module
```

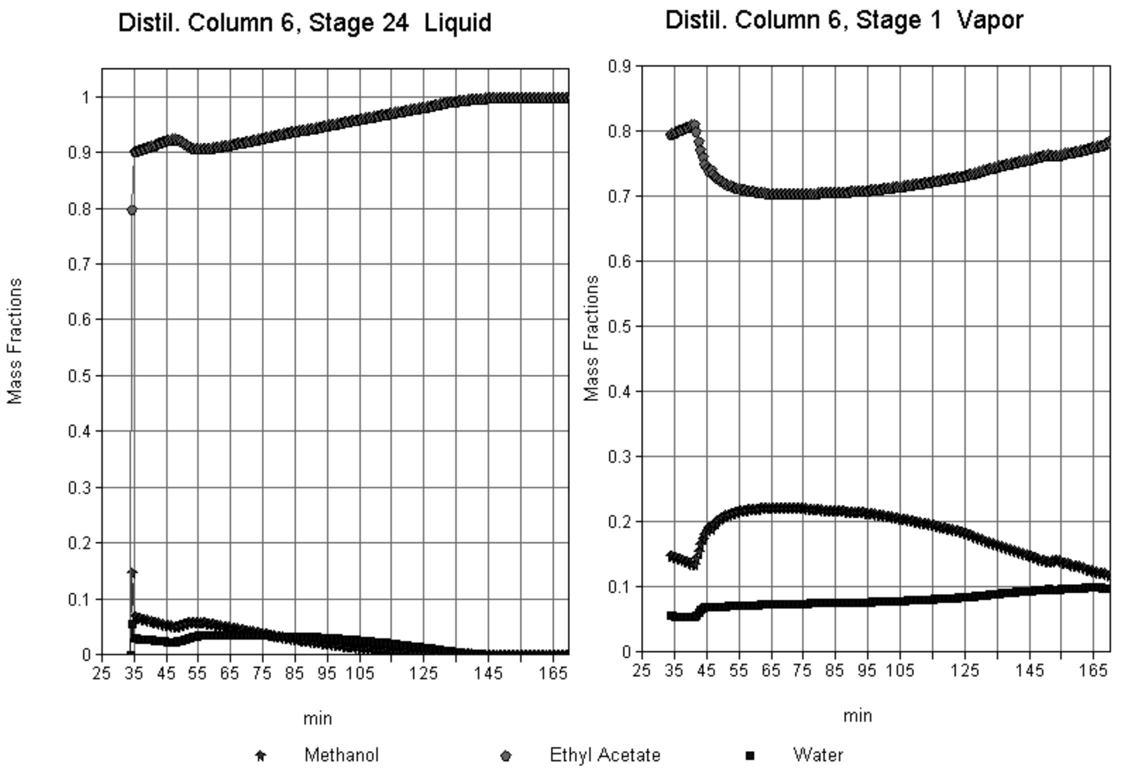
The parameters that have been entered as specifications of the distillation column are:

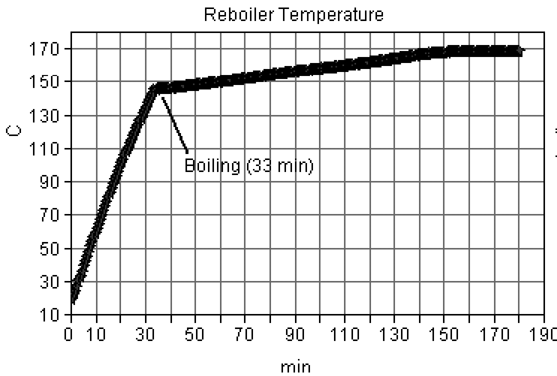


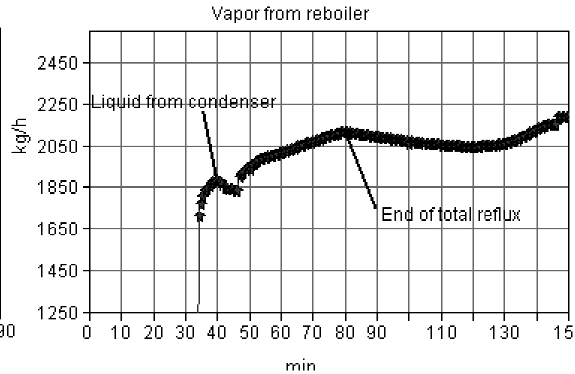
Plots:

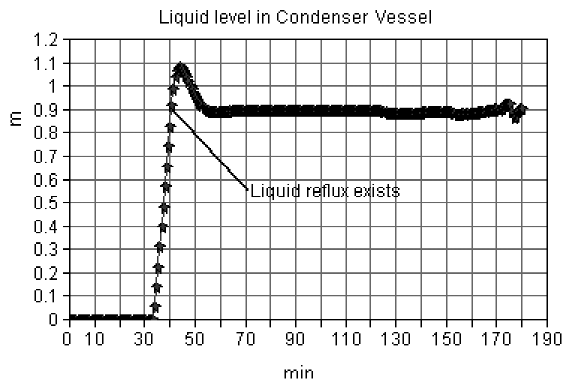
Several plots can be produced using the simulator of batch technology. These can help in the design phase and can help analyze the existing technology.

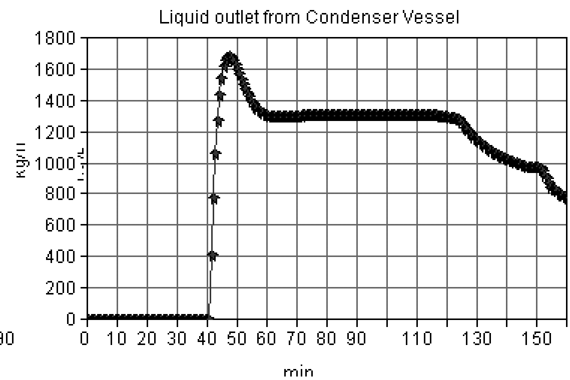
With the next set of profiles, we would like to show how you could use these results in the design of time schedule of the batch technology.


Distil. Column 6, Stage 24 Liquid
Distil. Column 6, Stage 1 Vapor
Mass Fractions
min
Methanol
Ethyl Acetate
Water


Reboiler Temperature
C
min
Boiling (33 min)


Vapor from reboiler
kg/h
min
Liquid from condenser
End of total reflux


Liquid level in Condenser Vessel
m
min
Liquid reflux exists


Liquid outlet from Condenser Vessel
min