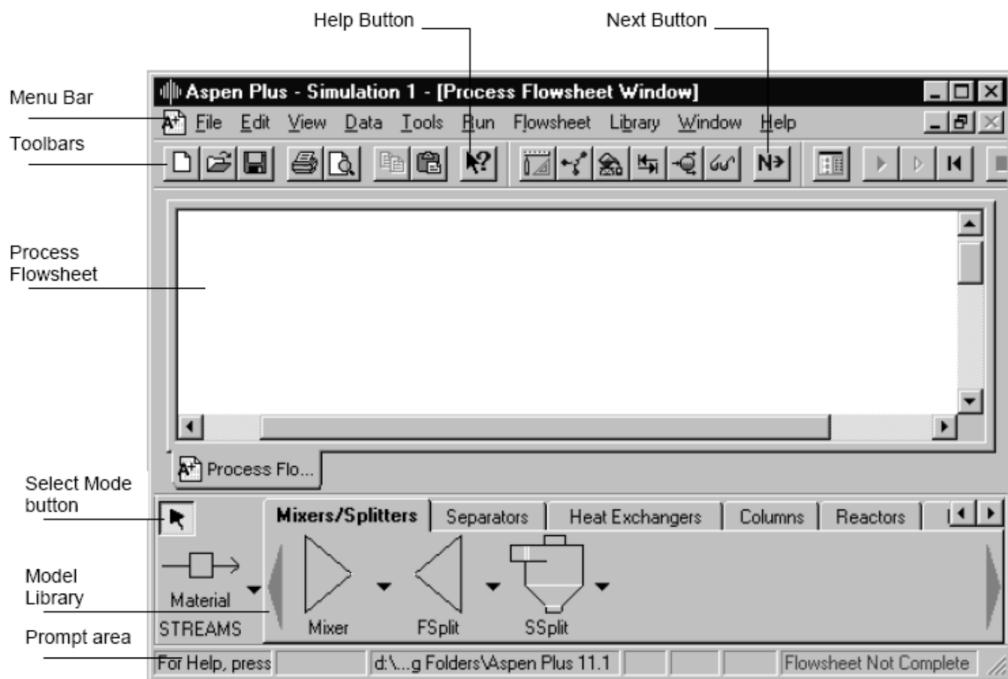


Exercise I: Introduction to Aspen Plus Graphic User Interface

Basic Graphic User Interface: This topic leads you through an Aspen Plus simulation to explain how to open a file, enter data, run a simulation, and examine results.

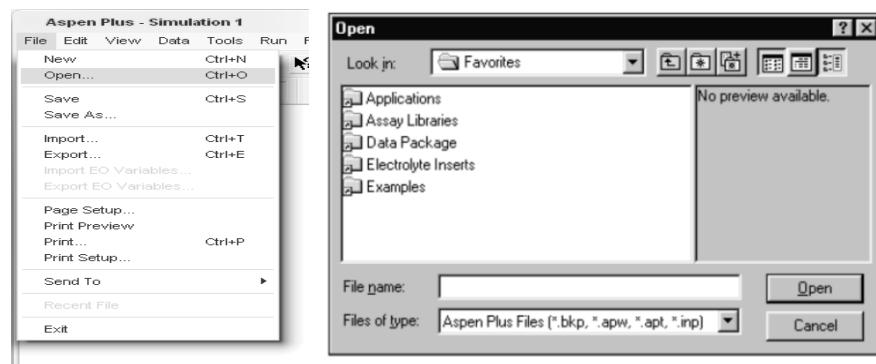


Opening an Existing Simulation and Running It:

File → Open

And Go to

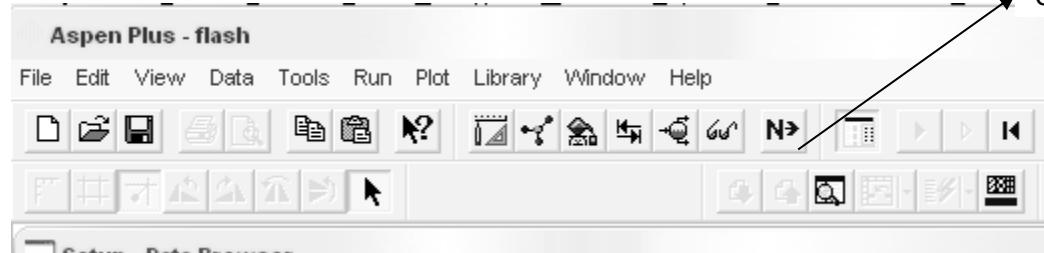
Program files → Aspen Plus 11.1 → Favorites → Examples → flash.bkp



If it asks to close the current run before opening the new run click → **NO**

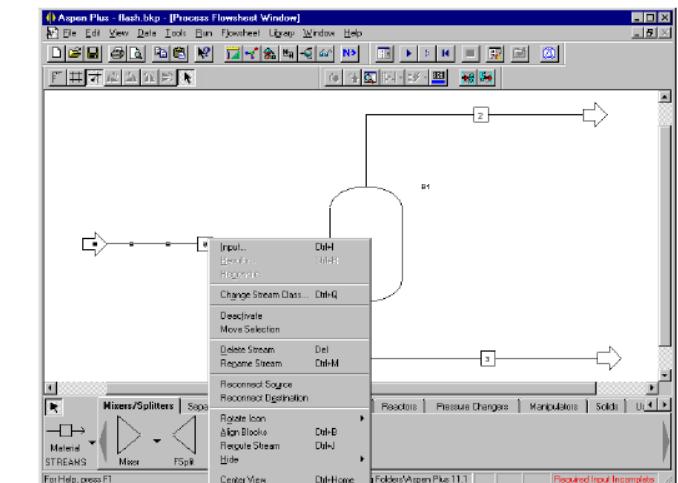
Process flowsheets display streams and unit operation blocks. The Flash simulation has one feed stream (stream 1), two product streams (streams 2 and 3), and one unit operation block (BI).

Giving Title and Name of the Particular Person:

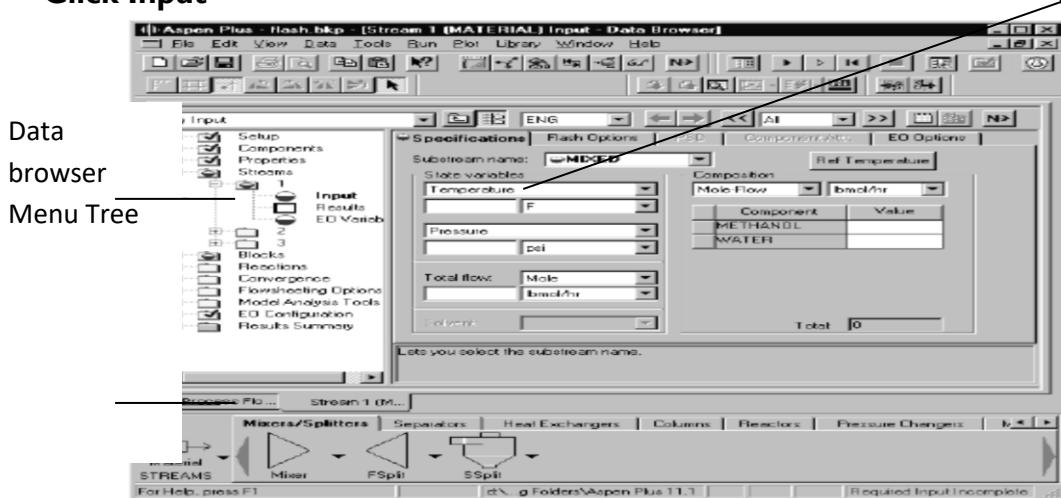


Click Setup → Accounting → Give: User Name & Project Name

Entering Data:



Click Input



Getting Help:

- Click , then click the box or sheet.

Parameter	Value	Units
Temperature	180	F
Pressure	20	psi
Methanol mole-flow	50	lbmol/hr
Water mole-flow	50	lbmol/hr

Leave Total moles empty and other options as default

When all required specifications have been entered, a check mark (✓) appears on the tab containing the sheet name. Check marks also appear in the Data Browser menu tree.

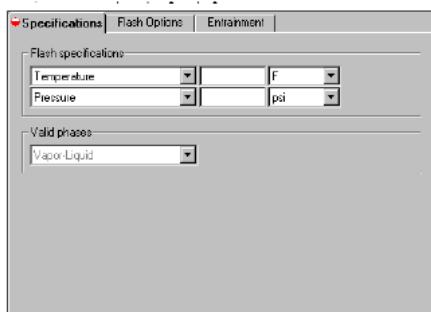
Expert Guidance - the Next Function

The Aspen Plus expert system, known as the **Next** function, guides you through all the steps for entering specifications for your simulation model. The **Next** function:

Click Next Function → .

- Guides you through the required and optional input for a simulation by displaying the appropriate sheets.
- Displays messages informing you what you need to do next.
- Ensures that you do not enter incomplete or inconsistent specifications even when you change options and specifications you have already entered.

After Clicking NEXT FUNCTION:



If you click Next function without completion error message will come.

Entering the specifications:

Heat duty	0 Btu/hr
Pressure	1 atm

Running the Simulation:



Examining Stream and Block Results

Click Check Results Button to View the Result Information-----



Property	Value
Temperature F	180.3
Pressure psi	14.70
Vapor Frc	1.000
Mole Flow lbmol/hr	10.757
Mass Flow lb/hr	308.627
Volume Flow cuft/hr	4908.881
Enthalpy MMBruthr	-0.963
Mole Flow	
METHANOL	8.262
WATER	2.494

Problem 1:

Now Change the Temperature to 90 degree centigrade (Right Click Stream 1 → Click Input → Change Temperature) and run the simulation view results.

In Second stream water will be less and Methanol will be more (Due to the raise in feed temperature some part of methanol will come our as vapors).

Problem 2:

Now change the temperature of Flash chamber to 83 degree centigrade and input feed temperature as 180 F and 20 PSI pressure.

Problem 3: Modifying the Methanol and Water Composition and Running It.

Methanol -60 and Water - 40.

Saving the file:

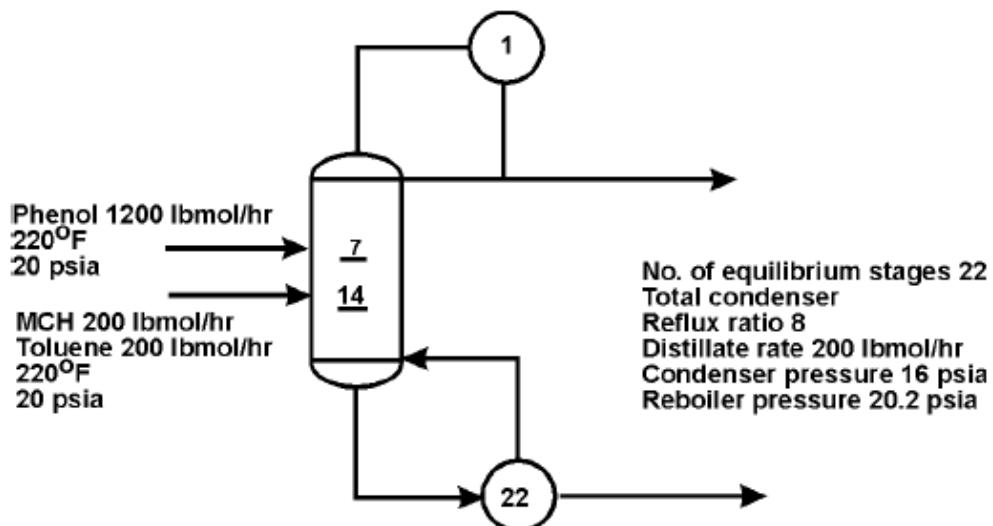
Click Tools → Options and see that “Always create backup copy” → *.apw (activated)

Click file → Save as → type name flash and save

(Aspen Plus will place a file called **Flash.apw** and a file called **Flash.bkp** in your Aspen Plus working folder)

Click File and Exit.

Exercise 2: Building and Simulation a Process Flow Diagram



MCH and toluene form a close-boiling system that is difficult to separate by simple binary distillation. In the recovery column in Figure 3.1, phenol is used to extract toluene, allowing relatively pure methylcyclohexane to be recovered in the overhead. The purity of the recovered methylcyclohexane depends on the phenol input flow rate. In this session, create an Aspen Plus simulation that allows you to investigate the performance of the column.

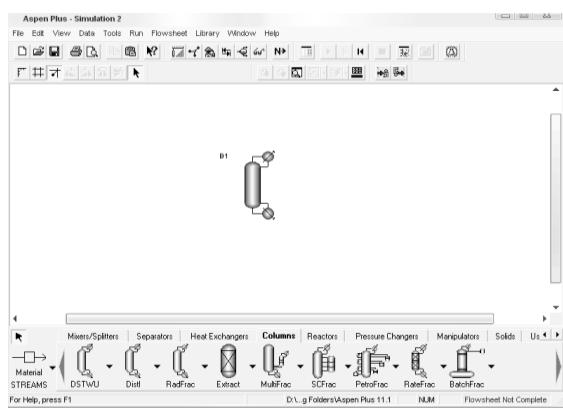
In this simulation, create an **Aspen Plus** process model for a **Methylcyclohexane (MCH)** recovery column

This simulation is divided into three sections:

1. Building the Process Model.
2. Adding Data to the Process Model.
3. Running the Simulation.

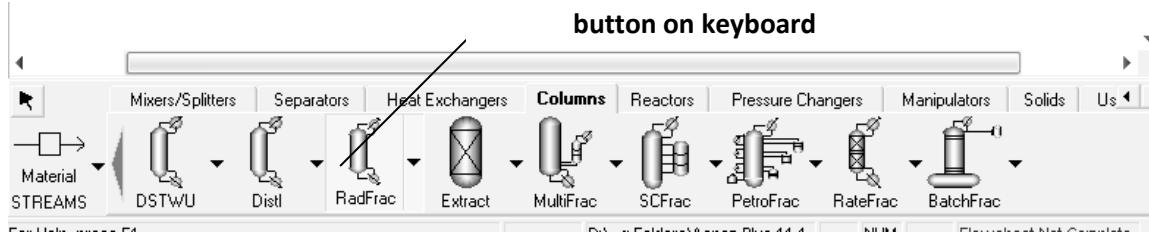
Start Aspen Plus New Project and select general with English Units

Select Columns Tab → Radfrac box → Click on Radfrac and drag it to the main window

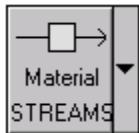


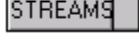
Click help  and Click on Radfrac in Columns Tab and try to read the Radfrac explanation in the help window.

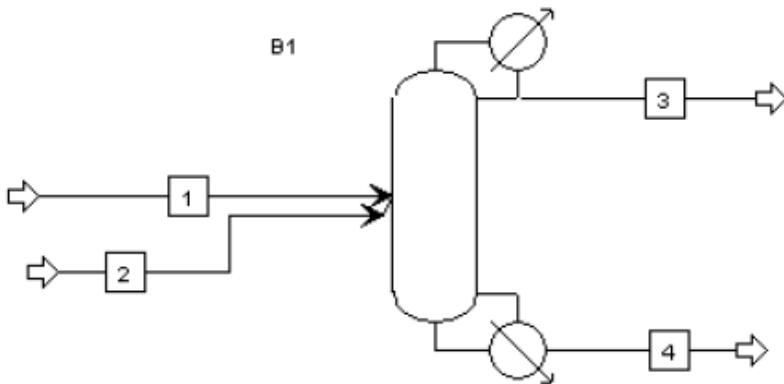
**Click on Radfrac and press F1
button on keyboard**



To Connect Streams to the Block:



Click  and try to connect the streams.



Click  to stop adding streams.

Click on the numbers → Right Click → Click Rename

Phenol	First Stream
MCH	Second Stream
Distil	Third Stream
Residue	Fourth Stream

Click Data and Date Browser which is helpful to enter our required data.

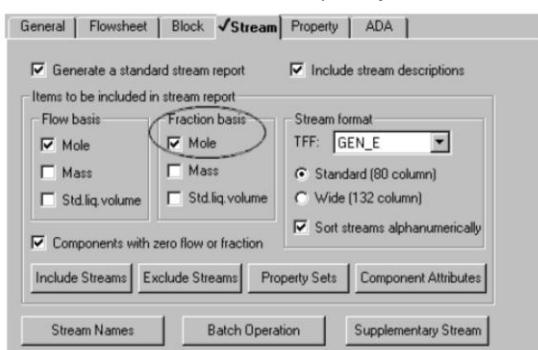
Specifying a Title for the Simulation

Click Data→Data Browser→Setup Option→Click Specifications→

Enter Title of the project as “Simulation of MCH” → Click Accounting→Enter your Name and Project Title.

Specifying Data to be Reported

Setup →Report Options→Streams tab→Fractions→Mole.
(Output will be in moles)



Setting Property Set

Click Property Set and there you can find five properties are available to know more about property sets.

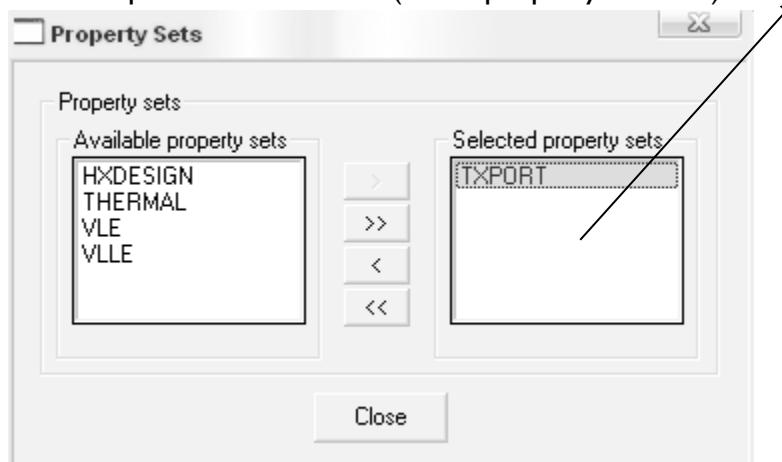
Click Help→Search → type the first property “Hxdesign”

Property Set	Description
HXDESIGN	Thermal and transport properties in SI units needed by heat exchanger design programs and Aspen Pinch, including: Mass vapor fraction Mass flow rate for total, vapor, and liquid phases Mass enthalpy for total, vapor, and liquid phases Mass density for total, vapor, and liquid phases Mass heat capacity for total, vapor, and liquid phases Pseudo-critical pressure for total, vapor, and liquid phases Viscosity for vapor and liquid phases Thermal conductivity for vapor and liquid phases Average molecular weight for total, vapor, and liquid phases Thermal properties, including:
THERMAL	

Read all property sets and try to find our suitable property set for our simulation process.

For our simulation let us consider “Txport”.

Click “Texport” and click Add (in the property window)



Add Button

Click Close.

Entering Components

Click Next button.

Click Find → Type “Toluene” → Click “Find Now” → Select Toluene (in selection window) → Click “Add”.

Click Find → Type “Phenol” → Click “Find Now” → Select Phenol (in selection window) → Click “Add”.

Again Type “Methylcyclohexane” → Select and Click ADD.

Component ID	Type	Component name	Formula
TOLUENE	Conventional	TOLUENE	C ₇ H ₈
PHENOL	Conventional	PHENOL	C ₆ H ₆ O
MCH	Conventional	METHYLCYCLOH	C ₇ H ₁₄ -6

Re-order Components

Components order

- TOLUE-01
- PHENO-01
- METHY-01

Close

After addition, click Reorder if the order is missing.

Selecting Thermodynamic Methods

Click Next button.

The screenshot shows two side-by-side configuration dialogs for 'Property methods & models'.

Process Type Dialog:

- Process type: ALL
- Base method: ALL
- Henry components: REFINERY, GASPROC, PETCHEM, CHEMICAL, COALPROC, POWER, SYNFUEL, ENVIRON, WATER, METAL, POLYMER, ELECTROL, TSWEET
- Free-water method: Water solubility
- Electrolyte calculation: None selected
- Chemistry ID: None selected
- Use true-component

Base Method Dialog:

- Process type: ALL
- Base method: ALL
- Henry components: AMINES, APISOUR, B-PITZER, BK10, BPSIDEAL, BWR-LS, BWRS, CHAO-SEA, ELECNRTL, ENRTL-HF, ENRTL-HG, FACT, GRAYSON
- Petroleum calculation: None selected
- Free-water method: Water solubility
- Liquid enthalpy: None selected
- Liquid volume: None selected
- Poynting correction
- Heat of mixing

For getting explanation about these process types and base methods

Process type Help:

Click Help→Help topics→Search→Type one Property type “Refinery” and press enter
Click “Recommended property methods for different applications”.

Try to read all property methods and choose the best one related to our simulation.

Base Method Help:

Click Help→Help topics→Search→Type “property methods” and press enter.
Click on “Available Property Methods”

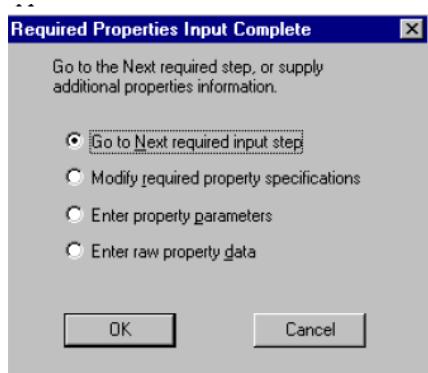
In that click on each property method and click on “Activity property method”

For using most popular “Redlich-Kwong” Equation we have to select “UNIFAC” in Base Method options.

Go to Help and type “Choosing property method” and click on “Choosing a property method” → Click “Recommended property method for different applications”.

After entering “UNIFAC” in base methods option and process type “All”.

Click Next  button.



Entering Stream 1 Data: Press OK.

Parameter	Value	Units
Temperature	220	F
Pressure	20	psi
Toluene flow rate	200	lbmol/hr
MCH flow rate	200	lbmol/hr

Click Next:

Entering Stream 2 Data:

Parameter	Value	Units
Temperature	220	F
Pressure	20	psi
Phenol flow rate	1200	lbmol/hr

Click Next (Click Help button  and click on each block for explanation)

We have to calculate all these parameters for that equipment

Parameter	Value	Units
Number of stages	22	—
Condenser	Total	—
Distillate rate	200	lbmol/hr
Reflux ratio	8	—

Click Next Button: Enter 14 (For Phenol) and 7 (For MCH).

Click Next Button and select Pressure Profile in View option and enter the following numbers as at stage one the pressure is 16 and at stage 22 the pressure is 20.2.

Stage	Pressure
1	16
22	20.2
*	

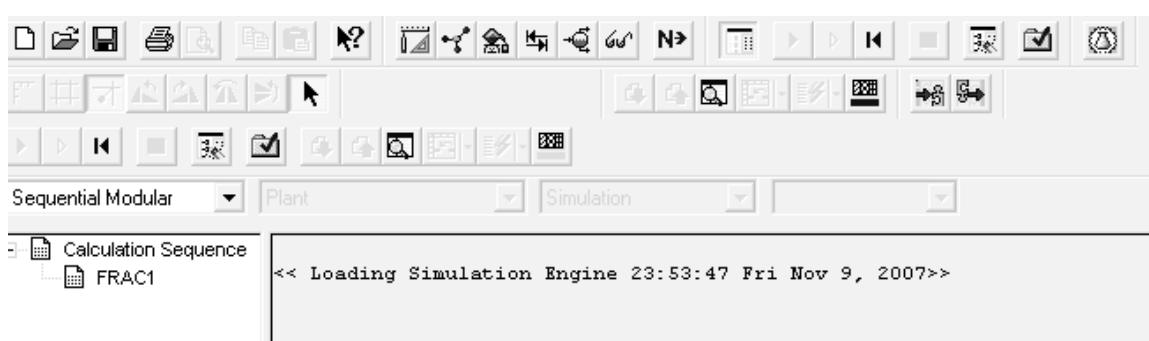
At the bottom right corner see the button “Required Input Complete”



After seeing the window click on Next Button and run the simulation.

After completion of simulation please try to find “Result Available”

Click on button to view the results.



View Results → Click Streams →

Distillate

Entering

Residue

Mole Flow lbmol/hr				
TOLUE-01	41.877	200.000		158.123
PHENO-01	< 0.001		1200.000	1200.000
METHY-01	158.123	200.000		41.877

If you closely observe the results....

See that some quantity of toluene is separated in the residue

Problem 2: Increase the quantity of phenol and run the simulation.

For 2000 lbmol/hr

Mole Flow lbmol/hr				
TOLUE-01	41.419	200.000		158.581
PHENO-01	< 0.001		2000.000	2000.000
METHY-01	158.581	200.000		41.419

For 900 lbmol/hr

Mole Flow lbmol/hr				
TOLUE-01	42.119	200.000		157.881
PHENO-01	< 0.001		900.000	900.000
METHY-01	157.881	200.000		42.119

Problem 3: Increase the temperature and see the removal of toluene in the residue.

Temp 130 degree centigrade

Mole Flow lbmol/hr				
TOLUE-01	41.836	200.000		158.164
PHENO-01	< 0.001		1200.000	1200.000
METHY-01	158.164	200.000		41.836

There is an increase of approx 0.041 lbmol/hr for 1200 phenol feed.

Problem 4: Increase the number of stages and see the output.

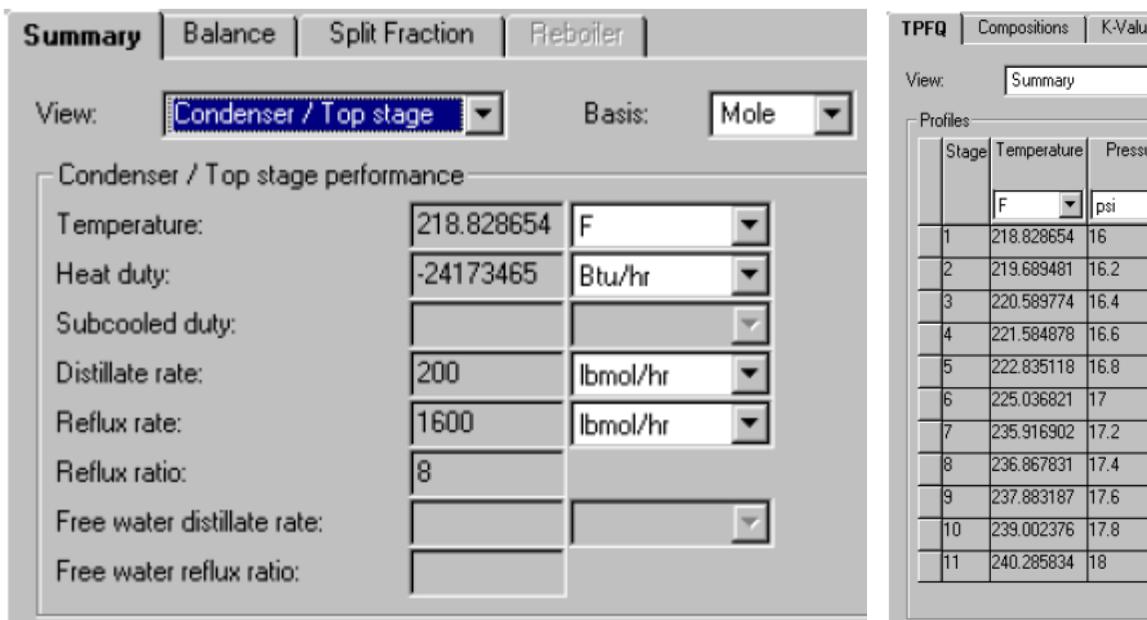
Problem 5: Change the type of boiler used and view the output.

Try to optimize the process and try to get more removal of toluene and finally note down the removal amount.

Examining the Simulation:

Click Results → Click block → View the results.

Click Profiles, to view results.



Creating Reports

File Export → select Report Files → Save.



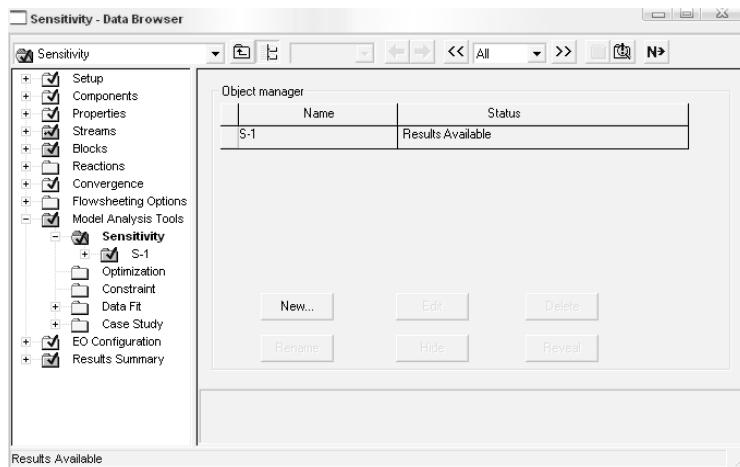
Save your file and exit aspen plus as given in the above section

Exercise 2: Performing a Sensitivity Analysis Using Aspen Plus and visualizing data
One of the benefits of a simulation is that you can study the sensitivity of process performance to changes in operating variables. With Aspen Plus, you can allow inputs to vary, and can tabulate the effect on a set of results of your choice. This procedure is called a sensitivity analysis.

Save Simulation under new name as **mhcnew.apw**

For determining the sensitivity of the distillate (With in the range of Phenol concentration what is the removal of MCH?)

Click Data → Model Analysis Tools → Click Sensitivity.



Click New → Type “S-1” → Click OK.

In the Design Sheet

Again Click New → Type MCHSEN → Click Ok → Select Stream → In reference Area (type option) → Select Mole Flow → Stream “Distill” → in component option “Methy-I”.

Because we want to monitor the MCH concentration in the distillate

For monitoring the condenser properties:

Press Next Button and click New → Type “QCOND”

Select Block → In type option → Select “Bloc-Var” → IN Block Field “Select “Frac I” → Variables (Condenser Duty).

After Completion Click on Variable Name and Click New → Type QREB → Select Block → Type Block Var → IN Block Field “Frac I” → Variable (Reboiler duty). → Close.

Click Next → Type Stream Variable → Stream (Phenol) → Variable (mole Flow) → Overall Range → Lower (1200) and Higher (2000) and Incr (100).

Line 1: Phenol

Line 2: Flow rate

Leave the other parameters as default and click next.

In tabulated form type the words

Column No	Tabulated Expression
1	MCHSEN
2	QCOND
3	QREB

Click Table Format and type the following words.

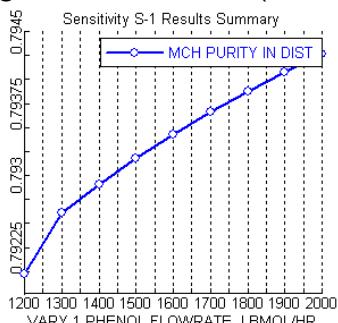
The parameters written in the table will come in the output window.

Specify optional labels				
Column number	1	2	3	
► Column labels	MCH	CONDENS	REBOILER	
	PURITY	DUTY	DUTY	
	IN DIST			
Unit labels				

Close it and run the simulation.

Click Results → Model Analysis Tools → Sensitivity → S-1 and click on results.

For plotting the results Click PHENOL → Select Plot (From the menu) → (X-Variable)
Again Click on MCH (in the table) → Click Plot → Y-Variable → Again click Plot → Display Plot.



Problems: Change the variables and numbers and monitor the concentration of Phenol, in Distillate and Residue etc....

Meeting Process Design Requirements

Open **mch.apw** file (present in example folder)

Give name of the project.

And

Giving Design Specifications and converging them through the specifications.

Click Data → Flow Sheet Options → Design Spec.

Click New → Type DS-1

Entering into design specification windows:

Again Click New → Type XMCH → in reference “Type” Option select “MoleFrac” → Stream (Distillate) → component (MCH).

Click Next to setup design specifications (Input as given in the figure).

Spec:	XMCH*100
Target:	98.0
Tolerance:	0.01

Click Next → in Vary Option (Give inputs as shown below)

Type:	Stream-Var
Stream name:	PHENOL
Substream:	MIXED
Variable:	MOLE-FLO\
Lower:	1200
Upper:	2000
Report labels:	Line 1: PHENOL Line 2: FLOWRA

Creating a Process Flow Diagram

PFD mode: Process Flow Diagram Mode

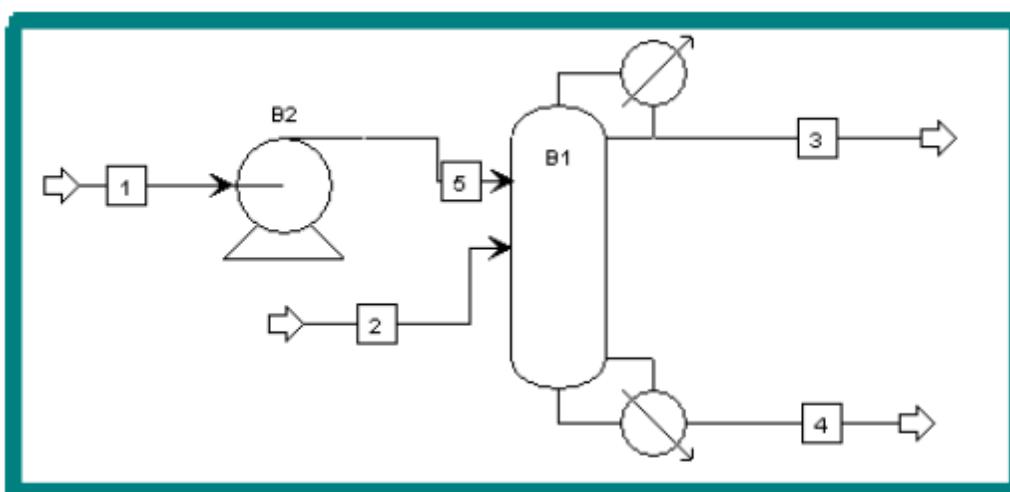
Select View → PFD Mode.

Adding a pump to the diagram → Click **Icon I** in the pump diagram and drag it to the main window.

Click on connection I and right click → Select “Reconnect Destination” → connect to the pump.

Click on materials and connect the pump to the column.

View the final figure:



Displaying Stream Data:

Tools→Options→Result Views→Check Temp and Pressure Options→Click OK.

Adding Stream Table:

View Choose Annotations (See that annotation option is checked)

Data→Result summary→Streams→Click “Stream Table to view it on the flow diagram.

Drawing and Naming:

View Toolbar→ Select Draw→and click Ok

Using drawing “A” symbol you can write any text and drawing ordinary lines is also possible using drawing toolbox.

Adjusting the window: Click View→ Zoomfull. (Drag the components and click Zoomfull to adjust.

Typed Keywords

Final Flow Diagram: Drawing Toolbox

The screenshot shows a software interface for a chemical process simulation. At the top, there is a toolbar with various icons for drawing tools and a font selection bar. Below the toolbar is a table titled "Methylcyclohexane Recovery Process" containing stream data for streams 1 through 4. To the right of the table is a flow diagram labeled "MCH Flow Diagram". The flow diagram illustrates a process flow starting with stream 1 entering a pump (1), then entering a heat exchanger (2) which is cooled by stream 2. Stream 2 then enters a heat exchanger (3) which is cooled by stream 4. Stream 4 exits and is shown exiting the system. Stream 3 then enters a separator (B1). From the separator (B1), two paths emerge: one going to a pump (5) and then to a heat exchanger (2), and another path that exits the system. Stream 5 then enters a heat exchanger (3) which is cooled by stream 4. Stream 4 exits and is shown exiting the system. Stream 3 then enters a pump (1) and returns to the inlet of heat exchanger (2). A legend indicates that circles with numbers represent Temperature (F) and rectangles with numbers represent Pressure (psi).

Methylcyclohexane Recovery Process					
Stream ID	1	2	3	4	
Temperature	220.0	220.0	218.8	325.3	
Pressure	20.00	20.00	16.00	20.20	
Vapor Frac	0.000	0.000	0.000	0.000	
Mole Flow	Ibmol/hr	400.000	1200.000	200.000	1400.000
Mass Flow	lb/hr	38065.736	112935.648	19605.002	121396.382
Volume Flow	cuft/hr	827.446	1792.795	449.995	2314.389
Enthalpy	MMBtu/hr	-12.702	-71.945	-14.509	-62.696
Mole Fw.	Ibmol/hr				
TOLUENE		200.000		5.219	194.781
PHENOL			1200.000	0.262	1199.738
MCH		200.000		194.519	5.481
Mole Frc.					
TOLUENE		0.500		0.026	0.139
PHENOL			1.000	0.001	0.857
MCH		0.500		0.973	0.004
*** VAPOR PHASE ***					
Density					
Viscosity					
*** LIQUID PHASE ***					
Density	lb/cuft	46.004	62.094	43.567	56.774
Viscosity	cP	0.288	1.021	0.323	0.443
Surface Ten	dyne/cm	16.805	31.995	14.950	23.805

Adjust the flowchart until you get the following Figure.

Remove the options like Click View → Annotations

View → Global Variable → (Remove the options and try to view the Flow Chart)

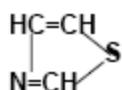
Exercise 3: Estimating Physical Properties of Non-Databank Components

This chapter guides you through the procedure for estimating physical properties for a component that is not present in the Aspen Plus databank.

If we are trying to simulate Thiazole and water in Aspen plus and the problem is, Thiazole (C3H3NS) is not in the Aspen Plus databank.

Some properties of the molecule

Molecular structure for Thiazole:



Molecular weight: 85

Normal boiling point: 116.8 °C

Vapor pressure correlation:

$$\ln p_i^{oL} = 16.445 - 3281.0/(T+216.255)$$

For p_i^{oL} in mmHg, T in °C for $69^{\circ}\text{C} < T < 118^{\circ}\text{C}$

Then we need this information.....

Parameter	Description
TC	Critical temperature
PC	Critical pressure
CPIG	Ideal gas heat capacity coefficients
DHFORM	Heat of formation
DGFORM	Gibbs free energy formation
DHVLWT	Watson heat-of-vaporization coefficients
VC	Critical volume
ZC	Critical compressibility factor

While starting Aspen Plus select Template and press OK.

In the Run type: Select Property Estimation → English with General Units → Press OK

The Data Browser appears. There is no process flowsheet for a Property Estimation run. First enter a title for the simulation. Then define a new component with the name *thiazole* and tell Aspen Plus to estimate all missing properties. Then enter the molecular structure of Thiazole and all known properties. Then run the estimation.

Give Title → Account → Your Name and Title “Property Estimation for Thiazole”

Click Components → Specifications → Enter a name Thiazole.

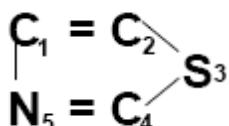
Next, tell Aspen Plus to estimate all missing properties.

Specifying Properties to Estimate:

Click Properties → Estimate Properties → Input.

Click Molecular Structure →

For entering the structure according to the number of atoms and the bonds



Enter the following information

Atom 1	Atom 2 (Connections)	
C—1	(is connected to) → C—2	(Bond Type is Double Bond)
C—2	→ S—3	(Single Bond)
S—3	→ C—4	(Single Bond)
C—4	→ N—5	(Bond Type is Double Bond)
N—5	→ C—1	(Single Bond)
Input	the	data

Define molecule by its connectivity					
Atom1		Atom2		Bond type	
Number	Type	Number	Type		
1	C	2	C	Double bond	
2	C	3	S	Single bond	
3	S	4	C	Single bond	
4	C	5	N	Double bond	
5	N	1	C	Single bond	
*					

Atom number - atom type correspondence						
	Atom number	1	2	3	4	5
	Atom type	C	C	S	C	N

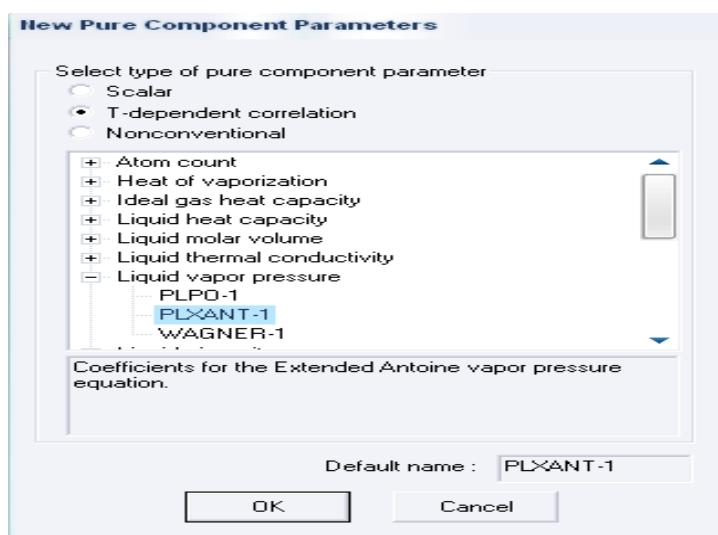
The structure is enough to estimate the properties but.....

Properties → Parameters → Pure Components—New → Select “Scalar”.

Click New → Give one name as TBMW → (In parameters at TB → Enter 116.8 as it is given below and Molecular weight (MW) etc...

Pure component scalar parameters				
	Parameters	Units	Data set	Component
	TB	C	1	THIAZOLE
►	MW		1	85
*				

Next specifying the coefficients for the Antoine vapor pressure correlation which we have.....



For finding the list of properties just click on the parameter and automatically it will display the explanation.

For our component Thiazole we have ...

The Antoine vapor pressure correlation (also given above) is:

$$\ln p_i^{\text{oL}} = 16.445 - 3281.0/(T+216.255)$$

for p_i^{oL} in mmHg, T in °C for $69^\circ\text{C} < T < 118^\circ\text{C}$.

You can get help on specifying the coefficients by clicking , then clicking PLXANT in the **Parameter** field near the top of this sheet. Follow the link to [Extended Antoine/Wagner](#).

in search button type the following keywords “Extended Antoine/wagner”.

Click on the link Extended Antoine/Wagner....

$$\ln p_i^{*J} = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i}T + C_{5i} \ln T + C_{6i} T^{C_{7i}} \text{ for } C_{8i} \leq C_{9i}$$

This is the corresponding equation and the constants to be supplied was C1,C2.....C9....

Plank-I Option....

Enter the following Data...

Components	THIAZOLE	
Temperature units	C	
Property units	mmHg	
1	16.445	
2	-3281	
3	216.255	
4	0	
5	0	
6	0	
7	0	
8	69	
9	118	

Run the simulation and views the results.

(The original Results will come with minute errors which can be neglected).

Problem: Using Thiazole in the Flash Drum Flow Chart.

Open flash aspen file → Click Setup Components →

File → Import → Thiazole (in the components list “Thiazole will be added”).

Click Setup → Specifications → Global → Select Flowsheet (At Run Type).

Click Properties → Estimation → Input → Do not estimate any property.

In streams → Stream 1 → Input → Give Methanol = 200, water = 200 and Thiazole = 40.

Temperature = 90 Degree Centigrade and Pressure 20 psi.

Blocks → BI → Input → Temp = 90 C and Pressure 20 psi.

Run the simulation and get the output.

Problem: Input only the Thiazole as Stream 1 and run the simulation....

Problem 3: Input the Thiazole and Water in stream 1 and run the simulation.....

Analyzing Properties

Mixing two components and analyzing thermodynamic properties.

Before starting a simulation study, it is important to understand the physical property and phase equilibrium behavior of the fluids in your process, and to confirm that the behavior predicted by the property models and data you are using is reasonable.

In this chapter you will use the interactive property analysis features in Aspen Plus to obtain a binary T-xy diagram for the acetone-chloroform system, using the NRTL activity coefficient model with parameters from the built-in binary pair databank. Then you will check your results against literature data.

Type NRTL in help search and read the explanation.

NRTL uses Ideal gas law...

New → General units with English → Property Analysis (At Run Type) → OK

In setup → specifications → Give any title ("Property Analysis") → Name of Account → Input data (METCBAR) (Metric units with Celsius for Temperature and bar for pressure)

Component → specification → (At component ID) Type Acetone and press Enter → type CHCL3 and press Enter.

Automatically all components will be activated.

Base method → Select NRTL.

If you click next it will show setup properties has to set click **Cancel**.

(Here it will show required inputs were not complete but you can analyze the properties).

Click Tools (in main menu) Not in data browser → analysis → Property → Binary.

Select **Txy** → and **Go to get the plot**.

Click Plot Wizard and select different Plots.

Exercise 4: Simulation of a Shell and Tube Heat Exchanger using ASPEN EDR

Design a shell and tube exchanger for the following duty. 20,000 kg/h of kerosene (420 API) leaves the base of kerosene side stripping column at 200°C and is to be cooled to 90 °C by exchange with 70,000 kg/h light crude oil (340 API) coming from storage at 40°C. The kerosene enters the exchanger at a pressure of 5 bar and the crude oil at 6.5 bar. A pressure drop of 0.8 bar is permissible on both streams. Allowance should be made for fouling by including a fouling factor of 0.0003 (W/m² 0C)-l on the crude stream and 0.0002 (W/m² 0C)-l on the kerosene stream, if the space we have can limit the length of the heat exchanger is 5 m long.

(Towler and Sinnott, 2nd Edition 2017, Page 1102)

Properties are all in average

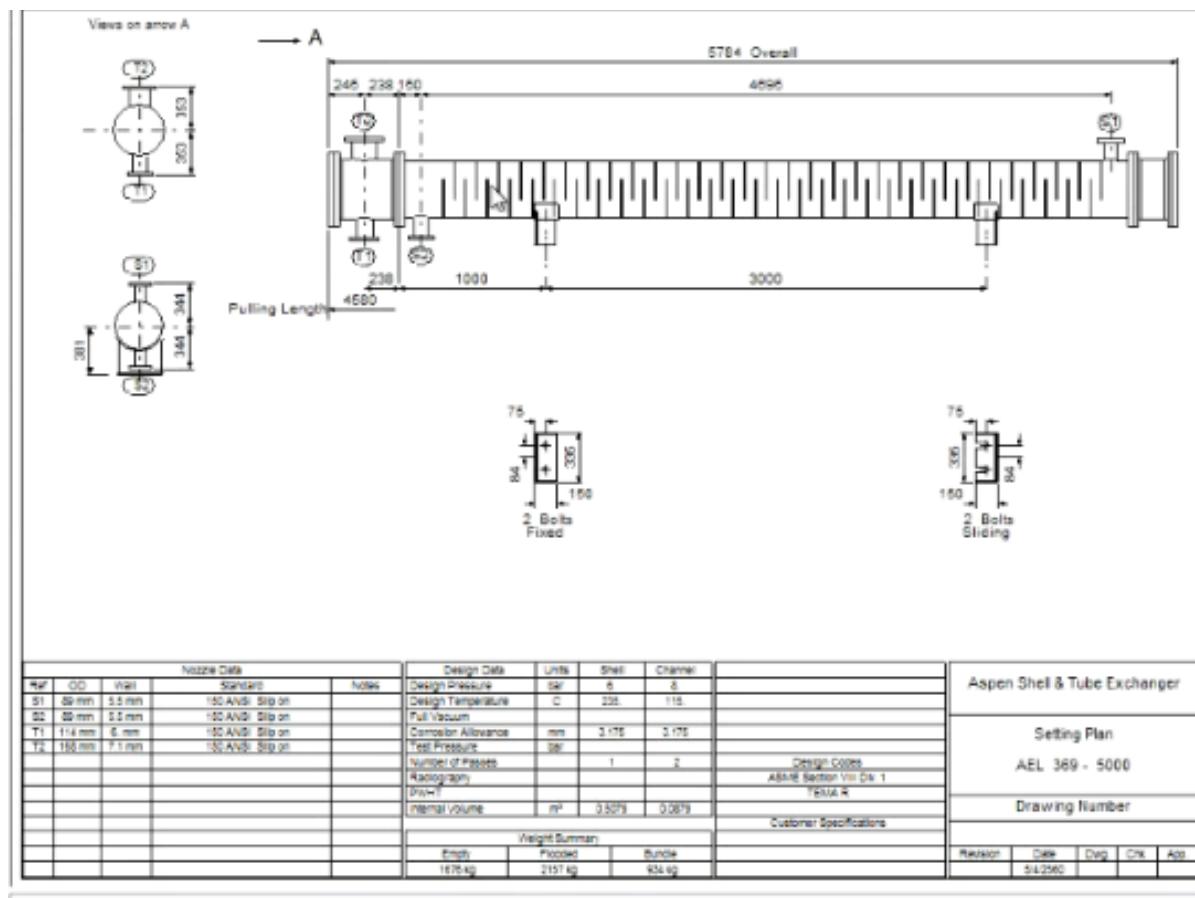
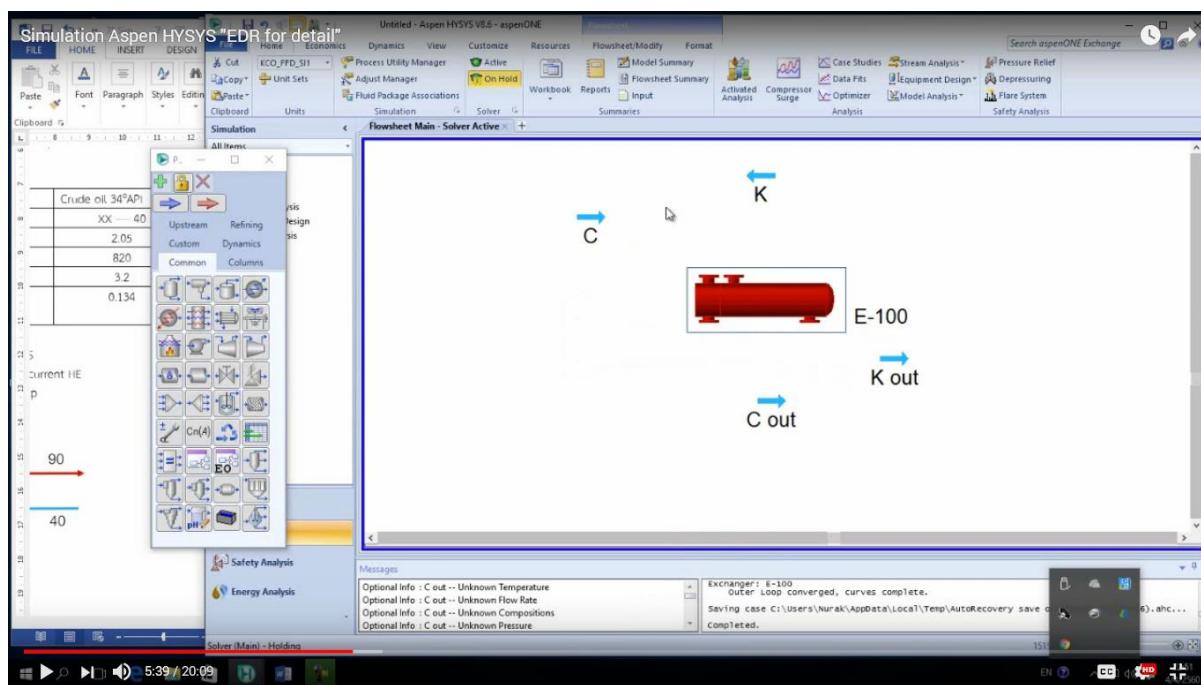
	Kerosene 42° API	Crude oil 34° API
T in and out, °C	200-90	xx-40
Cp (kJ/kg·°C)	2.47	2.05
Density, kg/m ³	770	820
Viscosity, nN/s·m ²	0.43	3.2
k _f , thermal conductivity, W/m·°C	0.132	0.134

1. How to input both chemicals into ASPEN-HYSYS?
2. Make a preliminary design for a counter-current Heat Exchanger
3. Optimize for the allowable pressure drop

Students can watch the below video and can perform this experiment.

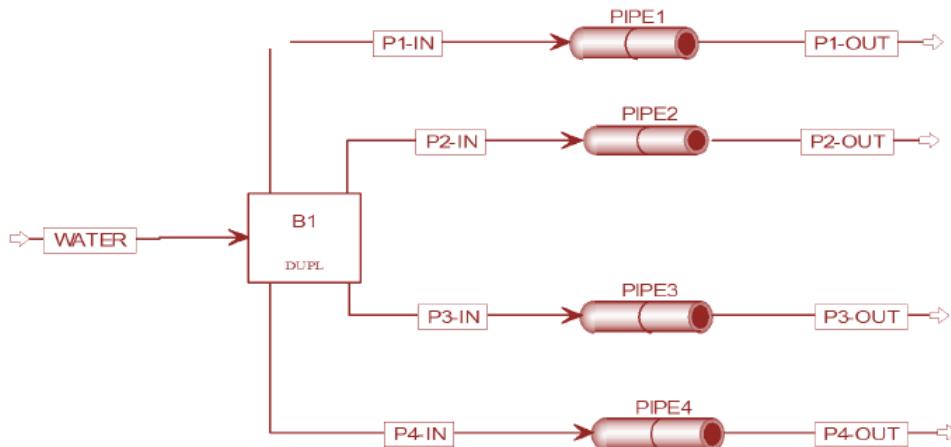
<https://www.youtube.com/watch?v=j8Tmdwk3ObE>

Chemical Process Simulation Laboratory



Exercise 5: Simulation of Pipes by Aspen Plus

Find the pressure drop in below pipes by simulating using Aspen Plus.



Find suitable property method using Method Assist and also find the Suitable Schedule Number and Nom Diameter for all four pipes with $p_1=0.08741667 \text{ ft}$; $p_2= 0.25566667 \text{ ft}$; $p_3= 0.07975 \text{ ft}$; $p_4= 0.24166667 \text{ ft}$ using trial and error method. The component is water with flow rate 1223.752 lbmol/hr, Temperature 100°F; Pressure 80 psia. The length of all pipes is 30ft and roughness is 0.00015ft and Erosion velocity coefficient is 100. Also generate report with all stream parameters.

Solution: Students will be given below manuscript where they can use for solving the above problem.

Anunay Gupta, S.M. Walke (2015) Simulation of Pipes by Aspen Plus, International Journal of Informative & Futuristic Research, Volume 2, Issue 8, Page No. 2498-2506

Research Paper

Volume 2

Issue 8

April 2015

International Journal of Informative & Futuristic Research

ISSN (online): 2347-1697

Simulation of Pipes by Aspen Plus

Paper ID	IJIFR/ V2/ E8/ 012	Page No.	2498-2506	Research Area	Chemical Engineering
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Key Words	Simulation, Design, Pipes, Steady State, Dynamic
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Research Paper

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Simulation of Pipes by Aspen Plus

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Abstract

Simulation of pipes in an Ammonia synthesis unit (Production of ammonia) process is gaining importance and so the process needs to be studied and better ideas suggested such that the production cost is reduced. With the advent of computers and simulating software's like "ASPEN PLUS" it is possible to design and optimize a particular process. Proper design can significantly reduce production cost as well as provide to make the process safe and reduce environment hazards. The material, unit operation and processes involved are been identified. Steady state simulation is done. Each unit is taken into consideration and the variables are been optimized. The units are sequentially optimized. Use of newer equipment's in the process is been going to be suggested. The distillation column will be optimized and number of trays will be seen for smooth production and to attain high efficiency in product.

1. Introduction

The purpose of analysis/simulation is to model and predict the performance of a process. It involves the decomposition of the process into its constituent elements (e.g. units) for individual study of performance. The process characteristics (e.g. flow rates, compositions, temperatures, pressures, properties, equipment sizes, etc.) are predicted using analysis techniques. These techniques include mathematical models, empirical correlations and computer-aided process simulation tools (e.g. ASPEN Plus). In addition, process analysis may involve the use of experimental means to predict and validate performance. Therefore, in process simulation, we are given the process inputs and flow sheet and are required to predict process outputs. The lab will focus on ASPEN Plus. It is a



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computer-aided software which uses the underlying physical relationships (e.g. material and energy balances, thermodynamic equilibrium, rate equations) to predict process performance (e.g. stream properties, operating conditions, and equipment sizes).

a) Simulation Modes:

There are two modes of simulation-

- 1) Steady state mode
- 2) Dynamic mode.

b) Steady State Mode and Dynamic Mode :-

Initially process simulation was used to simulate steady state processes. Steady state models perform a mass and energy balance of a stationary process (a process in an equilibrium state) it does not depend on time.

Dynamic simulation is an extension of steady-state process simulation whereby time-dependence is built into the models via derivative terms i.e. accumulation of mass and energy. The advent of dynamic simulation means that the time-dependent description, prediction and control of real processes in real time has become possible. This includes the description of starting up and shutting down a plant, changes of conditions during a reaction, holdups thermal changes and more.

Dynamic simulations require increased calculation time and are mathematically more complex than a steady state simulation. It can be seen as a multiply repeated steady state simulation (based on a fixed time step) with constantly changing parameters.

Dynamic simulation can be used in both online and offline fashion. The online case being model predictive control, where the real-time simulation results are used to predict the changes that would occur for a control input change and the control parameters are optimized based on the results.

c) Various Process Simulators:-

- Aspen Plus.
- Aspen Hysys.
- Aspen Custom Modeller by Aspen Technology.
- CHEMASIM.
- CHEMCAD.

d) Overview of Aspen Plus

Aspen PLUS is a market leading process modelling tool for conceptual design, optimization, business planning, asset management and performance monitoring for oil and gas processing, petroleum refining, and air separation industries. Aspen PLUS is a core element of AspenTech's aspen ONE Engineering applications. Aspen PLUS has established itself as a very intuitive and easy to use process simulator in oil and gas refining industry. Users with little prior knowledge of Aspen PLUS can pick up and train themselves in its modelling capabilities. Some of the very intuitive capabilities include a highly interactive process flow diagram for building and navigating through large simulations. The program also provides a very flexible and easy to use distillation column



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modelling environment. Additionally the interactive nature of PLUS enables users to build and use their models quickly and effectively. Aspen PLUS offers a comprehensive thermodynamics foundation for accurate calculation of physical properties, transport properties, and phase behaviour for the oil & gas and refining industries. Comprehensive library of unit operation models including distillation, reactors, heat transfer operation, rotating equipment's, controllers and logical operations in both the steady state and dynamic environments.

2. Description

Before Starting with simulation we have to select the available simulation templates as shown in fig.2.1. There are numerous options and the highlighted one is generally the solution to all and or can solve as seen by the no of available templates.

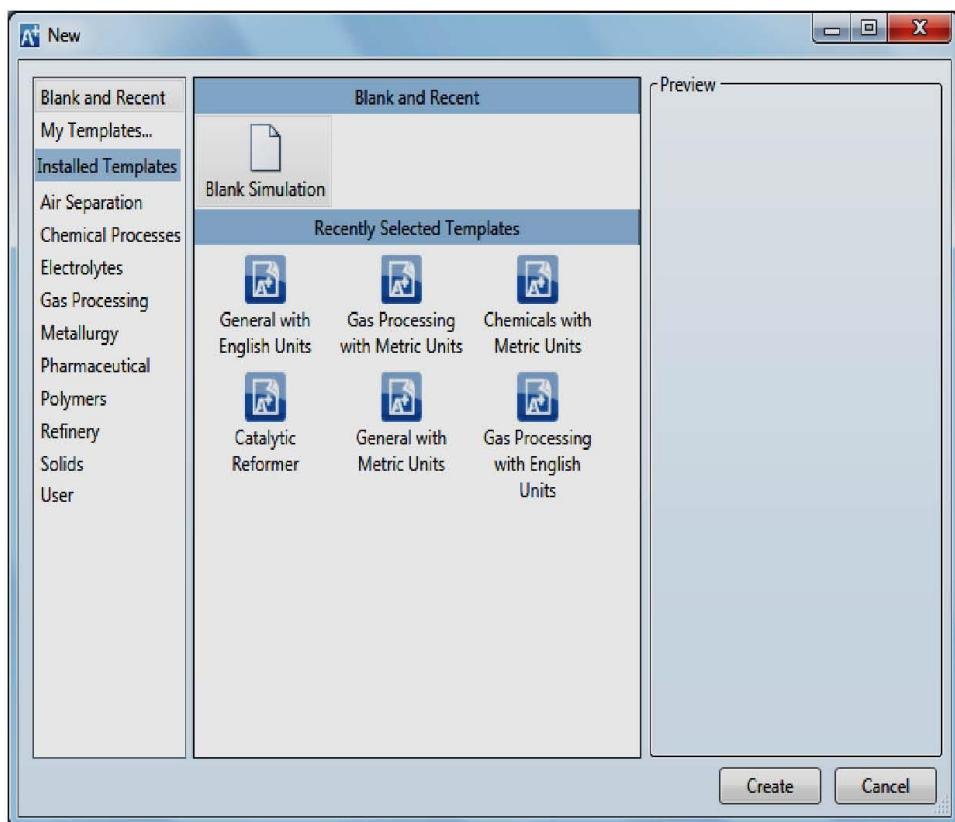


Figure2.1: Available Simulation Templates

Aspen has a huge database of commonly used (and some not so commonly used) components and their physical properties. It also has an option where a user can define components that are not included in the database. Under the Specifications option we will input our components in the Selection tab. While making the PFD material streams are specified and entered. This is the only option where we will need to input data under the Components tab as shown in fig 2.



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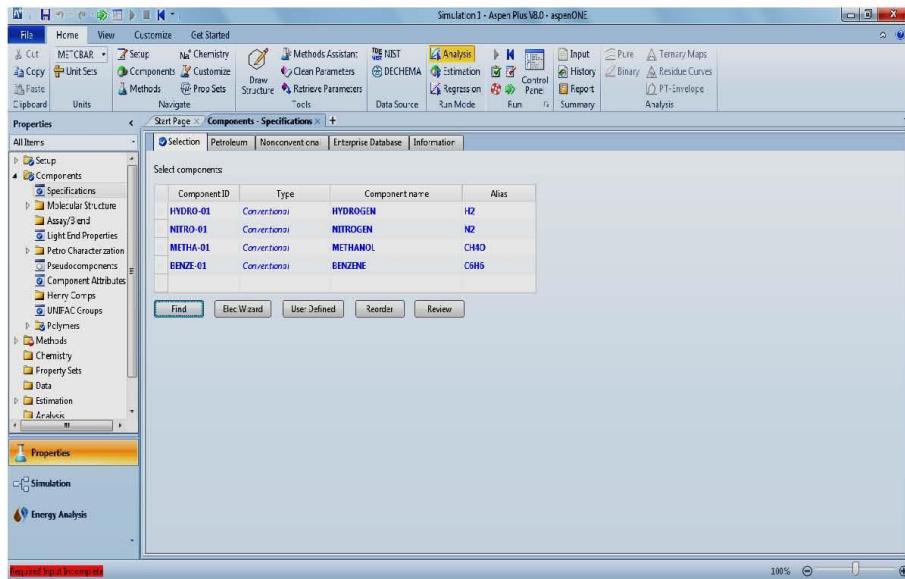


Figure 2.2: Component Selection

By knowing all the required data, process inputs we simulate the flow sheet. By knowing the specific volume with the help of equation of state we can determine the size and thus cost of the plant. Fig.2.3 represents the Aspen Plus screen where one will be able to draw the flow sheet and also simulate it by adding numerous inputs and also can check the energy analysis.



Figure 2.3: Aspen Plus Screen



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3. Working with Process Pipes

3.1. Pipes

A pipe is a tubular section or hollow cylinder, usually but not necessarily of circular cross-section, used mainly to convey substances which can flow — liquids and gases (fluids), slurries, powders, masses of small solids. It can also be used for structural applications; hollow pipe is far stiffer per unit weight than solid members.

In common usage the words *pipe* and *tube* are usually interchangeable, but in industry and engineering, the terms are uniquely defined. Depending on the applicable standard to which it is manufactured, pipe is generally specified by a nominal diameter with a constant outside diameter (OD) and a schedule that defines the thickness. Tube is most often specified by the OD and wall thickness, but may be specified by any two of OD, inside diameter (ID), and wall thickness. Pipe is generally manufactured to one of several international and national industrial standards. While similar standards exist for specific industry application tubing, tube is often made to custom sizes and a broader range of diameters and tolerances. Many industrial and government standards exist for the production of pipe and tubing. The term "tube" is also commonly applied to non-cylindrical sections, i.e., square or rectangular tubing. In general, "pipe" is the more common term in most of the world, whereas "tube" is more widely used in the United States.

Both "pipe" and "tube" imply a level of rigidity and permanence, whereas a *hose* (or hosepipe) is usually portable and flexible. Pipe assemblies are almost always constructed with the use of fittings such as elbows, tees, and so on, while tube may be formed or bent into custom configurations. For materials that are inflexible, cannot be formed, or where construction is governed by codes or standards, tube assemblies are also constructed with the use of tube fittings.

3.2 Pipe Materials

Pipe is made in many materials including ceramic, fiberglass, and many metals, concrete and plastic. In the past, wood and lead were commonly used.

Typically metallic piping is made of steel or iron, such as unfinished, black (lacquer) steel, carbon steel, stainless steel or galvanized steel, brass, and ductile iron. Iron based piping is subject to corrosion in highly oxygenated water stream. Aluminum pipe or tubing may be utilized where iron is incompatible with the service fluid or where weight is a concern; aluminum is also used for heat transfer tubing such as in refrigerant systems. Copper tubing is popular for domestic water (potable) plumbing systems; copper may be used where heat transfer is desirable (i.e. radiators or heat exchangers). Inconel and titanium steel alloys are used in high temperature and pressure piping in process and power facilities.

Lead piping is still found in old domestic and other water distribution systems, but it is no longer permitted for new potable water piping installations due to its toxicity. Many building codes now require that lead piping in residential or institutional installations be replaced with non-toxic piping or that the tubes' interiors be treated with phosphoric acid. According to a senior researcher and lead expert with the Canadian Environmental Law Association, "there is no safe level of lead [for human exposure]".

Pipe may be made from concrete or ceramic, usually for low-pressure applications such as gravity flow or drainage. Pipes for sewage are still predominantly made from concrete or clay. Reinforced concrete can be used for large-diameter concrete pipes. This pipe material can be used in many types of construction, and is often used in the gravity-flow transport of storm water.





3.3 Pipes in Aspen Plus

There are two modules available for modelling pipes in Aspen Plus: Pipes and Pipelines. The pipes module is used to model single segments of pipes with any associated fittings. Pipelines, on the other hand, are used to model larger pipes networks such as those encountered with oil and gas collecting systems.

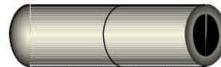


Figure 3.1: Pipes in Aspen Plus

Pipe specifications can be made in the **Setup | Pipe Parameters** tab for the pipe block. This sheet takes basic input about the pipe geometry. Temperature calculations are setup in the **Setup | Thermal Specification** tab where the choice on how to calculate the temperature profile is made. In this terms to include in the energy balance calculations is made (*i.e.*, and terms). Any fittings in the pipe can be defined in the **Setup | Fittings 1** tab, which also gives the ability to modify the factors used in the calculations, if needed.

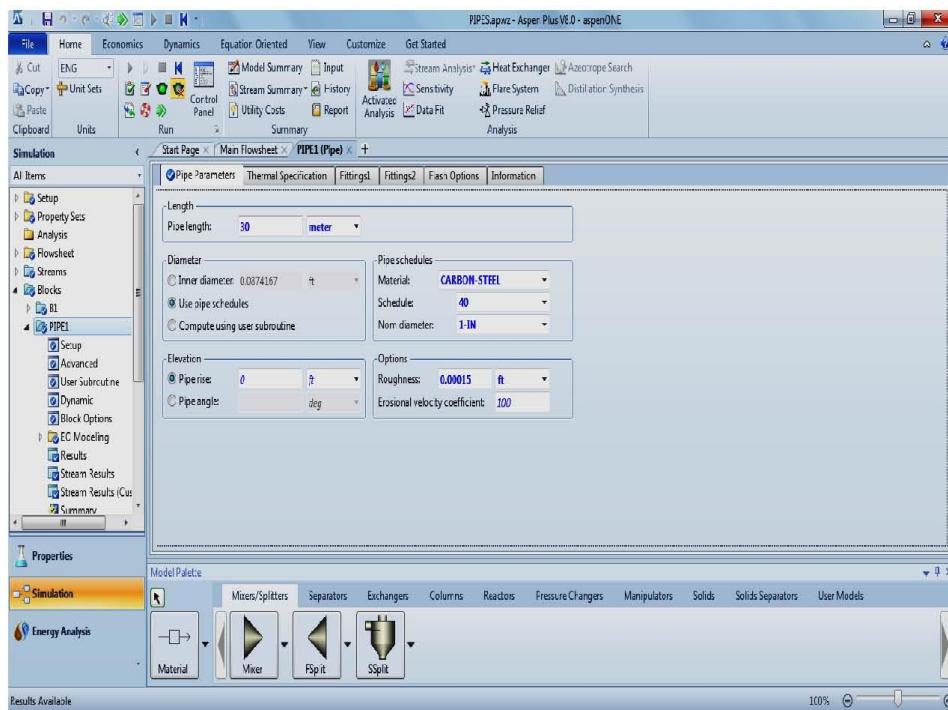


Figure 3.2: Pipe Specifications Tab in Aspen Plus

Finally, the **Setup | Fittings 2** tab gives the ability to include the entrance and exit effects and any contraction, expansion, or orifice presents in the pipe. Further calculations options for the pipe module can be made through the **Advanced | Calculation Options** and **Advanced | Methods** tabs available for the pipe block.





4. Simulation of Pipes in Aspen Plus

The fig below represents the basic example of simulation of a pipe in aspen plus. Water is the feed inlet which goes through the block B1(Duplicator) where it expands to four sub-streams i.e. Pipe 1, Pipe 2, Pipe 3 and Pipe 4. The inlet of the respective pipes are P1-IN, P2-IN, P3-IN, P4-IN and outlet of the pipes are P1-OUT, P2-OUT, P3-OUT and P4-OUT.

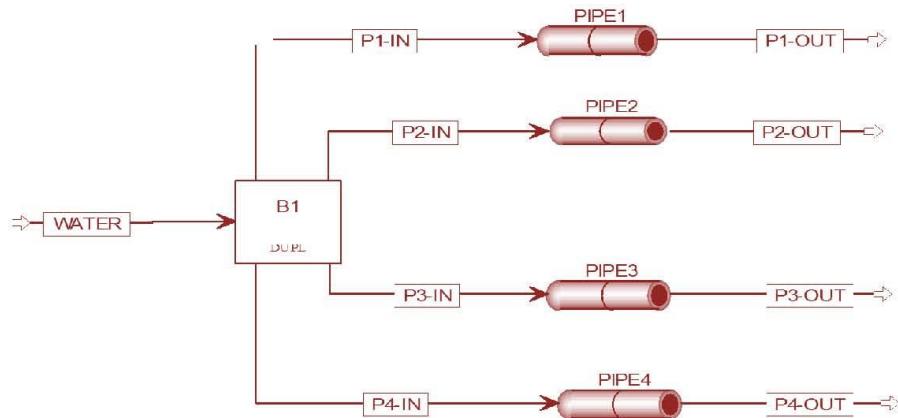


Figure 4.1: Simulation of pipe in Aspen plus

The following Table 4.1 shows the model summary of the following pipes

Table 1: Model Summary

Pipe				
Name	PIPE1	PIPE2	PIPE3	PIPE4
Property method	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA
Free-water phase properties method	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA
Water solubility method	3	3	3	3
Pipe length [meter]	30	30	30	30
Inner diameter [ft]	0.08741667	0.25566667	0.07975	0.24166667
Pipe rise [ft]	0	0	0	0
Pipe angle [deg]				
Roughness [ft]	0.00015	0.00015	0.00015	0.00015
Erosional velocity coefficient	100	100	100	100
Total pressure drop [psi]	47.93556	0.20819652	77.1780522	0.27512778
Frictional pressure drop [psi]	47.93556	0.20819652	77.1780522	0.27512778
Elevation pressure drop [psi]	0	0	0	0
Acceleration pressure drop [psi]	0	0	0	0
Enthalpy change [Btu/hr]	-2789.0424	-12.112494	-4490.6978	-16.006434
Equivalent length [ft]	98.4251969	98.4251969	98.4251969	98.4251969





All the required inputs are specified and the following outputs are been calculated as seen in the Table 2.

Table 2:-Simulation Results

RESULTS						
	P1-IN	P1-OUT	P2-IN	P2-OUT	P3-IN	P3-OUT
Temperature F	100	100	100	100	100	100
Pressure psia	80	32.06	80	79.79	80	2.82
Vapor Frac	0	0	0	0	0	0
Mole Flow lbmol/hr	1223.752	1223.752	1223.752	1223.752	1223.752	1223.752
Mass Flow lb/hr	22046.23	22046.23	22046.23	22046.23	22046.23	22046.23
Volume Flow cuft/hr	355.516	355.568	355.516	355.516	355.516	355.6
Enthalpy MMBtu/hr	-149.867	-149.87	-149.867	-149.867	-149.867	-149.872
Mole Flow lbmol/hr						
WATER	1223.752	1223.752	1223.752	1223.752	1223.752	1223.752

4. Conclusions

The goal of Plus is to provide a capability to design an entire process completely and accurately. Aspen Plus provides an extremely powerful approach to steady state modeling. It is an approach to modeling maximizes return on simulation time through increased process understanding. Aspen Plus offers a comprehensive thermodynamics foundation for accurate calculation of physical properties, transport properties, and phase behaviour and newer versions of Plus have almost doubled in its capabilities on physical properties. This has introduced the novel approach of steady state and dynamic simulations in the same platform & became the defacto standard in industry, and today enjoys universal acceptance. It let the engineers to estimate the Green House Gas Emissions associated with a process. Refinery Reactor Technology which includes Fluidized Catalytic, Hydrocracking and Hydro treating, Reforming and Isomerisation enables Aspen Plus to perform single unit, multi-unit as well as refinery wide simulations.

Acknowledgements

This work was done by Anunay Gupta as a part of there BE project work during June 2014 to Feb 2015,at the Department of Chemical Engineering, Bharati Vidyapeeth College of Engineering, Navi Mumbai, India, under the guidance of Dr. S.M. Walke. We are thankful to the authorities at Bharati Vidyapeeth College of Engineering, Navi Mumbai for providing all facilities for completing this work.

References

- [1] Mohd.Kamaruddin Abd Hamid "Plus: An introduction to Chemical Engineering Simulation".
- [2] Michael E Hanyak "Chemical Process Simulation and Aspen tech Plus Software" Version 2006 Bucknell university Lewisburg PA 17837 December 15 2007.
- [3] Aspen Plus Customization Guide, 2005.



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Exercise 6: Aspen Plus Biodiesel Model

This example is a model of a process for the alkali catalysed production of biodiesel from vegetable oil. It is intended to:

- Provide an example of how to model the different areas of this process
- Supply a starting set of components and physical property parameters for modeling processes of this type

The model is not intended for equipment design or for specifying other engineering documents without further review by a process engineer with experience of biodiesel processes.

The model includes:

- A nominal set of chemical species and property parameters for this process.
- Typical process areas including: transesterification, methanol recovery, water washing, FAME purification, catalyst removal, glycerol purification, feed stock recovery and the main streams connecting these units.
- Key process control specifications such as pure methanol flow rate, phosphoric acid flow rate, and specifications for distillation columns.

This model is based upon information included in the following paper:

Y. Zhang, M.A. Dube, D.D. McLean, M. Kates, "Biodiesel Production from waste cooking oil: I. Process design and technological assessment", *Bioresource Technology*, 89:1-16, 2003.

Key Simulation Parameters to be used:

The Aspen Plus simulation flowsheet is shown in Figure 1.

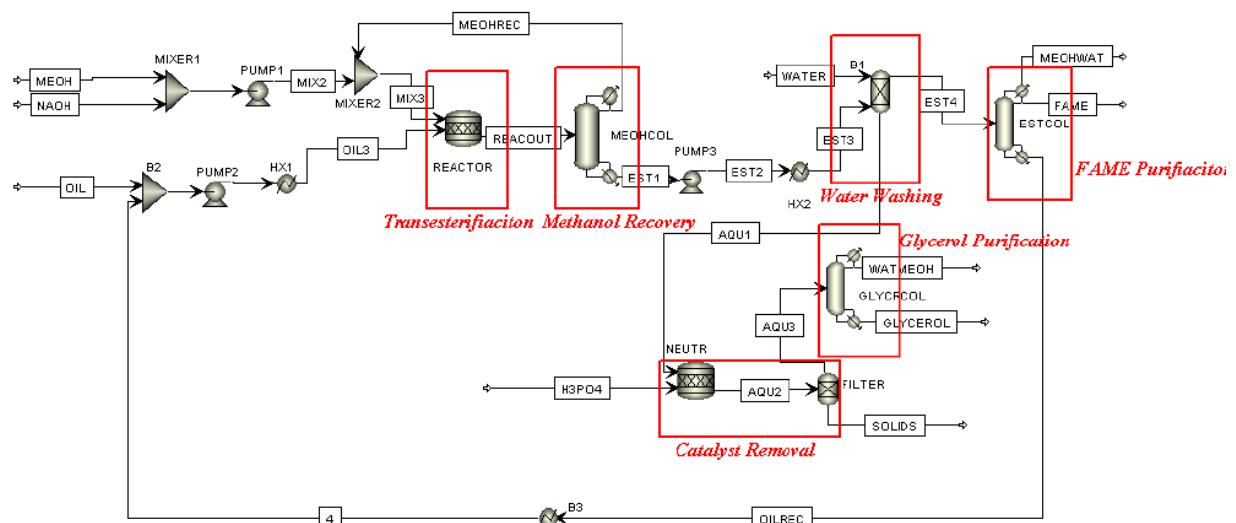


Figure 1. Biodiesel Flowsheet in Aspen Plus

The following are the list of compounds entering into the system.

Table 1. Components Used in the Biodiesel Model

ID	Type	Formula	Name
METHANOL	CONV	METHANOL	CH4O
OIL	CONV	TRIOLEIN	C57H104O6
FAME	CONV	METHYL-OLEATE	C19H36O2
GLYCEROL	CONV	GLYCEROL	C3H8O3
NAOH	CONV	WATER	H2O
WATER	CONV	WATER	H2O
H3PO4	CONV	WATER	H2O
NA3PO4	CONV	WATER	H2O

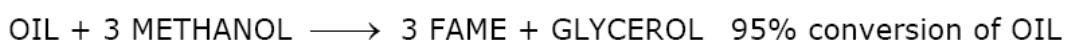
Table 2. General Unit Operations Used in the Bio-Diesel Process

Unit	Purpose
Transesterification	Oil reacts with alcohol in the presence of catalyst to yield biodiesel and glycerol
Methanol Recovery	Recover excess methanol
Water Washing	Separate FAME from glycerol and electrolytes
FAME Purification	Purify FAME and recover oil
Catalyst Removal	Remove excess catalyst
Glycerol Purification	Purify glycerol

The models used to calculate physical properties in Aspen Plus are grouped into property methods named after the central model, for example, Ideal, Redlich-Kwong-Soave, and NRTL (Non-Random Two Liquid). The property method used in this model is Dortmund modified UNIFAC. This is suitable for preliminary work. NRTL would probably give more accurate results, but requires estimation of NRTL binary interaction parameters.

The reactions modeled are:

Transesterification



Catalyst Removal



This model assumes fixed fractional conversions for each reaction. A more detailed model could model the reaction kinetics. This would require fitting of kinetic parameters to experimental data.

Table 3. Aspen Plus Unit Operation Blocks Used in the Biodiesel Model

Unit Operation	ASPEN-PLUS "Block"	Comments / Specifications
Transesterification	RStoic	Simplified simulation with stoichiometric reactions
Methanol Recovery	RadFrac	Rigorous multi-stage distillation model. 7 theoretical stages.
Water Washing	Liquid-Liquid Extractor	Rigorous multi-stage liquid-liquid extractor model. 6 theoretical stages
FAME Purification	RadFrac	Rigorous multi-stage distillation model. 6 theoretical stages.
Catalyst Removal	RStoic	Simplified simulation with stoichiometric reactions
	Sep	Simplified simulation for solid removal
Glycerol Purification	RadFrac	Rigorous multi-stage distillation model. 6 theoretical stages.

Streams - Streams represent the material and energy flows in and out of the process. Streams can be of three types: Material, Heat, and Work. Feeds to the biodiesel model are oil, methanol, sodium hydroxide, water and acid.

Design-Specs, Calculator Blocks - The simulation includes a Design Spec and Calculator Block as shown in Tables 4 & 5:

Table 4. Design Specs Used in the Biodiesel Model

Spec Name	Spec (Target)	Manipulated Variable
MEOHCONC	Mass fraction of methanol in reactor outlet is 0.092	Methanol feed stream flow rate

Table 5. Flowsheet Calculators Used in the Biodiesel Model

Name	Purpose
PO3FLOW	H ₃ PO ₄ feed flow is determined according to excess sodium hydroxide

Key Simulation Results

Table 6. Key Simulation Results

Plant capacity (pure FAME)	9.23	MM kg/yr
Oil feed	1050	kg/hr
Methanol feed	121.418	kg/hr
Catalyst feed	50	kg/hr
H ₃ PO ₄ feed	40.8	kg/hr
Water feed for washing	50	kg/hr
Transesterification reactor biodiesel composition	0.753	Mass fraction
Product FAME purity	0.997	Mass fraction
Product Glycerol purity	1	Mass fraction

The Biodiesel model provides a useful description of the process. The model can be used as a guide for understanding the process and the economics, and also as a starting point for more sophisticated models for plant design and specifying process equipment.

Exercise 7: An Analysis of Capital Cost Estimation Techniques for Chemical Processing

Students have to refer to the below thesis book and perform cost estimation.

Symister, O. J. (2016). An Analysis of Capital Cost Estimation Techniques for Chemical Processing (Doctoral dissertation), Master Degree Thesis Submitted to the Graduate School of Florida Institute of Technology, USA.

Summary Costs

Item	Material(USD)	Manpower(USD)	Manhours
Equipment&Setting	452100.	11629.	368
Piping	244064.	63931.	2103
Civil	9339.	8236.	328
Structural Steel	29488.	5262.	183
Instrumentation	55450.	5678.	182
Electrical	4590.	2703.	90
Insulation	0.	0.	0
Paint	555.	775.	35
Subtotal	795586	98214	3289

Total material and manpower cost = USD 893800.

[Sizing Data](#)
[Design Data](#)
[Summary Costs](#)

Sizing Data

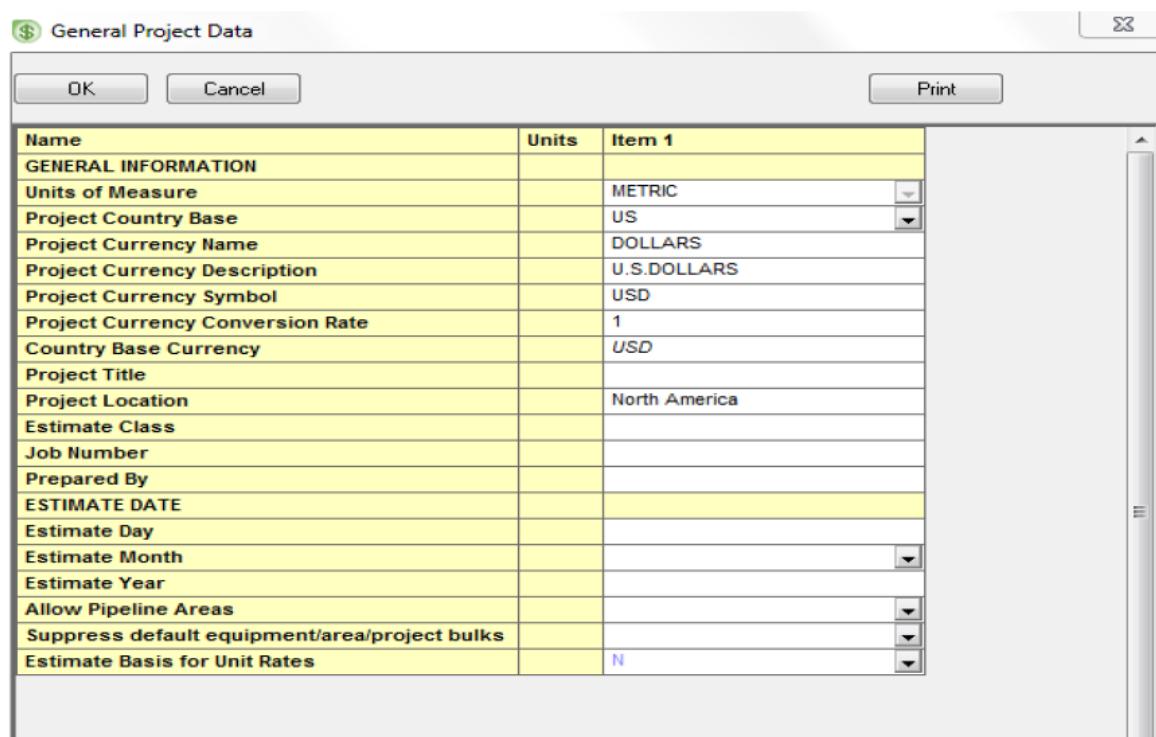
Description	Value	Units
-------------	-------	-------

Design Data

Parameter	Value	Units
Item type	CYLINDER	
Number of identical items	1	
EQUIPMENT DESIGN DATA		
Application	CONT	
ASME design basis	D1NF	
Liquid volume	211.982	M3
Design gauge pressure	1100.000	KPAG
Design temperature	30.000	DEG C
Operating temperature	30.000	DEG C
Fluid specific gravity	1.0000	
SHELL DATA		
Shell material	SS304	
Diameter option	ID	
Vessel diameter	3.0000	M
Vessel tangent to tangent height	30.000	M
Head type	HEMI	
MECHANICAL DESIGN DATA		
Wind or seismic design	W+S	
Fluid volume	20.000	PERCENT
Weld efficiency	100.000	PERCENT

Base material thickness	13.000	MM
Corrosion allowance	0.000000	MM
Head thickness Top	7.0000	MM
Head thickness Bottom	8.0000	MM
THICKNESSES REQUIRED		
Circumferential stress thickness	12.831	MM
Long tensile stress thickness	6.6875	MM
Long compressive stress thick	7.0744	MM
VESSEL SKIRT DATA		
Skirt material	CS	
Skirt height	4.5000	M
Skirt thickness	13.000	MM
NOZZLE AND MANHOLE DATA		
Nozzle ASA rating	150	CLASS
Nozzle material	SS304	
Nozzle A Quantity	1	
Nozzle A Diameter	400.000	MM DIAM
Nozzle A Location	S	
Nozzle B Quantity	1	
Nozzle B Diameter	450.000	MM DIAM
Nozzle B Location	S	
Nozzle C Quantity	1	
Nozzle C Diameter	350.000	MM DIAM
Nozzle C Location	S	
Nozzle D Quantity	1	
Nozzle D Diameter	200.000	MM DIAM
Nozzle D Location	S	
Nozzle E Quantity	8	
Nozzle E Diameter	50.000	MM DIAM
Nozzle E Location	S	
Number of manholes	1	

Manhole diameter	450	MM
WEIGHT DATA		
Shell	29600	KG
Heads	1700	KG
Nozzles	310	KG
Manholes and Large nozzles	160	KG
Skirt	4400	KG
Base ring and lugs	900	KG
Ladder clips	140	KG
Platform clips	300	KG
Fittings and miscellaneous	70	KG
Total weight	37600	KG
VENDOR COST DATA		
Material cost	191861	DOLLARS
Shop labor cost	71551	DOLLARS
Shop overhead cost	75566	DOLLARS
Office overhead cost	57626	DOLLARS
Profit	55497	DOLLARS
Total cost	452100	DOLLARS
Cost per unit weight	12.024	USD/KG
Cost per unit liquid volume	2132.724	USD/M3



The General Project Data window displays the following configuration:

Name	Units	Item 1
GENERAL INFORMATION		
Units of Measure	METRIC	
Project Country Base	US	
Project Currency Name	DOLLARS	
Project Currency Description	U.S.DOLLARS	
Project Currency Symbol	USD	
Project Currency Conversion Rate	1	
Country Base Currency	USD	
Project Title		
Project Location	North America	
Estimate Class		
Job Number		
Prepared By		
ESTIMATE DATE		
Estimate Day		
Estimate Month		
Estimate Year		
Allow Pipeline Areas		
Suppress default equipment/area/project bulks		
Estimate Basis for Unit Rates	N	

Figure 28: Geneal project data window

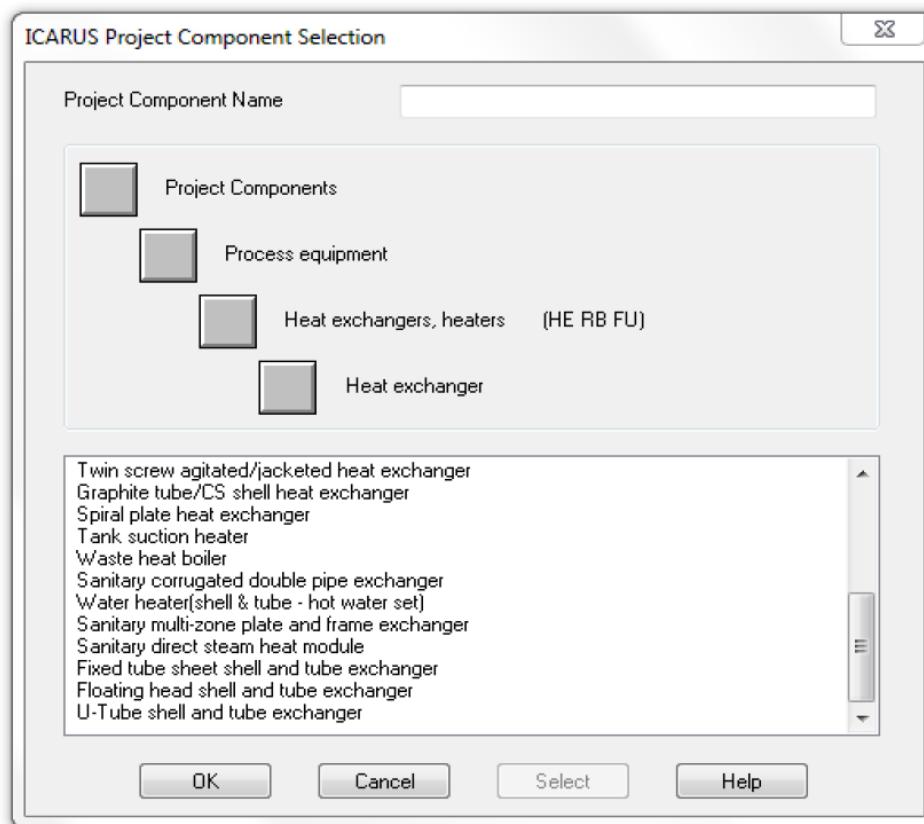


Figure 29: Project component selection window

Name	Units	Item 1
Item Reference Number		1
Remarks 1		
Remarks 2		
Item description	PV	
User tag number		
Structure tag		
Component WBS		
Quoted cost per item	USD	
Currency unit for matl cost	USD	
Source of quote	VB	
Number of identical items	1	
Installation option		
Code of account		
Icarus/User COA option		
Application	CONT	
Shell material	SS304	
Liquid volume	M3	
Vessel diameter	M	3
Vessel tangent to tangent height	M	30
Design gauge pressure	KPAG	1,100
Vacuum design gauge pressure	KPAG	
Design temperature	DEG C	30
Operating temperature	DEG C	
Skirt height	M	
Skirt thickness	MM	
Vessel leg height	M	
Wind or seismic design		
Fluid volume	PERCENT	20
Manhole diameter	MM	450
Number of manholes		1
Allowance for internals	PERCENT	0
Demister thickness	MM	
Demister area	M2	
Base material thickness	MM	
Corrosion allowance	MM	
Number of body flange sets	PAIR	
Weld efficiency	PERCENT	100
Stress relief		
Cladding material		
Cladding thickness	MM	
Stiffening ring spacing	MM	
Head type		
Head thickness Top	MM	
Head thickness Bottom	MM	

Figure 30: Equipment specification screen

Exercise 8: Integration of EXCEL into ASPEN Plus - Getting Started Customizing Unit Operation Models

Construct an Ultrafiltration Membrane model. Ultrafiltration is a pressure driven membrane process used to separate components based on molecular size and shape. The solvent and small solute species pass through the membrane and are termed the **permeate**. Large solute species, such as proteins, are retained by the membrane and are termed the **retentate**. The simulation that you will construct is shown below in Figure 1.1. There is one feed stream (a water-protein feed), one unit operation block (an ultrafiltration membrane), and two product streams (permeate and retentate).

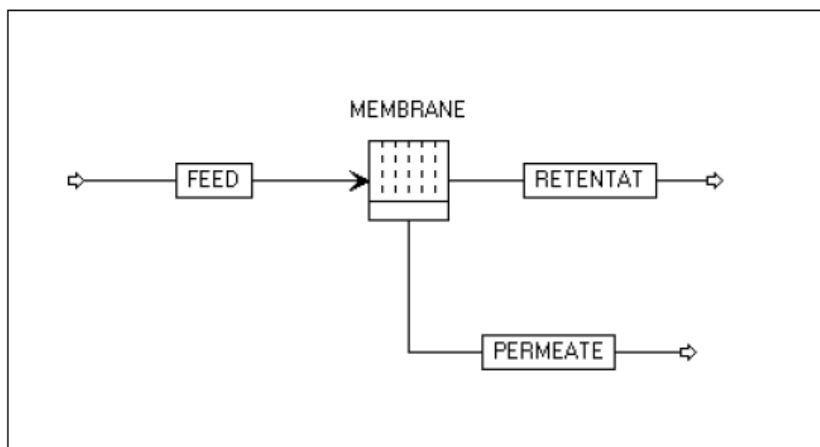


Figure 1.1 Ultrafiltration Membrane Model

Aspen Plus will write feed stream data and real and integer membrane parameters (such as physical dimensions) to Excel. Excel will calculate product stream data such as mole flow rates and solute concentrations using a user-specified set of equations. Aspen Plus will read the product stream data from Excel. Results will be displayed in the Excel file and on Aspen Plus results forms.

Students have to refer to the **ASPEN Document for solving this problem.**

https://userpages.umbc.edu/~dfrey1/ench445/Aspen_Excel_Tutorial.pdf

**Exercise 9: Dynamics and Control of Flow Driven Process using
ASPEN Plus**

**Students have to refer to the below Book Chapter 5 for solving the
above problem.**

**Process Simulation and Control Using Aspen by Amiya K Jana, PHI
Learning (2012), India**

Exercise 10: Aspen Energy Analyzer (Heat Exchanger Networks)

In this tutorial, you will design a heat exchanger network for a crude pre-heat train. A network will be created based on a process flow diagram proposed by a contractor. The concepts introduced here are used throughout the tutorial:

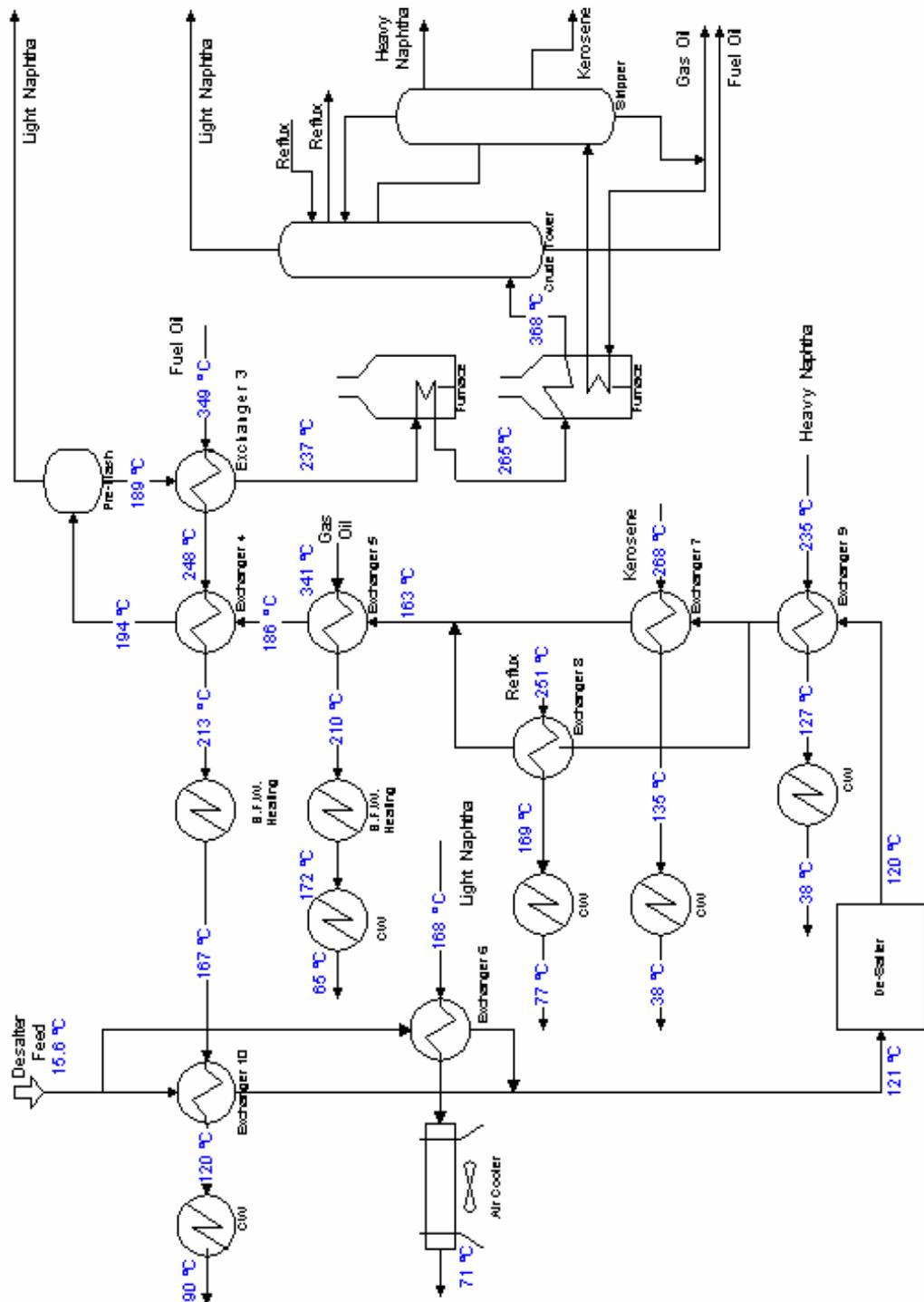
- creating process and utility streams,
- adding heat exchangers, and
- using the worksheet to manipulate the network.

Crude oil is often fractionated to produce saleable products such as heavy and light naphtha, kerosene, gas, and fuel oils. The proposed flowsheet was adapted from B. Linnhoff, D.W. Townsend, et al. The crude oil is split and heated in two heat exchangers, 10 and 6, by the Fuel Oil and Light Naphtha product streams, respectively. The crude feed is then mixed back together and passed through the desalter unit.

Effluent leaving the desalter is heated up further in heat exchangers 9, 7, 8, 5, and 4 by the product streams Heavy Naphtha, Kerosene, Reflux, Gas Oil, and Fuel Oil, respectively. An air cooler, coolers using cooling water, and boiler feed water heaters are used to further cool the product streams down to their target temperatures.

After the crude oil has been heated by the products, it is passed through a Pre-Flash operation to remove the Light naphtha cut. The heavier components from the Pre-Flash operation are heated by the hottest portion of the fuel oil in heat exchanger 3, and then passed through two furnaces. The crude tower takes the heated feed, and separates the Light Naphtha and the Fuel Oil cuts. The remaining cuts pass to the second column, the stripper. The stripper column also produces three other products: Gas Oil, Heavy Naphtha, and Kerosene.

Process Flowsheet

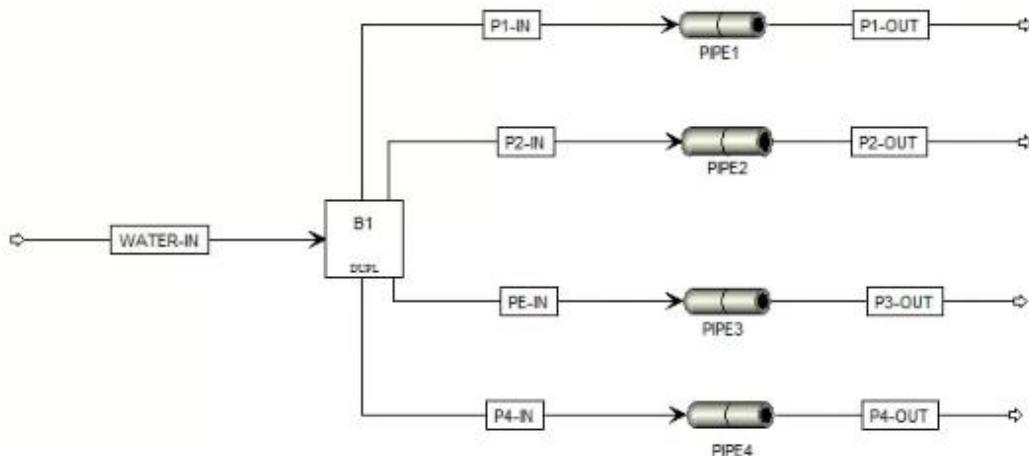


Refer to

<https://www.aspentechn.com/en/products/pages/aspen-energy-analyzer>

Appendix/Case Studies**Simulation of Pipes and Valves**

- I. Water was fed into four pipes using a Duplicator block as shown in the below diagram,



Property Method is Steam Table, Feed enters at 100°C and 80 psia and mass flow rate of 10000 kg/hr and all pipes lengths are 30 m and material of construction is Carbon-Steel. The below information can be used for the pipes.

	Pipe 1	Pipe 2	Pipe 3	Pipe 4
Schedule No.	40	40	80	80
Nominal Diameter	1 in	3 in	1 in	3 in

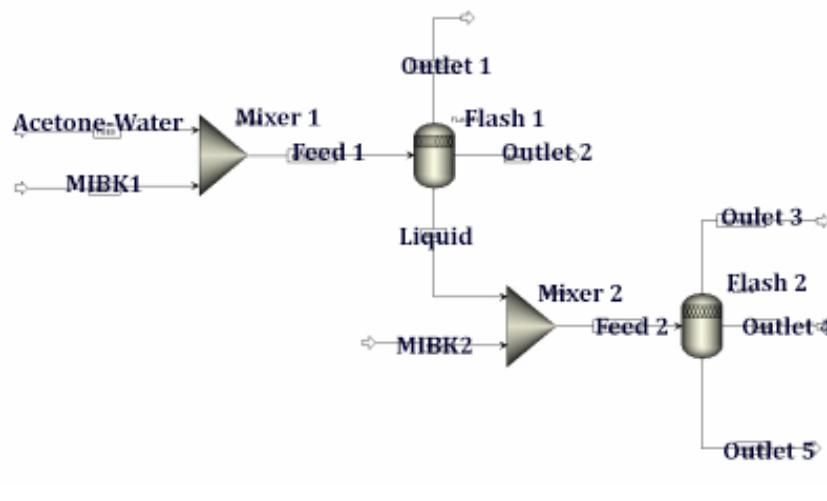
Part I:

- Find whether change in the materials of construction will affect the pressure drop. Using ASPEN Plus prepare the table showing pressure drops for each pipe.
- Find the effect of pressure drop at constant schedule number 40 and different nominal diameters. Tabulate the results for the following. (Pipe 1 to Pipe 4 – 40 Schedule No.) and Nominal Diameters (Pipe 1 to Pipe 4 - (Set 1: 0.25 in, 0.375 in, 0.5 in and 1 in), (Set 2: 2 in, 3 in, 4 in and 5 in), (Set 3: 6 in, 8 in, 10 in and 30 in) respectively. Give your inference about the result.
- Find the effect of Constant Nominal Diameter and different Schedule Numbers. Tabulate the pressure drop results for four pipes with constant nominal diameter (1 in) and with different schedule numbers Set 1: 10, 20, 40, 80; Set 2: 40, 80, 120 and 160 – For four pipes.
- Find the effect of length of pipe and pressure drop at 40 and 80 schedule number and nominal diameter 1 inch and 3 inch. Tabulate the results. (Set 1: 40 Schedule Number and Nominal Diameter 1 In for all four pipes) and Length should be varied from 1 m, 5 m, 10m and 30 m. Give your inference. Also find the effect of length on the schedule number and nominal diameter by repeating the same with 80 Schedule Number and 1 inch pipe with above lengths (1, 5, 10 and 30 m) and 40 schedule number and 3 inch pipe and 80 schedule number and 3 inch.
- Find the effect of pressure drop on roughness factor for different materials of construction.

Part 2: Connect values (Globe Value) to the above pipes and find the Chock Outlet Pressure. Use any “Calculation Type” and outlet pressure 2 bar and different series styles and various sizes.

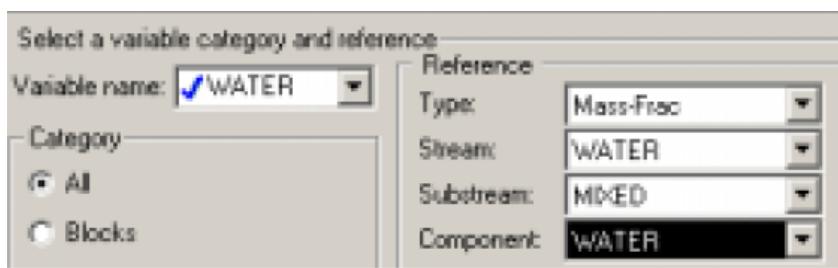
MEETING PROCESS DESIGN REQUIREMENTS USING DESIGN SPECIFICATIONS

A mixture containing 50.0 wt% acetone and 50.0 wt% water is to be separated into two streams – one enriched in acetone and the other in water. The separation process consists of extraction of the acetone from the water into methyl isobutyl ketone (MIBK), which dissolves acetone but is nearly immiscible with water. The overall goal of this problem is to separate the feed stream into two streams which have greater than 90% purity of water and acetone respectively. Fluid package is NRTL.



Process flow diagram for separation of water and acetone using MIBK.
Block: Flash3 Separator;
Mixer 1: Acetone and water mixture – 100 lbs/hr and MIBK – 100 lbs/hr and 75° F and 50 psi; **Mixer 2:** MIBK Flow rate is 50lbs/hr and 75° F and 50 psi. Flash3 Conditions are (75° F and 50 psig)

1. Simulate the entire result and explain the need for use of second flash separator. Find the increase in the mole fraction of water and acetone using the second separator. Also note whether any component has reached 90% purity (Mass Fraction) at Outlet 1, Outlet 2 and 3 and 4 and 5. (Table Format: Should contain, temperature, pressure mass flow and mass fraction for both flash separators and (Acetone-water), MIBK1, MIBK2, Outlet 1, Outlet 2, Liquid and Outlet 3, Outlet 4 and Outlet 5).
2. Meeting Process Requirements Using Design Specifications: USE: Flow-sheeting Option – Design Spec to do sensitivity analysis. (Variable Definition: Variable Name: Water; Category: All; Type Mass Fraction- Stream: Water; Sub stream (Mixed; Component: Water and Spec Tab Options: Water – Target – 0.9 and Tolerance: 0.001. Vary Tab Options -Type: Mass Flow; Stream: MIBK2; Sub Stream: Mixed; Component: Methy-01; Low 25; and High 100; Export the results. Find whether water has reached 90% (Mass Fraction), if yes then tabulate the results in the above Table Format. Also note down number of iterations ASPEN took for achieving the above result.

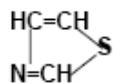


3. What is the flow rate of MIBK2 to achieve 95% purity of water in the above streams? MIBK range can be 25 lb/hr to 500 lb/hr can be used.

Estimate Physical Properties of Non-Databank Component and Use it in simulation

Find the following Critical Temperature (TC), pressure (PC), ideal gas heat capacity coefficient (CPIG), heat of formation (DHFORM), Gibbs free energy formation (DGFORM), Watson heat of vaporization coefficient (DHVLWT), critical volume (VC) and critical compressibility factor (ZC) for Thiazole component.

Molecular structure for Thiazole:



Molecular weight: 85

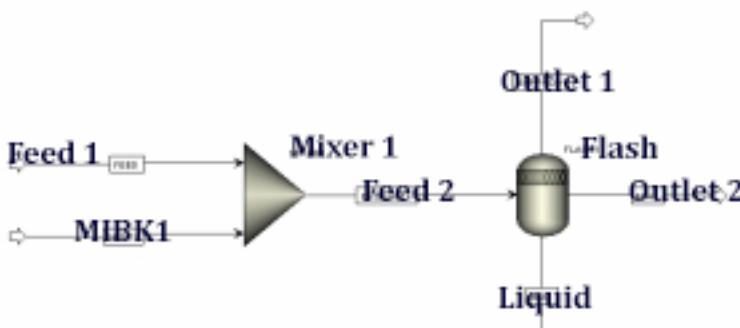
Normal boiling point: 116.8 °C

Vapor pressure correlation:

$$\ln p_i^{oL} = \frac{\text{C}_1 + \text{C}_2 T + \text{C}_3 T^2}{T + \text{C}_8 + \text{C}_9}$$

For p_i^{oL} in mmHg, T in °C for $69^\circ\text{C} < T < 118^\circ\text{C}$

1. Generate Txy Diagrams for Thiazole and Water Mixture with NRTL Fluid Package. Tabulate the Txy results in the Activity Coefficient and Mole Fraction of Thiazole and Water.
2. Perform flash separation of Thiazole 40 lb/hr, water 200 lb/hr and acetone 200 lb/hr at 90°C and 20 psia. Change the conditions of the flash separation starting from (90°C and 20 psia) to (150°C and 60psia) and try to achieve maximum separation of components during flash operation. Tabulate the results in the following form: (Temp, pressure, mole flow and mass fraction for each case and give the inference.
3. Using three phase flash separator (Flash3) to separate acetone from the above mixture. MIBK (methyl isobutyl ketone) can be used for separation of acetone from thiazole, water and acetone mixture. Find the optimal flow rate of MIBK (from 300 lb/hr to 1000 lb/hr) for separation of acetone from water and thiazole mixture. Use design specifications or sensitivity analysis for achieving the desired concentration. Tabulate the results in the format mentioned in problem 2 for all feeds including Feed1, MIBK1, Outlet1, Outlet2 and Liquid as shown in the below diagram.



Reactor Problem

Ethyl acetate is produced in an esterification reaction between acetic acid and ethyl alcohol.



The feed mixture, consisting of 52.5 mole% acetic acid, 45 mole% ethyl alcohol and 2.5 mole% water, enters the RCSTR model with a flow rate of 400 kmol/hr at 75°C and 1.1 atm. The reactor operates at 70°C and 1 atm. Both the reactions are first-order with respect to each of the reactants (i.e., overall second-order). For these liquid-phase reactions, the kinetic data for the Arrhenius law are given below:

$$\text{Forward reaction: } k = 2.0 \times 10^8 \text{ m}^3/\text{kmol} \cdot \text{s}$$

$$E = 6.0 \times 10^7 \text{ J/kmol}$$

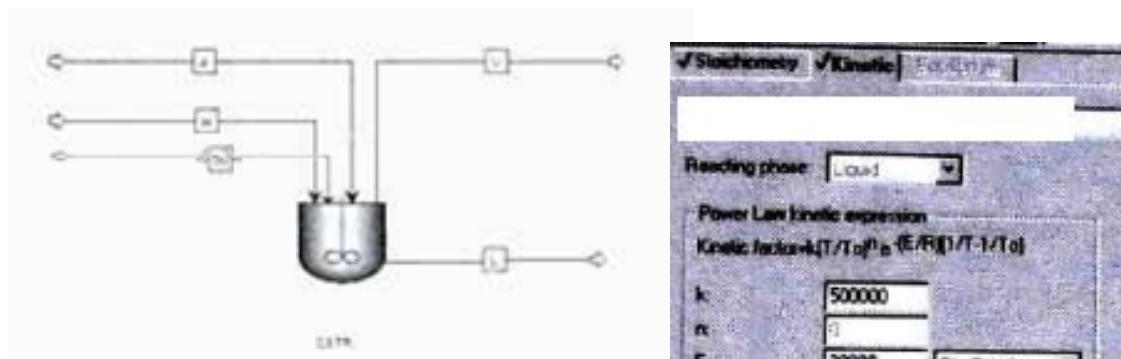
$$\text{Reverse reaction: } k = 5.0 \times 10^7 \text{ m}^3/\text{kmol} \cdot \text{s}$$

$$E = 6.0 \times 10^7 \text{ J/kmol}$$

$[C_i]$ basis = Molarity

Perform the Aspen Plus simulation using the NRTL thermodynamic model and reactor volume of 0.15 m³.

Use the below flow diagram (CSTR). Powerlaw Model can be used (See Diagram) .



Part 2:

Simulate the same results in Rstioc and RGibbs Models. – Use 80% Ethanol Conversion for Rstioc Model. Use default parameters for RGibbs Model.

Perform Sensitivity Analysis by changing the acetic acid flow rate and checking outlet ethyl acetate concentration. Or any other parametric change for enhancing the ethyl acetate output concentration.