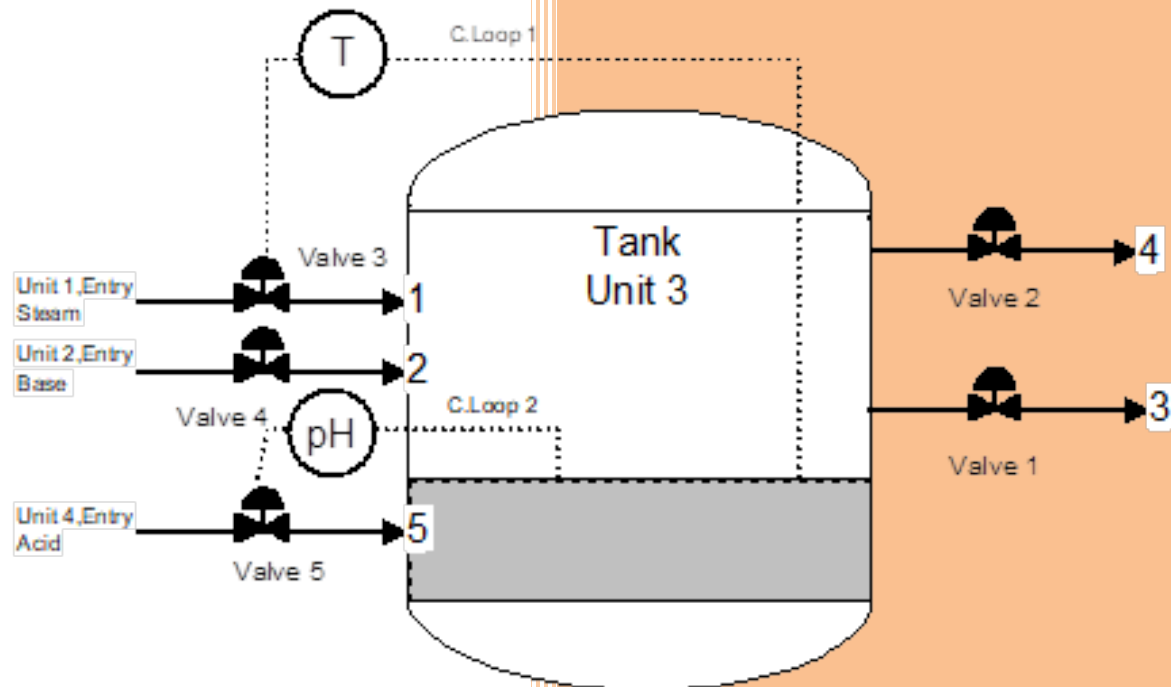


2018

A guide to using DynaChem 9.6



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Chapter 1 Dynamic Simulation

Overview

DynaChem is the primary dynamic simulation component of the ESP family of software. Specifically, DynaChem allows for description of one or more processing streams and, where applicable, process control. The entire system is solved on an unsteady-state (time-dependent) basis.

DynaChem is supported by the extensive OLI thermodynamics already discussed¹. The OLI databases also support DynaChem. The architecture of the program is such that the user need know only the names of the chemicals involved and not the detailed chemical reactions.

The philosophy of DynaChem is based upon discrete, modular computation of “Process” units. The term process is a general term in this case referring to any chemical system. This can range from a traditional chemical process to a geological system being altered by the environment.

¹ See “A Guide to Using the OLI Software”

Comparing Dynamic versus Steady-State Simulations

We have explored the capabilities of ESP and have seen the power of the tool. The only major aspect not covered in ESP is the effects of time on a process. It is true that some unit operations (i.e., Bioreactors) do vary with time but on the whole, ESP is a steady-state simulator.

It is helpful to look at some of the differences between a steady-state simulator and a dynamic simulator

	Dynamic	Steady-State
Variation with time	Yes	No
Effects of Upsets	Yes	No
Physical Configuration	Important	Unimportant
Graphical Display	Important	Less important
Interrupt Facilities	Important	Less Important
Flowsheeting	Important	Important

DynaChem Attributes

There are many attributes to DynaChem. These are but a few:

- Modular (flow sheeting capability with recycles)
- Dynamic (unsteady-state)
- Access to All OLI Thermodynamics and Chemistry
- Multiple and interaction process control loops
- Interactive forms-driven input and graphical output
- Interactive with process interrupt and real-time intervention
- Real-time process unit display and graphical display.

Applications

DynaChem has been used to study a variety of processes. These processes include (but are not limited to):

- pH Controlled Neutralization
- Multistage Column Controllability during startup and upsets
- Batch Distillation and Batch Reactors
- Vessel Pressure Control
- Evaporators
- Ion Exchange Columns
- Deepwell injection of Hazardous Waste
- Oil well formation protection

Concepts

DynaChem is based on two distinct concepts - a unit and a node. A unit, as opposed to a unit operation, can be one of three types:

1. Entry Unit
2. Tank
3. Pipe

Each unit will be described in a few moments. Each unit has the following characteristics:

- Each unit accumulates mass and energy
- Homogeneous
- At equilibrium
- Either constant volume (Pipe) or varying volume (Tank)

*There is a special type of node called and **Energy Node** which is just a collection point for energy in transit.*

*Heat exchangers can be built with **Energy Nodes**.*

A node is a collection point for mass and energy in transit between units. The concept of a node is analogous to the Stream Name in ESP/Process.

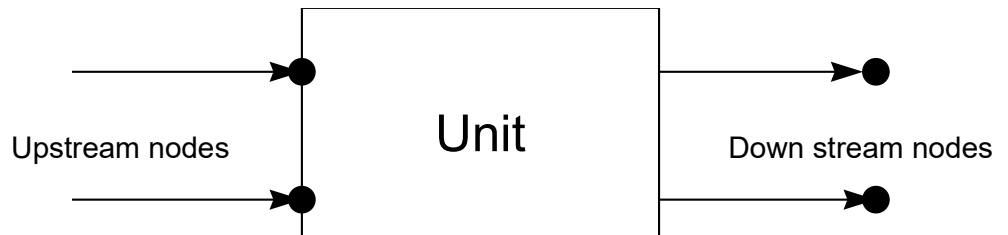


Figure 1-1 A generic view of a unit

How does time affect all of this?

DynaChem breaks the flow of time in to discrete packets called time increments. These packets arrive at a node and then are taken into the unit. When the calculation is done, the packet is placed at the downstream node.

Let's look at an example of packet movement.

Let's start with three tank units, each partially filled with liquid, and one entry unit. The process looks like this:

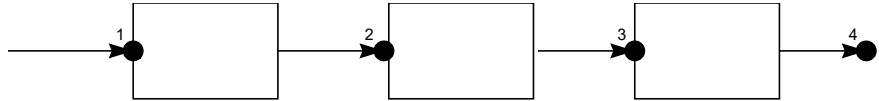


Figure 1-2 The process at time=0

On the first time increment (time=t1) some information at node 1 (the number above the black dot is the node number) is placed into the first tank. The equilibrium is established and the results are placed at node 2.

The gray tank indicates that a new equilibrium condition exists in that tank.

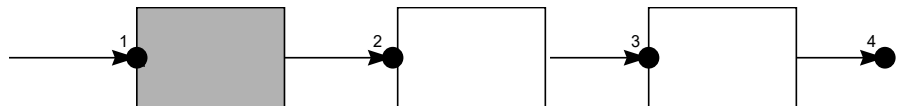


Figure 1-3 The process at time=t1

We now begin the second time increment (time=t2). Now since there is information at node 2, some information is placed into the second tank and equilibrium is established. The results are placed at node 3. There is still information at node 1 so that information is placed into the first tank and equilibrium is re-established. The results are placed at node 2 once again.

The different patterns in the tanks indicate different equilibrium conditions.

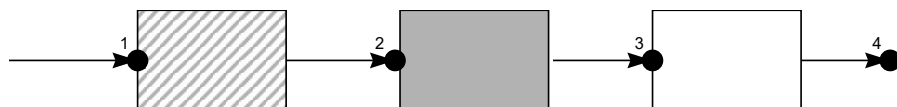


Figure 1-4 The process at time=t2

As we begin the third time increment (time=t3) material is available at node 3. As before, the information is placed in the third tank and equilibrium is established. The results are placed at node 4. As with the previous time increments, information from node 2 enters the second tank, computed and placed at node 3. Information at node 1 is placed into the first tank, computed and placed at node 2.

This will continue till the last time increment (user specified) is reached.

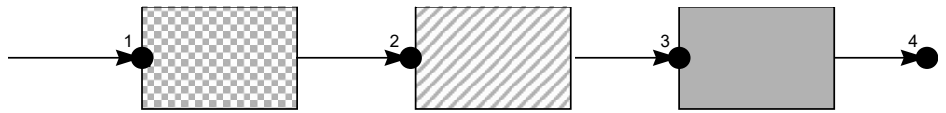


Figure 1-5 The process at time= t_3

The Units

Here we will briefly describe the DynaChem units.

The Tank

Tanks are varying volume units. The sum of vapor, liquids, and solids does not have to remain constant.

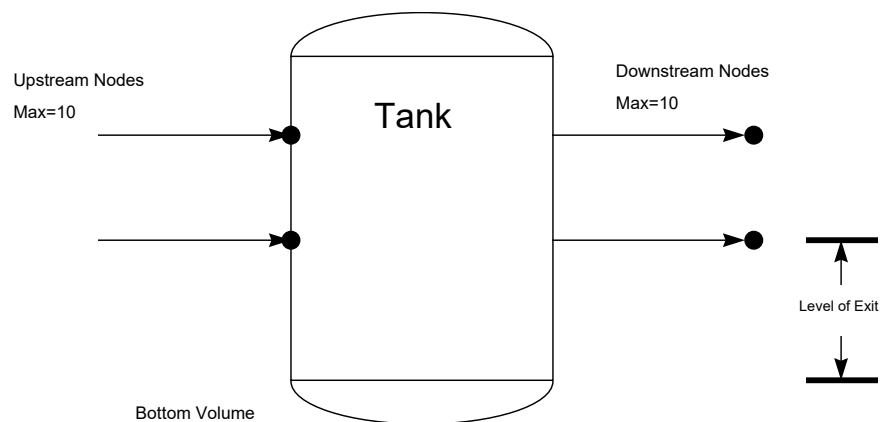


Figure 1-6 The DynaChem tank

You must specify the geometry of the tank (2 of 3 are required):

- Cross Sectional Area (CSA) in m^2
- Maximum Level in m
- Maximum volume in m^3

In addition, the level (in meters) of the exits must also be specified. A bottom volume (optional) can also be specified.

The initial conditions of the tank must also be specified:

- Temperature
- Pressure
- Initial Volume
- Composition

The tank can start empty.

*The letter m refers to meters.
All of DynaChem's units are
in metric units.*

Some properties of the exit streams are:

- Fluids flow through the exits up to the limit set by a valve
- Liquid and suspended solids will flow only through exits at or below the level in the tank.
- Liquid and suspended solids will flow preferentially through exits from bottom to top.
- Vapors flow preferentially through exits from top to bottom.
- All available fluid will exit through an unvalved line.

The Pipe

The pipe is a constant volume unit. The sum of vapors, liquids and solids must remain constant although the ratio of the phases may change.

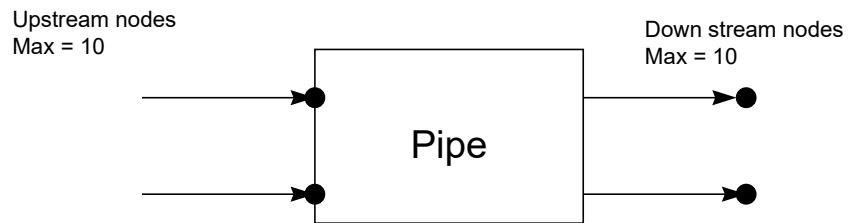


Figure 1-7 The DynaChem pipe

You must specify the geometry of the pipe (2 of 3 are required):

- Cross Sectional Area (CSA) in m^2
- Maximum Level in m
- Maximum volume in m^3

The initial conditions of the pipe must also be specified:

- Temperature
- Pressure
- Initial Volume
- Composition

The pipe can start empty.

In addition, the discharge temperature of the pipe may also be specified.

Some attributes of the exits are:

- Sufficient fluid will exit to main a constant resident volume
- Fluid (combined liquid, solid and vapor) will flow preferentially though exits with valves up to the capacity of each valve.
- Any remaining fluid will flow through the first entered unvalved exit.

The Entry Unit

*Scheduling flows is good
method of introducing upsets.*

This is a special unit in that no geometry is required. Rather this is how material enters the simulation. the entry units can be full flow, partial flow, and scheduled flow. Entry units do not necessarily require downstream valves.

Downstream nodes only

Max =1



Figure 1-8 The DynaChem entry unit

The attributes of the Entry unit are:

- Limits the flow to a node
- Maximum of 1 value per node
- May be either manual valves (stem position set by the user) or automatic valves (stem position set by a controller)
- Valve Specifications must be set, Capacity (Cv), linear or equal percentage, rangeability and or pressure functionality.

Control Loop

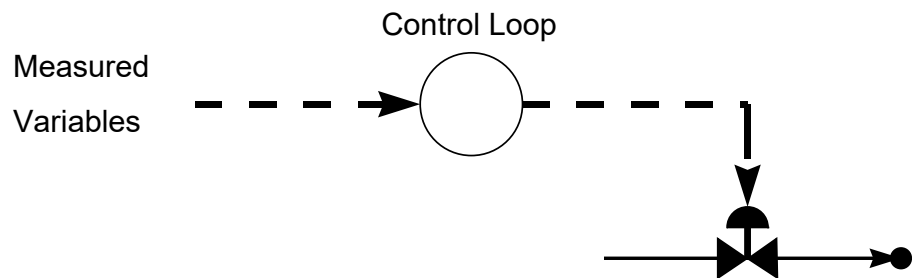


Figure 1-11 A simple Control Loop

Some of the attributes of a controller are:

- Retrieves a Measured Variable
- Computes the **Error**: Measured value-Set point value
- Adjusts the valve stem position based upon the specified control algorithm.
- The measured variables are: Temperature, Pressure, pH, Level, Flow, Composition.

Controller Algorithms

PID Controller (Proportional Integral Derivative).

- Specify Set Point

- Specify Controller Parameters: Gain (K_c), Integral Time, Derivative time, Valve Constant (Bias)
- Velocity Algorithm
- Positional Algorithm

This controller may be “Tuned” while DynaChem is executing.

- Any control Parameter may be changed during interrupt
- May change any set point or valve stem position during interrupt.

Ratio Control

- Specify Ratio
- PID Controller Set Point = Ratio * Measured 1 Value
- Can be “Tuned”

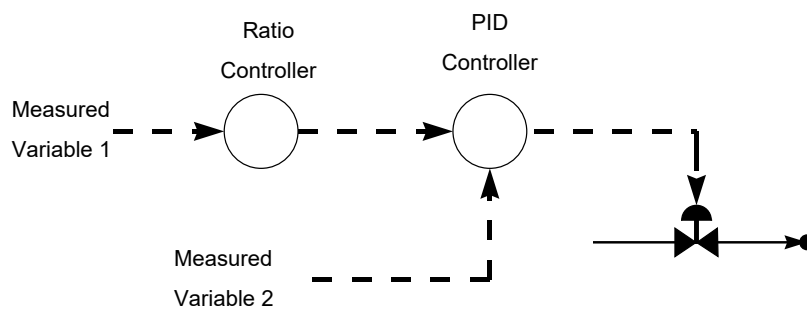


Figure 1-12 Ratio Control

Dead Band Control

- Specify Lower and Upper Set Points
- Between the Set points the **Error** is 0.0 (no action taken)

Summary

DynaChem is a powerful and flexible tool for simulating time-dependent processes. The simplicity of the units allows for a great deal of flexibility in creating processes.

Chapter 2 DynaChem Tour

Overview

In this section, we would now like to illustrate the use of DynaChem, the dynamic component of ESP.

The application we have chosen for illustration involves the pH- control neutralization of a basic (NH₃) stream using an acid. This example is a simplified illustration of an important environmental pretreatment application. In this illustration we will utilize both pH and temperature control.

Create the Chemistry Model Definition

First we must define the chemistry for this system. The name for the Chemistry Model we will use is **PHDYNA**. The system will be composed of **H₂O**, **CO₂**, **NH₃**, **HCL** and we will be considering the aqueous and vapor phase. We will also be using the Aqueous Framework and use no additional databanks.

We have created numerous chemistry models by this point. One nice feature of ESP is that its models can be used in DynaChem without modification

To create the Chemistry Model in ESP, simply select **ESP Process** and define a **New Process** called **PHDYNA**².

Then select **Chemistry Model** and define a **New Model** also called **PHDYNA**.

The **Inflows H₂O**, **CO₂**, **NH₃**, **HCL** can be entered, and then the **Phases** can be selected. Complete the generation of the chemistry model as you have done in previous chapters.

When you complete the Chemistry Model, simply <Esc> repetitively until you return to the main menu of ESP “**Selecting which Program.**” ProChem is in the OLI Toolkit.

² This process name will not be used in the DynaChem simulation.

Next we will use ProChem's dynamic modeling component, DynaChem, to <CONTINUE> the analysis.

ENTERING DynaChem

Having finished creating the chemistry model definition, the ESP enter the Toolkit and select the DynaChem component of ProChem. ProChem Menu listing ProChem's components will be displayed on your screen.

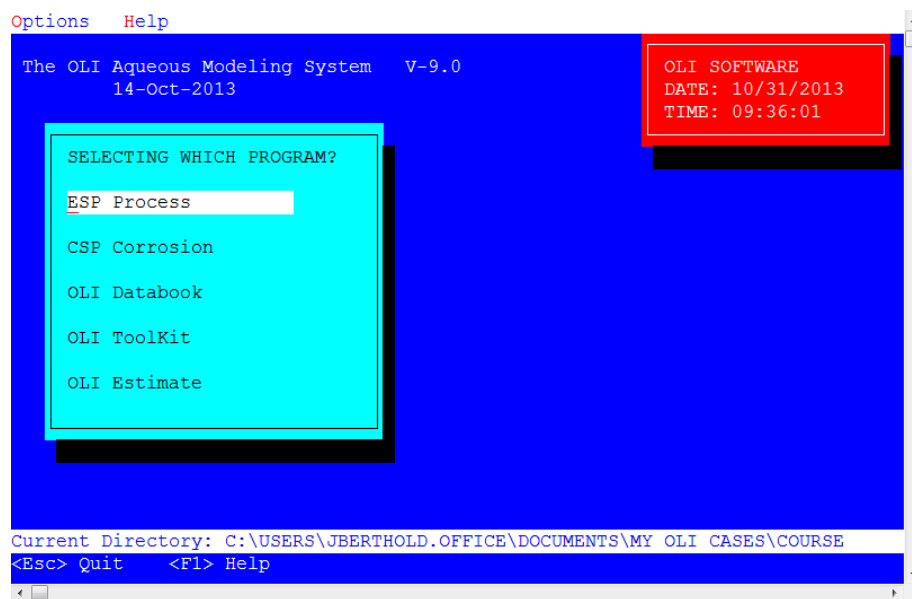


Figure 2-1 ESP Main menu, select OLI Toolkit

Select OLI ToolKit from the menu.

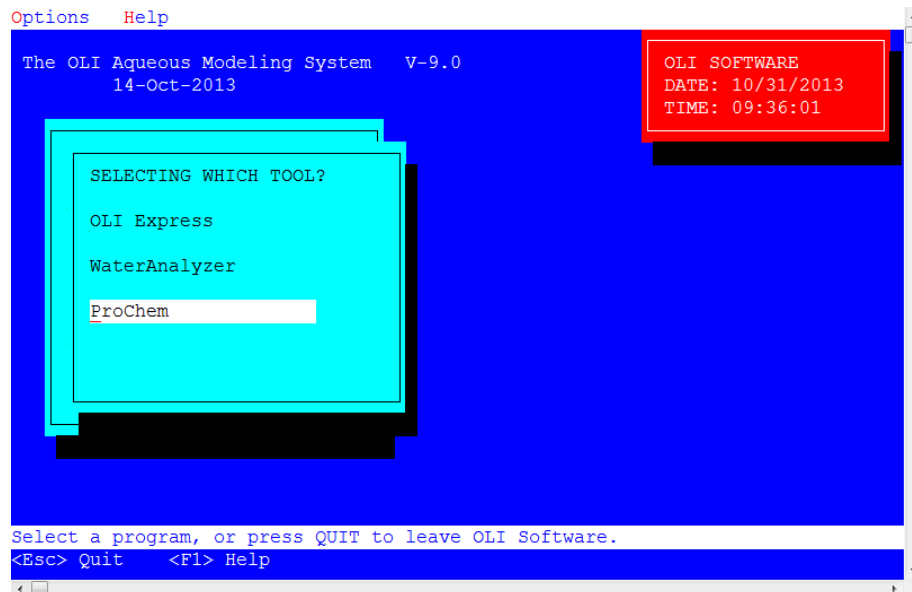


Figure 2-2 the OLI Toolkit Menu, select ProChem

Select ProChem from the menu.

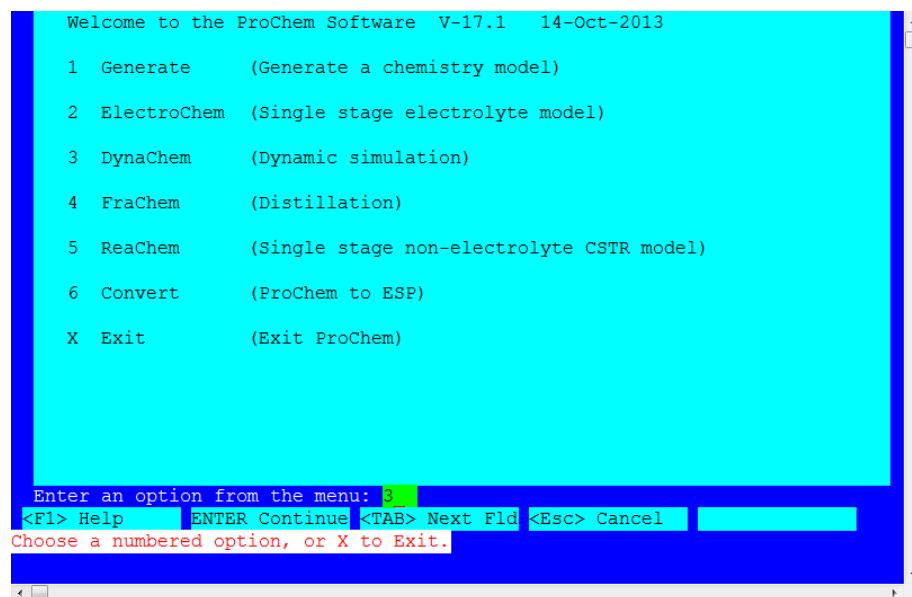


Figure 2-3 ProChem menu.

From the list of choices on ProChem's Menu, choose 3, DynaChem, and press <CONTINUE>.

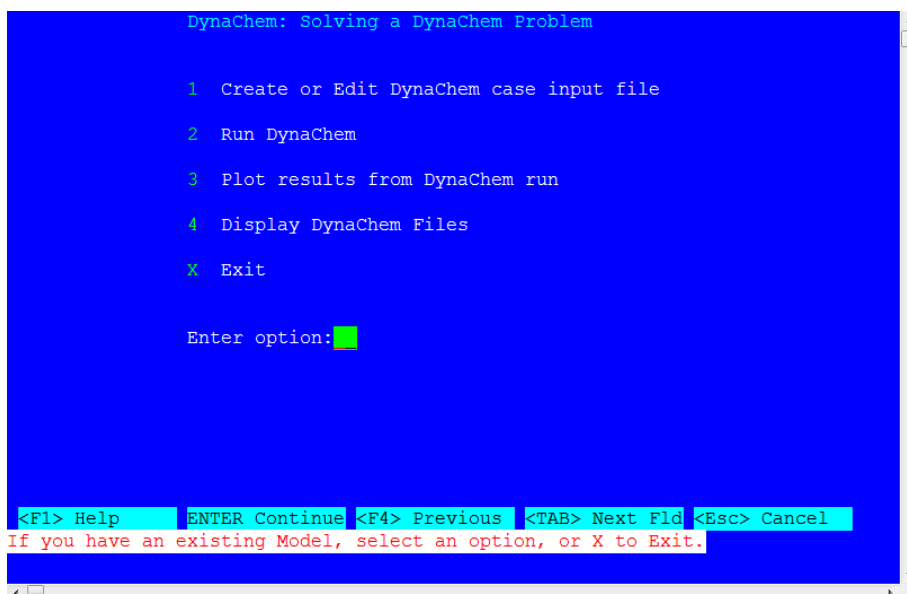


Figure 2-4 The DynaChem Main Menu

This menu lists all possible DynaChem functions, in the order you would access them. To start our DynaChem simulation please choose 1, **Create a DynaChem input file**, and press **<Enter>**.

You will see a screen that prompts for the ProChem model name. Enter **PHDYNA** to reference the **PHDYNA** Chemistry Model we generated. At the ProChem case prompt, press **<ENTER>** to accept the **PHDYNA** default as the case name, also. The screen should look like this:

The case name does not have to be the same (and frequently isn't) as the model name.

Note: the ESP process name you used in the model generation: **PHDYNA** does not actually exist on the disk. The case name illustrated here is actually a different file type.

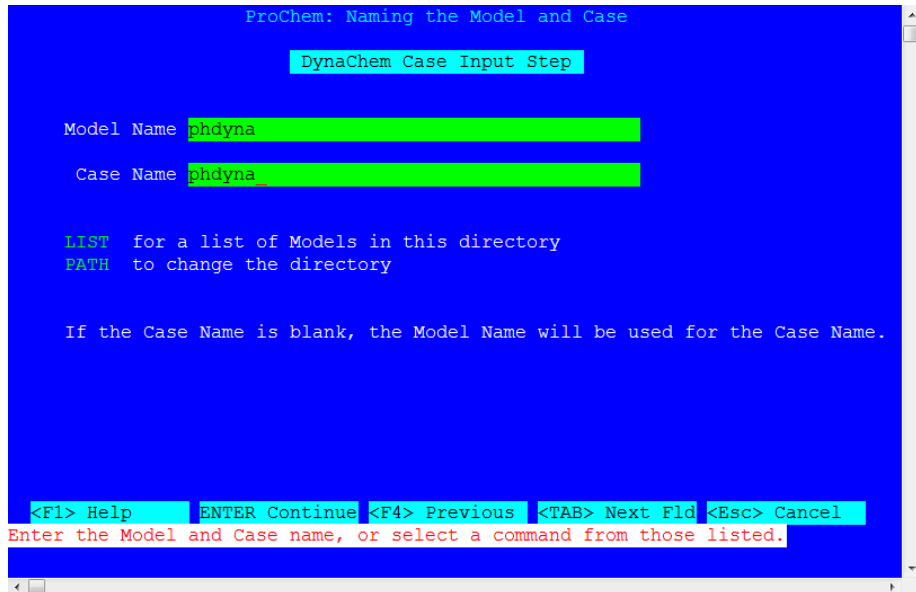


Figure 2-5 Selecting the DynaChem model and naming the DynaChem case

Creating a DynaChem Case

Once DynaChem has the Chemistry Model and Case name, the DynaChem Input Menu appears. It is shown below:

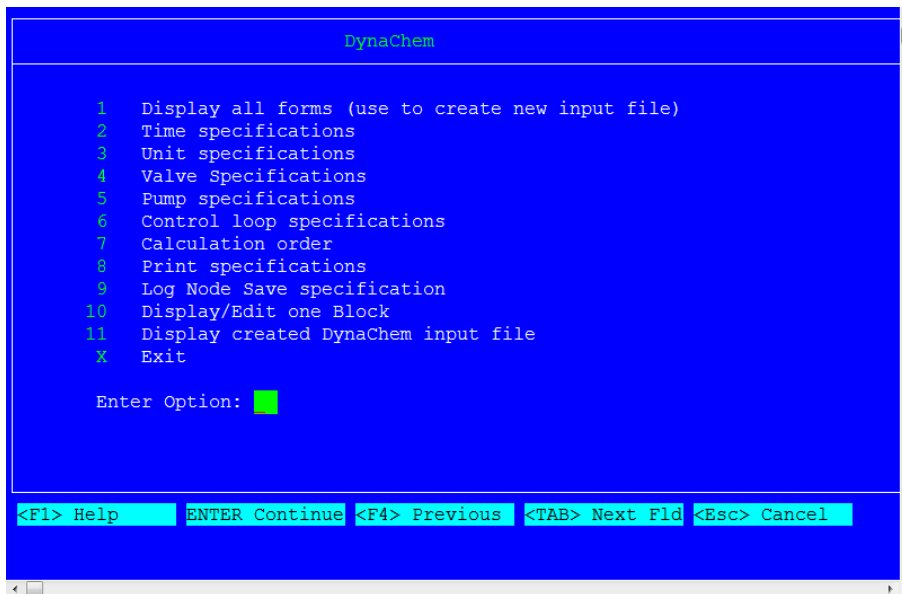


Figure 2-6 The DynaChem Case Edit Menu

When editing an existing DynaChem case, the user is able to edit distinct portions of the Case Input File, by selecting one of the option numbers from this menu.

Alternatively, and for this **PHDYNA** example, Option 1 can be selected to step through the basic options for DynaChem case input.

A schematic diagram for the neutralization tank is shown in Figure 2-7 on page 21. As shown in this diagram, there are three feed streams (steam feed, basic feed, and HCl feed), one mixing tank, five valves, and two control loops. The steam feed is for temperature control and the HCl feed is for pH control.

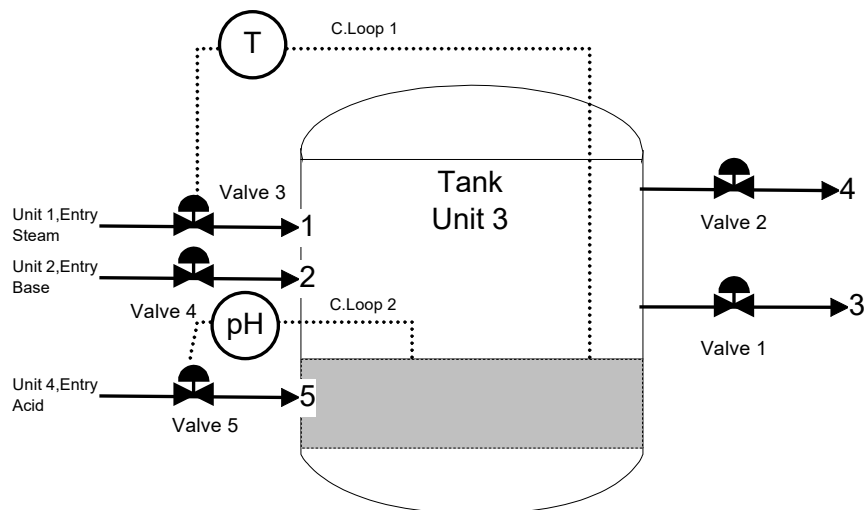


Figure 2-7 The diagram of the example process

- Enter a 1 now and press <ENTER> to CONTINUE.

DynaChem Input Option 2: Time Specifications

This screen allows the user to enter the case title, the time increment, and the end time. The use of DynaChem is to describe the dynamic behavior of the system with a discrete model. The smaller the time increment, the closer the discrete model approaches the real process. However, the smaller the time increment, the greater the computation time required to simulate a given period of time. Therefore, a compromise has to be made.

The proper time increment should be selected on the basis of producing no significant difference in the system response upon using further smaller values. For the **PHDYNA** example, a time increment of 0.0001 hour is used. The neutralization process will be simulated for a period of half an hour. Therefore, the END TIME is 0.5 hour.

This screen also allows the user to <CONTINUE> simulation from a previous run and to specify the time interval for saving results to the restart file.

The screen, including the user entries, is shown below.

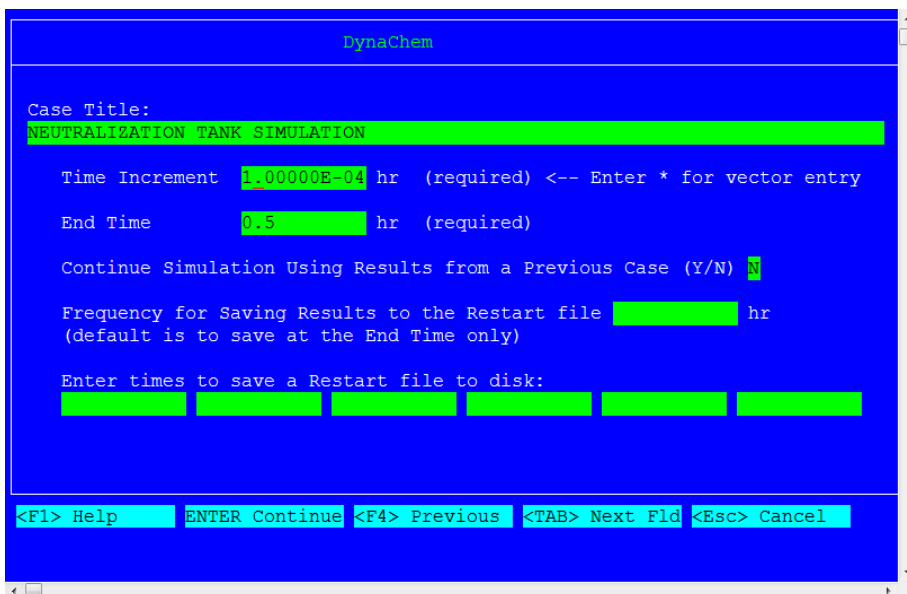


Figure 2-8 Entering Time Specifications

DynaChem Input Option 3: Unit specifications

This next screen prompts for the unit number, unit type and unit description. In DynaChem there are three basic unit types: ENTRY (feed streams), TANK, and PIPE.

For the **PHDYNA** example, there are four units. Unit number 1, 2, and 4 are assigned to the three feed streams. The mixing tank has unit number 3. These unit numbers are arbitrary and may be any integer from 1 to 100. For the feed stream, the unit type is ENTRY. For the mixing tank, the unit type is TANK.

The screen with the user entries should look like this:

DynaChem Unit Specifications		
Unit No.	Unit Type	Unit Description
1	ENTRY	STEAM FEED TO TANK
2	ENTRY	NH3-CO2 FEED TO TANK
3	TANK	Mixing Tank
4	ENTRY	HCL Feed to Tank

<Page Down> <Page Up>
 <F1> Help <ENTER> Continue <F4> Previous <TAB> Next Fld <Esc> Cancel

Figure 2-9 Top level unit specifications

After pressing <CONTINUE> and leaving the previous screen, you will see a series of eight screens corresponding to the four units. The first four screens prompt the user to provide physical configurations of all the units.

For an ENTRY unit, these include the downstream node number, the start time (default=0), the duration (default=0), and the ramp time (default=0). For a TANK unit, the user needs to give physical characteristics of the tank, the upstream and the downstream node numbers, and the exit levels. Detailed description of each entry can be obtained by pressing the HELP key.

You can also refer to the schematic diagram of the neutralization tank for the node numbers associated with each unit. Again, these node numbers are arbitrary and must be unique.

The last four screens require you to specify the initial states of each unit including temperature, pressure, flow rate, volume, and composition.

After the Unit Specifications Screen for Mixing Tank (3), four screens appear to prompt you to enter the quantity of solids and vapor suspended in the liquid solution, liquid entrained in the vapor and liquid dissolved in the solid solution. Press <ENTER> four times to <CONTINUE>.

Unit 1,Entry
Steam → 1

Figure 2-10 Entering Unit 1 (Steam Feed to Tank) with downstream node #1

Scheduled Entry Start Time (hr)	Scheduled Entry Duration (hr)	Time to ramp from 0 to full flow (hr)	Time to ramp from full flow to 0 (hr)

Figure 2-11 Specifying the start time for Entry 1

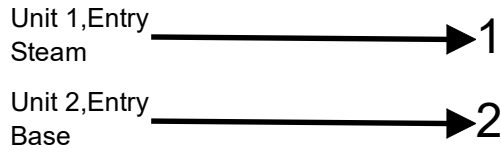


Figure 2-12 Adding Unit 2, the Basic NH3-CO2 feed with downstream node #2

DynaChem Entry Unit Unit: 2 NH3-CO2 FEED TO TANK

Down stream node numbers: 2

Up stream log node number (from previous run) :

Scheduled Entry Start Time (hr)	Scheduled Entry Duration (hr)	Time to ramp from 0 to full flow (hr)	Time to ramp from full flow to 0 (hr)

(default=0) (default=continuous) (default=0)

<Page Down> <Page Up>

<F1> Help ENTER Continue <F4> Previous <TAB> Next Fld <Esc> Cancel

Figure 2-13 Specifying the Start time for Entry 2

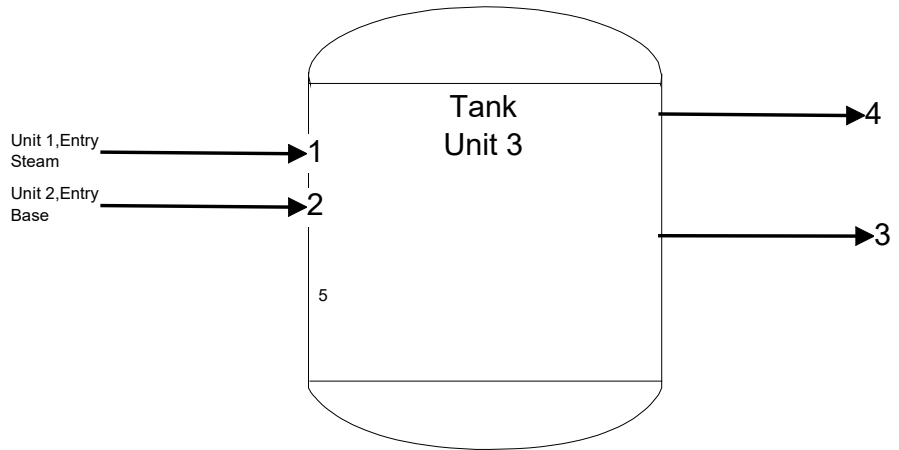


Figure 2-14 Adding the Unit 3 tank with upstream and downstream nodes, notice that Node #5 has not yet been defined

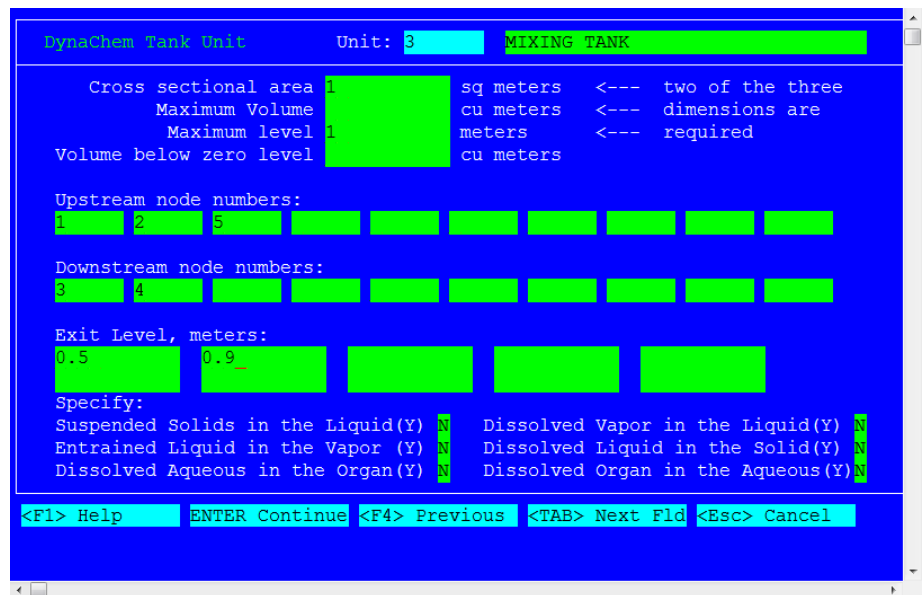
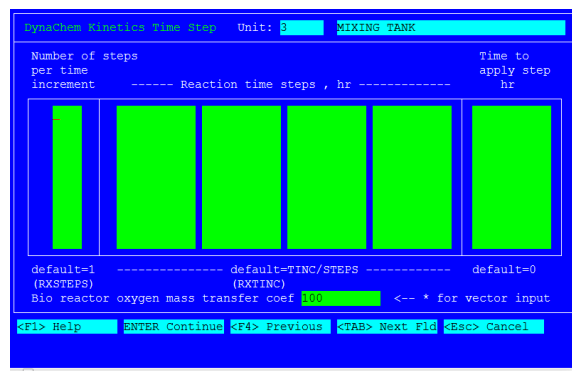


Figure 2-15 Specifying the configuration of the Tank Unit

Press <Enter> on the Kinetics Time Step screen since we do not have reaction kinetics in this model.



2-16 Press Enter on this screen

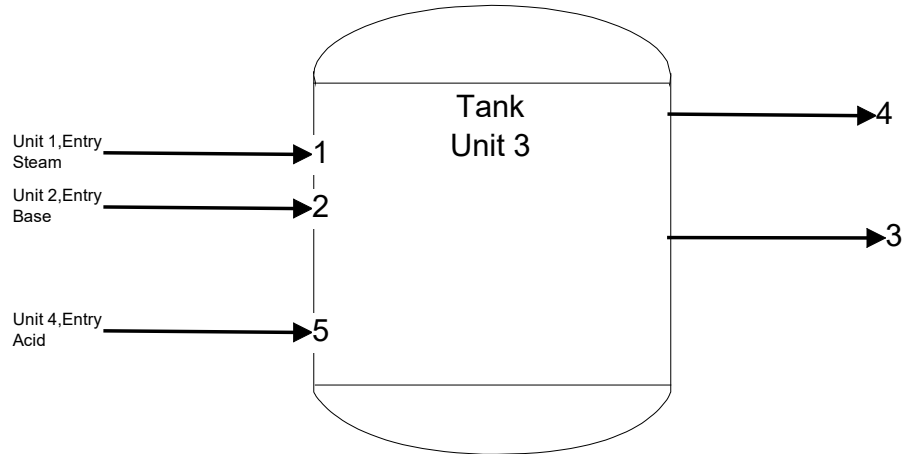


Figure 2-17 Adding the Unit 4 HCL Feed to Tank, node #5 is now defined

DynaChem Entry Unit Unit: 4 HCL FEED TO TANK

Down stream node numbers: 5

Up stream log node number (from previous run) :

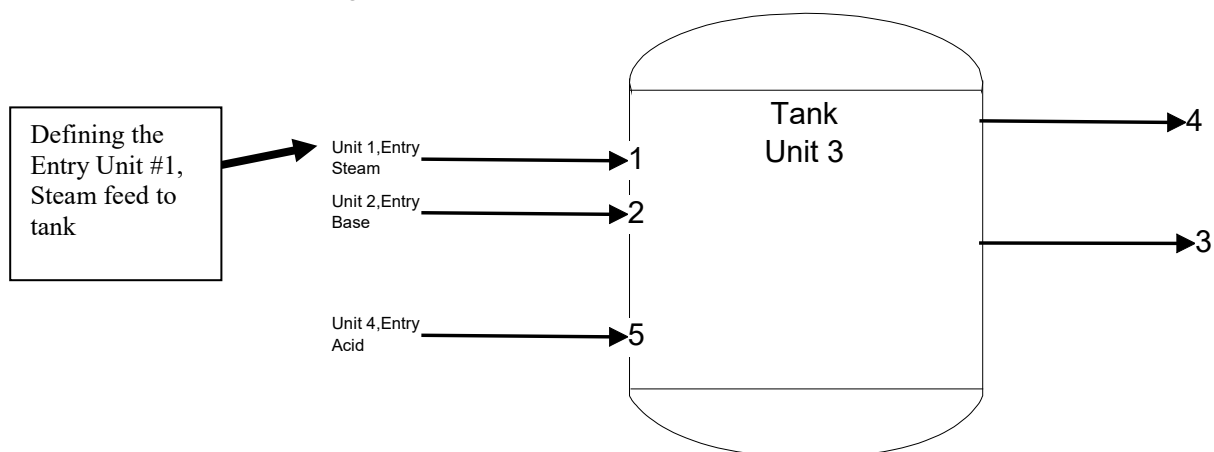
Scheduled Entry Start Time (hr)	Scheduled Entry Duration (hr)	Time to ramp from 0 to full flow (hr)	Time to ramp from full flow to 0 (hr)
0.02			

(default=0) (default=continuous) (default=0)

<F1> Help <Page Down> <Page Up>
 ENTER Continue <F4> Previous <TAB> Next Fld <Esc> Cancel

Figure 2-18 Specifying Entry 4

Figure 2-19



There are several items on this screen which are different from other screens.

No vapor time is the time after which the vapor phase is not considered. No equilibrium time is the time after which the equilibrium calculation is not performed for this stream. Non-standard refers to if the stream is not really aqueous.

These entries are really mole ratios were the amounts of each species is normalized to the total flow.

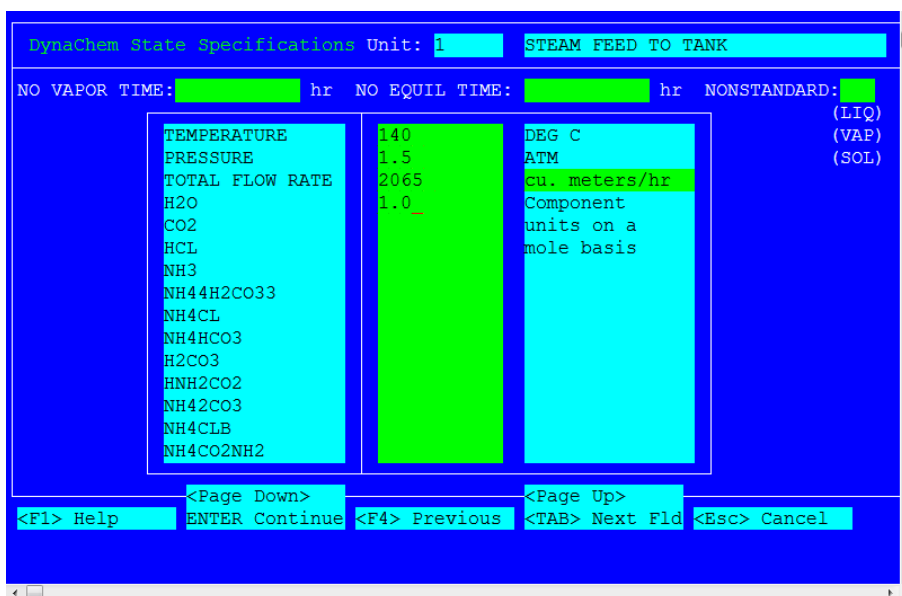


Figure 2-20 Entering the composition for the Steam Feed

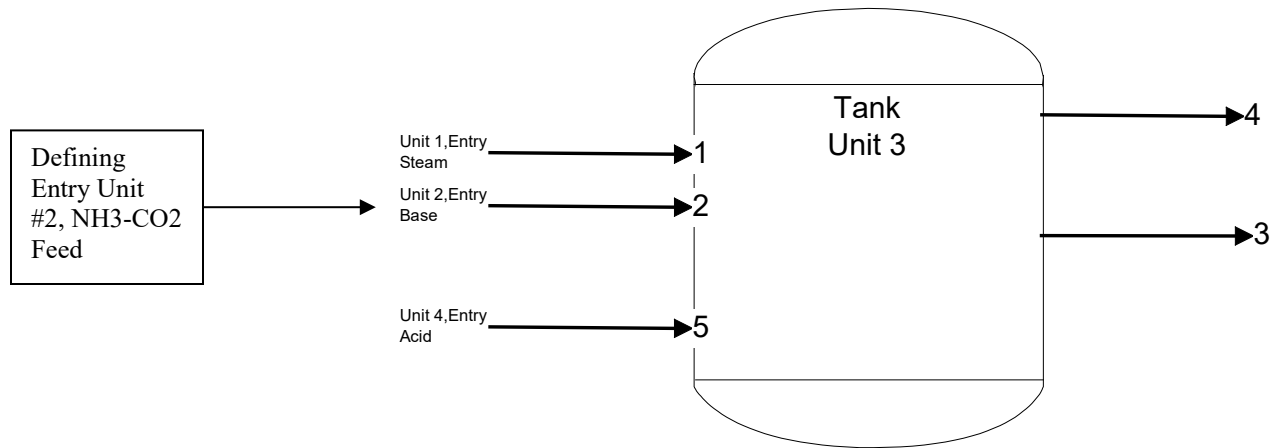


Figure 2-21

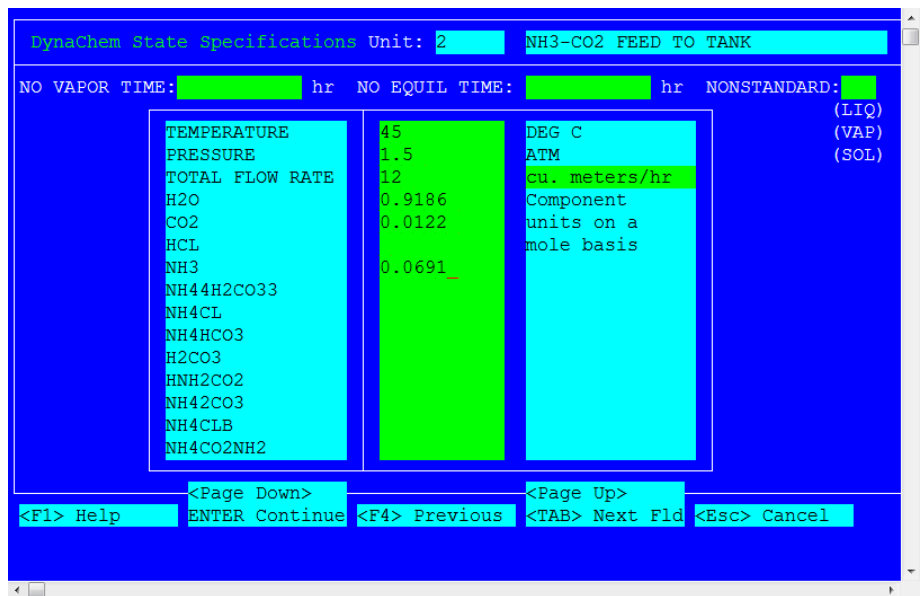


Figure 2-22 Entering the composition for the NH3-CO2 feed

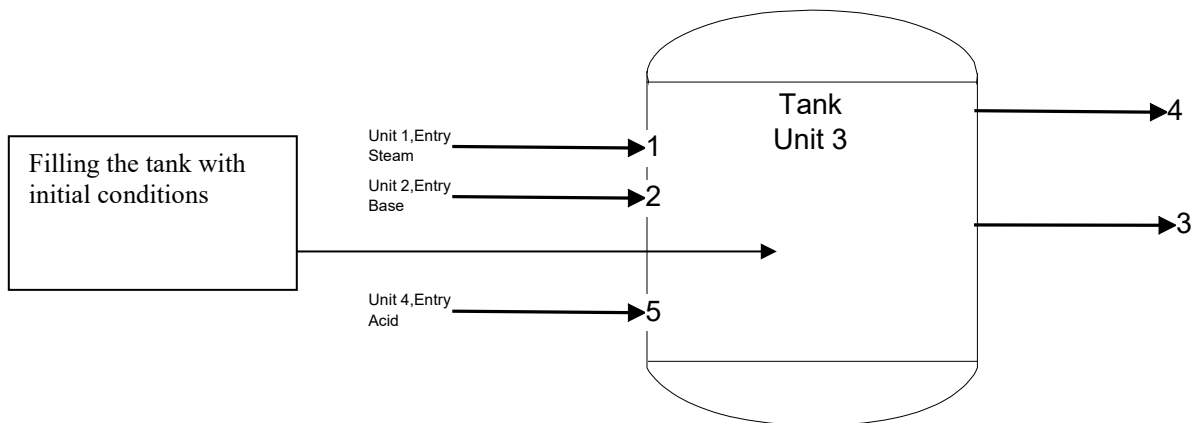


Figure 2-23 Filling tank

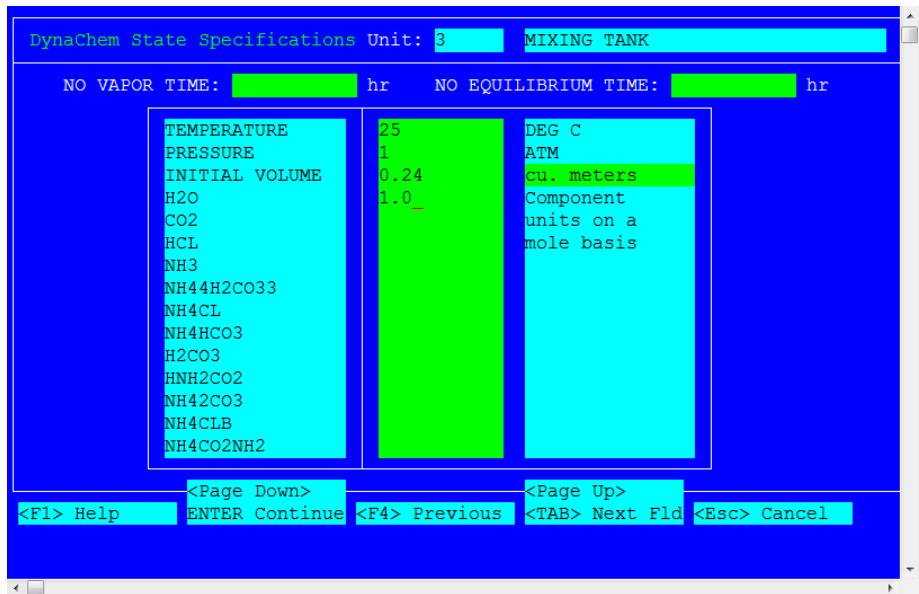


Figure 2-24 Entering the initial composition for the tank

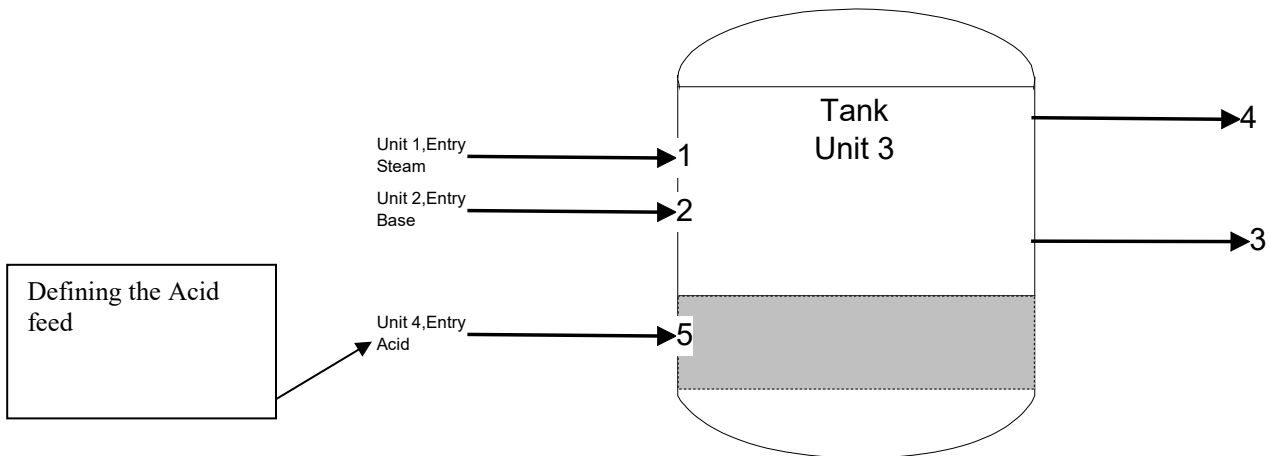


Figure 2-25 Entering the final feed conditions

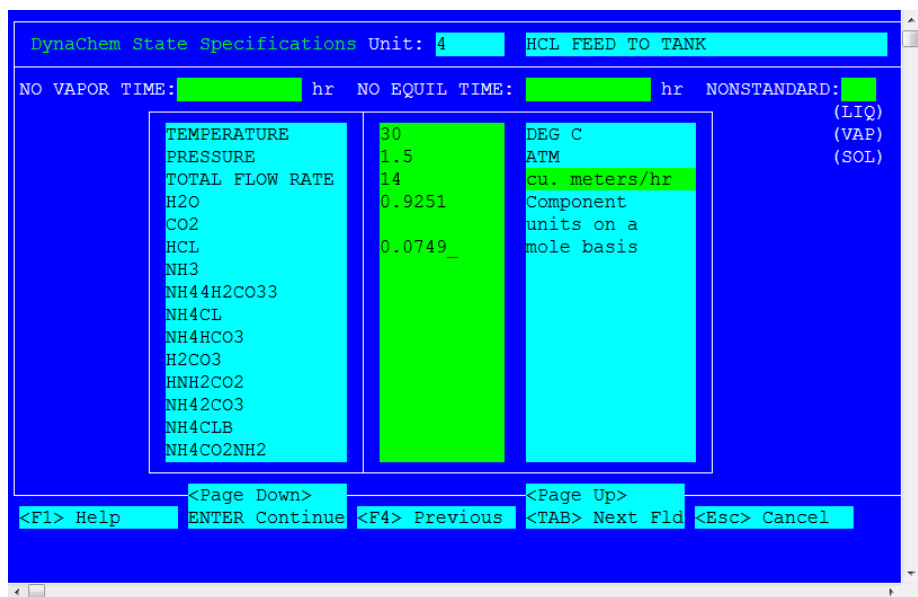


Figure 2-26 Entering the composition for the HCL feed

DynaChem Input Option 4: Valve Specifications

Valves are used to restrict the flow of mass and energy in order to achieve the desired process conditions. The screen on the next page requests general information about each valve. Inputs required for each valve are a unique valve number, the Downstream Node number, the capacity, and the valve type. The valve number need not be the same as the Downstream Node number. A linear valve type is the default.

Following the next page, there follow five consecutive screens, one for each of the five valves. For each valve, you need to specify Pressure Function, Rangeability, and Valve Override. The default Pressure

Function has been selected for each valve. For linear valve, the Rangeability is infinitely large. Just press NEXT FIELD to skip this entry field. All six screens exhibit the entries that you are required to make.

For Valves 1, 2, and 4 which are not associated with any control loops and remain fully open, the Valve Override is 1. For Valves 3 and 5 which are associated with the control loops and are initially closed, the Valve Override is 0.

Once finishing Valve Specifications, press <CONTINUE> to move to the next screen.

Valve No.	Downstream Node number	Capacity cu. meters/hr	Valve Type LINE/EQUA
1	3	33	LINE
2	4	100000	LINE
3	1	3000	LINE
4	2	10000	LINE
5	5	14	LINE

<Page Down> <Page Up>
<F1> Help ENTER Continue <F4> Previous <TAB> Next Fld <Esc> Cancel

Figure 2-27 Top level valve specification

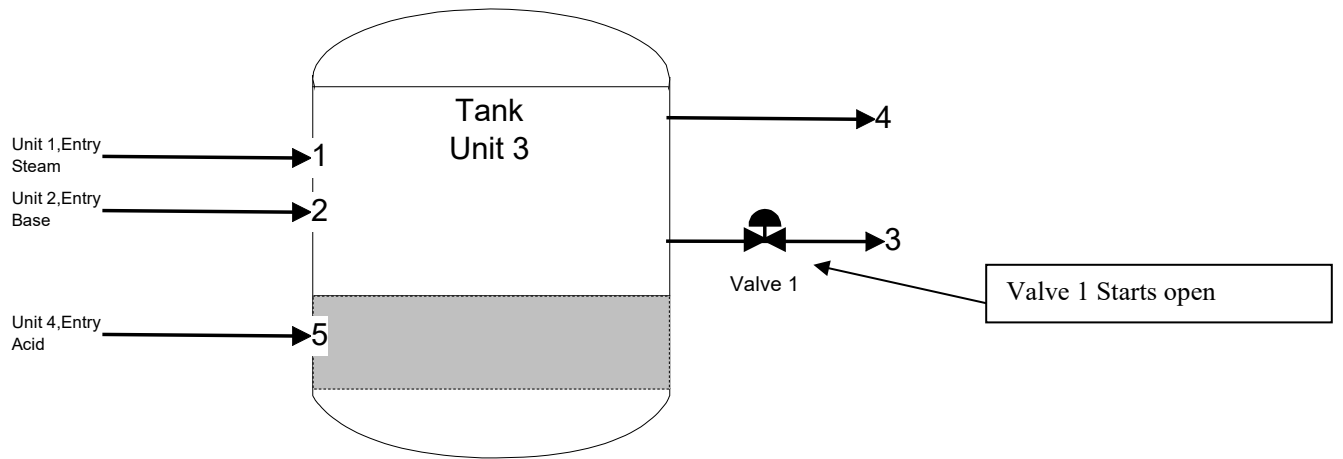


Figure 2-28 Adding Valve 1

Note: the current valve number is displayed on the top line.

The default valve override is 0. You will change the value to 1 here.

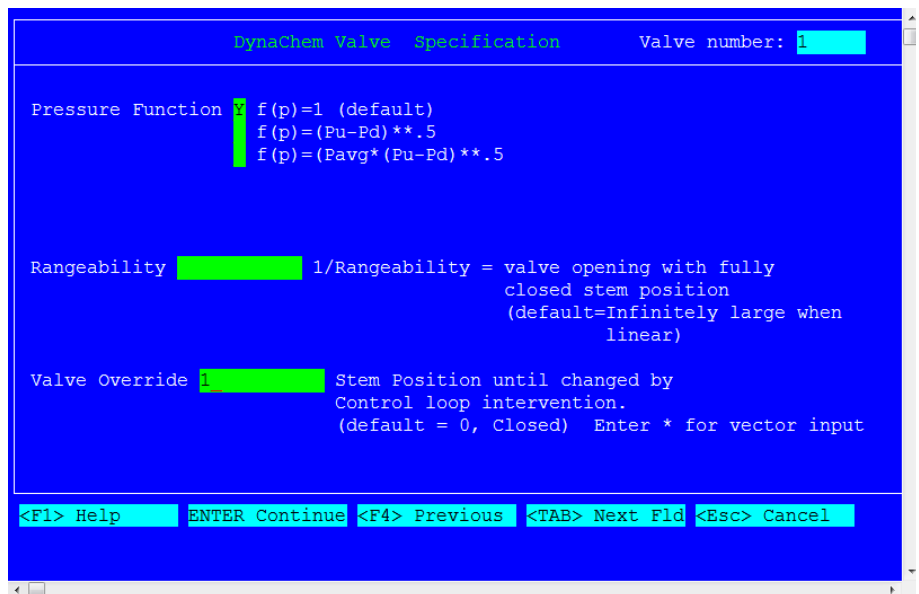


Figure 2-29 Specifications for Valve 1

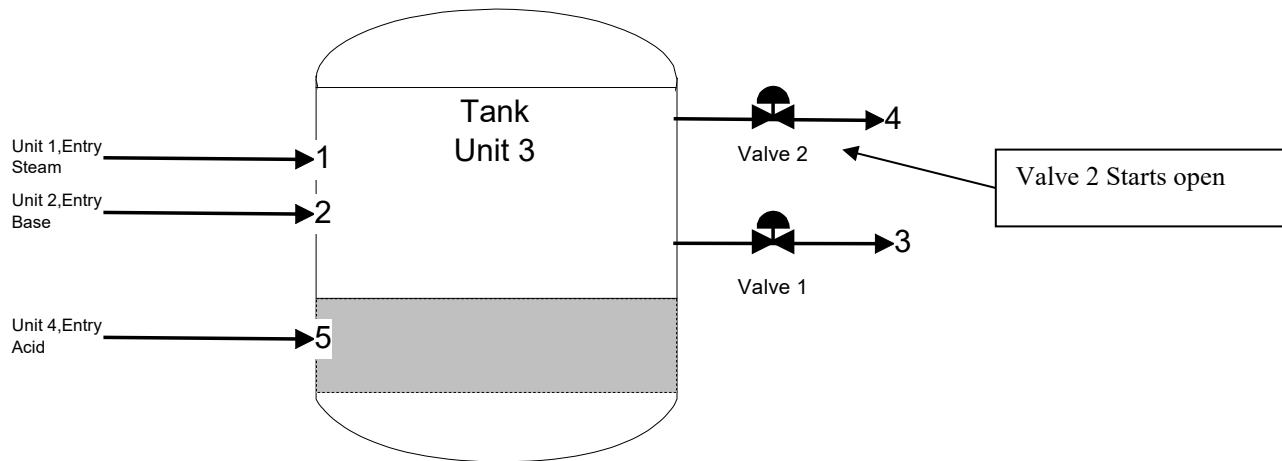


Figure 2-30 Specifying Valve 2

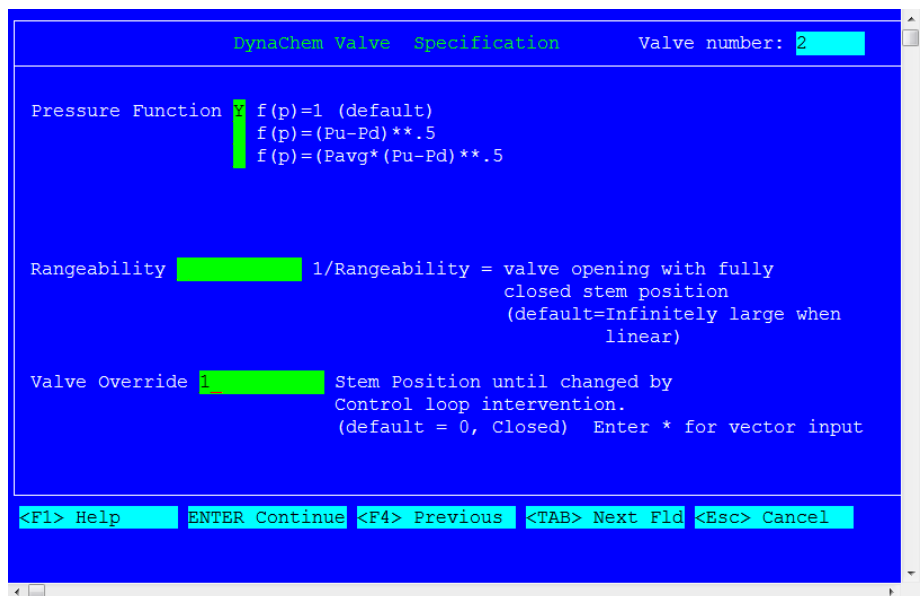


Figure 2-31 Specifications for Valve 2

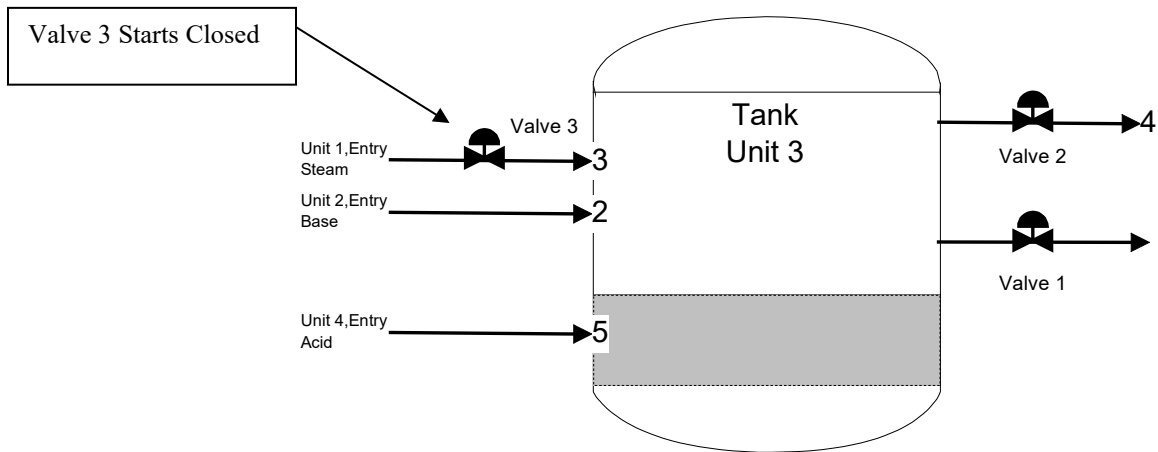
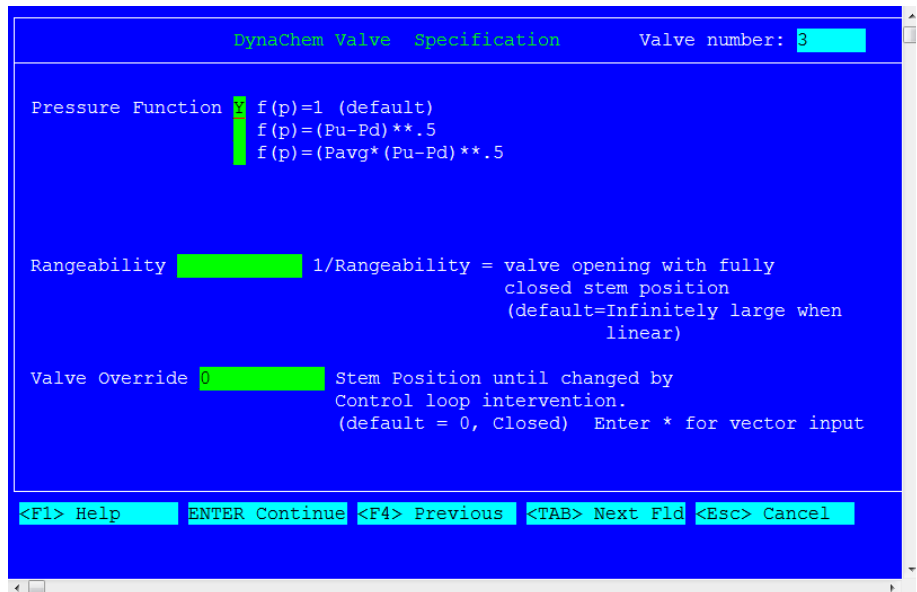


Figure 2-32 Specifying Valve 3 (starts Closed)



Note: we are using the default of zero for this valve.

Figure 2-33 Specifications for Valve 3

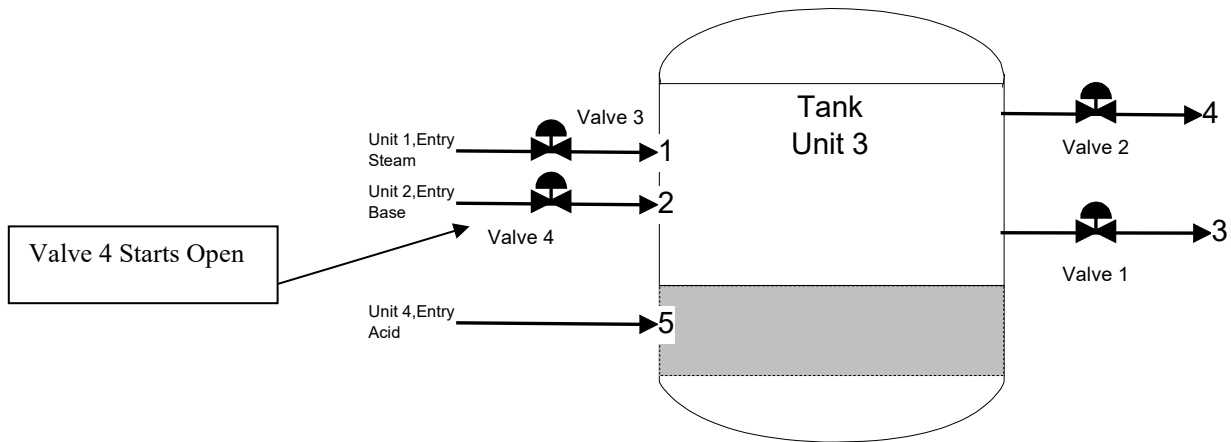


Figure 2-34 Specifying Valve 4

Once again we are using 1 to override the default of 0

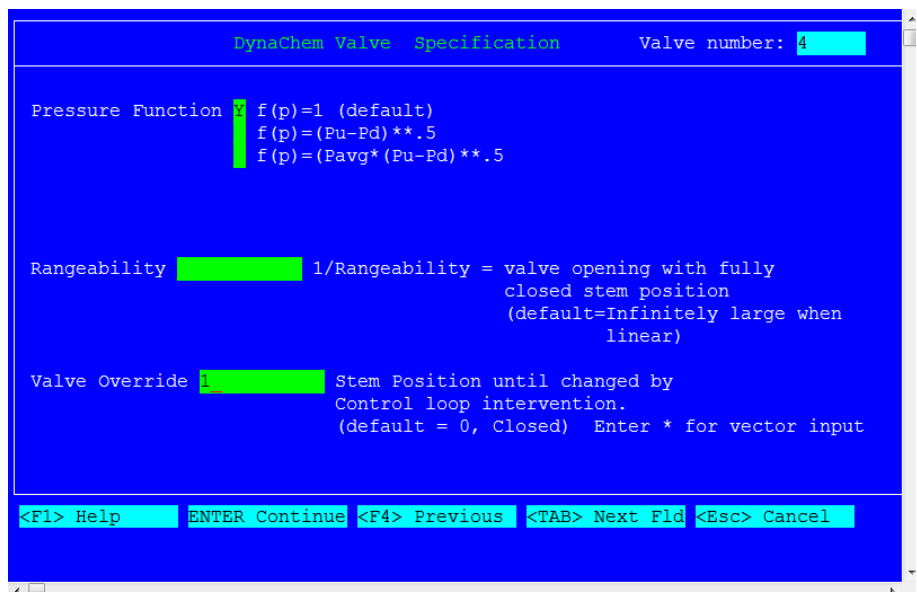


Figure 2-35 Specifications for Valve 4

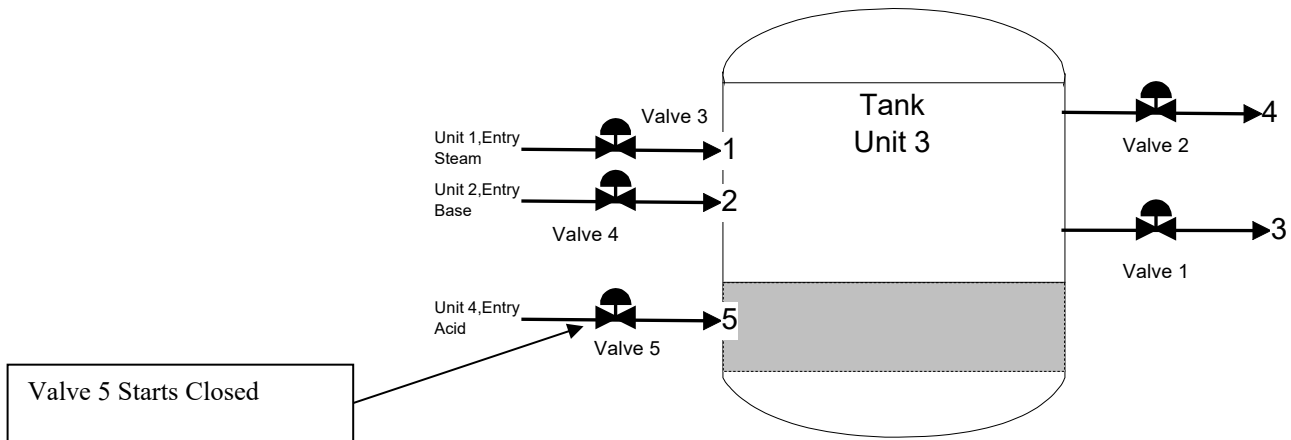


Figure 2-36 Specifying Valve 5 (Starts Closed)

Finally, we again are using the default value.

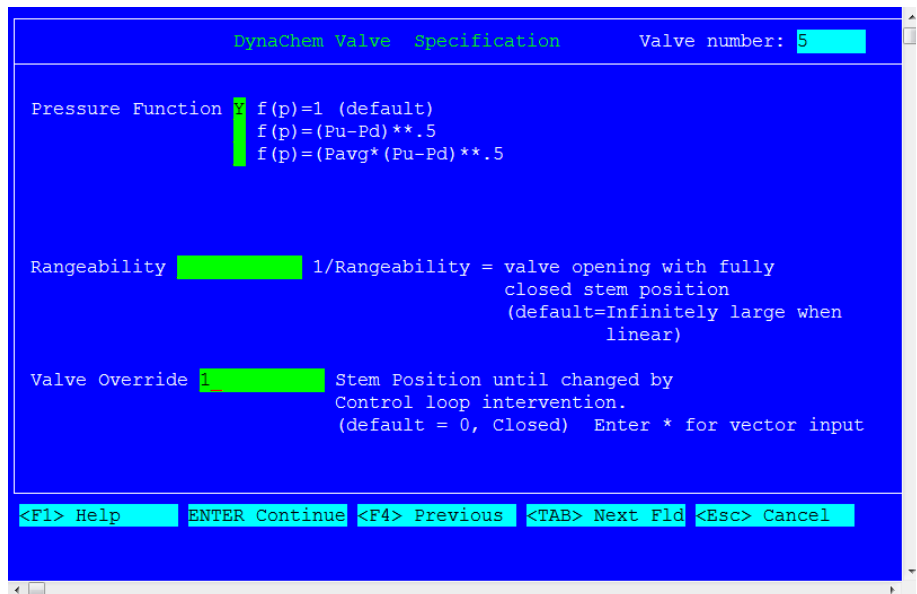


Figure 2-37 Specifications for Valve 5

DynaChem Input Option 5: Pump Specifications

Since there is no pump in the PHDYNA example, just press <CONTINUE> to move to the next data display.

DynaChem Input Option 6: Control Loop Specifications

For the **PHDYNA** example, there are two control loops. One is to control the temperature of the aqueous solution in the tank. The other is to control the pH. You will see three screens with the user entries, shown on the next three pages, for the Control Loop Specifications.

The first screen allows you to enter the Control Loop Number, the Control Loop Output ID Number, and the algorithm type of each control loop. Since Valve 3 controls the flow of steam, the Output ID Number for Control Loop 1 is 3. Likewise, the Output ID Number is 5 for Control Loop 2. For both control loops, the default Velocity Algorithm is chosen.

The second and the third screens prompt for the detailed settings of each control loop. For Control Loop 1, the set point temperature is 75 °C. For Control Loop 2, the set point pH value is 7.0. PI controllers are used for both control loops. The user needs to provide the controller gain and the integral time.

Control Loop No.	Control Valve	Control Loop Output ID Number	Algorithm Type
1	3	3	VELO
2	5	5	VELO

<F1> Help <Page Down> ENTER Continue <F4> Previous <TAB> Next Fld <Page Up> <Esc> Cancel

Figure 2-38 Control loop top menu

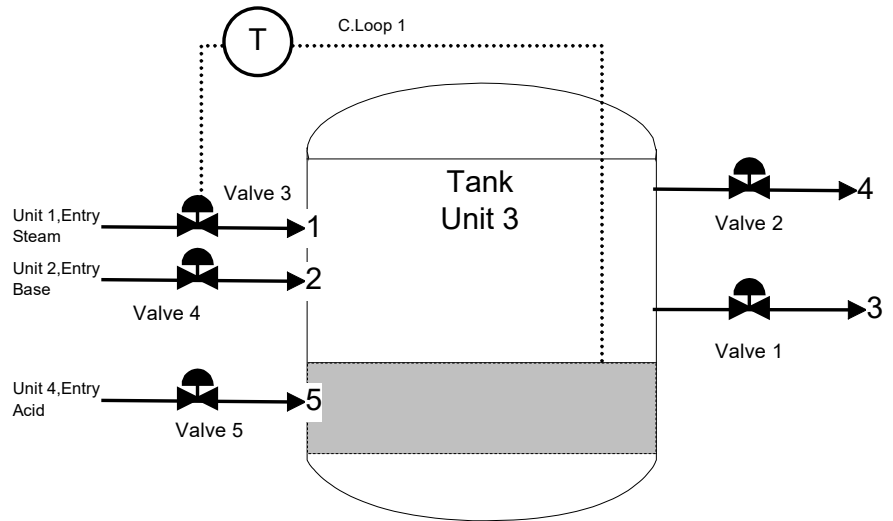


Figure 2-39 Configuring Control Loop 1 (Temperature)

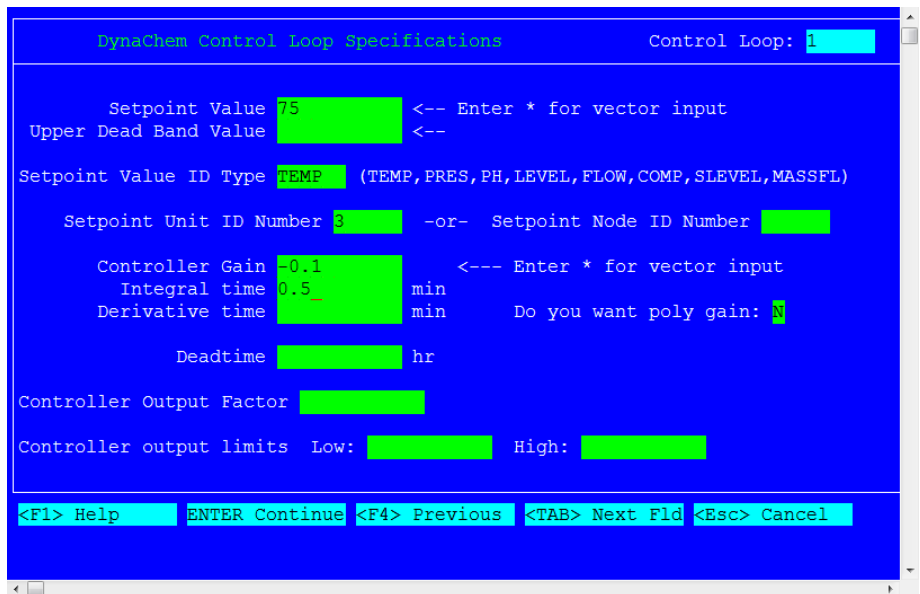


Figure 2-40 Control loop 1, temperature control

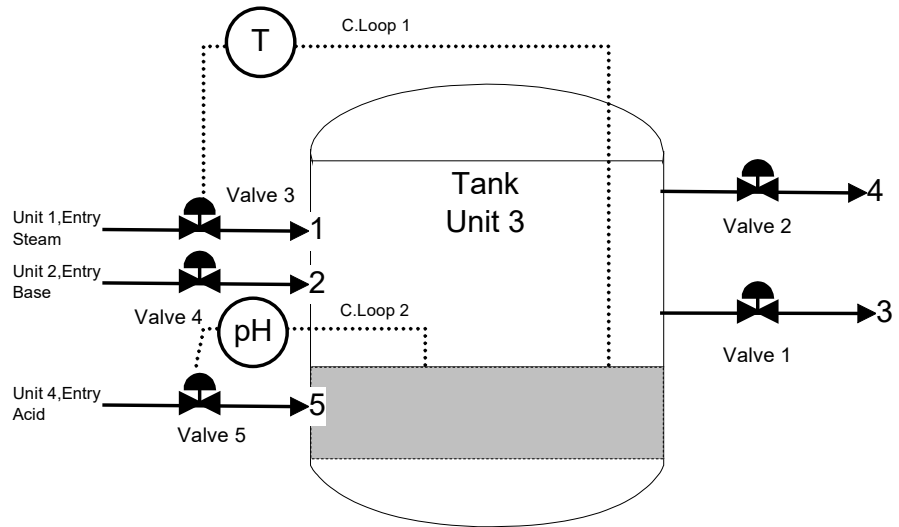


Figure 2-41 Configuring Control Loop 2 (pH)

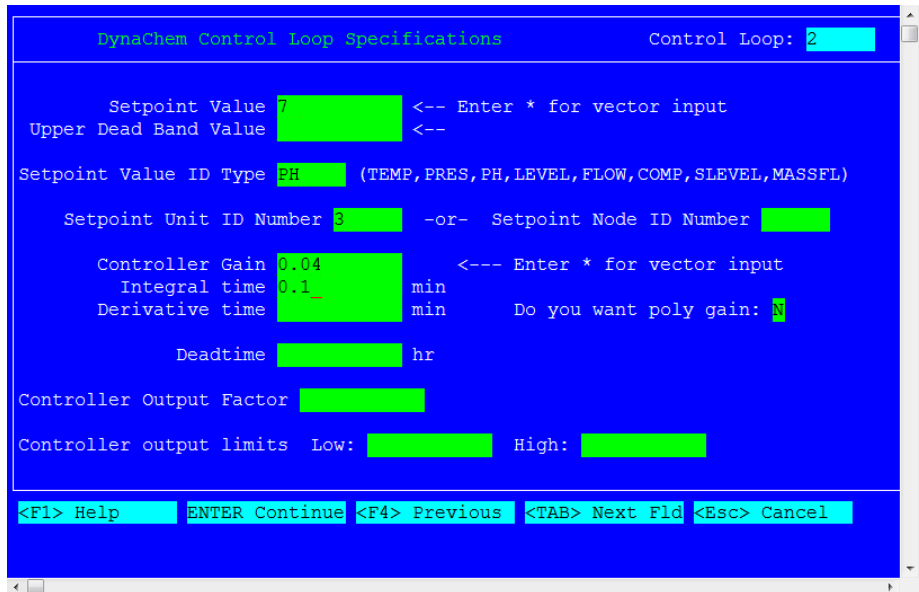


Figure 2-42 Control loop 2, pH control

DynaChem Input Option 7: Calculation Order

After specifying the control loops, you will see the screen for the calculation order. Specification of Node Order determines the order in which all computations are carried out.

As the Node Order may introduce the implicit dead time, the user should carefully examine the computation sequences to achieve the desired simulation. For details on the specification of the Node Order

and the resulting computations, you should refer to the DynaChem Handbook.

The screen should look like this:

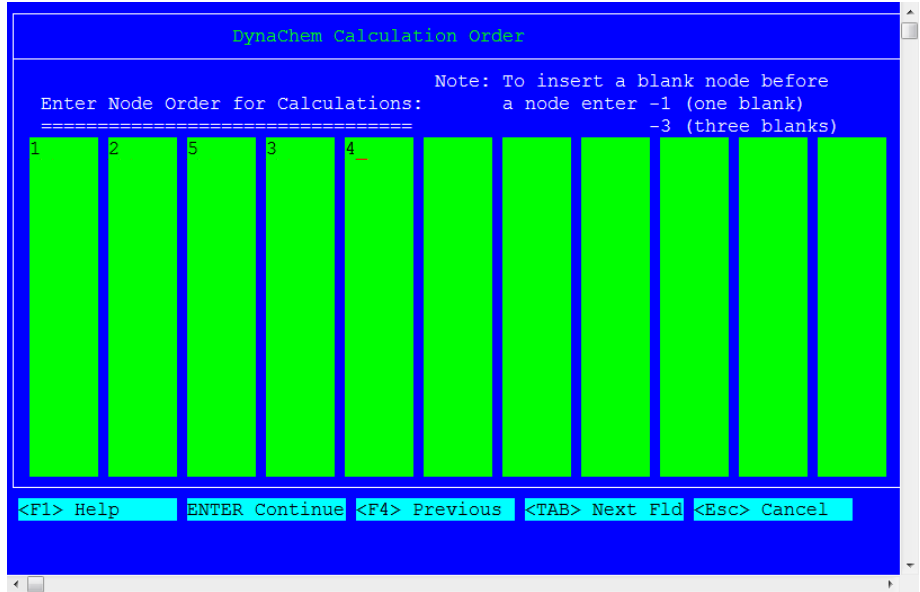


Figure 2-43 Specifying node order

DynaChem Input Option 8: Print Specifications

After the Calculation Order screen, you will see the Print Specifications screen. This screen allows you to set the frequency of printing of output, summary, and "trace" information. Frequency is in terms of number of time increments.

A frequency of 100 time increments is selected for the **PHDYNA** example. Since the standard terminal output is very brief, it is suppressed. The interactive capabilities of DynaChem are invoked. This shifts the user to the screen driven interactive process and allows you to change dynamically the operating and Specification parameters of the system.

The screen, including the user entries, is shown below:

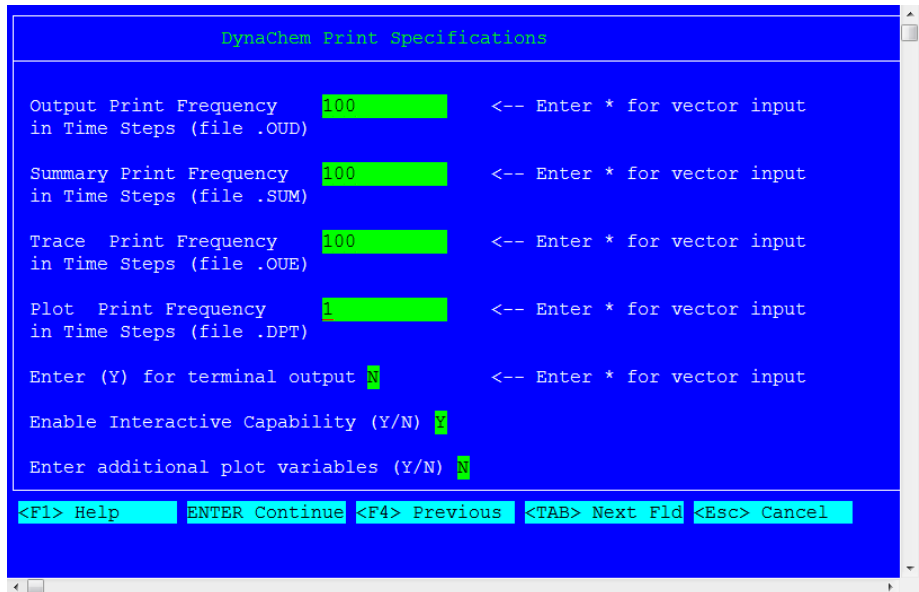


Figure 2-44 Specifying the frequency of output

DynaChem Input Option 9: Log Node Save Specification

Upon leaving the Print Specifications screen, you will see the Log Nodes screen. The Log Nodes capability allows the user to save all of the state variables for the specified nodes at each time step. The saved information may then be used in an ENTRY unit as a feed stream. In the **PHDYNA** example, we are not planning on using the result as input to another execution. Because this is the last screen for the DynaChem case input, pressing <CONTINUE> will return you to the DynaChem Input Menu.

The case description of **PHDYNA** is complete.

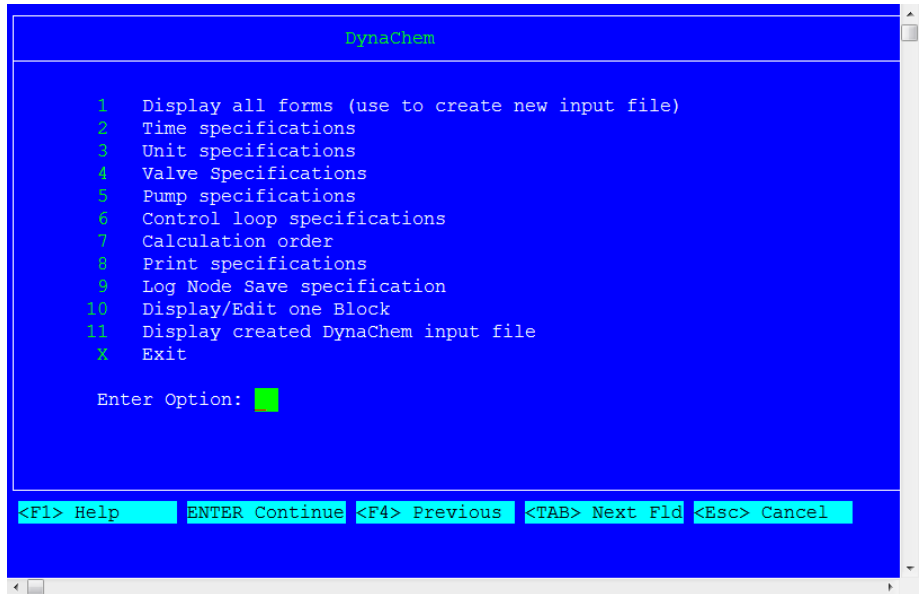


Figure 2-45 DynaChem input menu

Choosing Option 11 on the DynaChem Input Menu will display the case input file. For **PHDYNA**, it should look like:

There is more information available on this screen. Press the <Page Down> key to see the remainder of the file.

***Note:** The DynaChem program continues to undergo development. The numbers, format and content may be different from what is displayed here.*

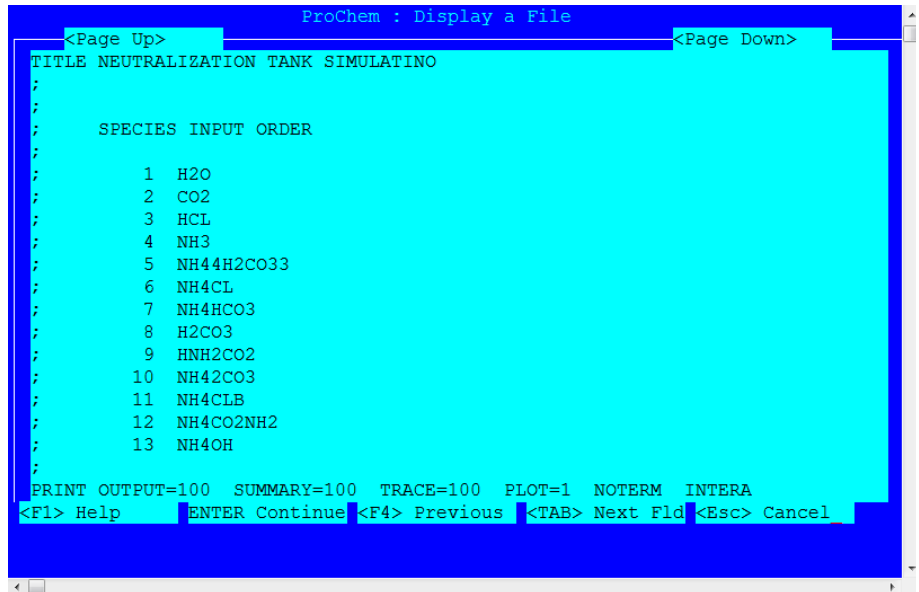


Figure 2-46 Displaying the Input Case

If you are satisfied with the input file that you saw displayed, you can exit this menu using X. ProChem at this time will write the Case Input File to your disk. The name for this file will be **PHDYNA.DIN**.

CANCEL will allow you to leave DynaChem without writing a file.

For the **PHDYNA** example, we do want the Case Input file written to disk. Therefore, enter an X on the Input Menu, and press <CONTINUE>.

Running DynaChem

We have fully defined the DynaChem case input, so the next step is to execute the case.

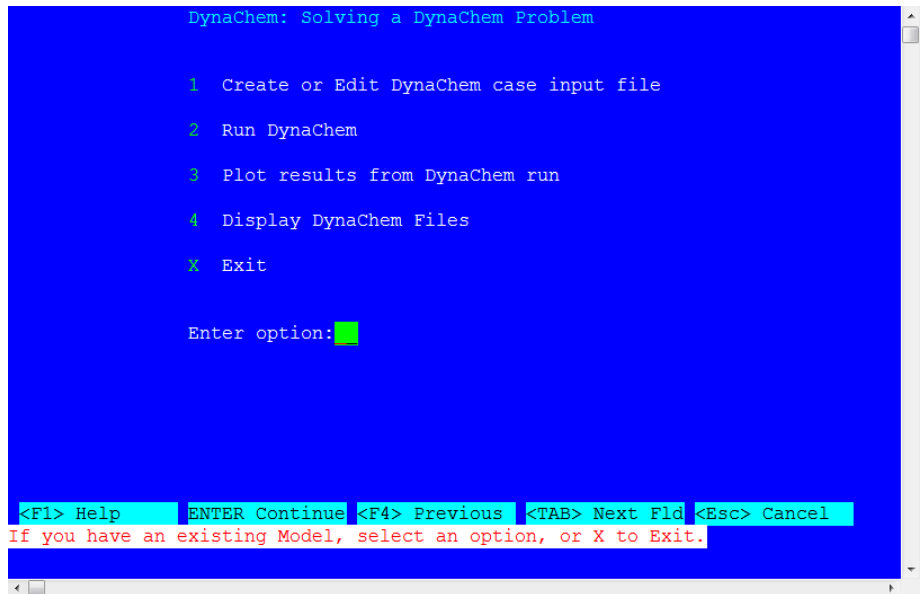
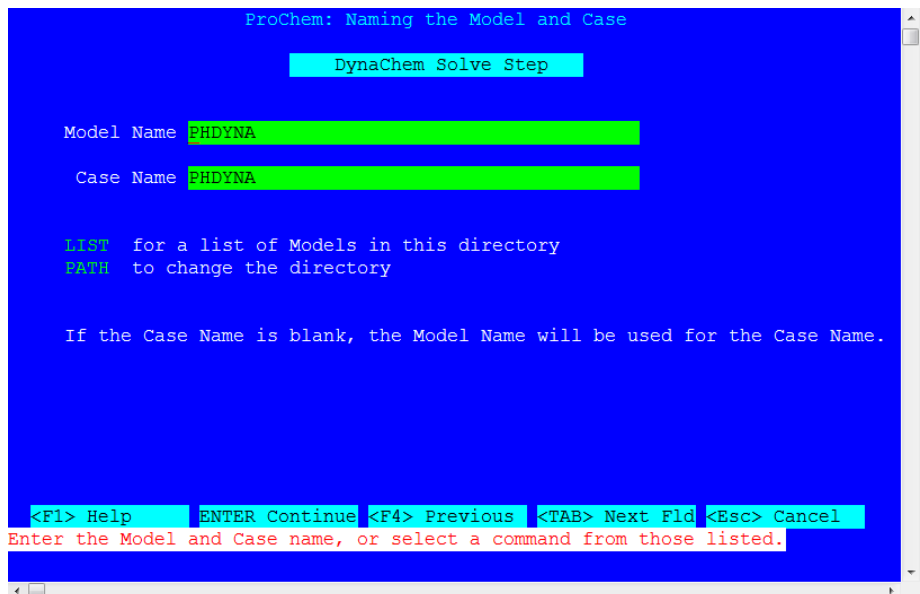


Figure 2-47 DynaChem main menu

Select 2 from this menu, "Run DynaChem", and press <CONTINUE>. The Model and Case name prompts will appear, with **PHDYNA** as the default prompt. In both cases, press <ENTER> to accept the **PHDYNA** name.



Since we have invoked DynaChem interactive capabilities, DynaChem will ask you to initiate execution of the case by making a choice from the following screen.

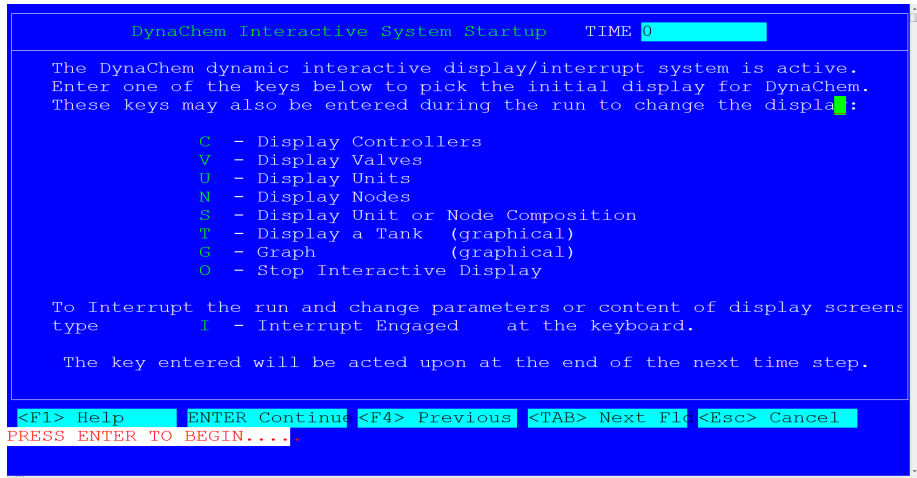


Figure 2-48 The DynaChem startup screen

This menu illustrates DynaChem's highly interactive calculations. Your selection of a particular display (e.g., "T") determines the information which will be displayed as the time dependant simulation proceeds. Regardless of the choice, the information on the particular display will be updated (refreshed) every time step. Once execution is initiated, the user can type any of the display keys noted on the menus (e.g., "G") and the alternative display is provided to the user.

In addition to the selection of a display, DynaChem has another very important feature; the ability to interrupt and suspend execution. At the time of such a suspension, the user can either display various information or, if desired, actually alter simulation parameters, unit configurations, display characteristics, etc.

To better illustrate all of this, please carry out the following sequence of entries:

- 1) Enter the letter T followed by <CONTINUE> as indicated on the menu.
- 2) You will now see a tank displayed. The tank will begin to fill. If you have a color monitor, the contents of the tank will be blue to reflect the initially basic pH of the system. The actual time, in hours, will be shown on the upper right corner of the screen. The pH will be displayed along the bottom. Flow rates and the

temperature and the volume of the liquid in the tank will also be displayed. Watch the valve movement on the lowest and uppermost feed streams. The valve stems will open and close to reflect the actions of the automatic controllers. Eventually you will see the tank fill to the level of the first exit stream and then the contents will go to neutral (yellow), overshoot to acid (red) and then back to neutral.

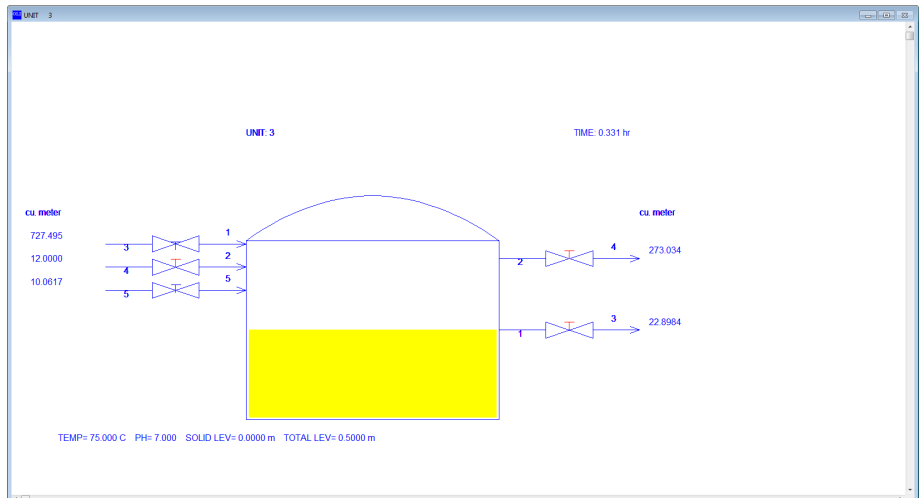


Figure 2-49 The DynaChem tank display

3) When time is about .1 hours, simply type the letter I and DynaChem will interrupt the execution. A menu offering various choices will then be displayed. This menu is shown on the next page.

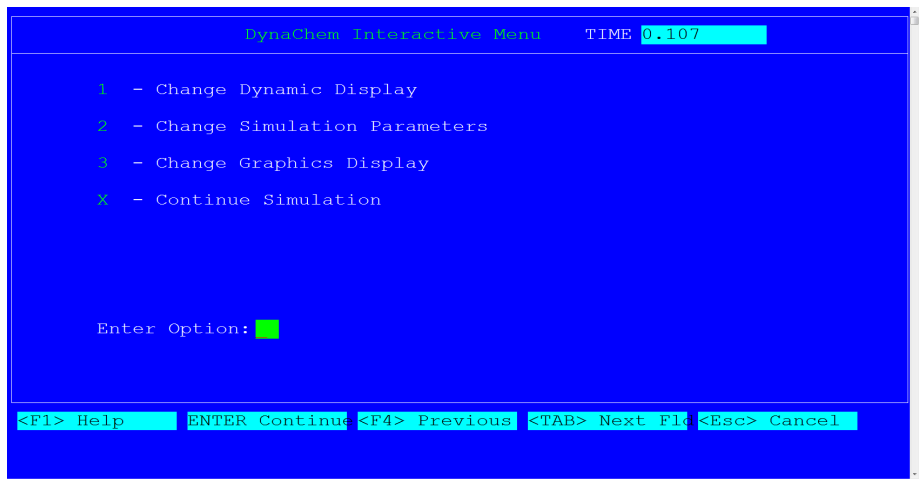


Figure 2-50 The Interactive Menu

To configure the Graphical Display to plot the pH and pH set point vs. time, simply type the number 3 and DynaChem will display a Plot Form.

The Plot Form should be set to the following values:

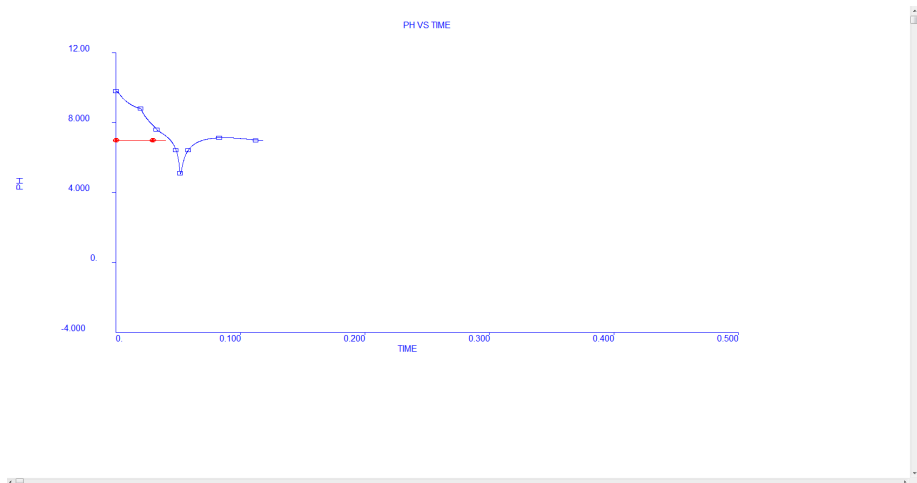
```

ProChem: Plot Form
TITLE-1 PH VS TIME
TITLE-2
X-LABEL TIME
Y-LABEL PH
X-SCALING MAN Y-SCALING MAN GRAPHICS DEVICE SCREEN
X-MINIMUM 0.0 Y-MINIMUM -4.00000
X-MAXIMUM 0.50000 Y-MAXIMUM 12.00000
X-SCALE TYPE LINEAR Y-SCALE TYPE LINEAR PLOT TYPE 2
X-AXIS VAR Y-AXIS VAR PARAMETRIC VAR VALUE
TIME PH UNIT
CSETPT CLOOP
OPTION: 1 Plot 2 Display Data 3 Excel 4 Display Params
5 Define Variable 6 Save 7 Recall Plot 8 Options 9 User Data
X Exit
<F1> Help ENTER Continue <F4> Previous <F3> Main Menu <Esc> Cancel
CHOOSE AN OPTION BETWEEN 1 AND 9, OR X TO EXIT

```

Figure 2-51 The DynaChem plot entry form

To restart the execution, exit the plot Form Screen and then the DynaChem Interactive Menu by **Entering** an X. On the graph you can read the time of the simulation right from the X-axis. The graph itself will **<CONTINUE>** to be drawn as the simulation Continues



When the time is at about 0.2 hours, simply type the letter I and DynaChem will interrupt execution. A menu, offering various choices will then be displayed.

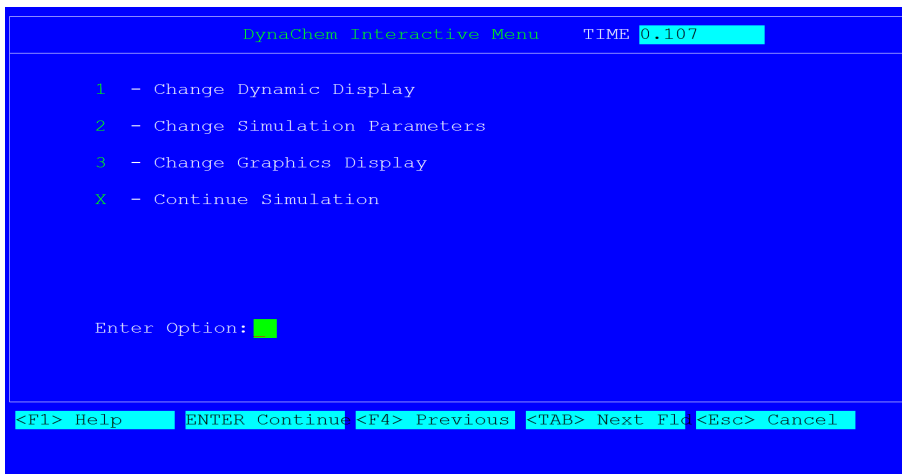


Figure 2-52 The interactive menu.

The DynaChem interactive menu offers a number of options. One of the most interesting is the ability to change simulation parameters. Please enter a 2, and the following menu will be displayed:

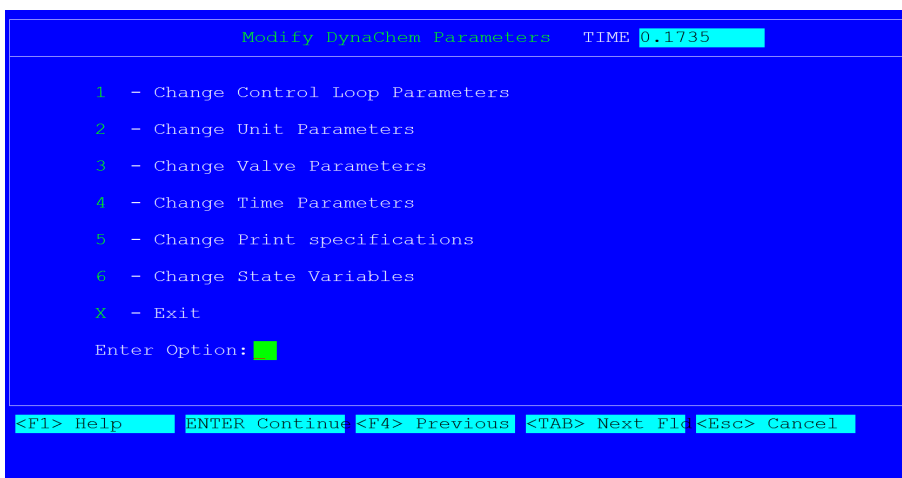


Figure 2-53 Modifying parameters while DynaChem is executing

In this case we wish to alter the set point on the pH controller; therefore we should enter Option 1 on the Modify DynaChem Parameters Menu.

The next screen you will see, as shown below, prompts for the Control Loop ID Number. Because pH is controlled via Control Loop 2, we should enter 2.

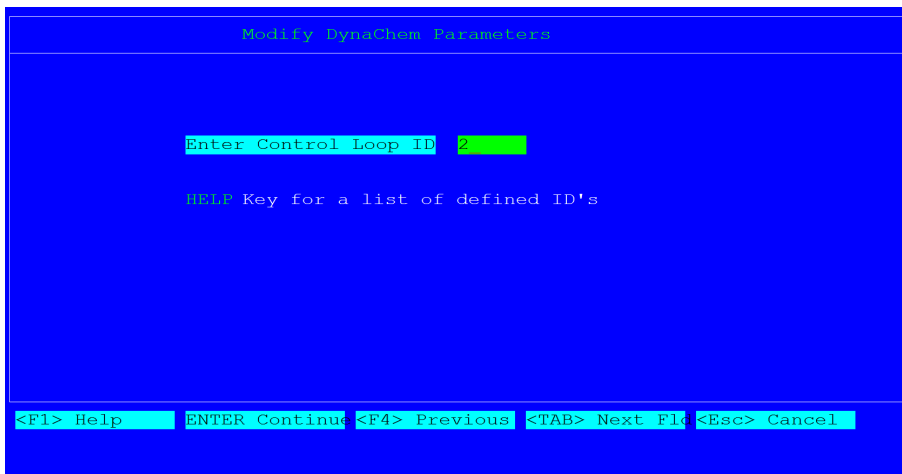


Figure 2-54 Selecting the pH controller (control loop 2)

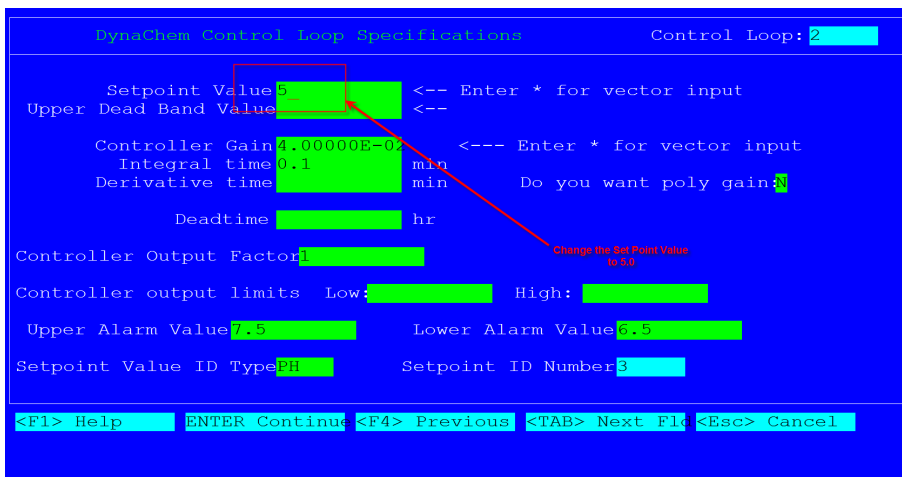


Figure 2-55 Changing the pH set point

To restart execution, we need only exit the Modify DynaChem Parameters Menu and then the DynaChem Interactive Menu by **Entering X**.

If you are in Graphical Display, you will see the pH of the liquid in the tank is dropping and will eventually be maintained at 5.0. The real time to reach the set points will be considerably less than the 0.5 hour. After the set points have been reached, you may allow the simulation to continue through the 0.5 hour requested or stop the simulation by first typing I and then pressing Esc.

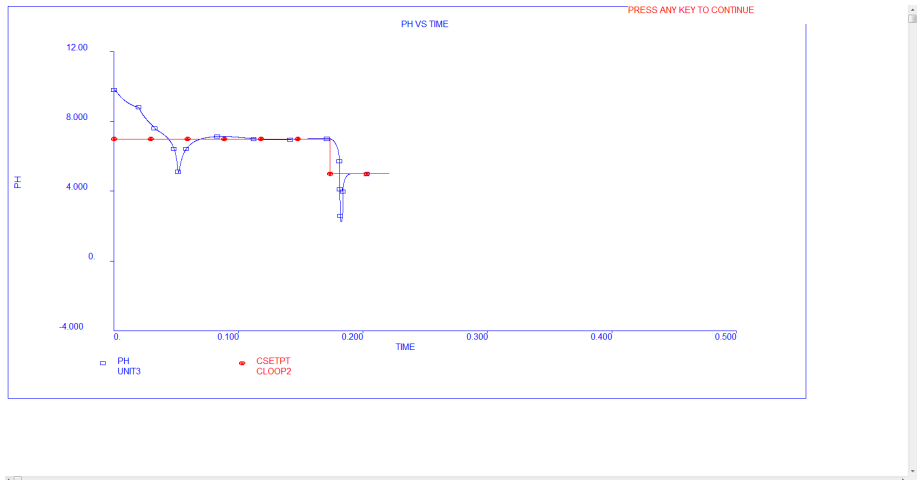
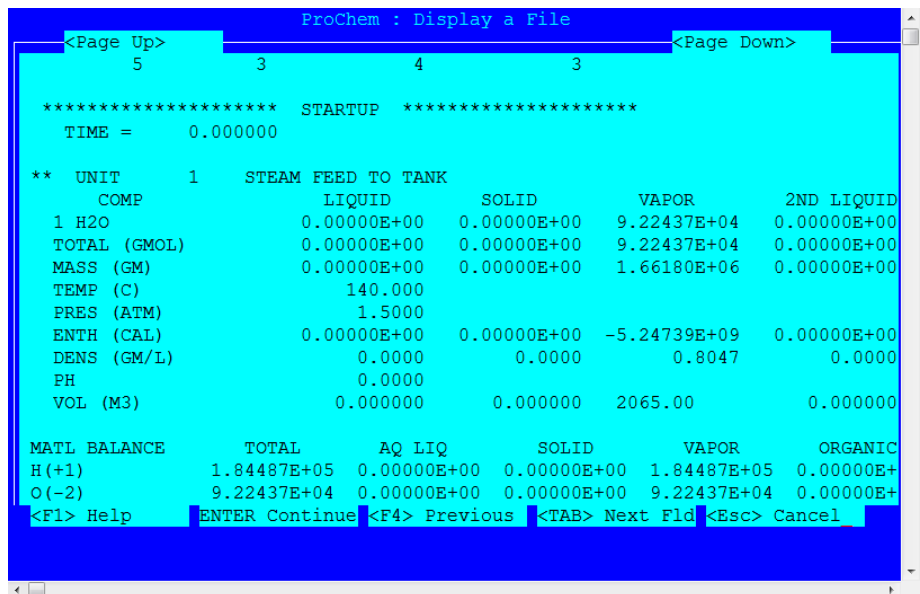


Figure 2-56 Response of pH controller after set point change

Since DynaChem is a dynamic simulator, it is quite important that DynaChem save the results of the important state variables at each time increment. At the completion of the run, the user will return to the DynaChem Menu. The DynaChem results are saved in a file with the file extension DOU. You can choose Plot, Option 3, to look at the profiles, or you can choose Option 4, and browse through the **PHDYNA** output (DOU) file.



2-57 The DOW file, we have used the page down function to show more of the file

