

Flash Operation

[Methanol & water]

→ Aim :

To carry out flash operation with the given data such as temperature and pressure. (Temperature = 180°F ; Pressure = 20 psi)

→ Problems :

- After one cycle of flash operation ; [initial T = 180°F ; P = 20 psi] change the temperature to 90°C. Run the simulation & view the results
- Change the temperature of flash chamber to 83°C ; Feed temperature = 180°F, 20 psi pressure.
- Modify methanol & water composition & run the simulation
Methanol = 60 ; water = 40.

→ Theory :

- A flash operation is a simple vessel (flash drum) that separates vapors from liquid at a given temperature & pressure. A liquid or liquid vapors mixture flows in, the vapors that boil off goes out the pipes at the top and the liquid that remains flows out at the bottom.
- A flash drum is used for rapid separation of a mixture into a liquid and vapors by flash evaporation caused by a sharp drop in pressure.

Flash Operation

[Methanol & water]

→ Aim :

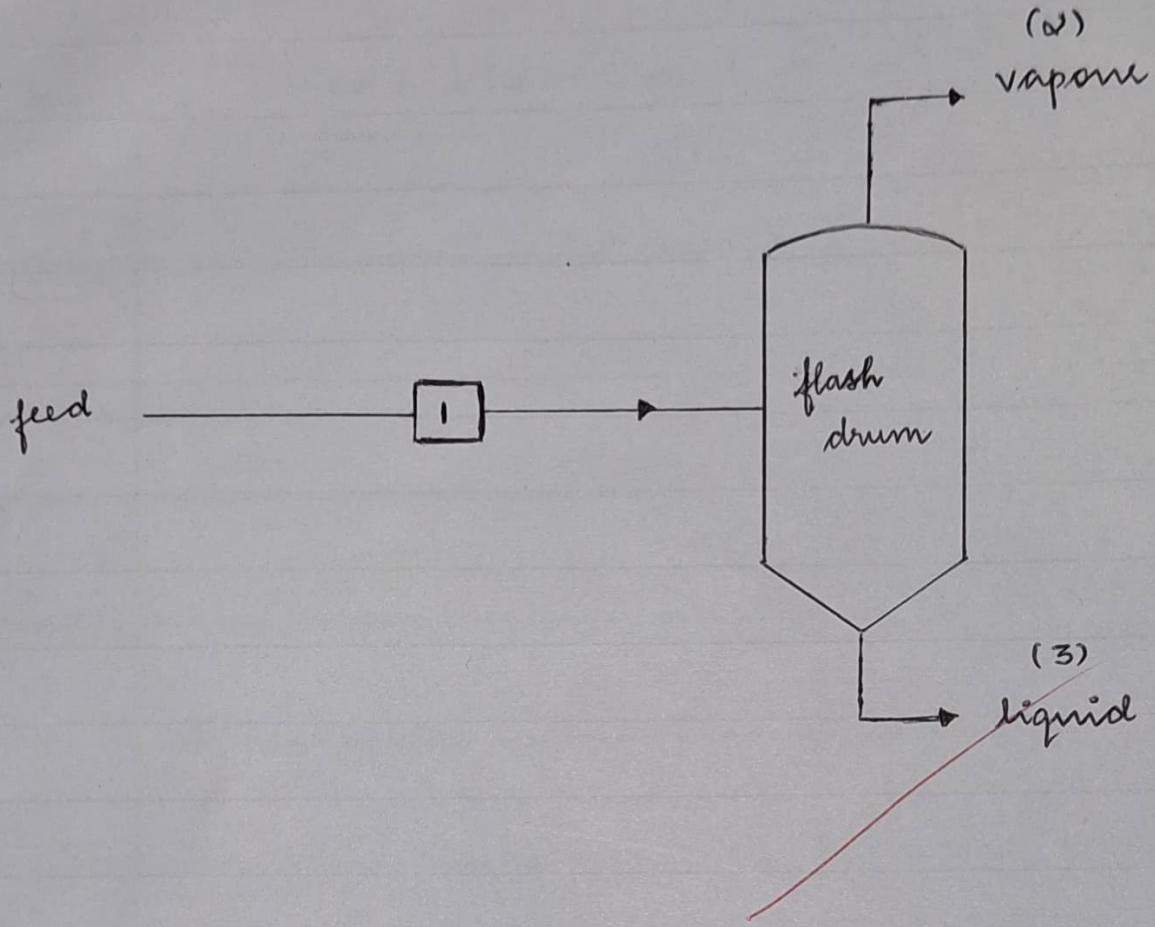
To carry out flash operation with the given data such as temperature and pressure. (Temperature = 180°F ; Pressure = 20 psi)

→ Problems :

- After one cycle of flash operation; [initial T = 180°F ; P = 20 psi]
Change the temperature to 90°C. Run the simulation & view the results
- Change the temperature of flash chamber to 83°C ; Feed temperature = 180°F , 20 psi pressure.
- Modify methanol & water composition & run the simulation
Methanol = 60 ; water = 40.

→ Theory :

- A flash operation is a simple vessel (flash drum) that separates vapour from liquid at a given temperature & pressure. A liquid or liquid vapour mixture flows in, the vapour that boils off goes out the pipes at the top and the liquid that remains flows out at the bottom.
- A flash drum is used for rapid separation of a mixture into a liquid and vapors by flash evaporation caused by a sharp drop in pressure.



→ Procedure :

- 1) Open C Drive in My PC, → Program files → ASPEN Tech
→ ASPEN Plus → Favorites → Examples → Getting Started
→ Process.
 - 2) Copy all the files present in "Process" onto Drive D in a New Folder. Rename the folder for your convenience.
 - 3) In Drive D ; open the folder "flash.bkp".

→ Starting ASPEN Hysys Plus

 - o Start → ASPEN Hysys Plus
 - o Search → ASPEN Hysys Plus (V14 or V11)
 - 4) Once flash.bkp is opened in the ASPEN Hysys Plus window, click on 'Setup' in the left side panel.
In the main window ; Select 'Accounting'.
Enter in the details such as username, account number, Project ID, Project Name [all your preferences]
 - 5) Click on "Simulation"
 - A flow diagram is displayed.
To carry out the operation mentioned in the AIM, one should double click on Stream 1 (inpnt)
Enter in the specifications :
 - Temperature : 180°F
 - Pressure : 10 psi
 - Component Value
 - Methanol 50
 - Water 50

Experiment No.

Date :

6. Click on Next Button and select Duty instead of Temperature
enter the values

$$\text{Duty} = 0 \text{ Btu/hr}$$

$$\text{Pressure} = 1 \text{ atm}$$

7. Click on Results \rightarrow Stream results.

The simulation results can be viewed in this tab. Scroll down
Enable mass flows, molar flows etc in the results tab
to have a detailed view of the simulation results.

\rightarrow Problem a:

- 1) Right click on Stream 1 (feed input).
- 2) Change the temperature to 90°C
- 3) View the results in Stream Results Tab.

\rightarrow Problem b:

- 1) Click on the Flash Drum in the flow diagram
Input the temperature as 83°C
- 2) Double click on Stream 1. Enter in the specifications
Temperature : 180°F ; Pressure : 20 psi
- 3) View the results in Stream Results Tab.

\rightarrow Problem c:

- 1) In Stream 1, the components & valve section has
methanol & water values as 50 & 50. Change it 60 & 40.
- 2) View the results in Stream Results Tab.

→ Saving the File:

- a) Click on Tools → Options
Activate (Always create backup copy) → * apw
- b) File → Save as → Flash → Save.

➤ Inference:

- As the methanol and water system is an azeotropic mixture ; the flash operation is not possible.
- At higher temperatures, maximum outlets will be seen in vapour phase.
- This operation is not suitable for the mentioned experiment

CSS/10

> Experiment Results:

Stream 1 2 3

		Stream 1	2	3
- Mole Flows	lbmol/hr	100	100	0
METHANOL	lbmol/hr	60	60	0
WATER	lbmol/hr	40	40	0
- Mole Fractions				
METHANOL		0.6	0.6	0
WATER		0.4	0.4	0
- Mass Flows	lb/hr	2643.14	2643.14	
METHANOL	lb/hr	1922.53	1922.53	
WATER	lb/hr	720.611	720.611	

a) Problem :

		1	2	3
- Mole Flows	lbmol/hr	100	85.6648	14.3352
METHANOL	lbmol/hr	50	47.401	2.59896
WATER	lbmol/hr	50	38.2637	11.7363
- Mole Fractions				
METHANOL		0.5	0.553332	0.181299
WATER		0.5	0.446668	0.818701
- Mass Flows	lb/hr	2502.87	2208.16	294.708
METHANOL	lb/hr	1602.11	1518.83	83.2763
WATER	lb/hr	900.764	689.332	211.432

Problem b)

		1	2	3
- Mole Flows	lbmol/hr	100	78.462	21.538
METHANOL	lbmol/hr	50	45.5909	4.40911
WATER	lbmol/hr	50	32.8711	17.1289
- Mole Fractions				
METHANOL		0.5	0.581057	0.204713
WATER		0.5	0.418943	0.795287
- Mass Flows	lb/hr	2502.87	2053.01	449.859
METHANOL	lb/hr	1602.11	1460.83	141.277
WATER	lb/hr	900.764	592.182	308.582

Problem c)

		1	2	3
- Mole Flows	lbmol/hr	100	10.7737	89.2263
METHANOL	lbmol/hr	50	8.27493	41.7251
WATER	lbmol/hr	50	2.49881	47.5012
- Mole Fractions				
METHANOL		0.5	0.768064	0.467632
WATER		0.5	0.231936	0.532368
- Mass Flows	lb/hr	2502.87	310.163	2192.71
METHANOL	lb/hr	1602.11	265.147	1336.96
WATER	lb/hr	900.764	45.0168	855.747

Simulation of MCH

> Aim:

To carry out the simulation of Methylcyclohexane, and to determine the results of the simulation.

> Theory:

Methylcyclohexane also known as cyclohexylmethane is an organic compound with the molecular formula $\text{CH}_3\text{C}_6\text{H}_11$. Classified as saturated hydrocarbon, it is a colourless liquid with a faint odour. It is used as a solvent. It is mainly converted in naphtha reformers to toluene.

Methylcyclohexane is usually dehydrogenated to toluene which increases the octane rating of gasoline.

Methylcyclohexane is flammable and is considered very toxic to aquatic life.

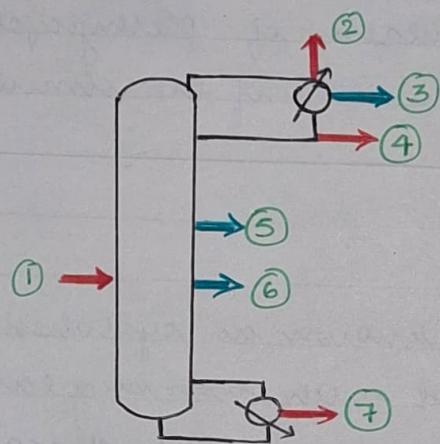
> Procedure:

- 1) Click on Start \rightarrow Aspen Hysys Plus \rightarrow Aspen Hysys Plus Plus V14 or V11.
- 2) Open a new simulation.
- 3) Click on File \rightarrow New \rightarrow User \rightarrow General with english units \downarrow last option
- open the selected template

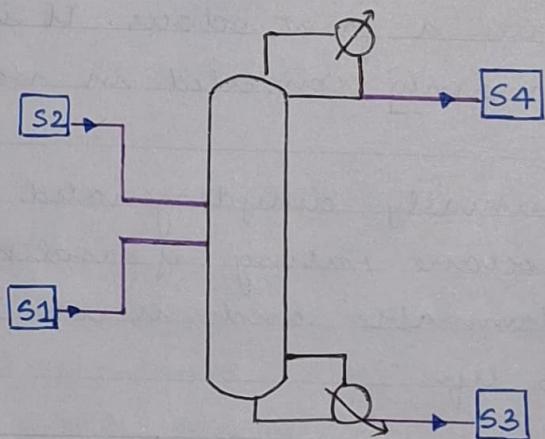
Step 4)



Step 5)



Step 6)



- 4) Click on Simulation to enter into the simulation Environment.

At the bottom of the page, click on column, select Bad Frac. Only single click to select.

Click once on the Simulation Blank Tab. A column is added.

- 5) An option i.e "Material" is present at the left bottom side in the same place where we selected column.

Click on the option 'Material'

- * Now, DO NOT CLICK ANYTHING, just move the cursor of the mouse onto the simulation environment. In other words, "HOVER THE CURSOR OF THE MOUSE" in the display tab of the simulation environment.
 - You will be able to see red and blue arrows that will be automatically added to the column.
 - (For our convenience, let us number the arrows 1 to 7 (rough work - just for understanding) as shown on the left hand side of the page).

- 6) Click on the following numbered arrows in order and drag them to create streams.

1st Drag \rightarrow Arrow No. 1 \rightarrow Stream 1 \rightarrow Phenol

2nd Drag \rightarrow Arrow No. 1 \rightarrow Stream 2 \rightarrow MCH

3rd Drag \rightarrow Arrow No. 4 \rightarrow Stream 3 \rightarrow Distil

4th Drag \rightarrow Arrow No. 7 \rightarrow Stream 4 \rightarrow Residue

Rename the streams as given above: 1: Phenol, 2 = MCH, 3 = Distil, 4: Residue.

Experiment No.

Date :

- 7) Click on "Properties" (above simulation option)
click on Setup.
Enter in all the accounting information.

Username : Raveena

Account no : 1905

Project ID : Exp 02

Project name : Simulation of MCH

- 8) Go Back to the simulation Environment. In the left side Panel click on Setup.

► Setup
↓ click on this

In the drop down Menu of Setup, click on Report options.
click on 'Stream' in the Report options Tab.
Enable "Mole" under the Fraction Basis option.

* ASPEN HYSYS PLUS consists of Property Sets that are essential for simulation.

eg: HXDESIGN, TXPORT

- 9) Click on properties ; scroll down, click on Components.
Click on specifications. Click on Find.

a) Type "Toluene". Enable "Equals". Search results will be displayed. Click on the component that is desired → add the selected component option.

b) Repeat the above step for "Phenol" & "Methylcyclohexane".

c) Click on Next

Experiment No.

Date :

10. Click on Methods → All methods filter → UNIFAC
Base Method

UNIFAC with Redlich-Kwong Equation of state & Henry's law

11. Click on Next, go to the simulation environment.
Double click on MCH stream (S2) and enter in the specifications such as:

Component	Value	Temp = 200 °F
Phenol	-	Pressure = 20 psi
Toluene	200	
MCH	200	

12. Double click on Phenol Stream (S1), enter in the specifications:

Component	Value	Temp = 200 °F
Phenol	1200	Pressure = 20 psi

13. Double click on the cylinder.

- i) In the configurations; enter the specifications:

No. of stages : 22

Condenser type : Total

Distillate Rate : 200 lbmol/hr

Reflux ratio : 8

- ii) Click on the 'streams'

Phenol : 14th stage

MCH : 7th stage *y_{input}*

- iii) Click on Pressure → View Pressure Profile
Input the data :

Stage	Pressure
1	16
N2	20.2

14. Click on Next. Ensure there is no error in simulation.
You can view the results under stream results

➤ Inference :

The simulation of Methylcyclohexane was carried out and the results were obtained as shown (on the left hand side)

→ Problem 1:

→ to 1000 lbmol/hr

Changing the quantity of phenol & view the result.

- i) In the flow diagram, double click on Phenol stream and change the component value from 100 to 1000 lbmol/hr.
- ii) Run the simulation & view the stream results.

→ Problem 2:

Changing the quantity of phenol to 900 lbmol/hr.

- i) In the flow diagram, double click on the Phenol stream and change the component value of phenol to 900.
- ii) Run the simulation and view the results.

→ Presułki

mole fraction mmole/l.m	Distil	MCH	Phenol	Residue
Tolu - 01	41.5796	200	0	158.402
Pheno - 01	7.9×10^{-5}	0	1200	1200
Methy - 01	158.402	200	0	41.5977

Problem 1) → 2000 lb mol/hr (phenol component value)

Problem 2) 900 lb mol/mr

Problem 3) → temp change to 130°C

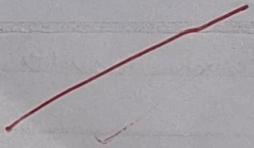
Material	Heat	Load	Work	Power	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids
					Units	DISTIL	MCH	PHENOL	RESIDUE
Average MW						96.9279	95.1643	94.113	94.0113
- Mole Flows		Ibmol/hr				200	400	1200	1400
TOLUE-01		Ibmol/hr				41.6792	200	0	158.321
PHENO-01		Ibmol/hr				8.07455e-05	0	1200	1200
METHY-01		Ibmol/hr				158.321	200	0	41.6793
+ Mole Fractions									
+ Mass Flows		Ib/hr				19385.6	38065.7	112936	131616
+ Mass Fractions									
Volume Flow		cuft/hr				436.433	827.177	1837.31	2313.23
+ Liquid Phase									
<add properties>									

Problem 4) No. of Stages = 40

Material	Heat	Load	Work	Power	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids
					Units	MCH	PHENOL	DISTIL	RESIDUE
Average MW						95.1643	94.113	96.9336	94.0105
- Mole Flows		Ibmol/hr				400	1200	200	1400
TOLUE-01		Ibmol/hr				200	0	41.4904	158.51
PHENO-01		Ibmol/hr				0	1200	8.31608e-05	1200
METHY-01		Ibmol/hr				200	0	158.51	41.4905
+ Mole Fractions									
+ Mass Flows		Ib/hr				38065.7	112936	19386.7	131615
+ Mass Fractions									
Volume Flow		cuft/hr				827.177	1837.31	436.506	2313.16
+ Liquid Phase									
<add properties>									

Problem 5) Change the boiler type & view the results.

Material	Heat	Load	Work	Power	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids
					Units	DISTIL	MCH	PHENOL	RESIDUE
Average MW						96.9341	95.1643	94.113	94.0104
- Mole Flows		Ibmol/hr				200	400	1200	1400
TOLUE-01		Ibmol/hr				41.4739	200	0	158.526
PHENO-01		Ibmol/hr				8.30396e-05	0	1200	1200
METHY-01		Ibmol/hr				158.526	200	0	41.474
+ Mole Fractions									
+ Mass Flows		Ib/hr				19386.8	38065.7	112936	131615
+ Mass Fractions									
Volume Flow		cuft/hr				436.513	827.177	1837.31	2313.22
+ Liquid Phase									
<add properties>									



→ Problem 3.

Increase the temperature of phenol. to 130°C .

- i) Double click on the phenol stream in the flow diagram sheet.
- ii) Change the temperature to 130°C .
- iii) Run the simulation and view the results.

→ Problem 4:

Increase the no. of stages and see the output.

- i) In the flow sheet, double click on the cylindrical vessel.
- ii) Change the no. of stages to a desired value.
- iii) Run the simulation & view the results.

→ Problem 5:

Change the boiler type and view the results.

$$\hookrightarrow \text{flow rate} = 600 \text{ lbmol/hr}$$

- i) Double click on the cylindrical vessel and change the type of reboiler used to Themosyphon.
- ii) Run the simulation, view the results.

→ Inference.

The simulation of methylcyclohexane was carried out under given and different conditions and results were obtained.

e

Sensitivity Analysis

> Aim:

To perform a sensitivity analysis using ASPEN Plus and to visualise the data.

> Theory:

One of the benefits of a simulation is that we can study the sensitivity of process performance to changes in operating variables. With ASPEN Plus, we can allow inputs to vary and can tabulate the effect on a set of results of our choice. This is called sensitivity analysis.

> Procedure :

1. In the files that were copied from C Drive, into the D Drive in a folder of our choice, make a copy of mch and rename it as mch-new.
2. Click on Data → Model Analysis Tools → click on Sensitivity. Click on New → Type S1 → click OK.
(All of this under Simulation Tab)
3. When you double click on S1 ; enter in the 'Vary' specifications under the manipulated variable :

Variable = 1

Type : Stream var

Stream : 2

Substream : Mixed

Experiment No.

Date :

Variable : Mole - flow

Unit : lbmol/hr.

- Right hand side :

• at quidistance

→ Start point : 1200

→ End point : 2000

→ Increment = 100

4) Under Define Tab of S1 ; input the specifications:

New → XMCH (variable → New → XMCH)

Under Preference :

Type : Mole-Frac

Stream : 3

Sub Stream : Mixed

Component : MCH

• Add New Variable : QCOND

Category : All

→ Under Preference :

Type : Block-var

Block : B1

Variable : cond-Duty

Sentence : Results

Units : Btu/hr

• Add New Variable : QREB

Category : All

7 Under reference :

Type : Block-var

Block : B1

Variable : Reb duty

Sentence : Results

Units : Btu/lhr

5) Check the Tabulate Tab under SI to see if all the 3 variables XMCH, QCOND and QREB are present.

6) Click on 'Options' tab under SI.

- "Do not reinitialise blocks" → Click on that option.
- Execute base case last → click on the option (down)

7) Click on "Custom" present under Plot on top right hand corner of the page.

A list of options will be displayed.

Select : XMCH ; QCOND Btu/lhr ; QREB Btu/lhr

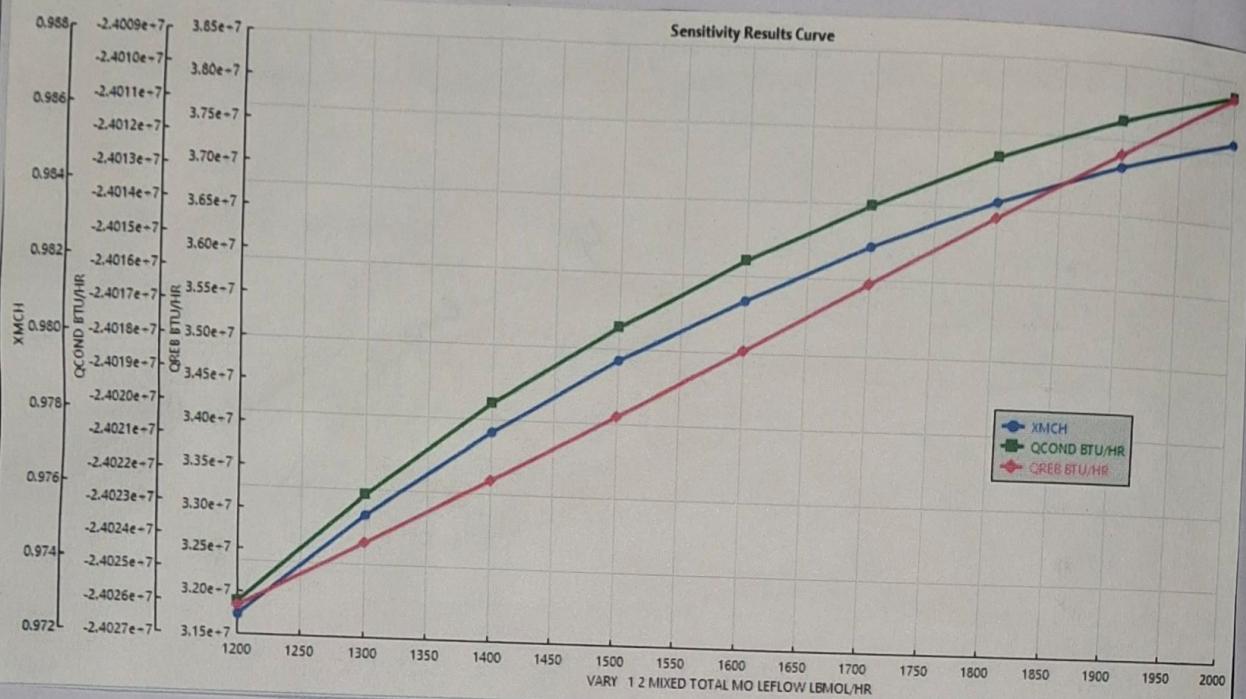
Click OK. (Results → Model Analysis Tools → Sensitivity → SI)

8) A graph is plotted. You can view the results.

You can also save the file as mch.sens.

✓
➤ Inference:

The sensitivity analysis was observed with change in operating variables and the effect on the process performance was also seen.



Meeting Process Design

Requirements

> Aim:

To meet the process design requirements based on given design specifications.

> Theory:

To ensure effectiveness of a process and to make sure that the process achieves its intended objectives and outcomes, one has to meet process design requirements.

→ Objectives include:

- a) Optimizing resource utilization, reducing wastes, increased efficiency, reduced errors.
- b) Customer satisfaction
- c) Encourages continuous improvement and adaptability.
- d) Compliance: to meet regulatory, legal and industry standards
- e) Consistency: to reduce variability in large scales.

> Procedure:

1. In the files present in the D Drive that we copied from C Drive, make a copy of mch and rename it as mch.specs.

Experiment No.

Date:

- a) Click on Data \rightarrow Flow sheeting options \rightarrow Design spec
Click on New \rightarrow Type DS - 1
3) Double click on DS 1. In the "Define" Tab, click on New. Input the following specifications:

Variable : XMCH \rightarrow category: all

- Under reference:

Type: Mole frac

Stream: 3

Substream: Mixed

- 4) Under "Spec" Tab, input the following specifications.

Spec : XMCH * 100

Target : 98.0

Tolerance : .01

- 5) Under "Vary" Tab, input the following specifications.

Type: Stream var

Stream: : 2

Substream: Mixed flow

variable: Mole flow

Units: lbmol/hr

- Report labels

Line 1

Line 2

- 6) Run the simulation and view the results.

Variable	Initial value	Final value	Units
► MANIPULATED	1519.08	1519.08	LBMOL/HR
XMCH	0.980005	0.980005	

Mch - specs

> Creating a flow diagram:

→ Connect stream 1 to pump and outlet of

1. Introduce a pump in the main flowsheet.

Pump to
flash
drum.

Enter in the specifications.

→ Discharge pressure: 25 psi

Connect it to the flash drum.

2. In the flash drum, in streams, enter in the pressures :

Stage 7	Stream 2
Stage 14	Stream S4
above stage	

Product streams :

Stage 1	Phase :	liquid
22		liquid

3. Click on streams in Results Summary.

Click on Send to flowsheet on top right hand corner

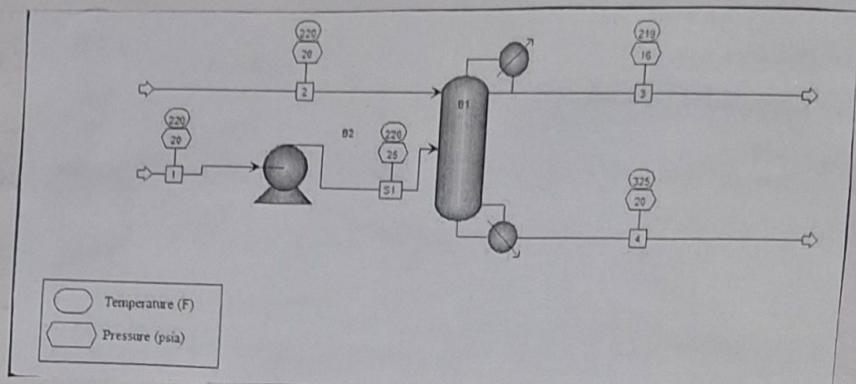
Click OK. ; enable temperature and pressure (on top)

4. You will be able to view the flowsheet along with results.

> Inference :

- Steps to create a flow diagram were analysed and the design specifications were met.

C

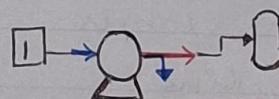


process flow diagram

Description	Units	1	2	3	4	S1
From						
To			B1	B1	B1	B1
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Maximum Relative Error						
Cost Flow	\$/hr					
- MIXED Substream						
Phase		Liquid Phase				
Temperature	F	220	220	218.829	325.302	220.053
Pressure	psia	20	20	16	20.2	25
Molar Vapor Fraction		0	0	0	0	0
Molar Liquid Fraction		1	1	1	1	1
Molar Solid Fraction		0	0	0	0	0
Mass Vapor Fraction		0	0	0	0	0
Mass Liquid Fraction		1	1	1	1	1
Mass Solid Fraction		0	0	0	0	0
Molar Enthalpy	Btu/lbmol	-21892.7	-60075.0	-72456.5	-44615.6	-31685.1
Mass Enthalpy	Btu/lb	-333.031	-636.337	-739.186	-475.369	-332.994
Molar Entropy	Btu/lbmol-R	-113.166	-72.4045	-154.57	-64.3603	-113.163
Mass Entropy	Btu/lb-R	-1.18916	-0.769335	-1.57684	-0.685745	-1.18914
Molar Density	lbmol/cuts	0.483572	0.669259	0.443812	0.605023	0.483553
Mass Density	lb/cut	46.0188	62.986	43.5046	56.7842	46.017
Enthalpy Flow	Btu/hr	-1.26771e+07	-7.2091e+07	-1.44917e+07	-6.24618e+07	-1.26756e+07
Average MW		95.1643	94.113	96.0248	93.8548	95.1643
♦ Mole Flows	Ibmol/hr	400	1200	200	1400	400
♦ Mole Fractions						
♦ Mass Flows	Ib/hr	38065.7	112936	19605	131396	38065.7
♦ Mass Fractions						
Volume Flow	cuft/hr	827.177	1793.03	450.641	2313.98	827.211
♦ Liquid Phase						

process flow diagram

results.



estimating physical properties of

Non Databank Components

→ dim:

To estimate the physical properties of a component which is unavailable in ASPEN Plus databank.

Thiazole ($C_3H_3N_1$) is the compound whose properties have to be estimated.

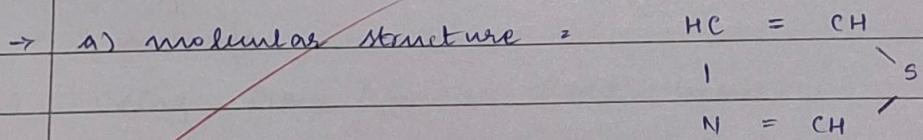
→ Theory:

Thiazole is a 5 membered heterocyclic compound that contains both sulfur and nitrogen.

Thiazole is a pale yellow liquid with a pyridine like odour and the molecular formula C_3H_3NS .

Thiazole ring is notable as a component of vitamin Thiamine (B1).

→ Properties of thiazole : (given)



b) molecular weight = 85 g/mol

c) Normal Boiling point = $116.8^\circ C$

- vapour pressure $\Rightarrow \ln P_i^{\circ L} = 16.445 - \frac{3281}{T + 216.255}$
 correlation $\downarrow \text{mmHg}$ $\downarrow ^\circ C$ for $69^\circ C < T < 118^\circ C$

Experiment No.

Date :

- properties to be determined :

Parameter	Description
T_c, P_c	Critical temperature & pressure
$C_{P, G}$	Ideal gas heat capacity co-efficient
DH_{FORM}	Heat of formation
DG_{FORM}	Gibbs free energy formation
V_c, κ_c	Critical volume, compressibility factor

> Procedure :

1. open Aspen Hysys Plus VII or VI4. Click on New simulation under File.
Select the template "General with English units".
2. Under properties, click on Components \rightarrow specifications \rightarrow user defined ; type in the following specifications.
Component ID : Thiazole
Click Next
Click on Draw / edit / import structure. or define molecule by its connectivity

\rightarrow 2 methods :

- a) Using Draw / import / edit structure :
Drawing pane will open. Draw the structure, input appropriate bonds. Import the same.
- b) Define molecule by its connectivity.

Experiment No.

Date :

Enter in the specifications.

Atom 1 no.	Atom 1 type	Atom 2 no.	Atom 2 type	Bond 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

- Under define molecule by its connectivity, also enter other data such as:

Molecular weight = 85

Normal Boiling point = 116.8 °C

Click Next

- Click on option 3) Extended Antoine vapour pressure co. efficient.

*	Component	Temp units	Property units
	Thiazole	°F	mmHg

Scroll right & enter in the values under 1, 2, 3, 4, 5, 6, etc.

By comparing it with the given Antoine equation

$$1 = 16.445$$

$$6 = 0$$

$$2 = -3281.0$$

$$7 = 0$$

$$3 = 216.255$$

$$8 = 69$$

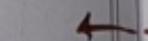
$$4 = 0$$

$$9 = 118$$

$$5 = 0$$

cancel the tab

click on finish → or



*	Parameter \Rightarrow PLXANT		
	component	Temp Units	Property units
	Thiazole	F	mmHg
→	You can click on "Help" to know more about the parameter "PLXANT".		
3.	Click on "Estimation" (left hand side panel); Enter the component Thiazole Under Parameter; enable : ZC, PC, Tr, Vc, DGFDFM Under method, type "Joback". or click on Joback.		

Experiment No.

Date :

4) Click on Estimation on the top panel

Click on Run

View the simulation results.

Problem 2 :

→ Input thiazole and water in stream 1 & run the simulation.

i) Under properties → under components add water and methanol

By clicking on find → type H₂O → enable equals add selected compound.

Do the same for methanol.

ii) Go to simulation environment. Add a "flash v" from separators.

iii) Go to the flowsheet, click on Stream 1

↳ drag streams
(ref LHS page)

→ Input the following specifications.

Flash type Temperature Pressure

Temperature 90 °C

Composition :

Pressure 20 psi

Mole flow mol/mn

Total flow basis Mole

Thiazole 40

Water 200

Methanol 200

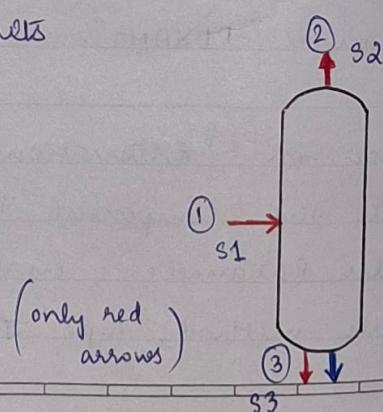
3) Click on Run. View the simulation results.

Component	THIAZOLE	Formula	C3H3NS	
Estimated pure component parameters				
PropertyName	Parameter	Estimated value	Units	Method
NORMAL BOILING POINT	TB	387.84	K	JOBACK
CRITICAL TEMPERATURE	TC	629.049	K	JOBACK
CRITICAL VOLUME	VC	0.2125	CUM/KMOL	JOBACK
CRITICAL COMPRES.FAC	ZC	0.282247		DEFINITI
IDEAL GAS CP AT 300 K		69908.6	J/KMOL-K	JOBACK
AT 500 K		105485	J/KMOL-K	JOBACK
AT 1000 K		150830	J/KMOL-K	JOBACK
STD. HT.OF FORMATION	DHFORM	1.6918e+08	J/KMOL	JOBACK
STD.FREE ENERGY FORM	DGFORM	1.9547e+08	J/KMOL	JOBACK
LIQUID MOL VOL AT TB	VB	0.0742774	CUM/KMOL	GUNN-YAM
UNIQUAC R PARAMETER	GMUQR	2.72973		BONDI
UNIQUAC Q PARAMETER	GMUQQ	1.816		BONDI
PARACHOR	PARC	168.6		PARACHOR

Simulation results

Material	Heat	Load	Work	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids
				Units		S1	S2	S3
Mass Liquid Fraction					0.0470072		0	1
Mass Solid Fraction						0	0	0
Molar Enthalpy	Btu/lbmol				-79845.6	-77442.5	-113755	
Mass Enthalpy	Btu/lb				-2619.55	-2489.6	-5254.08	
Molar Entropy	Btu/lbmol-R				-19.2673	-17.9595	-37.7222	
Mass Entropy	Btu/lb-R				-0.632117	-0.577357	-1.74229	
Molar Density	lbmol/cuft				0.00305293	0.00285112	2.54278	
Mass Density	lb/cuft				0.0930552	0.0886879	55.0534	
Enthalpy Flow	Btu/hr				-3.51321e+07	-3.18197e+07	-3.31236e+06	
Average MW					30.4807	31.1064	21.6509	
- Mole Flows	lbmol/hr				440	410.882	29.1183	
THIAZOLE	lbmol/hr				40	39.3939	0.606105	
WATER	lbmol/hr				200	176.14	23.8595	
METHA-01	lbmol/hr				200	195.347	4.65267	
+ Mole Fractions								
+ Mass Flows	lb/hr				13411.5	12781.1	630.437	
+ Mass Fractions								

Problem 2 Results



Experiment No.

Date :

> Inference

- The methods to estimate the properties of non data bank compounds were analysed and the simulation was carried out.
- Components such as water & methanol were also added and simulation was carried out.

✓

Mixing Two Components & Analyzing Thermodynamic Properties

> Aim :

To use the interactive property analysis features in Aspen Plus to obtain a binary T-xy diagram for acetone chloroform system using the NRTL activity coefficients model with parameters from the built in binary pair database.

> Theory :

Txy diagram is essential for understanding the vapour liquid equilibrium (VLE) of binary mixtures which is crucial in designing and optimizing various chemical processes.

It is a diagram to visualize the relation between T, x and y.

T = temperature

x = mole fraction of one component in a liquid phase

y = mole fraction of the same component in vapour phase.

> Procedure :

i) open Aspen Hysys Plus.

open a new simulation that is with the selected template of general with English Units.

2. Click on specifications under Components (left panel)
Add Acetone and chloroform by clicking on find and enabling equals.

3. click on specifications under methods (left panel)
Under global tab ;
Method filter = Common
Base method = NRTL

Free water method : steam-TA
water solubility : 3

4. click on analysis (top right hand corner)
Binary analysis tab will pop up.
→ Analysis type = Txy
Component 1 = acetone
Component 2 = chlo - 01

compositions

Basis : mole fraction

vary : acetone

• equidistant

Start point = 0

End point = 1

• No. of intervals = 50

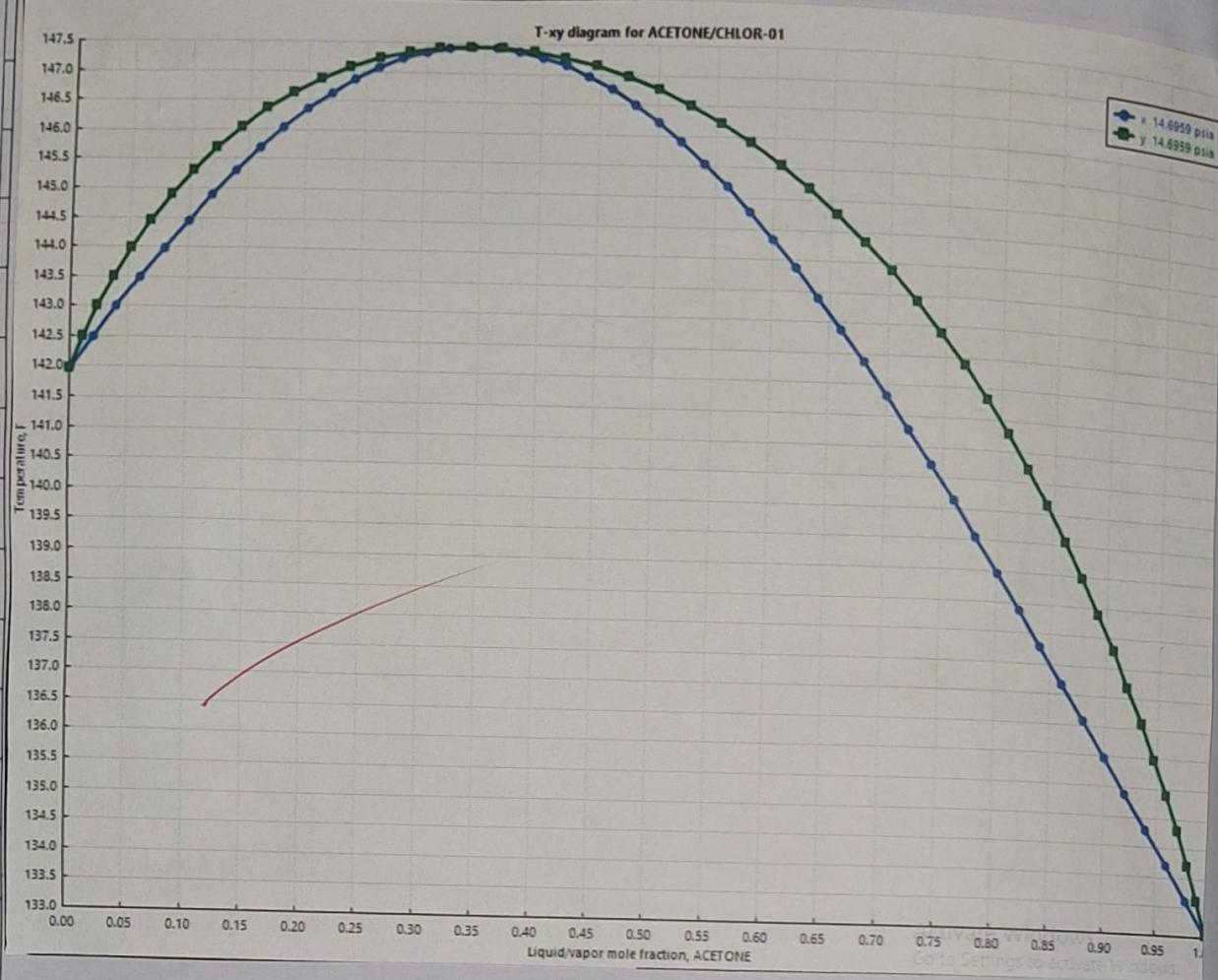
pressure

unit : psia

Enter values • dist of values

14.6959

5. Click on Run Analysis. The graph will be obtained.



Experiment No.

Date :

> Inference :

The thermodynamic properties of a binary mixture of acetone and chloroform were analysed with the help of a ~~Txy~~ diagram.

Simulation of a Shell & Tube Heat Exchanger using open loop

> Aim :

To design a shell and tube exchanger for the following duty 20,000 kg/hr 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 70000 kg/hr 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.

> Theory :

- A shell and tube heat exchanger is the most common type used in oil refineries and other chemical processes. It is suitable for higher pressure applications.
- Consists of a shell and bundle of tubes inside it.
~~One fluid runs through the tubes while the other over the tubes (i.e. in the shell region)~~
This is to transfer heat between the 2 fluids.
- The set of tubes is called a tube bundle and may be composed of several tubes → plain, longitudinally finned etc.

> Procedure :

1. Make sure Aspen EDR is installed and is working.
2. Open Aspen Hysys V14 or V11 on the desktop or whichever folder it is present in.
3. Click on Properties.
In the components list → add components → Select "hypothetical" instead of pure components.
→ click on the method "create a batch of hysys"
enter in the specifications : initial boiling point = 150°C
final boiling point = 150°C
→ Generate hysys.
click on NBP [1] 240° and NBP [1] 250° as the liquid density (kg/m^3) of both i.e. 818.0^+ and $\rho_d 2.60$ respectively are closely matched with the ones mentioned in question.
→ also add NBP [0] 150° and NBP [0] 160° .
4. Under fluid packages → Methods assistant for references and keep with fluid packages.
 - Based on component, based on process, we can select fluid packages.
→ Here we shall go for SRK.
5. Go to the simulation environment.
 - Add the 4 streams from the module palette.
Stream 3 has to be \leftarrow instead of \rightarrow . For this, click on Stream 3. Under "Showsheet or Modify" option on top panel, click on flip horizontal.

Experiment No.

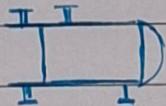
Date:

6. Add a heat exchanger from the model palette.

 will be added.

Right click on it - last but one option \rightarrow Change icon.

Click on the third one (as required in question)



7. Rename the material streams

Stream 1 - C

Stream 2 - C out

Stream 3 - K in

Stream 4 - K out

8. Double click on the heat exchanger.

Enter in the specifications.

Under Worksheet :

C inlet temp = 40°C

- Tube side inlet = C

Kin temp = 200°C

- Tube side outlet = C out

Kout temp = 90°C

- Shell side inlet = K in

C pressure = 650 kPa

- Shell side outlet = K out

Kin pressure = 50 kPa.

\rightarrow Under design \rightarrow Parameters.

Shell side pressure drop = 0.8 bar (80 kPa)

Mass flow (kg/h)

Tube side pressure drop = 0.8 bar (80 kPa)

C = 70000

Kin = 80000

*

\rightarrow Under worksheet \rightarrow composition

Under C : $NBP [1]^{240^*} = 0.5$

$NBP [1]^{250^*} = 0.5$

*
→ Under performance → plots

change plot type

X = heat flow

Y = temperature

Under K_{min} : $NBP[\alpha]_{150^*} = 0.5$ (mole fractions)
 $NBP[\alpha]_{160^*} = 0.5$

→ Under rating:

no. of shell passes = 1

Tubes passes per shell = 2

⇒ 1, 2 heat exchanger.

→ Under Design → Parameters → size exchanger → convert
click on yes.

9 → Double click on the shell and tube heat exchanger
again.

- Select rigorous shell and tube option in the displayed tab. Click on process.
- Enter the fouling resistance as mentioned in the question.

Under 1 = 0.0002 C-m²/W

Under 2 = 0.0003 C-m²/W

- Under rigorous shell and tube heat exchanger → click on Exchangers option on the right.

→ Enter in the following specifications by clicking on them.

~~Front end head type : 4 channel and removable cover~~

~~Rear end head type : 1 Removable channel with flat cover.~~

~~tube length = 5000 mm~~

~~Tube passes = 2~~

- Under Process → enter in the estimated outlet temp of 2 as 90°C

- Click on "View EDR browser"
 - A new tab will open up under which we should click on "Geometry"
 - Enter in these specifications :

Shell ID (in inches) = 14.536 / 15.25

- scroll down

Baffle spacing centre - centre = 76 mm

No. of baffles = 60.

No. of tubes / tube passes = 75 / 2

Shells in series = 1

Shells in parallel = 1

10. Under mechanical settings present next to the Geometry tab (on left) → click on setting plan → right click → print → pdf.

11. Under results → results summary → TEMA sheet → print → pdf.

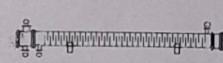
→ Inference :

- Using the specifications mentioned in the question, we were able to design a shell and tube heat exchanger and explore new options.
- A TEMA sheet consists of all the information related to the designed shell and tube heat exchanger.

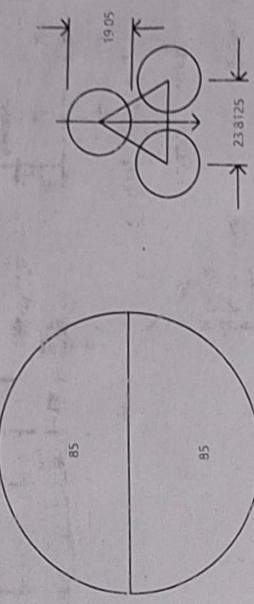
TEMA Sheet

TEMA Sheet

Heat Exchanger Specification Sheet

1	Company:					
2	Location:					
3	Service of Unit: Our Reference:					
4	Item No.: Your Reference:					
5	Date:	Rev No.:	Job No.:			
6	Size: 369 - 5000 mm	Type: AEL	Horizontal	Connected in: 1 parallel	1 series	
7	Surf/unit(eff.) 22.1 m ²	Shells/unit 1		Surf/shell(eff.) 22.1 m ²		
8	PERFORMANCE OF ONE UNIT					
9	Fluid allocation		Shell Side		Tube Side	
10	Fluid name		K in->K Out		C->C Out	
11	Fluid quantity, Total		kg/h 20000		70000	
12	Vapor (In/Out)		kg/h 0	0	0	0
13	Liquid		kg/h 20000	20000	70000	70000
14	Noncondensable		kg/h 0	0	0	0
15						
16	Temperature (In/Out)		°C 200	120.63	40	68.66
17	Bubble / Dew point		°C 229.05 / 229.52	226.01 / 226.49	/	/
18	Density	Vapor/Liquid	kg/m ³ / 608.66	/ 605.3	/ 803.45	/ 782.68
19	Viscosity		cp / 0.1557	/ 0.2846	/ 1.9775	/ 1.1923
20	Molecular wt, Vap					
21	Molecular wt, NC					
22	Specific heat		kJ/(kg-K) / 2.779	/ 2.39	/ 1.983	/ 2.102
23	Thermal conductivity		W/(m-K) / 0.0937	/ 0.1029	/ 0.1186	/ 0.1151
24	Latent heat		kJ/kg			
25	Pressure (abs)		kPa 500	472.975	650	546.389
26	Velocity (Mean/Max)		m/s 0.53 / 0.72		3.78 / 3.83	
27	Pressure drop, allow./calc.		kPa 80	27.025	80	103.611
28	Fouling resistance (min)		m ² -K/W 0.0002		0.0003	0.00039 Ao based
29	Heat exchanged	1136.8 kW		MTD (corrected)	100.94 °C	
30	Transfer rate, Service	509.7	Dirty 509.6	Clean 726.3		W/(m ² -K)
31	CONSTRUCTION OF ONE SHELL					
32			Shell Side		Tube Side	
33	Design/Vacuum/test pressure: g		kgPa 600 / /	800 / /		
34	Design temperature / MDMT		°C 235 /	115 /		
35	Number passes per shell			1	2	
36	Corrosion allowance		mm 3.18	3.18		
37	Connections	In mm 1	77.93 /	1	102.26 /	
38	Size/Rating	Out 1	77.93 /	1	154.05 /	
39	ID	Intermediate		/	/	
40	Tube #:	75 OD: 19.05 Tks. Average 2.11	mm Length: 5000	mm Pitch: 23.81	mm	Tube pattern: 30
41	Tube type: Plain	Insert:None		Fin#: #/m	Material: Carbon Steel	
42	Shell Carbon Steel	ID 14.536	OD 15.25	in	Shell cover	-
43	Channel or bonnet	Carbon Steel			Channel cover	Carbon Steel
44	Tubesheet-stationary	Carbon Steel			Tubesheet-floating	-
45	Floating head cover				Impingement protection	None
46	Baffle-cross Carbon Steel	Type Single segmental	Cut(%) 34.1	Horiz Spacing: c/c 76	mm	
47	Baffle-long	Seal Type		Inlet	178.98	mm
48	Supports-tube	U-bend	0	Type		
49	Bypass sea!		Tube-tubesheet joint	Expanded only (2 grooves)(App.A 'l')		
50	Expansion joint		Type None			
51	RhoV2-Inlet nozzle	2229	Bundle entrance 356	Bundle exit 150		kg/(m-s ²)
52	Gaskets - Shell side		Tube side	Flat Metal Jacket Fibre		
53	Floating head					
54	Code requirements	ASME Code Sec VIII Div 1		TEMA class R - refinery service		
55	Weight/Shell	1337.2 Filled with water	1864.1	Bundle	573.5	kg
56	Remarks					
57						
58						

Specifications



Shell inside diameter	mm	369.2144
Front head inside diameter	mm	387.35
Outer tube limit	mm	359.6894
Tube number (calcs.)		170
Tube number (layout)		170
Tube length	mm	5000
Tube O.D.	mm	19.05
Tube pitch	mm	23.8125
Tube pattern		30
Tube passes		2
Tie rod number		4
Tie rod diameter	mm	9.55
Sealing strips (pairs)		2
Baffle type		Single segmental
Centre to outer baffle cut	mm	58.7069
Centre to inner baffle cut		
Impingement protection		None
Shell Side Inlet Nozzle Inside Diameter	mm	77.9272
Shell Side Outlet Nozzle Inside Diameter	mm	77.9272

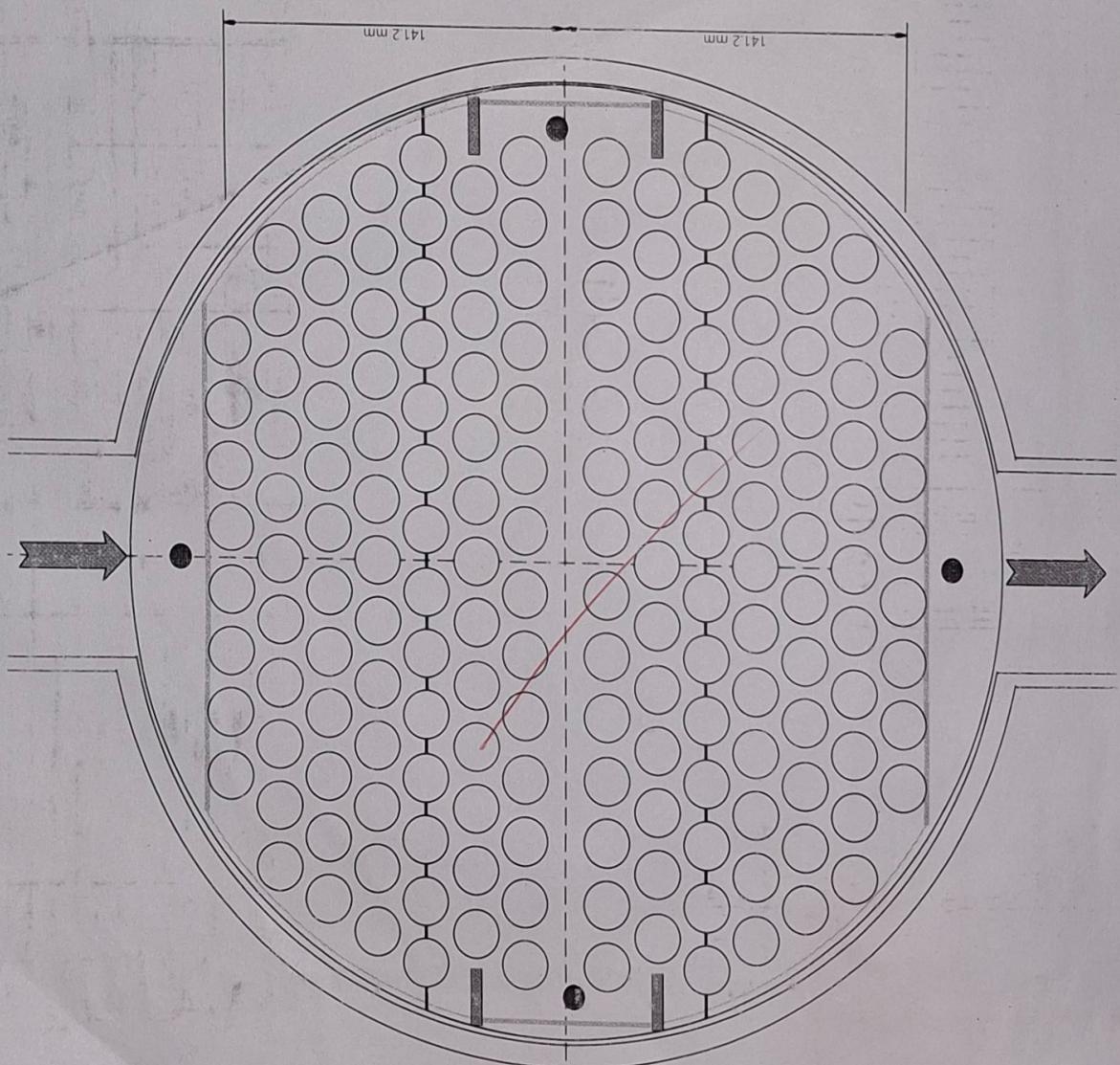
Notes:

Our Reference:
Your Reference:
Item No.:
Rev. No.:
Date:
Job No.:

Company Name

City, State

Company	Location:	ASME Code Sect. VIII Div 1	Tube Layout
	Service of Unit:	TEMA Form A/B	
	Item No.:	Steel - 800 - 5000	Dwg No.:
	Date:		2



Simulation of pipes in Aspen Plus

> Aim:

To find the pressure drop in the pipes by simulating them using Aspen Plus.

- Find suitable property method using Method Assist and also find the suitable Schedule Number and Nominal Diameter (Nominal) for all pipes with $p_1 = 0.08741667 \text{ ft}$, $p_2 = 0.05566667 \text{ ft}$, $p_t 3 = 0.07975 \text{ ft}$, $p_4 = 0.04166667 \text{ ft}$ using trial and error method.
- The component is water with flow rate $1003.752 \text{ lbmol/hr}$. Temperature is 100°F , pressure 80 psia .
- The length of all pipes is 30 ft and roughness is 0.00015 ft and erosion velocity coefficient is 100 .
- Also generate report with all stream parameters.

> Theory:

~~→ Nominal diameter:~~

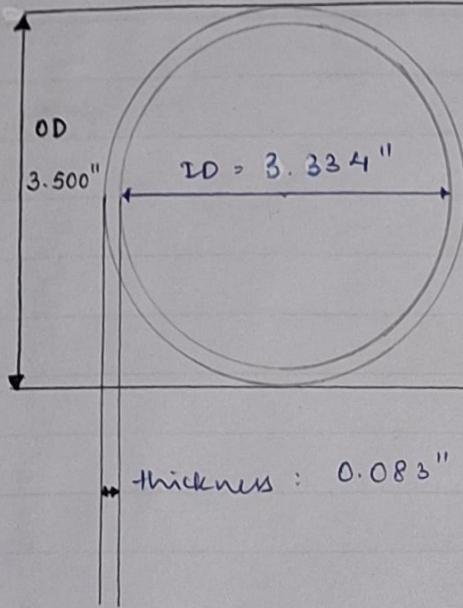
An approximate measurement of the diameter of a pipe or inside diameter of a shell.

- for pipes: it is an approx measurement of the diameter of a pipe. But its not exactly the inside diameter usually.

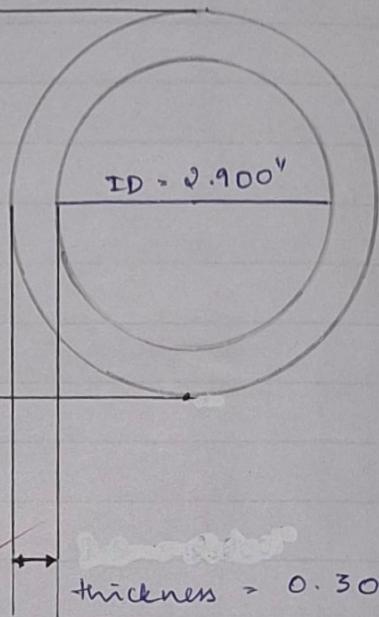
e.g: 4" schedule 80 pipe has a nominal size of 4", but its actual outside diameter is 4.5"

- Schedule Number: A dimensionless no. that defines the thickness of the pipe wall

NPS 3" Schedule 5



NPS 3" Schedule 80



> Procedure :

1. Open Aspen Plus. Open a new Blank Simulation.
2. Under Setup → Specifications: enter in the specifications.
 - Global : Title : Simulation of Pipes
3. Under Components → find the component Water.
Remember to enable "equals" (not contains)
4. Under Methods → click on Methods Assist if you are not sure which fluid package to go for.
 - Method filter : All
 - Base method : Steam TA.

• Methods Assist : → specify component type → specify (water only) → we can use Steam TA as specified under methods assist.
5. Go to Simulation.
 - In the bottom panel containing Equipment Symbols, click on "pipes" present under Pressure Exchangers. Insert 4 pipes onto the Simulation Environment.
 - Under equipment symbols panel → Manipulator. Under manipulator → click on "Duplicator". Insert the symbol.
→ DUPL (option 2)

6. Click on Material. Move the cursor on the screen.

Don't click on anything.

Refer figure (1). The arrow marks will appear.

7 Rename the pipes as pipe 1, pipe 2, pipe 3, pipe 4.

1st Drag : circle numbered 0 → Stream 1

2nd Drag : circle numbered ① → connect to ② → Stream 2

3rd Drag : circle numbered ① → connect to ③ → Stream 3

4th Drag : circle number ① → connect to ④ → Stream 4

5th Drag : circle numbered → ① → connect to ⑤ → Stream 5

6th Drag : circle number ⑥ → Stream 6

7th Drag : circle number ⑦ → Stream 7

8th Drag : circle number ⑧ → Stream 8

9th Drag : circle number ⑨ → Stream 9

• Rename the streams

Stream 1 - Water

Stream 2 - P1 in

Stream 3 - P2 in

Stream 4 - P3 in

Stream 5 - P4 in

Stream 6 - P1 out

Stream 7 - P2 out

Stream 8 - P3 out

Stream 9 - P4 out

Refer figure 2

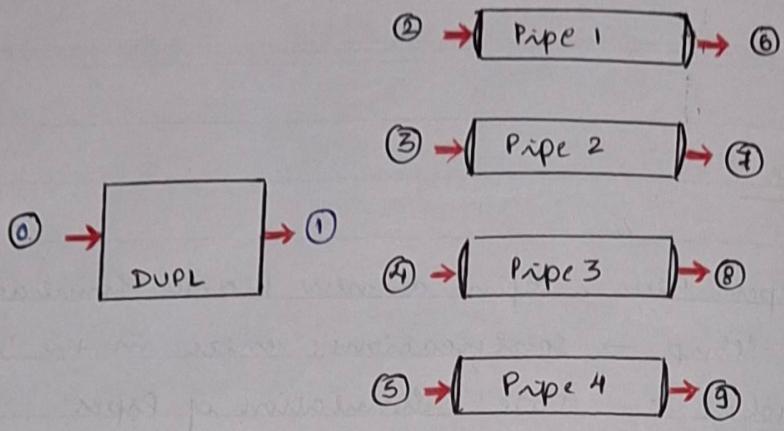


figure 1

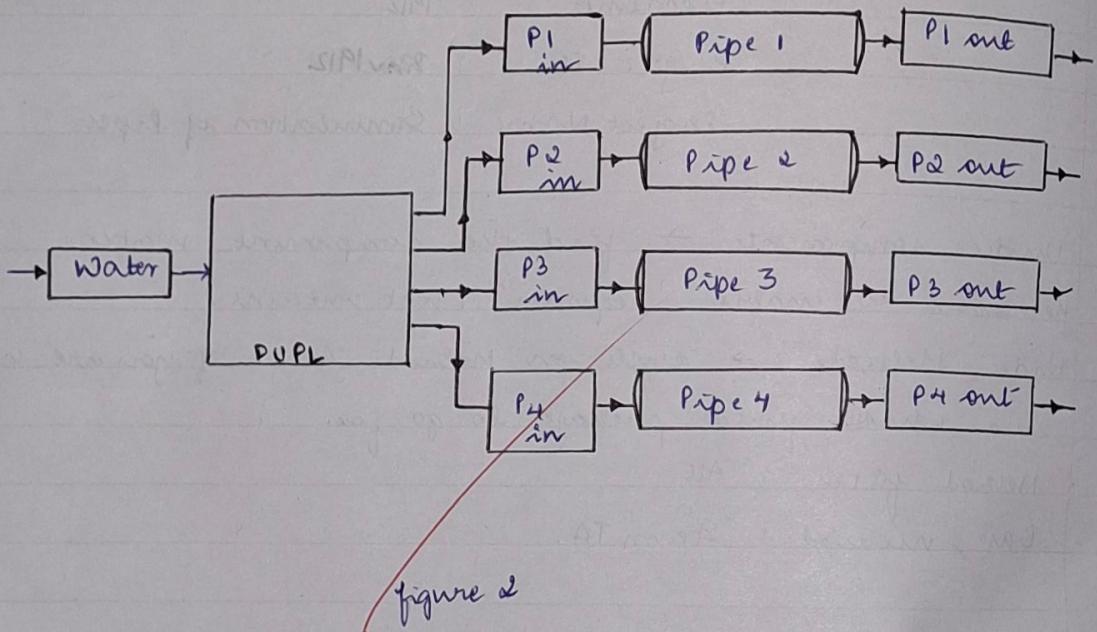


figure 2

(Units → English Units)

8. Click on P1 pipe → Under parameters.

Under diameter.

Click on "Use pipe Schedule"

Enter material: carbon steel

* Now, we have to obtain the values or specifications of pipes that are mentioned in the question i.e

$$P1 = 0.08741667 \text{ ft}$$

$$P2 = 0.05566667 \text{ ft}$$

$$P3 = 0.04975 \text{ ft}$$

$$P4 = 0.04166667 \text{ ft}$$

- To obtain the exact values, we must do trial and error method with the schedule number and nominal diameter. Keep changing until you get the exact value of 0.08741667 ft for pipe 1.

• After trial and error method we obtain "0.08741667" for 40 schedule Number 1 inch Nominal diameter.

→ Carry out the same for pipe 2, 3, 4 until you get the exact values as mentioned.

o Also enter in the specifications such as pipe length 30 ft; roughness = 0.00015 ft; erosion velocity co-efficient = 100.

9. Click on Stream 1 (water)

Enter the specifications

$$\text{Temperature} = 100^\circ\text{F}$$

$$\text{Pressure} = 80 \text{ psia}$$

$$\text{flow rate} = 1023.752 \text{ lb/mol/s.}$$

10. Run the simulation.

Click on OK.

You can view the results under Results Summary.

11. Under Results Summary, click on Models.

In the displayed tab, select "Send to Excel."

Click on "Export Tables to Excel".

12. Open Excel.

Make the content fit to page or else only half of it will be printed in a sheet.

To make the content fit into the page;

Click on  present at the bottom right next to the zooming option.

Adjust both the dotted blue lines up and down to make the content fit into a single page.

13. Click on print → pdf → Save.

> Inference.

- With the help of ASPEN Plus, pipes were simulated according to given specifications and pressure drop was obtained along with other results.

C
VSN

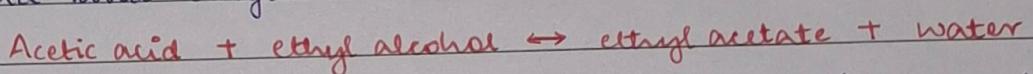
Results:

Name	PIPE1	PIPE2	PIPE3	PIPE4
Property method	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA
Henry's component list [ID]				
Electrolyte chemistry [ID]				
Use true species approach for electrolytes	YES	YES	YES	YES
Free-water phase properties method	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA
Water solubility method	J	J	J	J
Pipe method	FLUID	FLUID	FLUID	FLUID
Pipe length [ft]	30	30	30	30
Inner diameter [ft]	0.087416667	0.255666667	0.07975	0.241666667
Pipe rise [ft]	0	0	0	0
Pipe angle [deg]				
Roughness [ft]	0.00015	0.00015	0.00015	0.00015
Frictionless velocity coefficient	100	100	100	100
Outlet temperature [F]				
Heat transfer coefficient [Btu/hr-sqft-R]				
Heat flux [Btu/hr-ft ²]				
Enlargement diameter [ft]				
Enlargement angle [deg]				
Contraction diameter [ft]				
Contraction angle [deg]				
Orifice diameter [ft]				
Orifice thickness [ft]				
Conveying method				
Dilute phase conveying method	DILUTE	DILUTE	DILUTE	DILUTE
Muschelknaut solid friction parameter calculation	MUSCHELKNAUT	MUSCHELKNAUT	MUSCHELKNAUT	MUSCHELKNAUT
Solid-wall sliding friction parameter calculation	USER-SPEC	USER-SPEC	USER-SPEC	USER-SPEC
Salation velocity method	USER-SPEC	USER-SPEC	USER-SPEC	USER-SPEC
Consider initial acceleration	MOLERUS	MOLERUS	MOLERUS	MOLERUS
Fluid friction parameter method	YES	YES	YES	YES
Specified fluid friction parameter	0.02	0.02	0.02	0.02
Muschelknaut solid friction parameter	0.01	0.01	0.01	0.01
Solid-wall sliding friction parameter	0.55	0.55	0.55	0.55
Solid-wall impact friction parameter	0.015	0.015	0.015	0.015
Wall friction parameter f	0.4	0.4	0.4	0.4
Solid friction on tube bottom	0.2	0.2	0.2	0.2
Stogol solid friction parameter	0.08	0.08	0.08	0.08
Solid/fluid velocity ratio	0.8	0.8	0.8	0.8
Stress transmission coefficient				
Particle-wall friction				
Characteristic viscosity parameter [lb/sec]				
L/Equivalent length of elbows [ft]	0	0	0	0
Pressure drop coefficient per elbow	0	0	0	0
Voidage				
Sphericity	1	1	1	1
Particle diameter [ft]				
Total pressure drop of fluid flow [psi]	14.6100282	0.063458236	23.5219811	0.083858857
Frictional pressure drop of fluid flow [psi]	14.6100282	0.063458236	23.5219811	0.083858857
Elevation pressure drop of fluid flow [psi]	0	0	0	0
Acceleration pressure drop of fluid flow [psi]	0	0	0	0
Head duty of fluid flow [ft-lbf/lb]	-850.007102	-3.69188409	-136.852377	-4.87875634
L/Equivalent length of fluid flow [ft]	30	30	30	30
Solids loading of solids conveying				
Heat rate of solids conveying				
Total pressure drop of solids conveying				
Frictional pressure drop of dense phase conveying				
Elevation pressure drop of dense phase conveying				
Pressure drop due to elbows in dense phase conveying				
Slug length of dense phase conveying				
Slug velocity of dense phase conveying				
Calculated characteristic viscosity parameter				
Approach to salination velocity				
Total feed stream CO ₂ flow [lb/hr]	0	0	0	0
Total product stream CO ₂ flow [lb/hr]	0	0	0	0
Net stream CO ₂ production [lb/hr]	0	0	0	0

Dynamics & Control of a CSTR - Controlled Stirred Tank Reactor

Aim:

Ethyl acetate is produced in an esterification reaction b/w acetic acid and ethyl alcohol.



A 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 atm.

The reactor operates at 70°C and 1 atm.

Both the reactions are First Order with respect to each of the reactants (overall 2nd order) for these liquid phase reactions, the kinetic data for the Arrhenius law is given below:

$$\text{Forward reac}^n k = 2.0 \times 10^8 \text{ m}^3 / \text{kmol.s}$$

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

$$\text{Backward reac}^n k = 5.0 \times 10^7 \text{ m}^3 / \text{kmol.s}$$

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

~~Composition basis = Molarity.~~

~~o Reactor geometry data :~~

~~Vessel type : vertical~~

~~Head type : flat~~

~~Diameter = 0.45711 m~~

~~Volume = 0.15 m³~~

→ Simulate the reactor model using the SYSOPD thermodynamic model to compute the product compositions

- b) Report the default controllers during parameters and control actions used and constraints imposed on variables.
- c) Investigate the new performance of the default liquid level and temperature control algorithms and discuss the effect of loop interactions.
- d) Show the regulatory behaviors of both the controllers in presence of disturbance in feed temperature.

Theory:

A CSTR, continuous stirred tank reactor is a common model for chemical reactor in chemical engineering and environmental engineering. A CSTR often refers to a model used to estimate the key unit operation variables while using a continuous agitated tank reactor to reach a specified output.

The behaviour of a CSTR is often approximated or modelled by that of an ideal CSTR which assumes perfect mixing.

Procedure :

1. Open ASPEN Hysys Plus VII or VII present in the systems.
2. Open the template of metric units. (General with metric units). Open the selected template.
3. Under Setup, under Global, make sure you change the input mode to "Dynamic" instead of steady state.
Give the title of the experiment as Dynamic & control of a CSTR.

4. Input other specifications under the Accounting option of setup

Under Stream that is under Setup \rightarrow Report Options, make sure that Flow Basis: Mole and Fraction basis Mole is enabled.

5. Under components, add the 4 components acetic acid, ethanol, ethyl acetate and water. (enable: equals)

- Under specifications \Rightarrow method filter: all ;
Base method: SYSOP0

6. Enter into the simulation environment.

From the equipment symbols that is present at the bottom pane, click on reactors. Click on the CSTR.

Click on the displayed simulation environment in order to add the CSTR.

- Click on material; Arrow marks shall be shown.
Refer to the figure on the left and make your flow diagram look alike.

7. The incoming stream for the CSTR shall be the "Feed" stream. The outgoing stream shall be Product.

8. Double click on the Feed stream. Input the specifications as mentioned in the question \rightarrow flow rate, temperature, pressure.

Composition of the components :

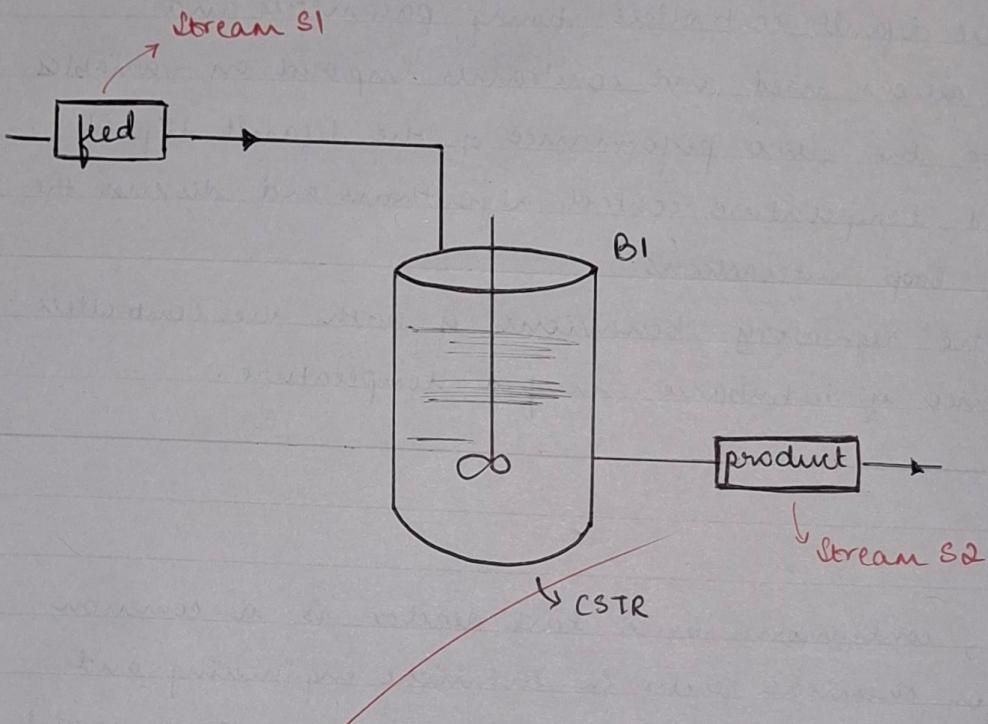
$$\text{• acetic acid} = 0.525$$

$$\text{• ethyl alcohol} = 0.45$$

$$\text{• water} = 0.025$$

- Temperature = 75°C , pressure = 1 atm

- Also enter the kinetic data for the above (the k values and E values) \rightarrow forward reaction.



9. Double click on the CSTR.

Input the specifications such as 75°C and latent pressure.
temp

As it is a dynamic setup, input the specifications such as vessel type, head type, diameter, volume (Blocks B1)

10. Under Reactions (in the left panel), click \rightarrow Kinetics.
Add New reaction let R1 \rightarrow Povcellaw, Click on R1.

	Component	Stoichiometric	Exponential
Reactants	Acetic acid	-1	1
	Ethyl alcohol	-1	1
Products	Ethyl acetate	1	
	Water	1	

Enter the above specifications under stoichiometry.

- Under kinetics, enter the value of k & E
(forward reaction)

11. Make sure all the specifications are input.
Run the simulation. View the results.

12. Now click on File \rightarrow Export \rightarrow Aspen Tech \rightarrow flow driven process.

Save the file as per your convenience.

13. Open Aspen Dynamics. (make sure it is installed)
Click on File \rightarrow import.

Select the file that you saved moments ago (the

one carried out in Aspen Hysys Plus). Click open or ok
Aspen dynamics will import the file.

15. In the display area, the flow sheet will be present along with a level controller and a temperature controller.

16. Double click on any one of them. (figure 1)

- By clicking on them, a dialogue box appears.

The 6th option consists of a graph icon.

The 5th option consists of a configuration option.

The dialogue box shows details such as set point, offset etc.

17. click on the configuration. (figure 2)

Adjust the settings such as set point, integral derivative values to obtain a desired graph.

One can also change values of gain time.

18. The same configuration settings will be applied for the other controllers.

You can view the graphs for the controller by clicking on the graph option.

~~You can add in more controllers and change their values as per your convenience.~~



figure 1
↓
level controller graph

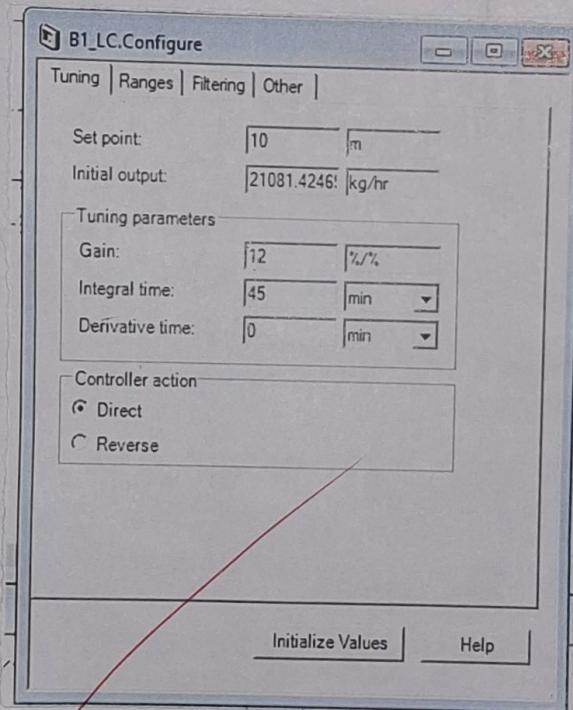
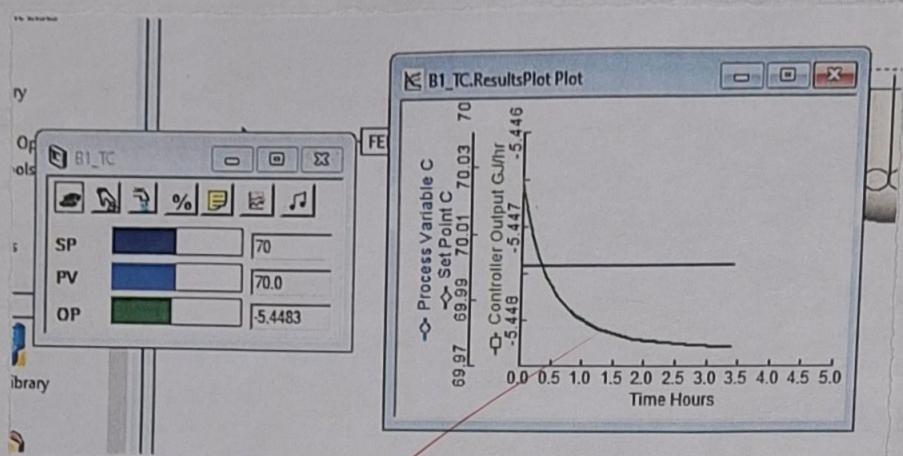
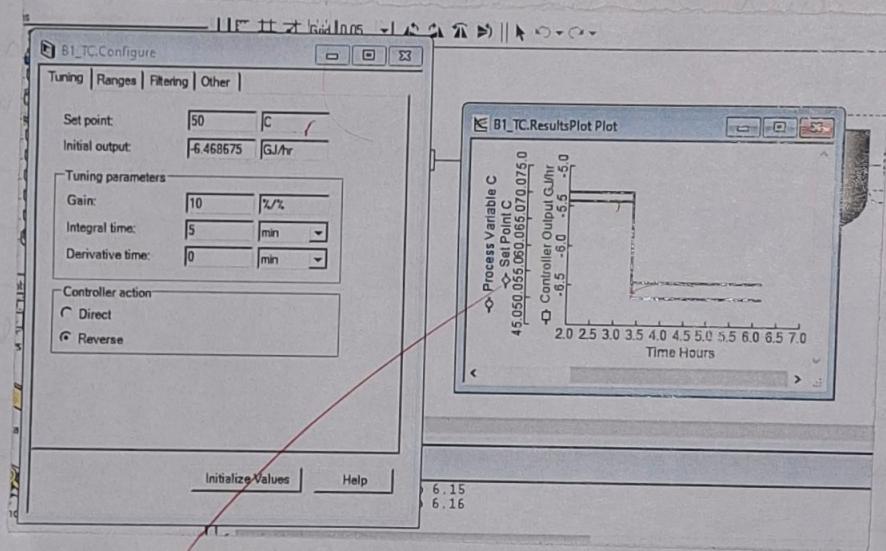


figure 2
level controller configuration



Temperature controller graph.



changing values in
temp. controller configuration

• Inference:

- We can analyse the effect of controllers in a reactive system.
- we can also manipulate the values and obtain desired or ideal graphs.
- we can add in additional controllers
- we can visualise a closed loop behaviour of the reactor system coupled with Aspen generated control schemes.

✓
20/12/24.