



KING FAISAL UNIVERSITY College Of Engineering

DEPARTMENT OF CHEMICAL ENGINEERING

CHE 410: COMPUTER AIDED PROCESS DESIGN LAB.

"Lab Manual"



Major Topics covered and schedule in weeks:

Торіс	Week #	Courses Covered
Introduction	1	3
Advanced skills in MS Excel	2	3
Application of Excel in Chemical Engineering Problem solving	3	3
Aspen Plus TM : Introduction & Properties Estimation	4, 5	6
Aspen Plus TM for Shell and Tube Heat exchangers	6	3
Aspen Plus TM Simulation of Separation Processes	7, 8	6
Aspen Plus TM Simulation of Reactor Models	9, 10	6
Aspen Plus Simulation of Chemical Plants	11	3
Chemical process simulation using Aspen Hysys	12, 13	6
Cost estimation using Aspen Plus	14	3
Final Exam	15	3

Specific Outcomes of Instruction (Lab Learning Outcomes):

- 1. Apply spreadsheet to solve common chemical engineering problems. (1)
- 2. Apply process simulators for properties estimation for process design. (1, 6)
- Design and simulate common process equipment using process simulators.
 (1,2)
- 4. Apply process simulators for process optimization and achieving specific design specifications. (1, 2, 6)
- 5. Design and simulate chemical processes using process simulators. (1, 2, 6, 7)
- 6. Communicate via class participation, written reports and oral presentations. (3, 5)

2

Student Outcomes (SO) Addressed by the Lab:

z	Outcome Description General Engineering Student Outcomes	Contribution
1.	an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics	Н
2.	an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors	
3.	an ability to communicate effectively with a range of audiences	L
4.	an ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts	
5.	an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives	Н
6.	an ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions	Н
7.	an ability to acquire and apply new knowledge as needed, using appropriate learning strategies	

PREFACE

This laboratory manual is prepared to serve as the primary instructional material for Computer Aided Process Design Laboratory (ChE 410) offered by the Department of Chemical Engineering to the undergraduate students. This lab is intended for the development of students' skills to solve common chemical engineering problems by spreadsheets and commercial process simulators.

This manual consists of two sections and Appendix. The first section contains three modules related to the application of MS Excel spreadsheets in chemical engineering calculations. The second section contains nine modules dedicated to the design and simulation of chemical engineering process equipment and process plant. The Appendix contains Economic Analysis of process plant, which will be of great help in Senior Design courses.

Syed Sadiq Ali

Table of Contents

Sn	Experiment Name	Page Number
i	Preface	4
ii	Acknowledgement	4
1	Application of Excel in Thermodynamics	6
2	Mass balances with Recycle Streams	25
3	Vapor-Liquid Equilibrium Using ASPEN Plus (I)	36
4	Vapor-Liquid Equilibrium Using ASPEN Plus (II)	45
5	Distillation using ASPEN Plus	57
6	Absorption using ASPEN Plus	72
7	Heat Exchanger Design Using ASPEN Plus	86
8	Reactor Design using ASPEN Plus (I)	97
9	Reactor Design using ASPEN Plus (II)	116
10	Process flow-sheet Simulation using ASPEN Plus (I)	133
11	Process flow-sheet Simulation using ASPEN Plus (II)	139
12	Chemical Process Simulation using Aspen Hysys	145
	APPENDIX	
A1	Cost Estimation and Analysis of process flow-sheet using ASPEN Plus	154

Experiment 1: Application of Excel in Thermodynamics

I. Objectives:

After the completion of this module, the students should be able to use EXCEL spreadsheet to solve routine chemical engineering problems and material & energy balance equations by using Solver.

II. Prerequisite Mathematical Skills

Essential commands and formulae entry in EXCEL

III. Prerequisite Engineering & Science Skills

- 1. Basic knowledge of Equations of State
- 2. Basic Knowledge of Material and Energy balance of chemical processes

Equations of State

Solving equations of state (EOS) allow us to find the specific volume of a gaseous mixture of chemicals at specified temperature and pressure. Without using equations of state, it would be virtually impossible to design a chemical plant. By knowing this specific volume, the size and thus cost of the plant can be determined, including the parameters such as diameter of pipes, the horse power of compressors and pumps, and the diameter of distillation tower and chemical reactor. Imagine how challenging it would have been to design a plant without knowing this important information. Determining the specific volume is the first step in the calculation of enthalpy and vapor-liquid properties of mixtures. Calculation of enthalpy is essentially important to perform energy balances to reduce energy use and help environment. In this module the calculations will be done for the vapor phase only.

Equations of State- Mathematical Formulation

The ideal gas EOS, which relates the pressure, temperature, and specific volume, is a familiar equation:

$$PV = nRT \text{ or } P\hat{v} = RT$$
 where $\hat{v} = \frac{V}{n}$

The term P is the absolute pressure, V is the volume, n is the number of moles, R is the gas constant, T is the absolute temperature and \hat{v} is the specific volume. This equation is quite adequate when the pressure is low (such as 1 atm). However, many chemical processes take place at very high pressure. For example ammonia is made at 220 atm or more. Under these conditions, the ideal gas EOS may not be a valid representation of the reality.

The rule of thumb is that the ideal gas is a good approximation for pressures upto 10 atm although this can change depending on the temperature. Accuracy of ideal gas EOS improves when used for processes which take place at high temperature.

Other equations of state have been developed usually in conjunction with the process simulators to address chemical processes at high pressure.

There are two key criteria:

(1) The equation is able to present the real p-V-T behavior

(2) The parameters must be easily found, including for mixtures.

The second criterion is no small criteria. There are more than 25 million compounds, leading to an infinite number of different mixtures. Obviously it is not possible to look up the properties of those mixtures on the web.

The first generalization of the ideal gas law was the van der Waals EOS:

$$P = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}^2}$$

Where b accounts for the excluded volume and a accounts for the force of interaction between two molecules.

This extension is just a first step, however, because it will not be a good approximation at extremely high pressures. Many more equations of state have been proposed in order to improve the representation. Some of the important Equations of State for pure components have been summarized in Table 1.1.

Model	EOS	а	b	α	ω	Z_c
Ideal gas	pV = nRT					
van der Waal	$p = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}^2}$	$a = 0.42188 \left(\frac{R^2 T_c^2}{p_c}\right)$	$b = 0.125 \left(\frac{RT_c}{p_c}\right)$			0.375
Redlich-Kwong	$p = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}\left(\hat{v} + b\right)}$	$a = 0.42748 \left(\frac{R^2 T_c^2}{p_c}\right) \alpha$	$b = 0.08664 \left(\frac{RT_c}{p_c}\right)$	$\alpha = \frac{1}{T_r^{0.5}}$		0.333
RK–Soave	$p = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}\left(\hat{v} + b\right)}$	$a = 0.42748 \left(\frac{R^2 T_c^2}{p_c}\right) \alpha$	$b = 0.08664 \left(\frac{RT_c}{p_c}\right)$	$\alpha = \left[1 + m\left(1 - T_r^{0.5}\right)\right]^2$	m = 0.480 + 1.574 ω - 0.176 ω^2	0.333
Peng-Robinson	$p = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}(\hat{v} + b) + b(\hat{v} - b)}$	$a = 0.45724 \left(\frac{R^2 T_c^2}{p_c}\right) \alpha$	$b = 0.07780 \left(\frac{RT_c}{p_c}\right)$	$\alpha = \left[1 + m\left(1 - T_r^{0.5}\right)\right]^2$	$m = 0.37464 + 1.54226\omega - 0.26992\omega^2$	0.307

Table 1.1: Equations of State for Pure Components

Reproduced from Introduction to Chemical Engineering Computing by B.A Finlayson

All these equations can be arranged into a cubic function of specific volume. The form of the Redlich-Kwong and Redlich-Kwong-Soave EOS is

$$\widehat{v}^3(p) - \widehat{v}^2(RT) + \widehat{v}(a - pb^2 - RTb) - ab = 0$$
(1)

When the temperature and the pressure of a gaseous mixture and the parameters a and b are given, then the specific volume, \hat{v} of the mixture can be calculated by solving the cubic EOS. The equation represents one algebraic equation with one unknown, i.e. the specific volume. Similarly the Peng-Robinson EOS results in

$$\hat{v}^{3}(p) + \hat{v}^{2}(bp - RT) + \hat{v}(a - 3pb^{2} - 2RTb) + (pb^{3} + RTb^{2} - ab) = 0$$
(2)

For the pure components, the parameters a and b are determined from the critical temperature and critical pressure and possibly the accentric factor. These are all tabulated quantities for pure components. For mixtures, it is necessary to combine the values of a and b for each component according to the composition of the gaseous mixture. Thus the following equations can be used to find a and b for a binary mixture.

$$a = y_1^2 a_1 + 2y_1 y_2 a_{12} + y_2^2 a_2$$
$$b = y_1 b_1 + y_2 b_2$$

Common mixing rules for the multicomponent mixtures in terms of the pure component properties $\{a_i, b_i, \alpha_1\}$ for the major equations of state are shown in Table 1.2. The only difference between the mathematical problem for a pure component and for a mixture is in the evaluation of the parameters *a* and *b*.

Model	ai	b _i	α	а	ь
Redlich-Kwong	$a_i = 0.42748 \left(\frac{R^2 T_{ci}^2}{p_{ci}}\right) \alpha_i$	$b_i = 0.08664 \left(\frac{RT_{ci}}{p_{ci}}\right)$	$\alpha_i = \frac{1}{T_{ri}^{0.5}}$	$a = \left(\sum_{i=1}^{NCOMP} y_i a_i^{0.5}\right)^2$	$b = \sum_{i=1}^{NCOMP} y_i b_i$
RK-Soave	$a_i = 0.42748 \left(\frac{R^2 T_{ci}^2}{p_{ci}}\right) \alpha_i$	$b_i = 0.08664 \left(\frac{RT_{ci}}{p_{cl}}\right)$	$\alpha_i = \left[1 + m_i \left(1 - T_{r_i}^{0.5}\right)\right]^2$	$a = \left(\sum_{i=1}^{NCOMP} y_i a_i^{0.5}\right)^2$	$b = \sum_{i=1}^{NCOMP} y_i b_i$
Peng-Robinson	$a_{ii}=0.45724\left(rac{R^2T_{ci}^2}{p_{ci}} ight)lpha_i$	$b_i = 0.07780 \left(\frac{RT_{ci}}{p_{ci}}\right)$	$\alpha_i = \left[1 + m_i \left(1 - T_{ri}^{0.5}\right)\right]^2$	$a = \sum_{i,j=1}^{NCOMF} y_i y_j a_{ij}$	$b = \sum_{i=1}^{NCOMP} y_i b_i$
	$a_{ij} = a_{ji} = \sqrt{a_{ii}a_{jj}} \left(1 - k_{ij}\right)$			Market State	

Table 1.2: Equations of State for Mixtures

IV. Solution of Cubic Equation of State by Excel

The mathematical problem that has to be solved in this module consists of a given set of chemicals along with its temperature and pressure, and the specific volume of the mixture has to be found out.

Once the parameters are known, the equation (1) or (2) which is nonlinear equation with one variable, must be solved to calculate specific volume, \hat{v} . Since these are cubic equations, it is possible to find the solution in a series of analytic steps, but it is not usually done because it is quicker to find the solution numerically using EXCEL.

This module will allow us to solve for the specific volume easily in less time interval than the hectic manual analytical steps.

V. Solving Equation of State Using Excel (Single Equation in One Unknown)

There are at least two methods to solve algebraic equations using Excel. The first one uses "**Goal Seek**" while the other uses "**Solver**". Both can be illustrated using a simple example:

Find 'x' so that 'f(x) = 0' $f(x) = x^2 - 2x - 8$

Solution using Goal Seek

Step1: Open a spreadsheet and put the following statement in cell B1

=A1*A1-2*A1-8

Cell B1 basically contains the equation f(x) that has to be zero at some value in A1. This value is the required value 'x'. The value in cell A1 has to be varied and adjusted in such a way that the value in cell B1 becomes zero.

Step2: Under "Data" and "What if analysis" choose "Goal Seek." When a small screen appears, fill in the spaces shown as below:

🗶 📄 🍤 - ((≊ ~ ∓					Book	1 - Micros	oft Excel						- (ar XX
File Ho	ime Insert	Page	Layout	Formulas	Data	Review	View As	pen Datashe	et Add	-Ins				∝ 🕜 🗖	ē X3
Get External Data *	efresh All + Connectio	nections verties Links ns	A ↓ A Z A Z ↓ Sort	Filter Sort & Filter	K Clear Reapply Advanced	Text to Columns I	Remove Duplicates Data T	🕈 Data Valid 🚰 Consolida 🖗 What-If Ar ools	ation - te nalysis - [•] []	Data Analysis Solver Analysis			
B1	-		<i>f</i> _x =A1	*A1-2*A1-8	1										~
A	В	С	D	E	F	G	н	1	J	К	L	M	N	0	
1	-8														
2															
3					Goal	Seek		? 🔀 🔄							
4					S <u>e</u> t ce	:	B1	1							
5					To <u>v</u> al	ue:	0								
7					By <u>c</u> ha	anging cell:	\$A\$1								
8															
9						ОК	Can	cel							
10															
11															
12															=
13															_
14															
15															
17															
18															
19															
20															
21															_
22															_
23															
24															
25															-
H I F H Sh	eet1 / Shee	t2 / She	et3 🦯 🞾						◀ [
Enter					1	_	1						.00% (_)	1	
🛃 start	92 Got	ogle Talk	- <u>0</u> 2M	licrosoft	- 🧿 Place	a Lands	Chapt	er#3	W 2 Mic	rosoft 👻	🔣 Micro	osoft Exc	EN 😰 🤇		12:08

Step3 Click OK. The following answer appears in the spreadsheet. -2.000000686 4.11369E-06 The value at cell B1 is 4.11×10^{-6} and not '0' as required but is small enough to be considered as relative tolerance for most purposes.

Solution using Solver

Step 1: Repeat the step same as done above for Goal Seek.

Step 2: Under the Data menu, click on "Solver".

Step 3:When the following window appears, choose the option to make the cell equal to a value of (or maximum or minimum) by changing another cell. If the appropriate cell location is inserted, the same answer will be obtained as with the Goal seek. This time, however, it is more accurate.

Solver Parameters				×
Se <u>t</u> Objective:	\$B\$1			E
То: <u>М</u> ах	() Mi <u>n</u>	◎ <u>V</u> alue Of:	0	
By Changing Variabl	e Cells:			
\$A\$1				E
Subject to the Cons	traints:			
			<u>^</u>	Add
				Change
			(Delete
				Reset All
			-	Load/Save
☑ Ma <u>k</u> e Unconstra	ined Variables Non-N	legative	-	
Select a Solving Met	thod: GR	G Nonlinear	•	Options
Solving Method				
Select the GRG No engine for linear S non-smooth.	nlinear engine for So olver Problems, and	lver Problems that ar select the Evolutionar	e smooth nonlinear. S y engine for Solver p	Select the LP Simplex problems that are
Help]		<u>S</u> olve	Cl <u>o</u> se

Solver Results						
Solver found a solution. All Constraints and optimic conditions are satisfied. © Keep Solver Solution © Restore Original Values	ality Re <u>p</u> orts Answer Sensitivity Limits					
Return to Solver Parameters Dialog	Outline Reports					
Solver found a solution. All Constraints and optimal satisfied. When the GRG engine is used, Solver has found at I solution. When Simplex LP is used, this means Solv optimal solution.	lity conditions are least a local optimal er has found a global					

CLASS PROBLEM

Find the specific volume of n-butane at 393.3 K using the following equations:

- I. Ideal gas
- Redlick- Kwong EOS II.

Use excel sheet to calculate the Specific Volume at the following pressures using the above equations and then plot the results.

Make a plot of P vs V for ideal gas and RK EOS and compare your results.

Pressure (atm)	5	10	15	20	25
Sepecific Volume(L/g-mol)					

Data Given: $T_C=425.2$ K; $P_C=37.5$ atm;

R=0.08206 L-atm/gmol.K

VI. Using Solver with set of equations

To apply solver write all the equations in the following form:

$$x + 2y + 3z - 366 = 0$$

$$4x + 5y + 6z - 804 = 0$$

$$7x + 8y - 351 = 0$$

- 1. Start a new sheet and name it example2
- 2. Start cell A1, enter "Solving set of equations: Solver method"
- 3. Put initial guesses of *x*, *y* and *z* in the cells B8:B10.
- 4. Now input in the equations (which are equal to zero). When these equations evaluate to zero, the problem is solved.

Cell	Contents
C8	=(B8+2*B9+3*B10-366)
C9	=(4*B8+5*B9+6*B10-804)/6
C10	=(7*B8+8*B9-351)

- 5. In cells C8:C10, enter the contents (equation) as shown in the table below.
- 6. In C11, point it to cells C9; C10, sum the absolute values of these solutions in a cell to create a single value for the solver to optimize.
- 7. In cell C11, type =SUM(ABS(B8:B10)) and press *Ctrl+Shift+Enter*
- 8. Open solver from data browser.
- Select cell \$C\$11 for the set cell option and cells \$C\$8:\$C\$10 as the cells to change as shown in Figure 2. Select the value of options and enter 0 in the value box.
- 10. On the subject to constraints, click on add, and, choose cell \$B\$8:\$B\$10=0.The dialogue box should appear as in Figure 2.
- 11. Click Solve to search for a solution.

When solver locates a solution to the problem, it displays the solver results dialogue shown in Figure 3. The results are shown in figure 4

	Solver Parameter	S	
Se <u>t</u> Objective:	SCS11		
To: <u>M</u> ax () Mi <u>n</u>	0	
By Changing Variable Cells			
\$B\$8:\$B\$10			
Subject to the Constraints:			
\$C\$8:\$C\$10 = 0		^	Add
			<u>C</u> hange
			<u>D</u> elete
			<u>R</u> eset All
		~	<u>L</u> oad/Save
Make Unconstrained Va	ariables Non-Negative		
S <u>e</u> lect a Solving Method:	GRG Nonlinear	v	O <u>p</u> tions
Solving Method			
Select the GRG Nonlinear Simplex engine for linear problems that are non-sm	engine for Solver Problems that Solver Problems, and select the E ooth.	are smooth nonli volutionary engir	near. Select the LP ne for Solver
Help		Solve	Cl <u>o</u> se

Figure 4: Solver Dialogue Box

Solver Results						
Solver found a solution. All Constraints and optim conditions are satisfied.	ality Re <u>p</u> orts					
 Keep Solver Solution Restore Original Values 	Answer Sensitivity Limits					
Return to Solver Parameters Dialog	Outline Reports					
<u>O</u> K <u>C</u> ancel	<u>S</u> ave Scenario					
Solver found a solution. All Constraints and optimality conditions are satisfied.						
When the GRG engine is used, Solver has found at solution. When Simplex LP is used, this means Solvoptimal solution.	least a local optimal ver has found a global					

Figure 5: Solver Dialogue box after running it.

+				
5				
6				
7				
8	1.47224E-11	25		
9	-6.25278E-12	22		
10	5.49107E-11	99		
11		7.59E-11		
12				
13				
14				/ / / / / / / / / / / / / / / / / / /
15				

Figure 6:Results of the calculation

If the solver cannot find a solution, the window in Figure 7 appears. If this happens, try running solver again. Solver can solve set of equations as long as the results are added together are roughly of similar magnitude. If not, the one result predominates the calculation, making it difficult or impossible for the solver to find a solution. If the results are of different order of magnitude, multiply the results by some factor to make their magnitudes roughly equal. Multiplying by a value will not change the results, because the wanted result is zero.

Solver Results							
Solver could not find a feasible solution.	Reports						
• Keep Solver Solution	Feasibility Feasibility-Bounds						
O Restore Original Values	Outline Reports						
OK Cancel	Save Scenario						
Solver could not find a feasible solution.							
Solver can not find a point for which all Constraints are satisfied.							

Figure 7:Solver Dialogue box without a solution.

CLASS PROBLEM

A mixture containing 45% benzene (B), 50% toluene (T) and 5% nitrobenzene (NB) by mass is fed to a distillation column. The overhead stream is composed of 95% B and 4% T. The bottom contains, 90% T. The feed rate is 2000 kg/h. Determine the overhead and bottom flow rate of the streams and the composition.



PRACTICE PROBLEMS

PROBLEM 1

Find the molar volume of methanol gas at 300° C using the following equation of state, $T_c = 512.6 K$, $p_c = 79.9 atm$, $\omega = 0.559$; units of a and b correspond to v in l/g mol.

(1) Ideal gas law;

(2) Redlich–Kwong equation of state;

(3) Redlich–Kwong–Soave equation of state.

Pressure (atm)	10	25	50	75	100	125
Sepecific Volume(L/g-mol)						

Plot the pressure and specific volume and make analysis on the nature of the plot. Give reasons why the ideal gas or Redlich-Kwong Equation of State are not expected to be valid choices.

PROBLEM 2

Consider a mixture of 25 percent ammonia, and the rest nitrogen and hydrogen in a 1:3 ratio. The gas is at 550 K. Use Excel to compute the specific volume using:

(1) Ideal gas law;

(2) Redlich–Kwong equation of state;

(3) Redlich–Kwong–Soave equation of state.

Plot the pressure and specific volume and make analysis on the nature of the plot. How do the three answers compare? Is the gas ideal or not? Comment on the reasons the RKS equation might be expected to be better.

Pressure (atm)	50	100	150	200	250	300
Sepecific Volume(L/mol)						

Data Given:

Component	Тс (К)	P _C (atm)	ω
NH ₃	406.6	111.23	0.252
N_2	126.1	33.5	0.040
H ₂	33.3	12.8	-0.215

PROBLEM 3

Calculate the molar volume of a binary mixture containing 30 mol% CO_2 and 70 mol% *i*-butane (2) at 400 K using the following equation of sates:

(1) Ideal gas law;

(2) Redlich–Kwong equation of state;

(3) Peng-Robinson equation of state.

Plot the pressure and specific volume and make analysis on the nature of the plot. How do the three answers compare? Is the gas ideal or not? Comment on the reasons the RKS equation might be expected to be better.

Pressure (atm)	20	40	60	80	100	120
Sepecific Volume(L/mol)						

Data Given:

Component	Тс (К)	P _C (atm)	ω
CO ₂	304.2	72.86	0.228
<i>i</i> -butane	408.1	36	0.177

PROBLEM 4

Ethane is dehydrogenated to ethylene and acetylene in the following pair of catalytic reactions:

$$C_2H_6 \rightleftharpoons C_2H_4 + H_2 \qquad [A \rightleftharpoons B+D]$$

$$C_2H_6 \rightleftharpoons C_2H_2 + 2H_2 \qquad [A \rightleftharpoons C+2D]$$

The reactions take place at 977^oC and 1 atm and proceed to a point such that the product gas composition satisfies the following equilibrium conditions:

$$\frac{y_B y_D}{y_A} = 3.75$$
 $\frac{y_C y_D^2}{y_A} = 0.135$

where y denotes the mole fraction. The product gas goes to a complex separation process that separates 95% of the unreacted ethane from the ethylene, acetylene and hydrogen and recycles the separated ethane to the reactor.



Calculate the flow rate and the composition of the product stream using Solver.

PROBLEM 5

One method for the manufacture of "Synthesis gas" (a mixture of CO and H₂) is the catalytic reforming of CH₄ with stream at high temperature and atmospheric pressure

$$CH_4 + H_2O(g) \rightarrow CO(g) + 3H_2(g)$$

The only side reaction to be considered is:

$$CO(g) + H_2O(g) \to CO_2(g) + H_2(g)$$

If the reactants is supplied in the ratio, 2 mol steam to 1 mol CH₄ to the reactor and the conversion of CH₄ is 90% and the product stream contains 17.4 mol % CO, calculate the flow rate and the composition of the feed stream supplied to the mixer and the flow rate and the composition of the product stream coming out from the separator. The separator after the reactor separates 99% of CH₄ and is recycled back to the reactor.



LITERATURE CITED:

- 1. Finlayson B.A (2012),. Introduction to Chemical Engineering Computing
- 2. Cutlip M.B., Shacham M., Problem Solving in chemical and Biochemical Engineering with PolymathTM, Excel, and Matlab[®].
- 3. R. Elliott and C. T. Lira, Introductory Chemical Engineering Thermodynamics, Prentice Hall PTR (2012).
- 4. Ovaris, W.J., "Excel for scientists and engineers", 2/e ,sybex, San Francisco (1996)
- 5. Felder Richard M., Rousseau Ronald W., Elementary Principles of Chemical Processes.
- 6. Smith J. M., Van Ness H. C., Introduction to Chemical Engineering Thermodynamics, 7th Edition.

Experiment 2: Mass balances with Recycle Streams

1. Objectives:

After the completion of this module, the students will be able to use EXCEL spreadsheets for solving material balance equations for the case when the unreacted feed with the product is separated and recycled back in the initial reactant stream.

2. Prerequisite Mathematical Skills

Essential command and formulae entry in EXCEL

3. Prerequisite Engineering & Science Skills

Basic Knowledge of Material and Energy balance of chemical processes

Engineers who design and run chemical plants use mass balances to decide which processes are cost-effective. Chemical engineering students are taught in their first course to look at the entire system as well as the individual pieces of equipment. Mass balance is the first step in the design of a process plant. Most processes involve a recycle stream. The reason is that all the reactants do not react, and businesses cannot afford to throw the rest away. Furthermore, any leftovers have to be disposed of in an environmentally friendly manner, which costs money. Thus, engineers take the unreacted reactants and put them back in the start of the process and try again. This makes the mass balances a little more complicated, and it leads to iterative methods of solution. In this module Excel will be used to solve mass balances with recycle streams.

4. MATHEMATICAL FORMULATION

The mathematical formulation of mass balances is really quite easy. The equations for three simple units is needed to be developed, which can then be combined in myriad ways. Once the mass balance is done for a simple unit, then with the help of Excel, the mass balance for a process can be done combining those simple units. Equations are given here for a mixer, separator, and reactor, and then those equations are used in Excel to perform mass balances on processes.

MIXER

A mixer is shown in figure 1. A mixer (called MIXR) adds all the flows in and transfers them to the output stream. The mass (or mole) balance is that the mass out equals the sum of the masses in.

$$n_i^{out} = \sum_{j=1}^{NSTRM} n_i^j$$

where n_i^j is the flow rate of component *i* in the j_{th} stream, and n_i^{out} is the flow rate of component *i* in the outlet stream.



Figure 1: Mixer

SEPARATOR

In this unit there is one input streams and two (or more) output streams as shown in figure 2. The split fraction sf_i is the fraction of component i going to the overhead stream. The mass balance for each component i is:

$$n_i^2 = n_i^{in} s f_i, \qquad n_i^1 = n_i^{in} (1 - s f_i)$$

If the split fractions of each component and the flow rate in are known, then the flow rates out of stream 1 and 2 for each component can be easily calculated.



Figure 2: Separator

REACTOR

As shown in figure 3, a reactor has one input stream and one output stream and a reaction occurs in the reactor. The reaction can be specified using the stoichiometric equation for the reaction as:

$$aA + bB \rightarrow cC + dD$$

If N moles of A react, then (b/a)N moles of B also react and form (c/a)N moles of C and (d/a)N moles of D. Let the conversion be specified as α . The equation for each component is:



Figure 3: Reactor

Case 1

Consider a simple process in which the reactor can convert 40% of the feed to it (perhaps due to equilibrium constraints), but the separation is complete and the unreacted A is recycled.

Find out the flow rates of all the streams.





SOLUTION

Method 1: Using Sequential method (Shown in figure 4)

- 1- Put the heading in Cell A1 to F1. Recycle in the Cell B1 is the stream that is mixing with S1 in the mixer.
- 2- In cell. A2 put the iteration no. In cell B2 put the flow rate of A (in stream S1).
- 3- In cell C2 put '0' considering that there is no recycle in first iteration. In cell D2 put "=B2+C2" since it is Stream S2 after mixer.
- 4- Since the conversion is 40%, hence the moles coming out of reactor is 60%. In cell E2 put "=0.6*D2". Since all the A is going at recycle put "=E2" in cell F2.
- 5- In the next row, in cell C3 put "=F2" to specify the value of recycle coming out of separator. For the rest of the columns drag the small plus pointer below to make calculations from the same formula.
- 6- After around 32 iterations the value of stream S5 will become equal to 'Recycle' stream going in mixer.

Method 2: Using circular reference iteration method (Shown in figure 5)

- 1. Put the heading in Cell H1 to L1.
- 2. In cell H2 put the flow rate of A (in stream S1). In cell I2 put "=L2".
- 3. Put "=H2+I2" in cell J2 and "=0.6*J2" in cell K2.
- 4. As "=K2" is put in cell L2 the Excel will automatically iterate and mention the final value as shown in figure 5. This is the circular reference iteration feature.

	A	В	С	D	E	F	G
1	Iteration no.	S1	Recycle	S2	S3	S5	
2	1	100	0	100	60	60	
3	2	100	60	160	96	96	
4	3	100	96	196	117.6	117.6	
5	4	100	117.6	217.6	130.56	130.56	
6	5	100	130.56	230.56	138.336	138.336	
7	6	100	138.336	238.336	143.0016	143.0016	
8	7	100	143.0016	243.0016	145.801	145.801	
9	8	100	145.801	245.801	147.4806	147.4806	
10	9	100	147.4806	247.4806	148.4883	148.4883	
11	10	100	148.4883	248.4883	149.093	149.093	
12	15	100	149.8825	249.8825	149.9295	149.9295	
13	20	100	149.9909	249.9909	149.9945	149.9945	
14	25	100	149.9993	249.9993	149.9996	149.9996	
15	29	100	149.9999	249.9999	149.9999	149.9999	
16	30	100	149.9999	249.9999	150	150	
17	31	100	150	250	150	150	
18	32	100	150	250	150	150	
19							

Figure 4: Solution of Sequential method.

	Н	I.	J	K	L	M
1	S1	Recycle	S2	S3	S5	
2	100	149.9988	249.9988	149.9993	149.9993	
3						

Figure 5: Solution of Circular reference iteration method.

Case 2

A process takes hydrogen and nitrogen in a ratio 3:1 to make ammonia. Flow sheet is shown in the figure below. Molar flow rate of nitrogen is 100 mol/hr. Find the flow rates of all the streams using 25% conversion per pass of nitrogen in the reactor. The product stream contains 98% ammonia and 2% each of nitrogen and hydrogen of the feed that is fed to the separator.



Figure 6: Block diagram for production of Ammonia.

P1	.8 *	\pm \times	$\sqrt{-f_x}$									
	А	В	С	D	E	F	G	Н	I	J	К	L
1	Conversion	0.25										
2				Recycle						S5		
3												
4					Mixer		Reactor		Separator			
5			S1			S2	R1	S3		S4		
6												
7		Stream	S1	Recycle	S2	R1	S3	S4	S5			
8		Nitrogen	100	297.6143	397.6143	-99.4036	298.2107	0.596421	297.6143			
9		Hydrogen	300	892.8429	1192.843	-298.211	894.6322	1.789264	892.8429			
10		Ammonia	0	4.057289	4.057289	198.8072	202.8644	198.8072	4.057289			
11												
12		Total	400	1194.515	1594.515	-198.807	1395.707	201.1928	1194.515		5.30577E-12	
13												

Figure 7: Solution for Case 2

Case 3

For case 2, the reactor conversion is changed to be the equilibrium conversion, which may not be 25%. The equilibrium equation is:

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \to NH_3$$
$$K_p = \frac{p_{NH_3}}{p_{N2}^{1/2}p_{H2}^{3/2}} = \frac{y_{NH_3}}{y_{N2}^{1/2}y_{H2}^{3/2}}\frac{1}{p}$$

Find out the flow rates of each species in all the streams. Data given: $K_p=0.05$, P=220 atm

SOLUTION (Shown in figure 8)

- 1- Prepare a spreadsheet as shown in figure 6.
- 2- A conversion value (initial guess) is put into cell B1.
- 3- Value of Kp and P are put into cells D20 and D21.
- 4- For the conversion value calculate the column '3'.
- 5- Column '4' can be obtained by summing the column '2' and '3'.
- 6- Column '5' is calculated assuming that the stream 5 takes 0.5% of nitrogen and hydrogen and 98% of the ammonia. H14=0.005*G14, H15=0.005*G15, and H16=0.98*G16.
- 7- Column '6' is obtained by subtracting column '5' from '4'.
- 8- The mole fractions of stream coming out of reactor are obtained by taking moles of a species in stream 4 and dividing by the total moles in stream 4.
- 9- Those mole fractions can be directly put in chemical equilibrium equation, as shown in Cell F19.
- 10-Notice that as conversion changes, mole balance changes. This in turn changes mole fractions, which no longer satisfy the chemical equilibrium equation.
- 11-We can use 'Solver' to set F10 to '0' by changing Cell B1 (Conversion).
- 12- The results are available now.
- **13-**Calculate the chemical equilibrium equation using the final mole fractions to cross check the results.

	А	В	С	D	Е	F	G	н	I.	J	К	
1	Conversion	0.740394										
2				Recycle					4	S5		
3					•							
					Mixor		Reactor		Senarator			
4				-	WINCI		Reactor	-	Separator		-	
5			S1			S2	R1	S3		S4		
6												
7		Stream	S1	Recycle	S2	R1	S3	S4	S5			
8		Nitrogen	100	34.82687518	134.8269	-99.825	35.00188	0.175009	34.82688			
9		Hydrogen	300	104.4817087	404.4817	-299.475	105.0067	0.525034	104.4817			
10		Ammonia	0	4.074489411	4.074489	199.65	203.7245	199.65	4.074489			
11												
12		Total	400	143.3830733	543.3831	-199.65	343.7331	200.35	143.3831		-3.7772E-08	
13												
14			Mole fract	ion out of the	reactor							
15			Nitrogen	0.101828673								
16			Hydrogen	0.30548917								
17			Ammonia	0.592682157								
18												
19			Total	1		-4.6E-08						
20			Кр	0.05								
21			Ρ	220								

Figure 8: Solution for Case 3 (Equilibrium conversion included).

PRACTICE PROBLEMS

PROBLEM 1

In a trans-alkylation reaction the toluene gets converted in to benzene and xylene. The reaction is mentioned below:

 $2C_7H_8 \rightarrow C_6H_6 + C_8H_{10}$

In the present problem the conversion is 58% per pass. 99.5% of the benzene is removed from the mixture coming out of the reactor using a splitter. The benzene stream also contains 0.1% toluene but none of the xylene. Then the 99.5% of toluene is removed in the second splitter from xylene and recycled back to the feed stream. The recycle stream contains 0.1% xylene.

Calculate the total flow rate of each stream and the mole fraction of the stream.

PROBLEM 2

Consider the reaction given below:



The reaction conversion is at the equilibrium with Kp = 0.1 and P = 300 atm.

$$K_p = \frac{p_C^2 p_D^3}{p_A p_B} = \frac{y_C^2 y_D^3}{y_A y_B} \frac{1}{P}$$

There are two separation units. In the first unit 95% of A is separated from the inlet stream. This stream also contains 2% of C (of the feed stream). In the second separation unit 98% of B is separated from the inlet stream. This stream also contains 3% of D (of the feed stream).

If the composition of inlet stream is 100 mol/hr each of A and B, calculate the extent of conversion and flow rate of the final product stream.

PROBLEM 3

The figure below shows the Ammonia process with vapor-liquid equilibrium and a purge stream.



Calculate all the streams inlet and outlet for the mixer, reactor, flash separator and recycle for all components. Set the conversion per pass in the reactor to 25%. Change the separator so that it is a phase separation. The K-values are

Nitrogen	4.8
Hydrogen	70
Ammonia	0.051
carbon dioxide	0.32

The flow rates of nitrogen and hydrogen into the process are one and three moles per time unit, respectively, but there is also 0.01 moles per time unit of carbon dioxide. Because of the carbon dioxide, you will add a purge stream as one per cent of the recycle stream.

LITERATURE CITED:

- Ovaris, W.J., "Excel for scientists and engineers", 2/e ,sybex, San Francisco (1996)
- 2. Finlayson B.A (2012),. Introduction to Chemical Engineering Computing
- 3. Cutlip M.B., Shacham M., Problem Solving in chemical and Biochemical Engineering with PolymathTM, Excel, and Matlab[®].

Experiment 3: Vapor-Liquid Equilibrium Using ASPEN Plus (I)

Isothermal Flash

1. Objectives:

After the completion of this module, the students will have:

- 1- Reviewed and expanded the chemistry and chemical engineering knowledge of vapor liquid equilibrium and its applications.
- 2- Learned to use Aspen Plus to perform flash vaporization.

2. Prerequisite Engineering & Science Skills

Knowledge of Vapor-Liquid Equilibrium of a mixture of chemicals.

3. PROBLEM DESCRIPTION

A 100 kmol/h feed consisting of 10, 20, 30 and 40 mole% of propane, n-butane, n-pentane and n-hexane, respectively, enters a flash drum at 105 psia and 200°F. The flash drum operates at 100 psia and 200°F. Compute the compositions of the exit streams using the RK-Soave property method.

SIMULATION APPROACH USING ASPEN PLUS

- Step 1 Open the Aspen Plus user interface and choose template; OK. When the window appears, choose with English units. This opens the Aspen Plus window.
- Step 2 Enter the components: propane, n-butane, n-pentane and n-hexane as shown in Fig. 1.
- Step 3 Specify the property method in the methods tab. Choose SRK in the base method. Then the program has to be specified which database has to be used for the binary interaction parameters in the SRK. Generally default database is used. Select property/Parameters/Binary and click all the red boxes to accept them.
- **Step 4** Specifications for properties are completely defined now. This can be confirmed by the message on the left –bottom of the screen as shown in Fig 2.
| Properties < Components - Specifications × + | | | | | | | | |
|---|---|--------------------------------------|---|-----------|----------------|------------|-----------|---------|
| All Items | • | 0 | Selection Petroleum Nonconventional Enterprise Database Information | | | | | |
| Setup Gomponents | * | Sel | ect component | ts: | - | | | |
| Specifications | | Component ID Type Component name Ali | | | | | | Alias |
| Molecular Structure | | | PROPANE | Cor | ventional | | PROPANE | C3H8 |
| Assay/ blend
Light End Properties | | BUTANE | | | nventional | | N-BUTANE | C4H10-1 |
| Petro Characterization | = | • | PENTANE | Cor | onventional | | N-PENTANE | C5H12-1 |
| Pseudocomponents | | • | HEXANE | Cor | ventional | | N-HEXANE | C6H14-1 |
| Component Attributes | | • | | | | | | |
| Henry Comps UNIFAC Groups Polymers Methods | | | Find | Elec Wiza | urd User Defin | ed Reorder | Review | |

Fig 1: Components specification

Properties <	/	Methods - S	pecification	ıs× 🛨						
All Items -		🥑 Global	Flowsheet	Sections	Referenced	Information				
Methods Specifications		Property m	ethods & o	ptions —		Method nar	ne:			
Selected Methods		Method filt	er:	соммон	-	SRK	-	Methods	Assistant	
🔺 🔯 Parameters		Base metho	od:	SRK	•	Madif				
Pure Components		Henry com	ponents:		Ŧ		/			
A Binary Interaction		Petroleun	n calculatio	n options -		EOS:		ESSRK	Ŧ	
ANDRIL 1		Free-wate	er method:	STEAM-TA	- 4	Data set:		1		
		Water sol	ubility:	3	•	Liquid gar	mma:		~	
						Data set:				
MULIJ-1		Electrolyt	e calculatio	n options -		Liquid mo	Liquid molar enthalpy:		Ŧ	
💽 RKSKBV-1		Chemistr	y ID:		-	Liquid mo	lar volume:	VLMXR03	Ŧ	
C RKSLBV-1		🔽 Use tr	ue compon	ents		Heat of mixing				
RKTKU-1						- Downti	na correction			
SRKKIJ-1							· · ·			
SRKLU-1						Use liq	uid reference	state enthalpy		
Electrolyte Pair										
< <u> </u>										
Required Properties Input Complete Check Status										

Fig 2: Method specification

- Step 5 Click on the Simulation to enter the Main Flow-sheet window. From the model Palette below choose separator section in which the flash (phase separation) unit appears. Among the five in built models, select Flash2 and place this on the window.
- **Step 6** Clicking on the 'material' highlights three red connection points. Add the input and output streams. The appearance of red arrow means the flow-sheet is not properly connected and an input or output stream is required to be connected in the flow-sheet. It has to be fixed before proceeding further. Rename the streams and block. Once the flow-sheet is complete "Required input incomplete" appears in red on the bottom left corner of the screen instead of "Flow-sheet incomplete". The result should appear something like Fig 3.
- Step 7 The boxes on the left that are red indicate that still the information is needed to be supplied. Start at the top and work down, turning the red boxes into blue boxes by filling the values in the required input forms.
- Step 8 In the list at the left, choose streams by clicking on it or the + in the front of it. Inside the folder, there are two or more folders, one for each stream. Choose the input stream (F) by clicking on it. Insert the temperature, pressure and flow rates of every component as shown the Figure 4. There is no need to provide any data for product streams L and V because these streams are asked to simulate in the present problem. This is the reason that only feed stream has the red mark.
- Step 9 In the list at the left, choose block (Flash). Choose specifications, and insert the operating temperature and pressure of the flash drum. This will change the status from 'required input incomplete' to 'Required input complete' in the bottom left corner of the screen.



	_					M	ole-Flow	•	l k
📑 Results		- State variables							-
🧭 EO Variables		Temperature:	200	F	-		Component	:	
📑 Stream Results (Cu	15	Pressure:	105	nsia	-		PROPANE		10
Þ 🚞 L			105	pond			BUTANE		20
V		Vapor fraction:					DENITANIS		
🔁 Blocks							PENTANE		31
ELASH	=	l otal flow basis:	Mole				HEXANE		40
📜 Utilities		Total flow rate:		kmol/hr	•				
🚞 Reactions		Solvent			-		Та	tal.	10
🛛 词 Convergence		Joiventa	l				10		
问 🔁 Flowsheeting Options									
问 🗀 Model Analysis Tools		• Reference Temperat	ure						
EO Configuration		 Component Attribut 	tes						
问 🔁 Results Summary	-								
	. (Particle Size Distribution 	tion						

Fig 4: Data specification for streams and blocks

Value

Running the Simulation and Checking the Results:

- Step 10 Run the simulation by clicking 'Next' or using shortcut F5. Be sure to check your results for both convergence and run status by viewing the Control Panel. Control Panel shows progress of the simulation. It presents all warnings, errors, and status messages as shown in Fig. 5.
- **Step 11** In doing so, it will be noticed that a system warning that arises due to changes in the simulation that was made. Follow the suggestions presented by Aspen and change to the STEAMNBS method as recommended (Hint: the change is under the properties tab). Reinitialize and re-run the simulation after making this change.
- **Step 12** Once the calculation is completed without any error, click the Results box and look at results/streams. On clicking stream table, the results will be reproduced on the screen as shown in Fig. 6.

Copy the sketch of the process in M.S. Word/Excel file. Copy the results of Stream table by clicking on the upper left box. And copy in Excel format. Your written report should include more than the process sketch and stream table. You still need to explain what problem you have solved and how you solved it, focusing on the chemical engineering information, not the detailed steps on the computer screen. You can generate the report of the simulation by clicking the report on the 'Report' tab.

To create a detailed report of the work that is done including Summary, System information, etc., select Export (Ctrl+E) from the File dropdown menu. Then Save the work as a report file. A detailed report will be generated. Subsequently, open the saved report file in MS Word to view the report.

/ Main Flowsheet × FLASH	(Flash2) × Control Panel × +						
Hide Sequence	Clear Messages Check Status Run Settings						
Calculation Sequence FLASH	<< Loading Simulation Engine 17:36:36 Fri Feb 14, 2014>>						
	->Processing input specifications						
	* WARNING IN THE "PROPERTIES" PARAGRAPH WHICH BEGINS ON LINE 33						
	FREE-WATER METHOD SHOULD BE STEAMNBS WHEN THE MAIN PROPERTY METHOD IS SRK. DEFAULT FREE-WATER METHOD IS STEAM-TA PLEASE SPECIFY THE RECOMMENDED FREE-WATER METHOD AND RUN AGAIN.						
	Flowsheet Analysis :						
	COMPUTATION ORDER FOR THE FLOWSHEET: FLASH						
	->Calculations begin						
	Block: FLASH Model: FLASH2						
	->Simulation calculations completed						
	*** Warning(s) were issued during Input Translation ***						

Fig 5: Control Panel view

Simulation	٠ _	Ma	in Flowsheet $ imes$ $ ightarrow$ FLASH (Fl	ash2) × Control Pane	el × Results Summar	y - Streams × +	
All Items	•	M	aterial Heat Load W	ork Vol.% Curves	Wt. % Curves Petrol	eum Polymers Solids	
Flowsheet	*	r					
🕨 📷 Streams		Dis	play: All streams 🔹 Fo	rmat: CHEM_E	 Stream Table 	Copy All	
Blocks							
🛅 Utilities				F -	L •	v	
🚞 Reactions							
🕨 📷 Convergence		2	Temperature C	93.3	93.3	93.3	
Flowsheeting Options			Pressure bar	7.24	6.89	6.89	
🕨 🚞 Model Analysis Tools			Vapor Frac	0.122	0	1	
🕨 词 EO Configuration			Mala Flaur Instal/ha	100	00.700	17.070	
🔺 🔯 Results Summary			Wole Flow kmol/nr	82.728		17.272	
🕎 Run Status	=		Mass Flow kg/hr	7215.03 6136.77		1078.26	
🕎 Streams			Volume Flow I/min	946.111 189.397		1113.69	
Convergence			Enthaloy MMBtu/br	-15.025	-12.870	-2.054	
🕎 Operating Costs		-	Enthalpy Wiwibtd/III	-15.025	-12.075	-2.034	
CO2 Emissions			Mole Flow kmol/hr				
🕎 Streams (Custom)			PROPANE	10	5.485	4.515	
🧭 Models			BUTANE	20	14.288	5.712	
Equipment Dynamic Configuration	Ļ		PENTANE	30	25.725	4.275	
			LIEVANE	40	27.22	2.77	
I Properties		-	TEARINE	40	57.25	2.11	

Fig 6: Results Summary

CLASS PROBLEM

PROBLEM 1: Computation of the Bubble Point

Compute the bubble point temperature at 18 bar of the following hydrocarbon mixture:

Component	Mole fraction
C1	0.05
C2	0.1
C3	0.15
i-C4	0.1
n-C4	0.2
i-C5	0.25
n-C5	0.15

Assume the mixture inlet temperature of 25 °C, pressure of 19 bar and flow rate of 120 kmol/h.Using SRK property method.

Solution: Bubble Point 37.68°C.

PROBLEM 2: Computation of the Dew Point

Compute the dew point temperature at 1.5 bar of the following hydrocarbon mixture:

Component	Mole fraction
C1	0.05
C2	0.1
C3	0.15
i-C4	0.1
n-C4	0.2
i-C5	0.25
n-C5	0.15

Assume the mixture inlet temperature of 25°C, pressure of 5 bar and flow rate of 120 kmol/h. Using SRK property method.

Solution: Dew Point 22.17°C.

PRACTICE PROBLEMS

PROBLEM 1

A liquid mixture, consisting of 60 mole % benzene and 30 mole % toluene, and 10 mole % xylene is flashed at 1 atm and 110°C. The feed mixture with a flow rate of 100 kmol/h enters the flash drum at 1 atm and 80°C. Using SYSOP0 property method,

- A. Compute the amounts of liquid and vapour outlets and their compositions
- B. Repeat the calculations when the flashed drum is operated at 1.5 atm and 120° C and then at 110° C. Compare the results.

PROBLEM 2

The stream from an ammonia reactor comes out at 700^{0} F and 3000 psia. The flow rates are given below.

Component	Mole flow (lbmol/hr)
Nitrogen	143.3
Hydrogen	450.4
Ammonia	221.6
Carbon dioxide	1.8

If the temperature is reduced to 60^{0} F in a flash unit, keeping the same pressure, determine the flow rate of each species in the vapor and the liquid stream and their composition. Use RKSWS method.

PROBLEM 3

Compute the bubble point and dew point pressure at 40°C of the following hydrocarbon stream:

Component	Mole fraction
C1	0.05
C2	0.1
C3	0.15
i-C4	0.1
n-C4	0.2
i-C5	0.25
n-C5	0.15

Use SRK thermodynamic model and consider the inlet temperature of 30°C, pressure of 4.5 bar and flow rate of 100 kmol/h. Make relevant comment on the results.

LITERATURE CITED:

- 1. Finlayson B.A (2012), Introduction to Chemical Engineering Computing
- 2. R. Elliott and C. T. Lira, Introductory Chemical Engineering Thermodynamics, Prentice Hall PTR (2012).

Experiment 4: Vapor-Liquid Equilibrium Using ASPEN Plus (II)

Non ideal Liquids-Test of Thermodynamic Model

1. Objectives:

After the completion of this module, the students will have:

- 1. Reviewed and expanded the chemistry and chemical engineering knowledge of vapor liquid equilibrium and its applications.
- 2. Learned to use Aspen Plus to perform vapor-liquid equilibrium calculations.
- 3. Learned to use the National Institute of Standards and Technology (NIST) Data Engine to extract the experimental VLE data and perform Consistency test.
- 4. Perform Regression analysis to fit EOS model on the experimental data.

2. Prerequisite Engineering & Science Skills

- Knowledge of Vapor-Liquid Equilibrium of a mixture.
- Preliminary knowledge of Aspen Plus.

3. PROBLEM DESCRIPTION

Estimate the thermodynamic properties for the mixture of water and ethanol at equilibrium using the Wilson property method.

ESTIMATION OF PROPERTIES USING ASPEN PLUS

Step 1:Start Aspen Plus and choose General with Metric Units.

- Step 2: Enter water and ethanol in the components list.
- Step 3: In the list at the left, choose Method specifications. First choose ideal property method (activity coefficient are all 1) in the Method name. Then again choose WILS-2 in the Method name. The Wilson method uses an ideal gas, Henry's Law, and Wilson binary parameters, which is applicable for alcohols.
- **Step 4:** It will be seen that the Parameters turn red and in the Parameters the parameters required for the Wilson method appears. As it is clicked the default value is accepted by Aspen and the red turns to blue. The parameters can be changed manually if a change in values are needed.
- Step 5: Go to Analysis tab on the top right corner of your screen. Choose binary. A BINRY-1 is added on the Analysis on the left side. The screen will appear as shown in Fig. 1. Click "Run Analysis". Get y-x graph plot. The y-x diagram for ideal method is shown in Fig. 2.

Properties	< /	BINRY-1 (BINARY) -	Input × 🛨					
All Items	-	🕝 Binary Analysis	Diagnostics					
🕨 🗾 Polymers	*							
🛭 🔯 Methods		Analysis type: Txy		•	Valid pha	ses		
Specifications		Components			Vapor-L	quid-Liquid		-
👂 📷 Selected Methods		Components	ETHANOL	-				
🕨 词 Parameters			LINANOL	-	Pressure			_
📜 Routes		Component 2:	WATER	-	Units:	bar		•
💿 NC Props					List of	values		
🚞 Tabpoly		Compositions			1 013	25		
🚞 Chemistry		Basis: Mo	le fraction	-				
👂 📴 Property Sets		Vary: ETH	IANOL	-	0 Overal	i range		
🚞 Data		Clist of values			Lower lim	iit:	Uppe	er limit:
Estimation	_				No. of po	ints:	A Incre	ments:
🔺 🔯 Analysis	=							
A konstruction in the second secon		Overall range			Property	options —		
📀 Input		Lower limit:	0		Property	method:	IDEAL	
Results		Upper limit:	1		Henry co	mponents:		
🕨 🗔 Customize		Number of points:	51		Chomista	/ID.		
Results	-	indiffuence of points.	51 V		Chemistry	, iD:		
< III >		Increments:			Calculatio	on approach:	True compo	onents

Fig 1: Binary analysis using Ideal gas method



Fig 2: Y-X behavior of ethanol using Ideal-gas EOS.

- **Step 6:** Add another analysis BINRY-2. Change Property method to WILS-2 in the BINRY-1 on the Analysis on the left side. Click Run Analysis. The y-x diagram for Wilson method is shown in Fig. 3.
- Step 7: Bring both the curves together in a single plot and make single Y-axis. It can be seen this is not a good fit. Ethanol and water forms an azeotrope according to Wilson method but not according to Ideal method. Hence the results has to be checked by experimental data for the confirmation.

When you have good comparison with the data, whether in the form of T-xy diagram, K-values, or activity coefficients, you have validated thermodynamics model for this binary pair. In a process, with many chemicals, you may have to do this for all binary pairs before deciding on the best thermodynamic model.



4. NIST Thermo Data Engine in Aspen Plus

The NIST Thermo-Data Engine provides experimental thermo-physical property data from various sources such as from thermodynamic journals, reference books, in-house data systems, and open and/or private on-line databases. Using NIST thermo data Engine, the experimental data can be compared with the results of the calculations made with the chosen equation of state.

- Step 1: Click on the NIST in the Home tab. Choose binary. Choose ethanol as first component and water as second one for a binary mixture. Then retrieve data. A window will open that contains experimental data for this system from a variety of sources. The table is shown in Fig. 5.
- Step 2: In this example, scroll down to Binary VLE/Isobaric/VLE47 since this is the best matching data. The data are from Jones et al (1943). Click Save Data tab and it will be seen that on the left side of the screen on the Data tab, a section is added named BLVE047 as shown in Fig. 6.
- **Step 3:** Click on Y-X graph to obtain Fig. 7. The data is close to Wilson method which can be checked by bringing both the graphs together.

CONSISTENCY TEST

A VLE data set must satisfy the constraint given by the Gibbs-Duhem equation. In order to check the validity of experimental data Consistency test is performed to check whether the data is consistent with the fundamental thermodynamic equations like Herington test, Van Ness test, Point test, Infinite dilution test, EOS test and Endpoint Consistency test.

Click on the "consistency" and the data will be evaluated for internal consistency (satisfying Gibbs-Duhem equation). The window with the results for BLVE047 is shown in Fig. 8. The Herington test plot is hown in Fig. 9. For the test to be passed the area above and below X axis should be equal.

For additional information about the test, use the help menu by pressing F1. And enter NIST TDE VLE consistency test. The data of VLE 47 can be copied in Excel and compared with the plot generated by WILS-2.

Start Page × BINRY-2 (BINARY) - Input	×	E Binary Ro	esults × +			
Experimental Data Consistency Test	1					
Binary diffusion coefficient 004 Binary diffusion coefficient 005	*	No.	Liquid Mole fraction ETHANOL	Temperature (K)	Vapor Mole fraction ETHANOL	Total pressure(N/sqm)
Binary diffusion coefficient 006	E	> 1	0	373.12	0	101000
Binary diffusion coefficient 007		> 2	0.018	368.62	0.179	101000
Binary diffusion coefficient 008		> 3	0.054	363.72	0.3375	101000
Binary diffusion coefficient 009		▶ 4	0.124	358.52	0.47	101000
Binary diffusion coefficient 010		> 5	0.176	356.82	0.514	101000
Binary diffusion coefficient 012		> 6	0.23	355.87	0.542	101000
Binary diffusion coefficient 013		7	0.288	355.12	0.57	101000
Binary diffusion coefficient 014		8	0.385	354.12	0.612	101000
Binary VLE		9	0.44	353.62	0.633	101000
▲ Isobaric		10	0.514	252.02	0.657	101000
Binary VLE 003		11	0.514	352.52	0.057	101000
Binary VLE 019		12	0.085	352.02	0.755	101000
Binary VLE 023		12	0.84	351.38	0.85	101000
Binary VLE 025		> 13	1	351.44	1	101000
Binary VLE 055						
Binary VLE 034						
Binary VLE 036						
Binary VLE 038						
Binary VLE 039						
Binary VLE 040		Jones, C.	A.; Schoenborn, E. M.; Colb	urn, A. P. Ind. Eng. Chem.	, 1943, 35, 666-72 Equilibrium s	till for miscible liquids data o
Binary VLE 047		ethylene	dichloride - toluene and eth	anol - water		
Binary VLE 058		📃 Display	Uncertainty			
Binary VLE 060	* }	Save Dat	ta Data Regression	Help	TDE ve	rsion: 6.0, Database version: 6

Fig. 5: Display of NIST data

Properties	۲.	BINRY-1 (BINARY) - Input × TDE Binary Results × Data - BVLE047 (MIXTURE) × +
All Items	-	Setup OData OConstraints Measurement Method OInformation
Elected Methods		
🕨 📷 Parameters		Category: All
🚞 Routes		- Components in mixture
🕢 NC Props		
📜 Tabpoly		Available components Selected components
🚞 Chemistry		ETHANOL
👂 📷 Property Sets		WATER
🔺 🔯 Data		
Ø BVLE047		
Estimation		
🔺 🔯 Analysis		
🔺 🔤 BINRY-1		
🖉 Input	E	
Results		
🔺 🔯 BINRY-2		
🕢 Input		
Results		
👂 📷 Customize	-	

Fig. 6: Saved NIST data





Overall data quality (QVLE) = 0.743

Test	Results	Score	Criteria to Pass
Herington test	Passed	R = 2.7144; A* = 4.2423	R < 10 or A* < 3
Van Ness test	Passed	DP = 0.287; DY = 0.00492	DP < 1 and DY < 0.01
Point test			d < 3
Infinite dilution test	Failed	11 = 57.72; 12 = 203.91	I1 < 30 and I2 < 30
EOS test			DP < 1.5 and DY < 0.01
Endpoint test	1	Fpure = 1	0.1 <= Fpure <= 1.0

Fig 8: Results of Consistency test for BLVE 047.



Fig 9: Herington test result for BLVE 047.

5. **REGRESSION ANALYSIS WITH ASPEN PLUS**

Let's choose one more method Peng Robinson and put it with experimental data. The result is shown in Fig. 10. It is seen clearly that the Peng-Robinson EOS does not fit the experimental results. It can be seen that there are no values in PRKBV-1 in Binary Interactions in Parameters. But suppose there are constraints by other factors in the design and Peng-Robinson has to be used.

Hence a Regression Analysis has to be done to calculate the modified parameters of Peng-Robinson so that it fits the Experimental data.

Click Regression (below Analysis button) and NEW.

Put Method: PENG-ROB, DATA SET: BLVE-047.

In Parameters enter the data as shown in Fig 11 and click RUN.

It can be seen in PRKBV-1 in Binary Interactions in Parameters that there are new values after Regression as shown in Fig. 12.

Now the Reng-Rob with new parameters can be compared with experimental data as shown in Fig. 13



Fig 10: Comparison of Experimental and Peng-Robinson Y-X data.

All Items 🔹	🕜 Setup	Setup Setup		Report	Algorithm	Diagnostics	Generic P
UNIFAC Groups Binary					-	-	-
Results	Paramete	rs to be r	regressed				
🔁 Routes							
OR Props	Type Name Element		Binary p	aramete	Binary paran	nete	
🔁 Tabpoly			PRKBV		PRKBV		
🔁 Chemistry					2		
Comperty Sets	Compo	nent or				-	
🔯 Data	Compo	nent of	ETHANG	<i>n</i>	WATER		
Ø BVLE047	Gro	up	WATER		ETHANOL	•	
🔁 Estimation 👘							
kegression							
🔺 🖾 R-1	Usa	qe	Rearess		Rearess		
🕝 Input 📃	Initial	value					
📑 Results	inicial	value					
🖄 Analysis	Lower	bound					
🔺 🔯 BINRY-1	Upper	bound					
🖉 Input	Scale f	actor					
🚫 Results 👻	Set Aji	= Aij	No		No		
< <u> </u>			4				

Fig 11: Regression data to be entered.



Fig 12: New Peng-Robinson Parameter after Regression.



Fig 13: Comparison of Experimental and Modified Peng-Robinson Y-X data.

PRACTICE PROBLEMS

PROBLEM 1

For a binary benzene/ethanol system at 1 atm perform the following steps and plot both T-xy and Y-X diagram:

- Test the consistency of the experimental VLE data. Include the results of various consistency test methods.
- Choose a suitable data set from the NIST TDE system. Mention the citation.
- Test whether Ideal gas, Peng Robinson, NRTL and Wilson model can be used to model the data.
- Perform regression of the Peng Robinson parameters to fit the above data.
- Produce a T-xy plot to compare the estimated results from part (d) with the experimental data provided.

PROBLEM 2

For a binary acetone/hexane system at 1 atm, perform the following steps and plot both T-xy and Y-X diagram:

- Test the consistency of the experimental VLE data. Include the results of various consistency test methods.
- Choose a suitable data set from the NIST TDE system. Mention the citation.
- Test whether Ideal gas, SRK, NRTL-2 and Unifac model can be used to model the data.
- Perform regression of the SRK model parameters to fit the above data.
- Produce a T-xy plot to compare the estimated results from part (d) with the experimental data provided.

LITERATURE CITED:

- Finlayson B.A (2012), Introduction to Chemical Engineering Computing.
- R. Elliott and C. T. Lira, Introductory Chemical Engineering Thermodynamics, Prentice Hall PTR (2012).

Experiment 5: Distillation using ASPEN Plus

1. Objectives:

After the completion of this module, the students will have:

- Reviewed and expanded knowledge of separation of fluids using distillation and its applications.
- Learned to use Aspen Plus to simulate distillation column by using DSTWU and RADFRAC method and perform related calculations.
- Perform Sensitivity Analysis of the process.

2. Prerequisite Engineering & Science Skills

- Knowledge of Vapor-Liquid Equilibrium of a mixture of chemicals.
- Knowledge of distillation as a method of separation of fluids.
- Knowledge of Aspen Plus.

3. MODES OF DISTILLATION IN ASPENPLUS

1. Short-cut distillation design

1. DSTWU

DSTWU performs shortcut design calculations for single-feed, two-product distillation columns with a partial or total condenser.

DSTWU assumes constant molal overflow and constant relative volatilities.

DSTWU uses Winn-Underwood-Gilliland method to estimate the minimum number of stages and optimum feed location at total reflux, minimum reflux ratio, required reflux ratio and optimum feed location for the specified number of stages, or the required number of stages and optimum feed location for the specified reflux ratio

DSTWU also estimates the optimum feed stage location and the condenser and reboiler duties. DSTWU can produce tables and plots of reflux ratio versus number of stages.

2. Distl

Shortcut distillation rating using the Edmister method for Columns with one feed and two product streams.

Determines separation based on reflux ratio, number of stages, and distillate-to-feed ratio.Distl assumes constant mole overflow and constant relative volatilities.

3. SCFrac

SCFrac is used to simulate complex distillation columns with a single feed, optional stripping steam, and any number of products. SCFrac also estimates the number of theoretical stages and the heating/cooling duty for each section. SCFrac can model complex columns, such as crude units and vacuum towers.

2. Rigorous distillation design

• RadFrac

RadFrac is a rigorous model for simulating all types of multistage vapor-liquid fractionation operations. It performs detailed rating and design calculations for single column. These operations include:

o Ordinary distillation

- o Absorption
- Reboiled absorption
- Stripping
- Reboiled stripping
- Extractive and azeotropic distillation

RadFrac is suitable for:

- *1* Two-phase systems
- 2- Three-phase systems (only in equilibrium mode)
- 3- Narrow and wide-boiling systems
- 4- Systems exhibiting strong liquid phase non-ideality

RadFrac (in equilibrium mode) can also model columns in which two liquid phases and chemical reactions occur simultaneously, using different reaction kinetics for the two liquid phases. In addition, RadFrac (in equilibrium mode) can model salt precipitation.

In equilibrium mode, RadFrac assumes equilibrium stages, but Murphree or vaporization efficiencies can be specified. Murphree efficiencies can be manipulated to match plant performance. In rate-based mode, RadFrac uses rate-based non-equilibrium calculations to model actual tray and packed columns, based on the underlying mass and heat transfer processes, and does not use empirical factors such as efficiencies and the Height Equivalent to a Theoretical Plate (HETP).

RadFrac can be used to size and rate columns consisting of trays and/or packing. RadFrac can model both random and structured packing.

• Multifrac

MultiFrac is a rigorous model for simulating general systems of interlinked multistage fractionation units. MultiFrac models can handle a complex configuration consisting of:

I- Any number of columns, each with any number of stages

II- Any number of connections between columns or within each column

III- Arbitrary flow splitting and mixing of connecting streams

MultiFrac can handle operations with:

- 1- Side strippers
- 2- Pumparounds
- 3- External heat exchangers
- 4- Single-stage flashes
- 5- Feed furnace

• PetroFrac

PetroFrac is a rigorous model designed for simulating all types of complex vaporliquid fractionation operations in the petroleum refining industry. Typical operations include:

- 1- Preflash tower
- 2- Atmospheric crude unit
- 3- Vacuum unit
- 4- Catalytic cracker main fractionator
- 5- Delayed coker main fractionator
- 6- Vacuum lube fractionator

• Extract

Extract is a rigorous model for simulating liquid-liquid extractors. It can have multiple feeds, heater/coolers, and side streams.

• BatchSep

BatchSep is a rigorous batch distillation model used for single batch columns. Typical operations include:

- 7- Ordinary azeotropic batch distillation
- 8- 3-phase distillation
- 9- Reactive distillation

CLASS PROBLEMS

PROBLEM 1

Use DSTWU to calculate the following for the mixture of methanol/water with a mole composition of 0.5/0.5 at 1 atm and 80° C. The feed flow rate is 100 lbmol/h. Purity of 99.5% is desired in both the bottom and distillate streams.

- a. Minimum reflux ratio.
- b. Minimum number of stages.
- c. Actual reflux ratio.
- d. Actual number of stages.

STEPS TO BE FOLLOWED

- **1.** Open a new file in Aspen and enter the components and the METHOD to be used in the properties section as 'NRTL-2'.
- 2. Click the Simulation section. Pick up a DSTWU column from the model palette and place it on the flow-sheet screen and add the input and output streams as shown in Fig. 1. Note that the columns shown inside DSTWU section have the same function but only icons are different.
- **3.** Now fill the required inputs for feed stream and the block till all the red marks turn to blue on the left side. The display is shown in Fig.2.
- **4.** When the required inputs are added the bottom left corner of the screen will display 'Required Inputs Complete'. Now Run the simulation.
- **5.** The result of the block can be seen in Fig. 3. The result of the streams can be seen from Stream Results.
- **6.** To add the mole fraction data in the Stream Results, go to Set Up, Report Options, Streams and Tick the fraction basis box for moles. The mole fraction can also be seen in Results as seen in Fig. 4.



Fig. 1: DSTWU Flowsheet

All Items		Specific	ations	Calcu	ulation Options	Cor	nvergence	Information	
 Flowsheet Streams Blocks B1 		Column specifications Pressure Condenser Number of stages: 5 Condenser Reflux ratio: Reboiler:						1	atm • atm •
Input Image: Block Options Image: December 2000 Image: December 2000		Key component recoveries Light key: Comp: METHANOL Recov: 0.995					Condenser specifications Total condenser		
Results Constraint Results Constraint Results Constraint Results (Custom) Constraint Results (Custom)	=						 Partial condenser with all vapor distillate Partial condenser with vapor and liquid distillate 		
Utilities Reactions		Heavy key Comp:	: WATER		-	•	Distillate va	por fraction:	D
 Convergence Flowsheeting Options 		Recov:	0.005						
Model Analysis Tools EO Configuration Results Summarv	r								

Fig. 2: Required Input in the DSTWU block

All Items	- Su	immary	Balance	Reflux Ratio Profil	e 🥝 Status	
Streams	*					
5 Blocks		Minimu	ım reflux rat	tio:	0.884634	
B1		Actual reflux ratio:			1.16291	
Block Options		Minimu	ım number	7.27416		
EO Modeling		Numbe	r of actual s	tages:	14.5483	
Stream Results		Feed sta	ige:		11.9089	
Stream Results (Custom)		Numbe	r of actual s	tages above feed:	10.9089	
Utilities		Reboile	r heating re	quired:	102616	cal/sec
Reactions		Conder	ser cooling	required:	270256	cal/sec
Convergence		Distillat	e temnerati	ire [,]	6/ 1203	C
Model Analysis Tools		Distillat	· · ·	<i></i>	400 507	с -
EO Configuration		Bottom	temperatu	re:	100.527	С
Results Summary	↓	Distillat	e to feed fra	iction:	0.5	
		HETP:				

Fig. 3: Results of the DSTWU block

|--|

		Units	1 •	2 •	3 -
►	Substream: MIXED				
$\left \right $	Phase:		Mixed	Liquid	Liquid
$\left \right $	Component Mole Flow				
$\left \right $	METHANOL	KMOL/HR	50	49.75	0.25
$\left \right $	WATER	KMOL/HR	50	0.25	49.75
arepsilon	Mole Flow	KMOL/HR	100	50	50
$\left \right $	Mass Flow	KG/HR	2502.87	1598.6	904.271
$\left \right $	Volume Flow	L/MIN	30720.5	35.7667	16.4685
$\left \right $	Temperature	с	80	64.1293	100.527
$\left \right $	Pressure	BAR	1.01325	1.01325	1.01325
►	Vapor Fraction		0.644928	0	0
►	Liquid Fraction		0.355072	1	1
►	Solid Fraction		0	0	0

Fig. 4: Stream Results with mole fraction

PROBLEM 2

Solve PROBLEM 1 using RADFRAC method. Let the desired composition of Methanol in the distillate be 99.9%.

STEPS TO BE FOLLOWED

- a. Open a new file in Aspen and enter the components and the METHOD and perform flow-sheeting.
- b. Fill the required inputs for feed stream and the block as shown in Fig. 5.
- c. Running the Simulation provides the Block and Stream Results.
- d. The Results tab display results for Condenser and Reboiler.
- e. The profile gives every detail of the column like flow rate, mole fraction, temperature, pressure in every tray.
- f. The change in composition, temperature, pressure and other parameters with respect to the tray can be viewed as graphs.
- g. Click Temp in the Plot section above. The temperature in the trays can be seen in Fig. 6.
- h. Likewise change in liquid composition of Methanol and Water according to trays can be seen in Fig. 7.
- i. To specify the composition click 'Design Specifications' in the block. Type is mole purity of the product and the value is 99.9%. In the Components select methanol and in the base components select both methanol and water. In the feed/product streams select Distillate.
- j. In the Vary section, vary "Reflux ratio" from 0.5 to 200. Check the results for composition and reflux ratio.

configuration	Greams	Pressure	Condenser	🕜 Reboiler	3-Phase	Inform
etup options —						
alculation type:	1		Equilibrium			
Number of stage	S:	-	15	•	Stage Wizard	
Condenser:		[Total			•
Reboiler:			Kettle			-
/alid phases:			Vapor-Liquid			-
Convergence:			Standard			-
)perating specif	ications					
Distillate to fee	ed ratio	•	Mole	▼ 0.5		
Reflux ratio		•	Mole	• 1.16		
ree water reflux	ratio:		0		Feed Basi	s
5: Required I	nput in the RA	ADFRAC blo	ock			
		Block C1	100: Lemperature Pr	otile		
⁰⁰ [_
95				•	Temperature C	
95				•	Temperature C]
90				•	Temperature C]
00 95 90 85					Temperature C]
00 95 90 85					Temperature C]
00 95 90 85 80					Temperature C]
00 95 90 85 80 75					Temperature C	
00 95 90 85 80 75					Temperature C	
00 95 90 85 80 75 70					Temperature C	
00 95 90 85 80 75 70 65					Temperature C	



Fig.7: Change in composition with respect to column trays.

4. SENSITIVITY ANALYSIS

Sensitivity Analysis is a tool for determining how a process reacts to varying key operating and design variables. It can be used to vary one or more flow-sheet variables and study the effect of that variation on other flow-sheet variables. It is a valuable tool for performing "what if" studies. The flow-sheet variables that are varied must be inputs to the flow-sheet. They cannot be variables that are calculated during the simulation.

In this problem let's do the Sensitivity Analysis for Feed Stage and number of stages to see the change in mole fraction of methanol at the distillate.

STEPS TO BE FOLLOWED

- Click 'Sensitivity' icon at the top.
- Click 'New'. In the 'Vary' tab the variable that has to be varied is entered. In this case vary the position of feed stage. Fill the inputs as shown in Fig. 8.
- 'Define' is the variable that will get varied with the change in variable in 'Vary'. In this case the mole fraction of light component in distillate will be defined. The inputs has to be filled as shown in Fig. 9.
- In the 'Tabulate' tab the values that is required to appear in the results as tables has to be filled. Click the 'Fill Variables' to fill default variables.
 It can be seen that the Simulation is ready to run. Run the Simulation. The results can be plotted as shown in Fig. 10.Analyze the Results.
- Repeat the Sensitivity Analysis taking variable as Reflux Ratio. The results are shown in Fig. 11.

NOTE: Only 1 Analysis can be done at a time. The other Analyses has to be either Deleted or Hidden. The Design specifications also has to be hidden or deleted.

√ary ⊖Def	fine 🛛 😜	Tabulate	Options	Cases	Fortran	Declarations	Information		
ctive	Cas	e study							
Manipulated	variables	(drag and o	drop variab	les from f	orm to th	e grid below)			
Variab	le	Active	Manij	Ianipulated variable					
1 🖉 B				lock-Var Block=C100 Variable=FEED-STAGE Sentence=FEE					
New		Delete		Co	ру	Paste			
Edit selected	variable								
Manipulated	variable -			M	lanipulate	d variable limits			
Variable:	1			- 0) Specify	limits			
Туре:	Block	-Var		•	Lower:	1			
Block:	C100			•	Upper:	15			
Variable:	FEED-	STAGE	- 👌	à	🔘 Num	ber of points: 1			
Sentence:	FEEDS			Increment: 1					
ID1:	ID1: F			 Clist of values 					
: Required	Input in	the 'Vary	' for Sens	sitivity A	Analysis.				
: Required	Input in Define	the 'Vary ƏTabulat	' for Sens	sitivity A	analysis.	tran Declaratio	ons Information		
Required	Input in Define	the 'Vary Tabulate	' for Sens	sitivity A	analysis.	tran Declaratio	ons Information		
: Required Vary 🛛 🖓 [) Measured	Input in Define	the 'Vary Tabulate (drag and c	r' for Sens e Option drop variab	sitivity A	nalysis. es For form to t	tran Declaration	ons Information		
Required Vary I	Input in Define variables able	the 'Vary Tabulate (drag and of Definition Male Fr	r' for Sens e Option drop variab	sitivity A	Analysis. es For form to t	tran Declaration	ons Information		
: Required Vary I I Measured Vari YD	Input in Define variables able	the 'Vary Tabulate (drag and of Definition Mole-Fr	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from t =D Substr	Analysis. es For form to t eam=MI	tran Declaration he grid below) (ED Component	ons Information		
: Required Vary I I	Input in Define variables able	the 'Vary Tabulate (drag and of Definition Mole-Fr	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from t	Analysis. es For form to t eam=MI	tran Declaration he grid below) (ED Component:	ons Information		
Required Vary I	Input in Define variables able	the 'Vary Tabulate (drag and of Definition Mole-Fr Delete	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from t D Substr	Analysis. es For form to t eam=MI	tran Declaration he grid below) (ED Component: Paste	ons Information = METHANOL Move Up		
Required Vary I	Input in Define variables able ed variabl	the 'Vary Tabulate (drag and of Definition Mole-Fr Delete e	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from t D Substr Copy	Analysis. es For form to t eam=MI	tran Declaration he grid below) (ED Component: Paste	ons Information = METHANOL Move Up		
Required Vary I	Input in Define variables able ed variabl	the 'Vary Tabulate (drag and of Definition Mole-Fr Delete e	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from f D Substr Copy Referenc	analysis. es For form to t eam=Ml	tran Declaration he grid below) (ED Component: Paste	ens Information		
Required Vary I	Input in Define variables able ed variabl	the 'Vary Tabulata (drag and of Definition Mole-Fr Delete	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from f D Substr Copy Referenc Type:	Analysis. es For form to t ream=Ml e	tran Declaration he grid below) (ED Component Paste	ens Information = METHANOL Move Up		
Required Vary I I Measured Vari YD New Edit selecter ariable: ategory All	Input in Define variables able ed variabl	the 'Vary Tabulata (drag and of Definition Mole-Fr Delete e	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from f D Substr Copy Referenc Type: Stream:	Analysis. es For form to t ream=Ml e	tran Declaration he grid below) (ED Component Paste	ens Information		
Required Vary I I Measured Vari YD New Edit selecter ariable: ategory All	Input in Define variables able ed variabl	the 'Vary Tabulata (drag and d Definition Mole-Fr Delete e	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from f D Substr Copy Referenc Type: Stream: Substream	e Trice and the search of the	tran Declaration he grid below) (ED Component Paste Aole-Frac	ens Information		
Required Vary I	Input in Define variables able ed variabl	the 'Vary Tabulata (drag and d Definition Mole-Fr Delete	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from f D Substr D Substr Copy Referenc Type: Stream: Substream Compone	e n:	tran Declaration he grid below) (ED Component Paste Nole-Frac) MIXED METHANOL	ens Information		
Required Vary I	Input in Define variables able ed variabl	the 'Vary Tabulate (drag and of Definition Mole-Fr Delete e	r' for Sens e Option drop variab on rac Stream=	sitivity A ns Case les from f D Substr D Substr Copy Referenc Type: Stream: Substream Compone	e n:	tran Declaration he grid below) (ED Component: Paste Mole-Frac) MIXED METHANOL	ens Information		
Required Vary I Measured Vari Vari Vari Vari Vari Vari Vari Vari Vari Vari Streams Model Utili	Input in Define variables able ed variabl	the 'Vary Tabulata (drag and o Definitio Mole-Fr Delete e	r' for Sens e Option drop variab on ac Stream=	sitivity A ns Case les from f D Substr D Substr Copy Referenc Type: Stream: Substream Compone	e form to t	tran Declaration he grid below) (ED Component: Paste Mole-Frac) MIXED METHANOL	ens Information		



Fig. 10: Change in composition of Methanol in distillate with the change in position of feed stage.



Fig. 11: Change in composition of Methanol in distillate with the change in reflux ratio.

PRACTICE PROBLEMS

PROBLEM 1

10 kmol/h of a mixture of benzene and toluene with a composition of 40% and 60% respectively at 368 K and 1 atm is fed to the distillation column for separation. Take reflux ratio as 2 with total condenser and 1 atm pressure for condenser and reboiler. Take Light key component recovery as 0.992 and Heavy key component recovery as 0.014.

- 1) Simulate the DSTWU column and use the data to simulate the RADFRAC column.
- 2) Use the design specification to obtain 99.5 % benzene in distillate by varying reflux ratio from 1.75 to 200.
- 3) Perform Sensitivity Analysis by varying the feed stage.

PROBLEM 2: DESIGN OF MULTICOMPONENT DISTILLATION COLUMN

A 2000 kmol/h of saturated liquid is fed to a distillation column at atmospheric pressure and 281.6 K. The feed mixture contains 0.056 *n*-propane, 0.321 *n*-butane, 0.482 *n*-pentane and 0.141 *n*-hexane. The column has a total condenser and a partial reboiler. Design a **DSTWU** column with a fractional recovery of 99.4% of *n*-pentane (light key) present in feed in the distillate and 99.7% of *n*-hexane (heavy key) present in feed in the bottom stream. The pressure throughout the column is 1 atm. Using the data of DSTWU column design a **RadFrac** column with a desired mole purity of n-hexane in the bottom be 99.9% (NOTE: Reflux ratio can be varied). Take Distillate to feed ratio as 0.86 (You can see the D/F ratio in DSTWU results as 0.86).

- 1. Mention the minimum reflux ratio, actual reflux ratio, minimum number of stages, actual number of stages in DSTWU results.
- 2. In addition to minimum reflux ratio, actual reflux ratio, minimum number of stages, actual number of stages mention the feed stage in the RadFrac results and also plot the variation in composition and temperature with respect to trays.

Perform the Sensitivity Analysis on *n*-hexane in the bottom by varying the feed stage in the first case and reflux ratio in the second case.

PROBLEM 3: DESIGN OF MULTICOMPONENT DISTILLATION COLUMN

The feed at 138 psia and 75⁰F and the composition given below is fed to a distillation column operating at 138 psia. The column has a total condenser and a partial reboiler at the column pressure. Design a **DSTWU** column with a fractional recovery of

99.5% of propane (light key) present in feed in the distillate and 99.9% of *i*-butane (heavy key) present in feed in the bottom stream. Using the data of DSTWU column, design a **RadFrac** column with a desired mole purity of propane in the distillate be 99% (NOTE: Reflux ratio can be varied). Take Distillate to feed ratio as 0.05 (You can see the D/F ratio in DSTWU results as 0.05).

COMPONENT	FLOW RATE (lb-mol/h)
Propane	100
<i>i</i> -butane	300
<i>n</i> -butane	500
<i>i</i> -pentane	400
<i>n</i> -pentane	500

- 1. Mention the minimum reflux ratio, actual reflux ratio, minimum number of stages, actual number of stages in DSTWU results.
- 2. In addition to minimum reflux ratio, actual reflux ratio, minimum number of stages, actual number of stages mention the feed stage in the RadFrac results and also plot the variation in composition and temperature with respect to trays.

Perform the Sensitivity Analysis on propane in the distillate by varying the feed stage in the first case and reflux ratio in the second case.

LITERATURE CITED:

- Finlayson B.A (2012). Introduction to Chemical Engineering Computing
- GhasemNayef, (2012), Computer Methods in Chemical Engineering
- Geankoplis C.J., (2009), Transport Processes and Separation Process Principles, Fourth Edition.

Experiment 6: Absorption using ASPEN Plus

1. Objectives:

After the completion of this module, the students will have:

- Reviewed and expanded knowledge of separation of fluids using distillation and its applications.
- Learned to use Aspen Plus to simulate packed bed and plate type absorption column by using RADFRAC method and perform related calculations.
- Perform Optimization Analysis of the process.

2. Prerequisite Engineering & Science Skills

- 1. Knowledge of Vapor-Liquid Equilibrium of a mixture of chemicals.
- 2. Knowledge of absorption as a method of separation of fluids.
- 3. Knowledge of Aspen Plus.

3. ABSORPTION IN ASPENPLUS

Absorption is a mass-transfer process in which a vapor solute in a gas mixture is absorbed by means of a liquid in which the solute is more or less soluble. The gas mixture consists mainly of an inert gas and a solute. The liquid also is primarily immiscible in the gas phase i.e. its vaporization into the gas phase is relatively slight. The **RadFrac and Multifrac** models are used for the design and simulation of the absorption column in Aspen Plus.
CLASS PROBLEM

Absorption of Acetone in an Absorption Tower (Example 10.6-4 Reference 1)

Acetone is being absorbed by water in a tower having a cross-sectional area of 0.186 m² at 293 K and 101.32 kPa (1 atm). The inlet air contains 2.6 mol% acetone and rest air. The total gas inlet flow rate is 15 kmol/h. Calculate the rate of water required so that the outlet air contains a maximum of 0.1% acetone. Perform the optimization if the permissible mole fraction of acetone in water is 0.5% for the following cases:

- 1. Tray tower
- 2. Packed tower as a single section with raschig packing of 15 mm.

NOTE: The Occupational Safety and Health Administration (OSHA) enforceable standard (permissible exposure limit or PEL) for acetone in workplace air is 1,000 ppm.

DESIGN OF TRAY TOWER: STEPS TO BE FOLLOWED

- Open a new file in Aspen and enter the components water, air and acetone. Choose the suitable METHOD to be used in the properties section.
- Click the Simulation section. Select 'ABSBR-1' from the RadFrac column Pallette and add the input and output streams as shown in Fig. 1. Note that all the column icons under the same model palette (in this case RadFrac) has the same function, only the resemblance of the icon differs. Here ABSBR-1 is chosen because it resembles more as absorption column.
- Now fill the required inputs for feed stream and then the block. Fill the variables of the block as shown in Fig 2. Note that there is no requirement of condenser and reboiler in absorption column. The feed stages and the product stages and the state should be mentioned correctly and carefully. In the pressure tab the stage will have the same pressure of the column, in this case '1 atm'.
- When the required inputs are added the bottom left corner of the screen will display 'Required Inputs Complete'. Now Run the simulation.
- In the Absorber select Tray Rating and add new rating. Let the tray spacing be default value and tray diameter has to be calculated from the tray surface area
- The composition of the acetone can now be plotted for each tray. The composition of acetone in water in each tray and the Stream Results can be seen in Fig. 3 and 4 respectively.

Since in the problem, it is asked to maintain the level of acetone less than 0.1% in air due to environmental concerns hence DESIGN SPECIFICATIONS has to be set.

• In the absorber block click 'Design Specifications' and set mole purity of acetone in air as 0.001. In the Vary section, vary the feed rate of water in from 10 to 40 kmol/h and RUN the simulation. The Stream and the block Results

shows the changes that has occurred due to the design specification. The flow rate of water required is 29.4 kmol/h. The Results can be seen in Fig. 5.

Let us add the Sizing and Rating in-order to get the dimensions of the column required.

- ➢ Go to 'Tray Rating' in 'Sizing and Rating' and press 'New'. Put the diameter of the Column as 0.4868 m (Since the Cross sectional Area is 0.186 m²) and other data as shown in Fig. 6.
- The results of the Column Specifications can be seen in Results of Tray Rating as shown in Fig. 7.



Fig. 1: Absorption column Flowsheet using RadFrac model.

a)

Configuration	Streams	Pressure	Condenser	Reboiler	3-Phase	Information
Setup options —						
Calculation type:		E	quilibrium		-	
Number of stages:		1	0		St St	age Wizard
Condenser:		1	None			•
Reboiler:		1	None			•
Valid phases:		١	/apor-Liquid			-
Convergence:		S	Standard			•
Operating specific	ations					
operating specific		Ŧ		Ŧ		
		~		-		
					Eee	d Racic

0	Configuration	🧭 Streams	P	ressure	Condenser	Reboil
Fee	d streams					
	Name	Stage			Convention	ı
	WATERIN	1		Above-S	Stage	
►	GASIN	11		Above-S	Stage	
Pro	duct streams –					
Pro	duct streams — Name	Stage		Phas	;e	Basis
Pro	duct streams – Name GASOUT	Stage 1	Vap	Pha: or	se I	Basis Viole

Fig. 2: Required Input in the Absorption block



Fig. 3: Mole fraction of acetone in liquid in each tray

		Units	GASIN -	GASOUT -	WATERIN -	WATEROUT -
►	Phase:		Vapor	Vapor	Liquid	Liquid
•	Component Mole Flow					
•	ACETONE	KMOL/HR	0.39	0.0560463	0	0.333954
•	WATER	KMOL/HR	0	0.414581	20	19.5854
•	AIR	KMOL/HR	14.61	14.5822	0	0.0278064
$\left \right $	Component Mole Fraction					
►	ACETONE		0.026	0.00372331	0	0.0167419
$\left \right $	WATER		0	0.0275417	1	0.981864
$\left \right $	AIR		0.974	0.968735	0	0.001394
•	Mole Flow	KMOL/HR	15	15.0528	20	19.9472
•	Mass Flow	KG/HR	445.624	432.892	360.306	373.038
•	Volume Flow	L/MIN	6013.68	6095.28	6.01251	6.29504
•	Temperature	С	20	22.9351	20	16.952
•	Pressure	BAR	1.01325	1.01325	1.01325	1.01325
•	Vapor Fraction		1	1	0	0

Fig. 4: Stream Results with mole fraction

		Units	GASIN -	GASOUT -	WATERIN -	WATEROUT -
►	Phase:		Vapor	Vapor	Liquid	Liquid
$\left \right $	Component Mole Flow					
►	ACETONE	KMOL/HR	0.39	0.0149545	0	0.375045
►	WATER	KMOL/HR	0	0.371055	30.2663	29.8952
►	AIR	KMOL/HR	14.61	14.5693	0	0.0406684
$\left \right $	Component Mole Fraction					
►	ACETONE		0.026	0.000999948	0	0.0123732
►	WATER		0	0.0248108	1	0.986285
►	AIR		0.974	0.974189	0	0.00134171
•	Mole Flow	KMOL/HR	15	14.9553	30.2663	30.3109
$\left \right $	Mass Flow	KG/HR	445.624	429.349	545.255	561.531
►	Volume Flow	L/MIN	6013.68	6020.31	9.0988	9.46992
•	Temperature	С	20	21.1993	20	19.7996
•	Pressure	BAR	1.01325	1.01325	1.01325	1.01325
•	Vapor Fraction		1	1	0	0

Fig. 5: Stream Results after specifying Design Specifications.

Specification	s Design / P	drop Layout	Downcomers			
Trayed section Starting stage: Tray type:	1 Bubble Cap	÷	Ending stage: Number of pass	es:	1 1	< > < >
Tray geometry Diameter: Tray spacing:	0.4868 0.6096	meter ▼ meter ▼	Deck thickness:	10 GAU	GE	T
- Weir heights — Panel A	Panel B	Panel C	Panel D			
meter •	meter	- meter -	meter -			

Fig. 6: Required inputs for tray rating.

Tray	y rating summary —			
Þ	Section starting stage:	1		
Þ	Section ending stage:	1		
Þ	Column diameter:	0.4868	meter	
Þ	Maximum flooding factor:	0.185493		
Þ	Stage:	1		
Þ	Panel:			
•	Section pressure drop:	0.00330299	bar	Ŧ

Downcomer results

Maximum backup / Tray spacing:	0.178689		
Stage:	1		
Location:			E
Backup:	0.108929	meter	
Maximum velocity / Design velocity:			
Stage:	1		
1			٣

Fig. 7: Column specifications after Rating.

4. OPTIMIZATION ANALYSIS

Optimization is tool to maximize or minimize a user-specified objective function by manipulating decision variables (feed stream, block input, or other input variables). The analysis has the option of imposing equality or inequality constraints on the optimization. Equality constraints within an optimization are similar to design specifications. The constraints can be any function of flow-sheet variables computed using Fortran expressions or in-line Fortran statements. The tolerance of the constraint must be specified.

STEPS TO BE FOLLOWED

Click 'Optimization' icon at the Model Analysis Tools.

- □ Click 'New'. In the 'Define' tab the variable that are needed in the final result has to be entered. In this case enter the mole fraction of acetone in the Gas Out and Water Out and the flow rate of Water In as shown in Fig. 8.
- □ In the 'Objectives and Constraints' enter 'WATERIN' which has to be minimized. Note that the words should be exact as it was in 'Define'. Two constraints one each for 'YACETONE' and 'XACETONE' has to be defined by pressing 'New' in Constraints and shift them to Selected section as shown in Fig. 9.
- □ In the 'Vary' tab let us vary Water at the inlet from 10 kmol/h to 100 kmol/h. as shown in Fig. 10.
- □ In the 'Constraints' below 'Optimization' select input in 'C1' and enter the 'XACTONE' i.e. the mole fraction of Acetone in Water coming out as shown in Fig. 11. In the 'Spec' section put the required inputs as shown in Fig. 12. Similarly add details in constraint 'C2' for YACETONE (mole fraction of Acetone in gas out) and the Spec as shown in Fig. 13.
- Run the Simulation. The results can be seen in Results under Optimization'O1' as shown in Fig. 14. Analyse the Results. Check the Stream Results.

NOTE: Only 1 Analysis can be done at a time. The other Analyses has to be either Deleted or Hidden. The Design specifications also has to be hidden or deleted.

0	Define	Objective	e & Constraints	⊖Vary	Fortran	Declarations	Information	
٢) Measur	ed variables (drag and drop va	riables fron	n form to t	he grid below)		
	\	/ariable	Definition					
	YACETO	NE	Mole-Frac Stre	am=GASOl	JT Substre	am=MIXED Com	ponent=ACETC)NE
	XACETO)NE	Mole-Frac Stre	am=WATE	ROUT Subs	tream=MIXED C	component=AC	ETONE
	WATER	IN	Mole-Flow Stre	am=WATE	RIN Substr	eam=MIXED Co	mponent=WAT	ER Units=kmol/hr
Þ								
	New		Delete	Сору		Paste	Move Up	Move Down
٢) Edit sele	ected variable	2					
Va	ariable:	VACE	FONE -	Referer	ice			
-C	ategory -			Туре:	L.	Mole-Frac	•	•
6				Stream:	•	GASOUT	•	
	All			Substre	am:	MIXED	-	•
C	Blocks			Compo	nent:	ACETONE	•	-
0	Streams	;						

Fig. 8: Inputs in the Define section of Optimzation Analysis.

 🕜 Define	🥝 Objective	& Constra	ints	⊖Vary	Fortran	Declarations
V Optimizat	tion is active					
 Maximize Minimize 	WATERIN					
Selected co	nstraints —					
Available		>	Sele	cted		
		>> < << New	C-1 C-2	2		

Fig. 8: Inputs in the Objectives and Constraints section of Optimzation Analysis.

	🕜 Define	🕜 Objectiv	e & Constraints	⊘ Vary	Fortran	Declarations	Information		
(Manipul	ated variable	s (drag and drop	variables fr	rom form t	o the grid below)		
	V	ariable	Active	Manipulat	ed variable	2			Low
	1		V	Mole-Flov	v Stream=	WATERIN Substr	eam=MIXED Co	omponent=WATER	10
	New		Delete		Сору	P	aste		
	Manipulat	cted variable ted variable -	: 		Manipu	ılated variable li	mits		
	Variable n	umber: 1		-	Lower:		10	kmol/hr	~
	Туре:	Mo	le-Flow	-	Upper:		100	kmol/hr	~
	Stream:	W	TERIN	•	Step siz	e:		kmol/hr	~
	Substream	n: MI	XED	-	Maxim	um step size:			
	Compone	ent: W/	TER	-	Pan	ort labels			
	Units:	km	ol/hr	-	🕑 кер				

Fig. 10: Inputs in the Vary section of Optimzation Analysis.

(Define	Gpec	Fortran Dec	arati	ions Info	ormation			
		Variable	Definition						
	XACET	ONE	Mole-Frac S	trear	n=WATER(OUT Sub	stream=MIXEI	D Compon	ent=ACET(
(New Edit sel	ected variabl	Delete		Copy		Paste	N	love Up
	/ariable:	S XACI	TONE	•	Type:	.c	Mole-Frac		-
ſ	Category				Stream:		WATEROUT		-
	🔘 All				Substroop				
	🔿 Blocks				Constream	16			
	~ -				Compon	ent:	ACETONE		•
	Stream	s							

Fig. 11: Required Inputs in the constraint 'C1' of Optimzation Analysis.

Venne	🕜 Spec	Fortran	Decla	arations	Information	
Constraint	expression	s ———				
Specificatio	on:			XACETO)NE	
Less than	or equal to	D	•	0.005		
Tolerance:	-			0.0000)1	
Vector con	straint info	rmation —				
📃 This is a	a vector con	nstraint				
17. Doquiro	d Spacificati	one in the o	natroin	t 'C1' of (Intimzation Analy	zoio
, 12. Required	i Specificati		Jiistiaiii		prinization Analy	/515.
🕜 Define	🕑 Spec	Fortran	Decla	rations	Information	
-						
Constraint	expressions	;		VACETO	ur.	
Specificatio	n:			TACETO	NE	
opeencade						
Less than	or equal to)	-	0.001		
Less than Tolerance:	or equal to)	•	0.001 0.00000	1	
Less than Tolerance:	or equal to		•	0.001	1	
Less than Tolerance: Vector cons	or equal to straint infor	rmation —	•	0.001	1	
Less than Tolerance: Vector cons	or equal to straint infor vector cor	rmation — nstraint	•	0.001	1	
Less than Tolerance: Vector cons This is a . 13: Required	or equal to straint infor vector cor d Specificati	rmation — nstraint ons in the co	onstrain	0.001 0.00000 t 'C2' of C	1 Optimzation Analy	/sis.
Less than Tolerance: Vector cons This is a . 13: Required	or equal to straint infor vector cor d Specificati	mation — nstraint ons in the co	onstrain	0.001 0.00000 t 'C2' of C	1 Optimzation Analy	/sis.
Less than Tolerance: Vector cons This is a . 13: Required 1 - Results ×	or equal to straint infor vector cor d Specificati Results Sumn	rmation — nstraint ons in the co nary - Run Sta	onstrain tus × Y	0.001 0.00000 t 'C2' of C B1 (RadFrac	1 Optimzation Analy) - Composition - Pl	/sis. ot ×
Less than Tolerance: Vector cons This is a . 13: Required 1 - Results × esults Stat	or equal to straint infor vector cor d Specificati Results Summ	mation — nstraint ons in the co nary - Run Sta	onstrain tus × Y	0.001 0.00000 t 'C2' of C B1 (RadFrac	1 Optimzation Analy) - Composition - PI	/sis. ot ×
Less than Tolerance: Vector cons This is a 13: Required 1 - Results × :sults Stat	or equal to straint infor vector cor d Specificati Results Summ us	rmation — nstraint ons in the co nary - Run Sta Initial value	onstrain tus × r	0.001 0.00000 t 'C2' of C B1 (RadFrac Final v	1 Optimzation Analy) - Composition - Pl value	/sis. ot × Units

77.8402



77.8402

WATERIN

KMOL/HR

DESIGN OF TRAY TOWER: STEPS TO BE FOLLOWED

- Follow all the steps of tray tower. But instead of selecting 'Tray Rating' in 'Sizing and and Rating', select 'Packing Rating' for Packed bed column. Select 'New'.
- Let the packing be same throughout, hence input packing section from 1 to 10 (Since we had tken 10 trays in Set Up). Select 'Raschig' type ceramic 15 mm packing (Vendor: Raschig). Take the section diameter as column diameter and HETP as Tray Spacing previously i.e. 0.6096 m. Run the Simulation.
- Analyse the Results. It could be seen that the results are little different for the packed tower.

PRACTICE PROBLEMS

PROBLEM 1: Absorption of heavier hydrocarbons using *n*-decane in a Packed Tower

Heavier hydrocarbons have to be separated from a mixture of feed in the table below at 25° C and 1 atm using *n*-decane at 25° C and 1 atm in a PACKED BED column operating at 101.32 kPa (1 atm) maintaining the flow rate of absorber (*n*-decane) so that the mole fraction of butane in the distillate remains less than 0.1%. Calculate the required diameter of the column. Take number of stages as 10. Mention the amount of light hydrocarbons recovered in the distillate in your results.

COMPONENT	MOLE FLOW (kmol/h)
Methane	280
Ethane	150
<i>n</i> -propane	240
<i>n</i> -butane	170
<i>n</i> -pentane	150

Perform Optimization Analysis to maximize *n*-pentane in the bottom by varying temperature of the absorbent from 10^{0} C to 60^{0} C. Comment on the results.

Specs of Packing Sizing: Raschig from Vendor Raschig 15 mm ceramic and HETP 0.6091 m.

PROBLEM 2: Absorption of SO₂ from air in a Packed Tower

 SO_2 is being absorbed from air at 20^oC and 1 atm in a packed bed tower using water at 20^oC and 1 atm. The inlet air contains 8 mol% SO_2 and rest air. The total gas inlet flow rate is 150 kmol/h. Calculate the rate of water required so that the outlet air contains a maximum of 0.5% SO_2 .

Perform the optimization to minimize the mole fraction of SO_2 at water outlet by varying the temperature of the water at the inlet.

Packing Sizing Specs: Number of stages are 7. Packing is 15 mm of type Raschig (Vendor: Raschig) and material is ceramic and HETP is 0.6096 m.

LITERATURE CITED:

- Geankoplis C.J., (2009), Transport Processes and Separation Process Principles, Fourth Edition.
- □ GhasemNayef, (2012), Computer Methods in Chemical Engineering.
- □ ASPEN Help.

Experiment 7: Heat Exchanger Design Using ASPEN Plus

1. **Objectives:**

After the completion of this module, the students will have:

Learned to use Aspen Plus to perform Shortcut and detailed design of Shell & Tube Heat Exchangers

2. Prerequisite Engineering & Science Skills

- Knowledge of design of heat exchangers.
- Knowledge of Aspen Plus.

3. HEAT EXCHANGERS

The most commonly used type of heat transfer equipment is the ubiquitous shell and tube heat exchanger. The design of Heat Exchangers is discussed in detail in Reference 1. The general equation for heat transfer across a surface is:

$$Q = UA\Delta T_m$$

where

Q = heat transferred per unit time, W;

U = Overall heat transfer coefficient, $W/m^{20}C$;

A = heat transfer area, m²;

 ΔT_m =Mean temperature difference, the temperature driving force, ⁰C.

The overall coefficient is the reciprocal of the overall resistance to heat transfer, which is the sum of several individual resistances and is given by:

$$\frac{1}{U_0} = \frac{1}{h_0} + \frac{1}{h_{0d}} + \frac{d_0 \ln(\frac{d_0}{d_i})}{2k_w} + \frac{d_0}{d_i} \times \frac{1}{h_{id}} + \frac{d_0}{d_i} \times \frac{1}{h_{id}}$$

where

 U_o = the overall coefficient based on the outside area of the tube, W/m28C;

 h_o = outside fluid film coefficient, W/m²⁰C;

 $h_i = inside fluid film coefficient, W/m^{20}C;$

 h_{od} = outside dirt coefficient (fouling factor), W/m²⁰C;

 h_{id} = inside dirt coefficient, W/m²⁰C;

 k_w = thermal conductivity of the tube wall material, W/m²⁰C;

 $d_i = tube inside diameter, m;$

 $d_o = tube outside diameter, m.$

The procedure for the design of shell and tube heat exchanger is mentioned in the flowchart in Fig.1.



Fig.1: Design procedure for Shell and Tube Heat Exchangers.

4. Heat Exchangers in Aspen Plus

Heater: Heater is used to heat or cool a stream. **HeatX:**HeatX can perform these types of calculations:

- 1. Shortcut design or simulation
- 2. Detailed rating or simulation for most types of two stream heat exchangers
- 3. **Rigorous** design, rating, or simulation by interfacing with the Aspen Exchanger Design and Rating (EDR) programs: Shell&Tube, AirCooled, or Plate

The **shortcut** method always uses a user specified (or default) value for the overall heat transfer coefficient.

The **detailed** method uses rigorous heat transfer correlations for film coefficients and combines the resistances due to shell and tube side films with the wall resistance to calculate the overall heat transfer coefficient. You need to know the geometry to use the detailed method.

MHeatX:MHeatX represents heat transfer between multiple hot and cold streams.

HxFlux:HxFlux is used to perform heat transfer calculations between a heat sink and a heat source, using convective heat transfer. The driving force for the convective heat transfer is calculated as a function of log-mean temperature difference or LMTD.

In this module HeatX type will be used for shortcut and Detailed design of heat exchanger.

CLASS PROBLEM

Design a Shell and Tube heat exchanger to heat 3441.5 lb-mol/h of methanol (24.7 psia) at 77 F using water (24.7 psia) with flow rate 2315.5 lb-mol/h, with a temperature rise from 144 F to 113 F.

DATA GIVEN

SHELL: Number of tube passes is 4; inside shell diameter is 17.25 in.

TUBES: Tube number is 200, pattern square, length 10 ft, pitch 1 in., inner diameter 0.482 and outer diameter 0.75.

Baffles: Number of baffles all passes is 12, baffle cut 0.25, baffle to baffle spacing 6 in.

NOZZLES: Shell inlet and outlet nozzle diameter is 4 in. Tube side inlet and outlet nozzle diameter is 3 in.

SHORTCUT DESIGN METHOD

Step 1:Start Aspen Plus and choose General with Metric Units.

Step 2: Complete the Properties tab. Use WILS-2 method.

- **Step 3:** Select the Simulation and from the Model Pallette select Exchangers and then select HeatX.
- Step 4: When the streams are connected to the exchanger block, the hot stream is the stream that has to be cooled and it has higher temperature and it should be allocated in the input where the arrow specifies "Hot required" as the stream is touched to the arrow as shown in Fig. 1. Similarly the cold stream (it has lower temperature) has to be heated and it should be allocated in the input where the arrow specifies "Cold required" as the stream is touched. Complete the flow-sheet as shown in Fig. 2.
- Step 4: Add the details of the input streams of Methanol and Water.
- Step 5: Add the details of the block. Select Shortcut for the Calculation method In the Exchanger Specification Select "Hot stream outlet temperature" and put minimum approach temperature as 10 F as shown in Fig. 3. It could be seen that all required data inputs have been done. Run the Simulation.
- Step 6: Check Thermal Results. The results are shown in Fig. 4.



Fig 1: Method of connection of streams to arrows according to temperature.



Fig 2: Flow-sheet of Heat Exchanger using HeatX.

Specifications	Streams	LMTD	Pressure Drop	🕑 U Methods	Film Coefficients
Model fidelity	Не	ot fluid	Sho	rtcut flow directi	on
Shortcut	0	🔵 Shell	۲	Countercurrent	
🔘 Detailed	(🖲 Tube	\bigcirc	Cocurrent	
🔘 Shell & Tube			\bigcirc	Multipass, calcula	te number of shells
🔘 Kettle Reboiler			\bigcirc	Multipass, shells i	n series 1 🏯
Thermosyphon	I				
O Air Cooled					
O Air Cooled O Plate					
 Air Cooled Plate Calculation mode 	Design		-		
 Air Cooled Plate Calculation mode Exchanger specific 	Design		•		
Air Cooled Plate Calculation mode Exchanger specific Specification H	Design ation lot stream o	outlet ter	- mperature		•
Air Cooled Plate Calculation mode Exchanger specific Specification H Value	Design ation lot stream o	outlet ter	• mperature 113	F	•
Air Cooled Plate Calculation mode Exchanger specific Specification Value Exchanger area	Design ation lot stream o	outlet ter	• mperature 113	F sqm	•
 Air Cooled Plate Calculation mode Exchanger specific Specification H Value Exchanger area Constant UA 	Design ation ——— lot stream o	outlet ter	mperature 113	F sqm cal/sec-K	

Fig 3: Details of Heat Exchanger block.

/	Main Flowsh	eet ×⁄C10	0 (HeatX) - Thern	al Results × C100	(HeatX) - Setup ×	- +	
	Summary	Balance	Exchanger Details	Pres Drop/Velociti	es Zones Uti	ility Usage	🥝 Status
	- Heatx resul	ts					
	Calculation	Model	Shortcut				
			h	nlet	0	utlet	
	Hot stream	:	WATERIN		WATEROUT		
	Temperatu	re	62.2222	с 🗸	45	С	•
	Pressure		1.70301	bar 🔻	1.70301	bar	•
	Vapor fract	ion	0		0		
	1st liquid /	Total liquid	1		1		
	Cold stream	n	METHIN		METHOUT		
	Temperatu	re	25	с -	34.5554	с	-
	Pressure		1.70301	bar 🔻	1.70301	bar	-
	Vapor fract	ion	0		0		
	1st liquid /	Total liquid	1		1		
	Heat duty		91806.9	cal/sec 🔹			

Fig 4: Thermal Results for Shortcut heat exchanger design.

DETAILED DESIGN METHOD

Step 1: Repeat steps 1 - 4 of Shortcut Design Method.

- **Step 2:** In the Block, in Calculation Select Shell and Tube and press "Convert" in the new window that appear as shown in Fig. 5.
- Step 3: Add all required data and press "Size" and then Accept Design and then Run the program.

Step 4: Click EDR browser for detailed results.

ABBREVIATIONS:

EDR:	Exchange Design and Rating
TEMA:	Tubular Exchanger Manufacturers Association



Fig 5: Required inputs in Specification sheet of Detailed design.

PRACTICE PROBLEMS

PROBLEM 1: DESIGN OF EG COOLER

Freon at 7 atm and 240 K flowing at a rate of 87.35 kmol/h is used to heat ethylene glycol at 2 atm and 315 K and flowing at a rate of 100 kmol/h. Design a Shell and Tube heat exchanger so that the temperature of Freon rises to 300 K and the hot fluid is at tube side. Use Property method "NRTL-2". Take minimum approach temperature as 10K.

Use

1. Shortcut method

2. Use same file for detailed design of Shell and Tube Exchanger.

DATA GIVEN

PRESSURE DROP: Method: Darcy's law, Max. Pressure drop: 0.4

U METHODS: Film co-efficient and U correction factor as 0.9.

FILM CO-EFFICIENT: from geometry; Fouling factor: 0.1; Scaling factor: 0.9.

SHELL: Number of tube passes is 4; inside shell diameter is 0.5 m. TUBES: Tube number is 100, pattern triangle, length 8 ft, pitch 1 in., inner diameter 0.5 in and outer diameter 0.75 in.

Baffles: Number of baffles all passes is 12, baffle cut 0.25.

NOZZLES: Shell inlet and outlet nozzle diameter is 4 in. Tube side inlet and outlet nozzle diameter is 3 in.

PROBLEM 2 DESIGN OF PROPANOL CONDENSER

Saturated n-propanol at 2 bar and 245 F flowing at a rate of 750 kmol/h is to be condensed in a shell and tube heat exchanger using water at 1 bar and 50 F flowing at a rate of 4700 kmol/h. Design the exchanger so that the temperature of water rises to 200 F and the hot fluid is at tube side. Use Property method "NRTL-2". Take minimum approach temperature as 10F.

Use

- 3. Shortcut method
- 4. Use same file for detailed design of Shell and Tube Exchanger.

DATA GIVEN

PRESSURE DROP: Method: Darcy's law, Max. Pressure drop: 0.5

U METHODS: Film co-efficient and U correction factor as 0.9.

FILM CO-EFFICIENT: from geometry; Fouling factor: 0; Scaling factor: 0.9.

SHELL: Number of tube passes is 4; inside shell diameter is 50 in. TUBES: Tube number is 180, pattern triangle, length 7 ft, pitch 2 in., inner diameter 1.8 in and outer diameter 1.95 in. Baffles: Number of baffles all passes is 12, baffle cut 0.25.

NOZZLES: Shell inlet and outlet nozzle diameter is 8 in. Tube side inlet and outlet nozzle diameter is 6 in.

LITERATURE CITED:

D. GhasemNayef, (2012), Computer Methods in Chemical Engineering

E. ASPEN HELP

Experiment 8: Reactor Design using ASPEN Plus (I)

1. Objectives:

After the completion of this module, the students will have:

- a. Reviewed and expanded knowledge of chemical reaction engineering.
- b. Learned to use Aspen Plus to perform the reactor design.

2. Prerequisite Engineering & Science Skills

- 1. Knowledge of chemical reaction engineering.
- 2. Knowledge of performing calculations used in the design of a reactor.
- 3. Knowledge of Aspen Plus.

3. MODES OF REACTOR DESIGN IN ASPENPLUS

1. RStoic

Description: Stoichiometric reactor.

Purpose: Models stoichiometric reactor with specified reaction extent or conversion. It is used where reaction kinetics are unknown or unimportant but stoichiometry and extent of reaction are known.

2. RYield

Description: Yield reactor.

Purpose: Models reactor with specified yield. It is used where stoichiometry and kinetics are unknown or unimportant but a yield distribution is known.

3. REquil

Description: Equilibrium reactor.

Purpose: Performs chemical and phase equilibrium by stoichiometric calculations. It is used for reactors with simultaneous chemical equilibrium and phase equilibrium.

4. RGibbs

Description: Equilibrium reactor with Gibbs energy minimization.

Purpose: Performs chemical and phase equilibrium by Gibbs energy minimization. It is used for reactors with phase equilibrium or simultaneous phase and chemical equilibrium. Calculate phase equilibrium for solid solutions and vapor-liquid-solid systems.

5. RCSTR

Description: Continuous stirred tank reactor.

Purpose: RCSTR rigorously models continuous stirred tank reactors. RCSTR can model one-, two-, or three-phase reactors. RCSTR assumes perfect mixing in the reactor, that is, the reactor contents have the same properties and composition as the outlet stream. RCSTR handles kinetic and equilibrium reactions as well as reactions involving solids.

6. RPlug

Description: Plug flow reactor.

Purpose:RPlug is a rigorous model for plug flow reactors. RPlug assumes that perfect mixing occurs in the radial direction and that no mixing occurs in the axial direction. RPlug can model one-, two-, or three-phase reactors. RPlug can also be used to model reactors with thermal fluid (cooling or heating) streams (co-current or counter-current).

RPlug handles kinetic reactions, including reactions involving solids. Reaction kinetics must be known when RPlug is used to model a reactor. The reaction kinetics can be provided through the built-in Reactions models or through a user-defined Fortran subroutine.

7. RBatch

Description: Batch reactor.

Purpose:RBatch is a rigorous model for batch or semi-batch reactors.

In this module, RStoic will be used for shortcut design and RCSTR and RPlug will be used of detailed design of reactor.

CLASS PROBLEM 1

Design of Reactor for the chlorination of propylene

Epichlorohydrin is used in is used in the production of glycerol, plastics, epoxy glues and resins, and elastomers.

Chlorination of propylene is one of the steps in the production of Epichlorohydrin. Following vapor-phase, irreversible reactions, exothermic reactions take place during the chlorination of propylene:

 $C_{3}H_{6} + Cl_{2} \xrightarrow{k_{1}} CH_{2} = CH - CH_{2}Cl + HCl$ $C_{3}H_{6} + Cl_{2} \xrightarrow{k_{2}} CH_{2}Cl - CHCl - CH_{3}$

The first produces allyl chloride and hydrogen chloride with a reaction rate r1 (kmol/s.m³). The second produces 1,2-dichloropropane with a reaction rate r_2 (kmol/s.m³)

$$\begin{aligned} r_1 &= k_1 P_{C_3} P_{Cl_2} = (8.992 \times 10^{-8} e^{-15111/RT}) P_{C_3} P_{Cl_2} \\ r_2 &= k_2 P_{C_3} P_{Cl_2} = (5.107 \times 10^{-12} e^{-3811/RT}) P_{C_3} P_{Cl_2} \end{aligned}$$

Where partial pressure P_j are in pascals and activation energies are in cal/mol. The reactor is specified to have a diameter of 1 m and a length of 10 m and pressure 3 atm. The valves are fitted before and after the reactor which develops a pressure drop of 2 atm. The feed flows at a rate of 0.025 kmol/s at 400 K and 5 atm with 10 mol% chlorine and 90 mol% propylene.

SIMULATION USING RSTOIC REACTOR

- **Step 1:**Open a new file in Aspen and enter the components ethane, hydrogen and ethylene. Choose the suitable METHOD to be used in the properties section. Here it is 'PENG-ROB'.
- **Step 2:**Click the Simulation section. Select 'RStoic' from the Reactors Pallette and connect the input and output stream. The flow-sheet will appear as in Fig. 1.
- **Step 3:**Fill the required inputs for feed stream and the block stream. The inputs required for the Specifications is shown in Fig. 2. In the Reactions section as the New is clicked the window in Fig. 3 appears. In the left the reactants along with stoichiometric co-efficient have to be filled and in the right hand side the products along with their stoichiometric co-efficient have to be filled. In the bottom the conversion of the reaction has to be filled.
- **Step 4:** For the second reaction click New in the "Reaction no." tab and the stoichiometry table for Reaction 2 will appear. Fill the required inputs as shown in Fig. 4.

The stream results can be seen on Fig. 5 and Fig. 6.





Specifications	⊖Re	actions	Combu	istion	Heat of I	Reaction	19
Operating condition Flash Type:	ons —	Temper	ature	- P	ressure	•	
 Temperature:		400		K		•	
Pressure:		3		at	tm	•	
Duty:				co	ıl/sec	Ŧ	
Vapor fraction:							
Valid phases							
Vapor-Only		-					

Fig 2: Required inputs in Specifications in RStoic Set Up.

eactants		Pro	oducts	
Component	Coefficient		Component	Coefficient
PROPYLEN	-1	▶	C3H5CL	1
CL2	-1		HCL	1
roducts generation				

Fig 3: Required inputs in Reaction 1 in RStoic Set Up.

			Pro	ducts	
	Component	Coefficient		Component	Coefficient
	PROPYLEN	-1		C3H6CL2	1
	CL2	-1			
roc	lucts generation				
roc	Jucts generation	kmol/hr			

Fig 4: Required inputs in Reaction 2 in RStoic Set Up.

_				
		Units	S1 -	S2 -
►	From		V1	RSTOIC
$\left \cdot \right $	То		RSTOIC	V2
$\left \cdot \right $	Substream: MIXED			
$\left \cdot \right $	Phase:		Vapor	Vapor
$\left \cdot \right $	Component Mole Flow			
$\left \cdot \right $	C3H5CL	KMOL/HR	0	7.2
$\left \cdot \right $	PROPYLEN	KMOL/HR	81	72
$\left \cdot \right $	CL2	KMOL/HR	9	0
$\left \cdot \right $	HCL	KMOL/HR	0	7.2
$\left \cdot \right $	C3H6CL2	KMOL/HR	0	1.8
$\left \cdot \right $	WATER	KMOL/HR	0	0
$\left \cdot \right $	Mole Flow	KMOL/HR	90	88.2
$\left \cdot \right $	Mass Flow	KG/HR	4046.68	4046.68
$\left \cdot \right $	Volume Flow	L/MIN	16027.2	15748.3
\rightarrow	Temperature	С	125.155	126.85
$\left \cdot \right $	Pressure	BAR	3.03975	3.03975
$\left \cdot \right $	Vapor Fraction		1	1
$\left \cdot \right $	Liquid Fraction		0	0

Fig 5: Stream Results of RStoic reactor.

		Units						
1		01110	FD 🔻	FEED -	PDT -	PRODUCT -	S1 -	S2 -
ŀ	From				PLUG	V2	V1	RSTOIC
$\left \right $	То		PLUG	V1			RSTOIC	V2
$\left \right $	Substream: MIXED							
$\left \right $	Phase:		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Þ	Component Mole Flow							
Þ	C3H5CL	KMOL/HR	0	0	0.0711567	7.2	0	7.2
Þ	PROPYLEN	KMOL/HR	81	81	74.8382	72	81	72
Þ	CL2	KMOL/HR	9	9	2.83817	0	9	0
Þ	HCL	KMOL/HR	0	0	0.0711567	7.2	0	7.2
Þ	C3H6CL2	KMOL/HR	0	0	6.09068	1.8	0	1.8
Þ	WATER	KMOL/HR	0	0	0	0	0	0
Þ	Mole Flow	KMOL/HR	90	90	83.9093	88.2	90	88.2
Þ	Mass Flow	KG/HR	4046.68	4046.68	4046.68	4046.68	4046.68	4046.68
$\left \right $	Volume Flow	L/MIN	16099.5	9533.6	14961.7	47698.8	16027.2	15748.3
Þ	Temperature	с	126.85	126.85	126.85	125.073	125.155	126.85
Þ	Pressure	BAR	3.03975	5.06625	3.03975	1.01325	3.03975	3.03975
Þ	Vapor Fraction		1	1	1	1	1	1
Þ	Liquid Fraction		0	0	0	0	0	0

Fig 6: Complete Stream Results.

SIMULATION USING RCSTR REACTOR

- **Step 1:**Click the Simulation section. Select 'RCSTR' from the Reactors Pallette and connect the input and output stream. The flow-sheet is shown in Fig. 7.
- **Step 2:**Fill the required inputs for feed stream and the block stream. The inputs required for the Specifications is shown in Fig. 8. In the Reactions section as the New is clicked, a new window appears which prompt for a new set of reactions. As the OK is clicked, the type is asked which is the type of reaction rate used in the reactor. Since in this case it is Power law, select Power law and click OK, the reaction set 'R-1 in this case' appears on the Available reaction sets. Bring it to Selected Reaction sets by clicking arrow. In this way number of reaction sets can be defined depending on the number of reactions in the process.
- **NOTE:** As the reaction set is created, a Reaction set appears in the 'Reactions' on the left hand side which is outside the block of the unit. This means that the reaction set is not dependent on the unit and an independent unit which can be used for other reactors if present in the process undergoing the same reaction. Now this R-1 in the 'Reactions' section has to be specified.
- **Step 3:** In the R-1 section the stoichiometry has to be filled the same way as done earlier for RStoic reactor and can be seen in Fig. 9. In the exponent fill the value according to the reaction rate. Now click 'New' in 'Reaction no.' tab and fill the required input for Reaction 2 as shown in Fig. 10.
- **Step 4:** In the Kinetic Section, T₀ is the reference temperature, which will automatically be specified if left blank. 'k' is the reaction rate constant 'A' and 'E' is the activation energy. Fill the values required here as shown in Fig. 11. Click the reaction in the top and select second reaction and fill the required inputs as shown in Fig. 12. The units of the values required should be consistent with the units required in the simulation. To see the required units ASPEN HELP can be used. The units can be seen in Fig. 13.

The stream results can be seen on Fig. 14. Calculate the overall conversion of propylene.



Fig 7: Flow-sheet of CSTR reactor.

Specification	ns	Streams	Re	actions	PSD	Compone	nt Attr.	Utili
Operating con	ditio	ns —						
Pressure:			3			atm	•	•
Temperatu	re:		40	0		К –		•
🔘 Duty:	Duty:					cal/sec		,
O Vapor fract	Vapor fraction:							
Holdup —								
Valid phases:		Vapor-O	nly					•
Specification t	ype:	Reactor v	olume					•
- Reactor					Pha	se		
Volume:	Volume: 7.85 I			•	Pha	se:		
Resi. time:			hr	~	Volu	ume:		

Fig. 8: Required inputs in Specifications in RCSTR Set Up.

0				Edit	Rea	ctic	n		×		
R	eact	ion No.: 🥑 1	•		R	Reaction type: Kinetic •					
ſ	Rea	ctants				Pro	ducts				
		Component	Coefficient	Exponent			Component	Coefficient	Exponent		
		PROPYLEN	-1	1			C3H5CL	1			
		CL2	-1	1			HCL	1			
				N		(Close				

Fig. 9: Required inputs in Reaction 1 in RCSTR Set Up

0				Edit I	Rea	Reaction			
R	eact	ion No.: 🥑 1	•		R	leact	tion type: Kine	etic	•
ſ	Rea	ctants	-		n n	Pro	ducts		
		Component	Coefficient	Exponent			Component	Coefficient	Exponent
		PROPYLEN	-1	1			C3H5CL	1	
		CL2	-1	1			HCL	1	
					Jl				
				N		(Close		

Fig. 10: Required inputs in Reaction 2 in RCSTR Set Up

Stoichiometry	⊘ Kinetic	Equilibrium	Activity	Informati	on		
1) PROPYLEN(MIXED) + CL2(MIXED)> C3H5CL(MIXED) + HCL(MI) -							
Reacting phase:	Vapor	-	Rate	basis:	Reac	(vol) -	
Power Law kinetic	expression —					Г	
If To is specified: Kinetic factor $=k(T/To) n e^{-(E/R)[1/T-1/To]}$							
If To is not specified: Kinetic factor $=kT n e -E/RT$					Edit Reactions		
k:	8.992e-08						
n:	0					Solids	
E:	15111	cal/mol		•			
То:		С		•			
[Ci] basis: Partial pressure -							

Fig. 11: Required inputs in Kinetics of Reaction 1 in RCSTR Set Up

	Stoichiometry	🧭 Kinetic Equ	uilibrium	Activity	Informati	ion		
	2) PROPYLEN(MIXE	D) + CL2(MIXED)	> C3H	6CL2(MIXE	D)	-		
	Reacting phase:	Vapor	-	Rate	basis:	Reac (vo) -	
Power Law kinetic expressionIf To is specified:Kinetic factor= $k(T/To)$ $n \in -(E/R)[1/T-1/To]$ If To is not specified:Kinetic factor= kT Edit Reaction:								
	k:	5.107e-12						
	n:	0					Solids	
	E:	3811	cal/mol		•		Condo	
	To:		С		-			
	[Ci] basis:	Partial pressure			•			

Fig. 12: Required inputs in Kinetics of Reaction 2 in RCSTR Set Up

When [Ci] Basis is	Units are: (To is not specified)	Units are: (To is specified)	
Molarity	$\frac{\frac{\text{kgmole} \cdot \text{K}^{\text{m}}}{\frac{\text{sec} \cdot \text{m}^{3}}{\left(\frac{\text{kgmole}}{\text{m}^{3}}\right)^{\Sigma_{\text{m}}}}}$	$\frac{\frac{\text{kgmole}}{\text{sec} \cdot \text{m}^3}}{\left(\frac{\text{kgmole}}{\text{m}^3}\right)^{\Sigma\alpha_i}}$	
Molality	$\frac{\frac{\text{kgm ole} \cdot \text{K}^{\text{m}}}{\text{sec} \cdot \text{m}^{3}}}{\left(\frac{\text{kgm ole}}{\text{kg H}_{2}\text{O}}\right)^{2\alpha}}$	$\frac{\frac{\text{kgm ole}}{\text{sec} \cdot \text{m}^3}}{\left(\frac{\text{kgm ole}}{\text{kg} \text{ H}_2 \text{O}}\right)^{\text{Z4}_1}}$	
Mole fraction, Mass fraction, or Mole gamma	$\frac{\text{kgmole} \cdot \text{K}^{\text{m}}}{\text{sec} \cdot \text{m}^3}$	$\frac{\text{kgmole}}{\text{sec}\cdot\text{m}^3}$	
Partial pressure or fugacity	$\frac{\frac{\text{kgmole} \cdot K^{\text{m}}}{\frac{\text{sec} \cdot m^{3}}{\left(\frac{N}{m^{2}}\right)^{\Sigma \alpha_{i}}}}$	$\frac{\frac{\text{kgm ole}}{\text{sec} \cdot m^3}}{\left(\frac{N}{m^2}\right)^{\Sigma\alpha_i}}$	
Mass concentration	$\frac{\frac{\text{kgmole} \cdot \text{K}^{\text{m}}}{\frac{\text{sec} \cdot \text{m}^{3}}{\left(\frac{\text{kg}}{\text{m}^{3}}\right)^{\Sigma \alpha_{i}}}}$	$\frac{\frac{\text{kgmole}}{\text{sec} \cdot \text{m}^3}}{\left(\frac{\text{kg}}{\text{m}^3}\right)^{\Sigma q}}$	

Fig. 13: Units required in Power law.

		Units			
		Units	FD 👻	PDT -	
\rightarrow	From			PLUG	
\rightarrow	То		PLUG		
\rightarrow	Substream: MIXED				
\rightarrow	Phase:		Vapor	Vapor	
\rightarrow	Component Mole Flow				
\rightarrow	C3H5CL	KMOL/HR	0	0.0711567	
\rightarrow	PROPYLEN	KMOL/HR	81	74.8382	
\rightarrow	CL2	KMOL/HR	9	2.83817	
\rightarrow	HCL	KMOL/HR	0	0.0711567	
\rightarrow	C3H6CL2	KMOL/HR	0	6.09068	
\rightarrow	WATER	KMOL/HR	0	0	
\rightarrow	Mole Flow	KMOL/HR	90	83.9093	
\rightarrow	Mass Flow	KG/HR	4046.68	4046.68	
\rightarrow	Volume Flow	L/MIN	16099.5	14961.7	
\rightarrow	Temperature	С	126.85	126.85	
\rightarrow	Pressure	BAR	3.03975	3.03975	

Fig. 14: Composition results for CSTR.

CLASS PROBLEM 2

For the previous problem, the reactions has to be carried out in plug flow reactor (PFR) here.

Plot the product flow rate of products and reactants, and temperature down the length of the reactor assuming:

- I. Isothermal at the inlet temperature
- II. Cooled Reactor with Co-current coolant flow

Flow rate and temperature of the coolant (water) entering the reactor at the same end of the process are specified to be 0.05 kmol/s and 350 K at 10 atm.

III. Cooled Reactor with Counter-current coolant flow

The flow rate and temperature of the coolant leaving the reactor at the same end as the process are specified to be 0.05 kmol/s and 450 K.

Take U = $150 \text{ W/m}^2\text{-K}$

SIMULATION USING RPlug REACTOR

- **Step 1:**Click the Simulation section. Select 'RPlug' from the Reactors Pallette and connect the input and output stream.
- **Step 2:**Fill the required inputs for feed stream and the block stream. The flow-sheet will appear as in Fig. 15. The inputs required for the Specifications and Configuration are shown in Fig. 16 and Fig. 17 respectively.
- Step 3: Define the reactions same as it was done in CSTR simulation. Run the Simulation.

The Composition results and the stream results can be seen on Fig. 18 and Fig. 19 respectively.

Step 4: For co-current or counter current coolant flow, the coolant flow line has to be added in the reactor in flow-sheet as shown in Fig. 20. In the Specification change the reactor type to co-current (or counter current) and fill the required inputs and Run the Simulation.

Check the composition, temperature (Fig. 21-24) and conversion for co-current and counter current reactors.


Fig 15: Flow-sheet of Isothermal RPlug reactor.

🕜 Spe	cifications	Configuration	Streams	Reactions	Pressure	Holdu
Reactor Opera Oco Cor Ter	type: Read ting conditi nstant at inl nstant at sp nperature p	ctor with specified on et temperature ecified reactor temp rofile	temperatur verature	e C	•	•
	Locatio	C Temperature				

Fig. 16: Required inputs in Specifications in RPlug Set Up.

Specifications	Configuration	Streams	Reactions	Pres
Multitube reactor	Number of	tubes:		
📃 Diameter varies al	ong the length of	the reactor		
Reactor dimensions	5			
Length:	10	meter	•	
Diameter:	1	meter	•	
Elevation				
Reactor rise:	0	meter -		
Reactor angle:	0	deg 🦷		
Valid phases				
Process stream:	Vapor-Only		-	
Thermal fluid stream	m: Vapor-Liquid		-	[

Fig. 17: Required inputs in Configuration in RPlug Set Up.



Fig. 18: Composition results for Isothermal PFR.

Heat duty:	-73681.6	cal/sec
Reactor temperature		
Minimum:	125.154	c ·
Maximum:	125.154	c ·
Residence time:	0.511239	min •
Thermal fluid inlet		
Temperature:		,
Vapor fraction:		

Fig. 19: Block results for PFR.



Fig 20: Flow-sheet of co-current/counter current RPlug reactor.







Fig. 22: Composition results for co-current PFR.



Fig. 23: Temperature profile counter-current PFR.



Fig. 24: Composition results for counter-current PFR.

PRACTICE PROBLEMS

PROBLEM 1

In a process, ethylene (E) reacts with benzene (B) to produce the desired product ethyl benzene (EB). There is a consecutive reaction that produces an undesirable product diethyl benzene (DEB). A third reaction combines benzene and diethyl benzene to form ethyl benzene.

The reactions are represented as:

$E + B \rightarrow EB$	(1)
$E + EB \rightarrow DEB$	(2)
$DEB + B \rightarrow 2EB$	(3)

The reaction takes place in the vapor phase and are assumed to be irreversible. The reaction rates of the three reactions are assumed to be those given here:

$$r_1 = C_E C_B (1 \times 10^6) e^{(-22500)/RT}$$

$$r_2 = C_E C_{EB} (6 \times 10^5) e^{(-22500)/RT}$$

$$r_3 = C_{DEB} C_B (6 \times 10^6) e^{(-20000)/RT}$$

The units of "r' are kmols⁻¹m⁻³.Concentrations have units of kmol/m³. Activation energies have units of kcal/kmol. Temperature is in Kelvin. There feed streams contains 30 kmol/h of pure ethylene and 225 kmol/h of benzene at 383° C and 1985 kPa. The reactor operates at adiabatic condition (Heat duty = 0). The excess of benzene is used to keep the ethylene concentration low so that the formation of DEB is supressed. Simulate the process to find out the flow rate and composition of the product steam if the reactor volume is 25.6 m³ (1.72 m × 11 m).

- I. Find out the heat duty, residence time, and composition of the product stream and the mole fraction of EB and conversion of ethylene for CSTR.
- II. Find out the heat duty, residence time, and composition of the product stream and the mole fraction of EB and conversion of ethylene for PFR.
- III. Compare the results for both the reactors.

Use Chao-Seader EOS to estimate properties.

PROBLEM 2

Maleic Anhydride (MA) is formed by the oxidation of benzene. The following reactions occur in a PFR reactor at vapour phase operating at constant temperature in the production of MA:

$$C_{6}H_{6} + 4.5O_{2} \xrightarrow{k_{1}} C_{4}H_{2}O_{3} + 2CO_{2} + 2H_{2}O$$

$$C_{6}H_{6} + 7.5O_{2} \xrightarrow{k_{2}} 6CO_{2} + 3H_{2}O$$

$$C_{4}H_{2}O_{3} + 3O_{2} \xrightarrow{k_{3}} 4CO_{2} + H_{2}O$$

$$C_{6}H_{6} + 1.5O_{2} \xrightarrow{k_{4}} C_{6}H_{4}O_{2} + H_{2}O$$

All the reactions are highly exothermic. For this reason, the ratio of air to benzene entering the reactor is kept very high. The composition of feed is as follows:

COMPONENT	MOLE FLOW (kmol/h)
Benzene	42.3
Nitrogen	2205
Oxygen	585
Temperature	450°C
Pressure	225 kPa

The reaction rate is:

$$r_i = k_i C_{Benzene}$$
 where $i = 1, 2$ and 4
 $r_3 = k_3 C_{MA}$

The reaction kinetics are

$$k_{1} = (7.7 \times 10^{6})e^{(-25143)/RT}$$

$$k_{2} = (6.31 \times 10^{7})e^{(-29850)/RT}$$

$$k_{3} = (2.33 \times 10^{4})e^{(-21429)/RT}$$

$$k_{4} = (7.2 \times 10^{5})e^{(-27149)/RT}$$

The reactor operates at constant temperature of the feed inlet. The reactor is a multitube reactor which contains 12100 tubes 7 m long and 1 inch in diameter.

LITERATURE CITED:

I. Fogler H.S., (2011), Essentials of Chemical Reaction Engineering.

II. GhasemNayef, (2012), Computer Methods in Chemical Engineering

III. ASPEN HELP

Experiment 9: Reactor Design (II) using ASPEN Plus

1. Objectives:

After the completion of this module, the students will have:

- I. Reviewed and expanded knowledge of chemical reaction engineering.
- II. Learned to use Aspen Plus to perform the rigorous reactor design.

2. Prerequisite Engineering & Science Skills

- 1. Knowledge of chemical reaction engineering.
- 2. Knowledge of performing calculations used in the design of a reactor.
- 3. Knowledge of Reactor Design in Aspen Plus.

CLASS PROBLEM

Design of Packed Bed Reactor for the production of ethylene oxide [1]

Ethylene oxide is a chemical used to make ethylene glycol (the primary ingredient in antifreeze). It is also used to make polyethylene oxide, and both the low-molecular-weight and high-molecular-weight polymers have many applications including as detergent additives. Because ethylene oxide is so reactive, it has many other uses as a reactant. However, because of its reactivity, danger of explosion and toxicity, it is rarely shipped outside the manufacturing facility but instead is often pumped directly to a nearby consumer.

A feed stream with the composition given below at 240° C and 26.5 bar is used to produce ethylene oxide in a catalytic packed bed reactor. The reactions involved in the process are given below. The Ergun equation hold good for the pressure drop analysis and the reactor has to be cooled co-currently using water at 95°C and 3 bar flowing at a rate of 8000 kmol/h. Take U = 500 W/m²K.

SIZE OF REACTOR: Tubular reactor 10 m tall with 4722 tubes and 7.38 cm diameter tubes.

CATALYST: Silver on inert support of 7.5 mm diameter spheres and have bulk density of 1250 kg/m³ and particle density of 2065.4 kg/m³ and void fraction is 0.4.

COMPONENT	MOLE FLOW (kmol/h)
Ethylene	1047.91
Ethylene Oxide	6.47
Carbon dioxide	31.71
Oxygen	6331.12
Nitrogen	28191.39
Water	30.98

Reactions Involved:

$$C_2H_4 + 0.5O_2 \to C_2H_4O$$
 (1)

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$$
 (2)

$$C_2H_4O + 2.5O_2 \rightarrow 2CO_2 + 2H_2O$$
 (3)

The reaction expressions are:

$$r_{1} = \frac{1.96exp(-2400/_{RT})p_{ethylene}}{1+0.00098exp(11200/_{RT})p_{ethylene}}$$

$$r_{2} = \frac{0.0936exp(-6400/_{RT})p_{ethylene}}{1+0.00098exp(11200/_{RT})p_{ethylene}}$$

$$r_{3} = \frac{0.42768exp(-6200/_{RT})p_{ethylene}^{2}}{1+0.000033exp(21200/_{RT})p_{ethylene}^{2}}$$

The units for the reaction rates are moles/ m^3 s. The pressure unit is bar. The activation energy numerator is in cal/mol.

PACKED BED REACTOR DESIGN:

- Step 1:Open a new file in Aspen and enter the components. Choose the suitable METHOD to be used in the properties section. Here it is 'PENG-ROB'.
- **Step 2:**Click the Simulation section. Select 'RPlug' from the Reactors Pallette and connect the input and output stream.
- **Step 3:**Fill the required inputs for feed stream. In the PFR block stream, select Adiabatic reactor in specifications. The configuration of the reactor is multitube reactor with the specifications given in the problem. In the Reactions tab create a new set of reactions R1 of LHHW type. In the Catalyst section, enter the data required. In the Pressure section, select "Use Frictional correlation to calculate process stream pressure drop" and from the list below select "Ergun".
- Step 4: Now in the Reactions on the left hand side, select R1 and then New in R1. Enter the first reaction as shown in Fig. 1. Let us enter the first reaction completely so that the reaction input method is clear, then the second and third reactions can be entered easily. In the kinetics tab select Reacting phase "Vapor" and rate basis as Catalyst weight. The LHHW rate expression is defined as the following equation in ASPEN PLUS:

$r = \frac{[Kinetic \ factor][Driving \ force \ expression]}{[Adsorption \ expression]}$

Hence three values have to be defined: Kinetic factor, Driving force expression and Adsorption expression. The kinetic factor has to be defined the same way as it was done for power law earlier. The values can be seen in Fig. 2. The units should match the units as required by APSEN PLUS. To check the units HELP can be used.

To enter the driving force expression click "Driving Force". The driving force in ASPEN PLUS is defined by following equation:

Driving force =
$$K_1 \prod_{i=1}^N C_i^{\alpha_i} - K_2 \prod_{j=1}^N C_j^{\beta_1}$$

and the K is defined as

$$\ln(K) = A + \frac{B}{T} + C \times \ln(T) + D \times T$$

By comparison, the driving force in this problem is " $p_{ethylene}$ ". In the driving force expression window make [C_i] basis as partial pressure as required by the problem. Term 1 is the first term of the Driving force equation which should be equal to $p_{ethylene}$. Hence K₁ should be 1 and α_i should be 1. Hence enter the values as shown in Fig. 3-a. The term 2 has to be 0. Hence select Term 2 and enter the exponent ' β_1 'as '0' but if we enter A=0 then K=1 but K=0 for Term 2 =0. Hence we enter the value of A such that K=0. Let us enter A = -9×10^6 which makes K=0. The values as shown in Fig. 3-b.

To enter the Adsorption expression click "Adsorption". The Adsorption expression in ASPEN PLUS is defined by following equation:

Adsorption term =
$$\left[\sum_{i=1}^{M} K_i \left(\prod_{j=1}^{N} C_j^{nu_1}\right)\right]^m$$

and the K is defined as

$$\ln(K) = A + \frac{B}{T} + C \times \ln(T) + D \times T$$

By comparison, the adsorption term in this problem is "1+K.pethylene". Hence the term no. 1 should be 1. It is possible when $K_1(\prod_{j=1}^N C_j^{nu_1})=1$. The overall exponent 'm' is 1. Component ethylene in term 1 is '0'. For K=1 in term 1 A=0. Term no.2 is K.P_{ethylene}, hence component ethylene in term 1 is '1'. Since $K = 0.00098exp(\frac{11200}{RT})$, hence

$$ln(K) = ln(0.00098) + \frac{11200}{RT}$$

After putting the values the adsorption window appears as shown in Fig. 4.

Step 5: Run the simulation and check the results.

- **Step 6:** Now add the other reactions in R-1 list accordingly. The values are shown in Fig. 5-8.
- Step 7: Add the cooling system in the flow-sheet. Take co-current exchanger.
- **Step 8:** Run the Simulation and check the results for composition, temperature and pressure.

This parameter	Is entered for	In this location
r = rate of reaction	_	_
k = pre-exponential factor (See <u>Units</u>)	k	Kinetic sheet
T = absolute temperature	-	-
$T_o =$ reference temperature	T _o	Kinetic sheet
n = temperature exponent	n	Kinetic sheet
<i>m</i> = adsorption term exponent	Exponent	Adsorption Expression dialog box
E = activation energy	E	Kinetic sheet
R = gas law constant	-	-
K = constant (See <u>Units</u>)	Coefficients A, B, C, D	Adsorption Expression dialog box
K ₁ = constant (See <u>Units</u>)	Coefficients A, B, C, D for driving term constants, Term 1	Driving Force Expression dialog box
K ₂ = constant (See <u>Units</u>)	Coefficients A, B, C, D for driving term constants, Term 2	Driving Force Expression dialog box
N = number of components	-	-
M = number of terms in adsorption expression	-	-
C = component concentration	-	-
<i>i</i> , <i>j</i> = indices	-	-
α = exponent	Exponent 1	Driving Force Expression dialog box
β = exponent	Exponent 2	Driving Force Expression dialog box
nu = exponent	Term exponents for each component	Adsorption Expression dialog box
Π = product operator	-	-
Σ = summation operator	-	-

a	ctants		Proc	ducts			
	Component	Coefficient		Compo	onent	Coeffi	cient
	ETHYLENE •	-1	•	EO	-	1	
	02 •	-0.5	►				

Fig 1: Required inputs in Stoichiometry for the first reaction.

🕜 Stoi	chiometry	Ginetic Equilibri	um 🛛	Activity Info	rmation	
) ETH	LENE(MIXED)	+ 0.5 O2(MIXED)	> EO(N	/IXED)		•
eacting	j phase: Vapo	r	-	Rate basis:	Cat (wt)	-
LHHW	kinetic expres	sion —				
r -	[Kine	tic factor][Driving fo	ce expr	ession]		
		[Adsorption expre	ssion]			
Kinetic	factor					
lf To is	specified:	Kinetic factor =k	(T/To)	n e -(E/R)[1/T-	1/To]	Solids
lf To is	not specified:	Kinetic factor =k	T ⁿ e ^{>}	-E/RT		
k:	0.00196					Driving Force
n:	0					Adsorption
E:	2400	cal/mol	•			
To:		С	•			

Fig 2: Required Kinetic factor inputs for the first reaction.

a)

•		Driving	Force	Expre	ssion		×
Reacting pl	ase: Va	ipor					
[Ci] basis:	M	olarity			•		
Enter term:	Те	erm 1			•		
Term 1 — Concentra for reacta	ition expo	onents		Concent for proc	tration expo lucts:	onents	
Cor	nponent	Exponent		C	omponent	Exponent	
ETH	LENE	1		► EO		0	
► 02		0					
Coefficien	ts for driv	ing force constar	nt:				
A: 0		B: 0		C: 0		D: 0	
				Clos	ie		

b)

9			Driving	Ford	e Exp	pression		
R	eact	ing phase: V	'apor					
[0	Ci] b	asis: P	artial pressure			•		
E	nter	term:	ferm 2			•		
ſ	Terr	m 2						
	Con for I	centration exp reactants:	onents		Con for p	centration expo products:	onents	
		Component	Exponent			Component	Exponent	
		ETHYLENE	0			EO	0	
		02	0					
	Coe	fficients for dri	ving force constan	t:				
	A:	-9e+06	B: 0		C: 0		D: 0	
						Close		

Fig 3: Required inputs in driving force expression for first reaction.

		Adsorptio	- Expression	
Reac	ting phase: 🛝	/apor		
[Ci] b	asis: P	artial pressure		
Adso	rption expressi	on exponent:	1	
Cor	ncentration exp	onents		
	Component	Term no. 1	Term no. 2	Term no. 3
Þ	ETHYLENE	0	1	
►				
- Ads	sorption consta	ints		
- Ads	sorption consta Term no.	ints1	2	
Ads	sorption consta Term no. Coefficient A	Ints 1 0	2 -6.928	
Ads	Term no. Coefficient A Coefficient B	Ints 1 0 0	2 -6.928 5636.07	
Ads	Term no. Coefficient A Coefficient B Coefficient C	Ints 1 0 0 0	2 -6.928 5636.07 0	
- Ads	orption consta Term no. Coefficient A Coefficient B Coefficient C Coefficient D	Ints 1 0 0 0 0 0 0 0	2 -6.928 5636.07 0 0	

Fig 4: Required inputs in adsorption expression for first reaction.

a)

0	Oriving Force Expression					×	
Reacting	g phase: 🛛 🛛	Vapor					
[Ci] basi	is: F	Partial pressure 🔹					
Enter te	erm: 1	ferm 1			•		
Term	1						
Conce for rea	entration exp actants:	onents		Con for	centration expo products:	onents	
	Component	Exponent			Component	Exponent	
) > E	THYLENE	1			CO2	0	
)) (02	0		۲	WATER	0	
Coeffi	Coefficients for driving force constant:						
A: 0		B: <i>0</i>		C: ()	D: 0	
	Close						

b)

9	L 0 etauto (L)	Driving	Force	Ex	pression		×
Reac	ting phase:	Vapor					
[Ci] Ł	oasis:	Partial pressure			•		
Enter	r term:	Term 2			•		
Ter	m 2						
Cor for	ncentration ex reactants:	kponents		Cor for	centration expo products:	nents	
	Componer	nt Exponent			Component	Exponent	
►	ETHYLENE				CO2		
	02				WATER		
Coe	Coefficients for driving force constant:						
A:	-9e+06	B: <i>O</i>	(C: ()	D: 0	
	Close						

Fig 5: Required inputs in driving force expression for second reaction.

9	Adsorption Expression ×					
React	ting phase: Vapor					
[Ci] b	asis:	Partial	pressure			
Adso	rption expres	sion exp	onent:	1		
Cor	centration e	xponent	s	_		
	Componer	nt Terr	m no. 1	Te	erm no. 2	Â.
►	ETHYLENE	0		1		
4					Þ	*
Ads	orption cons	tants —	1		2	
	Coefficient	۵			-6.928	
	Coefficient	R	0		5636.07	
•	Coefficient C		0		5050.07	
	Coefficient D		0		0	
< <u> </u>						
	Close					

Fig 6: Required inputs in adsorption expression for second reaction.

a)

0	Oriving Force Expression					×		
React	ting phase:	Vapor	Vapor					
[Ci] b	asis:	Partial pressure			•			
Enter	term:	Term 1			•			
Ten	m 1 ———							
Cor for	ncentration ex reactants:	xponents		Cor for	centration expo products:	nents		
	Componer	nt Exponent			Component	Exponent		
	EO	2			CO2			
	02	0			WATER			
Coe	Coefficients for driving force constant:							
A:	0	B: <i>0</i>		C: (0	D: 0		
	Close							

b)

۷	Driving Force Expression				
Reacting phase:	Vapor				
[Ci] basis:	Partial pressure	•			
Enter term:	Term 2	•			
_ Term 2					
Concentration er for reactants:	xponents	Concentration exponents for products:			
Compone	nt Exponent	Component Exponent			
EO		> CO2			
02		WATER			
Coefficients for a	driving force constant:				
A: -9e+06	B: 0	C: 0 D: 0			
	*	Close			

Fig 7: Required inputs in driving force expression for third reaction.

Adsorption Expression							>
Reac	Reacting phase: Vapor						
[Ci] b	asis:	Par	rtial p	pressure			
Adso	orption expres	sior	n exp	onent:	1		
Co	ncentration e	хро	nents	;	_		_
	Compone	nt	Tern	n no. 1	Te	erm no. 2	-
►	EO		0		2		
4						Þ	*
Ads	sorption cons	tant	ts —	1		2	_1
	Coefficient	А		0		-10.32	
•	Coefficient B			0		10669.4	
Þ	Coefficient C		0		0		
Þ	Coefficient D		0		0		
•	< <u> </u>						
	Close						

Fig 8: Required inputs in adsorption expression for third reaction.

PRACTICE PROBLEMS

PROBLEM 1

Chloroform reacts with water in presence of oxygen and produces hydrochloric acid and carbon dioxide by the following reaction:

 $2CHCl_3 + 2H_2O + O_2 \rightarrow 6HCl + 2CO_2$

The composition of feed stream is as follows:

COMPONENT	MOLE FLOW (kmol/h)
Chloroform	10
Water	15
Oxygen	7.5
Temperature	500°C
Pressure	10 bar

The reactor operates at constant temperature of 510^{0} C and the pressure drop in the system can be related by the Ergun equation.

SIZE OF REACTOR: The reactor is 10 m tall and 2.5 m in diameter.

CATALYST: The catalyst have particle density of 2500 kg/m³ and void fraction is 0.45.

The reaction expressions are:

$$r_{1} = \frac{7.44 \times 10^{6} exp \left(-9.0854 \times 10^{7} /_{RT}\right) p_{A}}{1 + 5.97 \times 10^{6} exp \left(\frac{2440}{RT}\right) p_{B} + 1.23 \times 10^{6} exp \left(\frac{5330}{RT}\right) p_{A}}$$

where A is chloroform and B is HCl.

The units for the reaction rates are kmoles/m³ s. The pressure unit is bar. The activation energy for kinetic factor is in J/kmol and activation energy values for adsorption factor are in cal/mol. R = 1.987.

Plot the composition along the reactor length and find out the extent of conversion.

PROBLEM 2: Design of reactor for water-gas shift reaction

The water-gas shift (WGS) reaction has been traditionally used to produce hydrogen from syngas, which comprises CO and H₂. The reaction that takes place is as follows: $CO + H_2O \rightarrow CO_2 + H_2$

COMPONENT	MOLE FLOW (kmol/h)
Carbon monoxide	35
Carbon dioxide	30
Hydrogen	40
Water	95
Temperature	320°C
Pressure	15 bar

The composition of feed stream is as follows:

The reactor operates at adiabatic conditions and the pressure drop in the system can be related by the Ergun equation.

SIZE OF REACTOR: The reactor is 5 m tall and 0.5 m in diameter.

CATALYST: The catalyst have particle density of 2081 kg/m³ and void fraction is 0.5.

The reaction expressions are:

$$r_1 = 0.2986 \exp\left[\frac{-40739}{RT}\right] \left(y_{CO} y_{H_2O} - \frac{y_{CO_2} y_{H_2}}{K_A}\right)$$

where

$$K_A = exp\left[-4.33 + \frac{4577.9}{T}\right]$$

A is chloroform and B is HCl.

The units for the reaction rates are kmoles/(kg cat.s). The activation energy is in kJ/kmol.

Plot the composition along the reactor length and find out the extent of conversion.

PROBLEM 3: Partial oxidation of Methanol

The partial oxidation of methanol produces formaldehyde and water. The reaction is as follows:

$$CH_3OH + 0.5O_2 \rightarrow HCHO + H_2O$$

The flow rate of feed stream is 30 kmol/hr and its composition is as follows:

COMPONENT	MOLE FRACTION
Methanol	0.35
Water	0.005
Oxygen	0.145
Nitrogen	0.5
Temperature	150°C
Pressure	3 bar

The reactor operates at constant temperature of 190° C and the pressure drop in the system can be related by the Ergun equation.

SIZE OF REACTOR: The reactor is 5 m tall and 1 m in diameter. CATALYST: The catalyst have particle density of 2200 kg/m³ and void fraction is 0.45.

The reaction rate expression is given as:

$$r_{1} = \frac{K_{A}P_{M}P_{O}^{0.5}}{1 + K_{M}P_{M} + K_{W}P_{W} + K_{O}P_{O}^{0.5} + K_{B}P_{M}P_{O}^{0.5} + K_{C}P_{W}P_{O}^{0.5}}$$

where

P_M is the partial pressure of methanol

 $P_{\rm O}$ is the partial pressure of oxygen

 $P_{W} \mbox{ is the partial pressure of water } \label{eq:pw}$

#	k ₀ (kmol/kg cat.s)	Ea (J/mol)
K _A	1.72×10 ⁻¹²	-31100
K _M	2.57×10 ⁻⁹	-56780
Kw	5.43×10 ⁻¹²	-86450

Ko	4.47×10 ⁻⁸	-60320
K _B	1.15×10 ⁻¹⁶	-36704
K _C	2.43×10 ⁻¹⁹	-146770

R = 8.314 J/mol.K.

Plot the composition along the reactor length and find out the extent of conversion.

LITERATURE CITED:

- A. Turton, Bailie, Whiting, and Shaeiwitz, 2012, Analysis, Synthesis, and Design of Chemical Processes, Prentice Hall, Fourth Edition.
- B. Fogler H.S., (2011), Essentials of Chemical Reaction Engineering.
- C. ASPEN HELP

Experiment 10: Process flow-sheet Simulation (I) using ASPEN Plus

1. Objectives:

After the completion of this module, the students will have:

- I. Reviewed and expanded knowledge of chemical reaction engineering.
- II. Learned to use Aspen Plus to simulate the Process flow-sheet.

2. Prerequisite Engineering & Science Skills

- I. Knowledge of chemical process flow-sheeting.
- II. Knowledge of Aspen Plus.

CLASS PROBLEM

Production of Ethylene Glycol

Propylene oxide is combined with water to produce propylene glycol in a continuous stirred tank reactor (CSTR). The reaction involved is as follows:

$$C_3H_6O+H_2O\rightarrow C_3H_8O_2$$

The reactor outlet is then fed to distillation tower. The propylene glycol is recovered in the bottom stream of the tower. The distillate of the tower is sent to other column to recover propylene oxide from water at the top. The feed streams containing 150 lbmol/hr of PO and 610.6 water are mixed in a mixer before feeding to the reactor. The temperature and pressure of both the streams are 75^{0} F and 16.17 psia respectively for both the feed. The reaction kinetics are as follows:

 $k = 4.72 \times 10^9 e^{32400/RT}$ where E is in Btu/lbmol.

The reactor is provided with a vent in order to vent the gases if formed by increase in the temperature in the reactor. The reactor has a volume of 280 ft³ and temperature 100^{0} F and pressure 16.17 psia.

The columns are DSTWU type with total condensers. The pressure of condenser and reboiler are maintained at 16.17 psia in both the columns and the recovery of light component is 0.995 and heavy component is 0.001 in the distillate in both the columns. Take initial guess for number of stages as 10.

Re-run the simulation after changing the temperature of reactor to 120^{0} F.

SIMULATION OF PROPYLENE GLYCOL PRODUCTION FLOW-SHEET

- **Step 1:**Open a new file in Aspen and enter the components. Choose the suitable METHOD to be used in the properties section. Here it is 'UNIFAC'.
- **Step 2:**Click the Simulation section. Draw the flow-sheet as shown in Fig. 1. In the reactor block add a vent stream to vent the gases if produced.
- Step 3: Fill the required inputs for feed stream.
- Step 4: Complete the blocks with the data described in the problem.
- Step 5: In the reactor block, in the 'Specifications' section, select valid phases as vapor liquid. In the 'Streams' section select gas for vent and liquid for product.
- Step 6: Run the simulation and check the results.
- **Step 7:** It could be seen that there is no molar flow in the reactor vent. This means that the temperature is low enough to produce the gases in the reactor.
- **Step 8:** Change the temperature of reactor to 120⁰F and re-run the Simulation and check the results of reactor streams.



Fig 1: Required flow-sheet of the propylene glycol production plant.

PRACTICE PROBLEMS

PROBLEM 1:Production of vinyl-chloride monomer (VCM)

Vinyl chloride monomer (VCM) is produced through a high pressure, non-catalytic process involving the pyrolysis of 1,2-dichloroethane (EDC) according to the following reaction:

$CH_2Cl - CH_2Cl \rightarrow HCl + CHCl = CH_2$

The cracking of EDC occurs at 500° C and 30 bar in a direct fired furnace. 1000 kmol/hr of pure EDC feed enters the reactor at 20° C and 30 bar. EDC conversion in the reactor (Here Stoichiometric) is maintained at 55%. The hot gases from the reactor are sub-cooled by 10 degrees before fractionation.

Two distillation columns (Here Radfrac) are used for the purification of the VCM product. In the first column, 99.5 % anhydrous HCl is removed overhead and sent to the oxy chlorination unit. In the second column, VCM product is removed overhead and the bottoms stream contains unreacted EDC. Overheads from both columns are removed as saturated liquids. The desired composition of both the components is 99.5%. The HCL column is run at 25 bar and the VCM column is run at 8 bar.

Complete the PFD and print the Custom Stream Results.

NOTE: To sub-cool liquid in cooler select "Degrees of subcooling" in the Temperature tab. Take number of trays in both the columns as 15. For other data of the column, first run the column as DSTWU unit and use the results for Radfrac unit.

PROBLEM 2 Production of Cumene

Cumene (isopropyl benzene) is produced by reacting propylene with benzene by the following reaction:

$$C_3H_6 + C_6H_6 \rightarrow C_9H_{12}$$

$$r_1 = C_{ben.}C_{prop.}(3.5 \times 10^7)e^{(-24900)/RT}$$

The main reaction is followed by a side reaction which produces *p*-di-iso-propyl benzene (C₁₂H₁₈):

$$C_3H_6 + C_9H_{12} \rightarrow C_{12}H_{18}$$

$$r_2 = C_{prop.}C_{cumene}(2.9 \times 10^9)e^{(-30150)/RT}$$

 $r_2 = C_{prop.}C_{cumene}(2.9 \times 10^5)e^{(-50150)/M}$ The units of "r' are kmols⁻¹m⁻³. Activation energies have units of cal/mol. The feed flow rate is 1000 kmol/h. The composition of feed is as follows:

COMPONENT	MOLE FRAC. (-/-)
Benzene	0.75
Propylene	0.2
Propane	0.05
Temperature	50°C
Pressure	3125 kPa

The feed has to be pre-heated up to 350°C before entering the reactor. The effluent coming out of the reactor has to be cooled up to 65°C. The effluent enters the distillation column (DSTWU) where benzene, propene and propane gets separated and exits as liquid overhead and the bottom stream containing cumene and p-di-isopropyl benzene enters other distillation column (DSTWU) operating at 200 kPa where cumene is separated as overhead liquid and p-di-iso-propyl benzene as bottom product. The desired composition of light key and heavy key in both the columns are 99.5% and 0.1%.

Complete the PFD and print the Custom Stream Results. Also plot the variation of composition of the reactor with length.

SIZE OF REACTOR: Tubular reactor 4 m tall with 2800 tubes and 2 in diameter tubes and the reactor operates at vapor phase and at constant temperature.

LITERATURE CITED:

- I. Turton, Bailie, Whiting, and Shaeiwitz, 2012, Analysis, Synthesis, and Design of Chemical Processes, Prentice Hall, Fourth Edition.
- II. Jana Amiya K., Process Simulation and Control using Aspen, Second Edition.
- III. Felder Richard M., Rousseau Ronald W., Elementary Principles of Chemical Processes.

Experiment 11: Process flow-sheet Simulation (I) using ASPEN Plus

1. Objectives:

After the completion of this module, the students will have:

- I. Reviewed and expanded knowledge of chemical reaction engineering.
- II. Learned to use Aspen Plus to simulate the Process flow-sheet.

2. Prerequisite Engineering & Science Skills

- I. Knowledge of chemical process flow-sheeting.
- II. Knowledge of Aspen Plus.

CLASS PROBLEM

Ammonia Synthesis

The ammonia synthesis process has to be performed in the Ammonia production plant using the feed at 27 atm and 280° C with following composition:

COMPONENT	MOLE FLOW (kmol/h)
Hydrogen	5160
Nitrogen	1732
Methane	72
Argon	19
Carbon monoxide	17

Customer requirement specifies that the liquid ammonia purity should not be less than 96 mole %. Moreover, the plant should produce at least 3250 kmol/hr of liquid ammonia for profitable operation. A purge stream is used in this process to create an exit for the impurities or by-products contained in the process.

Reaction Involved:

$N_2 + 3H_2 \rightarrow 2NH_3$

The reactor is RStoic with a fractional conversion of 40% of nitrogen and operates at 270 atm and 481.85° C. The compressors used are isentropic and their outlet pressure is 271 atm. The product from the reactor is cooled to 27° C before entering the flash column. The heat duty flash column is zero. The splitter purges 10% of the effluent and recycles the rest in to the system.

SIMULATION OF AMMONIA SYNTHESIS PROCESS FLOW-SHEET

- Step 1:Open a new file in Aspen and enter the components. Choose the suitable METHOD to be used in the properties section. Here it is 'RKS-BM'.
- Step 2:Click the Simulation section. Draw the flow-sheet as shown in Fig. 1.

Step 3: Fill the required inputs for feed stream.

Step 4: Complete the blocks with the data described in the problem.

- **Step 5:** Run the simulation and check the results. If there is convergence error increase the number of iterations in Convergence and again Run the Smulation.
- **Step 6:** It could be seen that the mole fraction of NH₃ at the outlet is less than the required specifications. Hence the Optimization has to be done to achieve the target.
- **Step 7:** In the Optimization, vary the purge to minimize flow of NH₃ at the top product of flash separator and put the constraint that mole fraction of NH₃ at bottom be greater than 0.96 and flow mole greater than 3250 kmol/h.
- Step 8: Run the Simulation and check the results for Optimization.
- **Step 9:** To check the Stream go to Results Summary and then Streams. All the Streams can be viewed together. By clicking Stream Table tab the results can be viewed with the flow-sheet.



Fig 1: Required flowsheet of the ammonia synthesis plant.

PRACTICE PROBLEMS

PROBLEM 1: n-heptane is converted to toluene in a vapour phase hydroforming process by the following reaction:

$C_7H_{16} \rightarrow C_6H_5CH_3 + 4H_2$

The feed that is available from some other plant contain 100 kmol/hr of n-heptane and 3 kmol/hr of methane at 175° C and 1 atm. The reaction takes at 10 atm and 420° C (Use Stoichiometric reactor) where 50% conversion is achieved. The reactor effluent is cooled to 35° C and then separated in a flash drum. The bottom stream which contains mainly n-heptane and toluene is sent to a distillation column to separate toluene from n-heptane. The n-heptane is recycled back and mixed with the feed after heating up to the feed temperature.

Take compressor as isentropic

In the distillation column take initial guess for number of stages as 10. The light key is heptane with recovery of 99% and heavy key is toluene with recovery of 0.01. The condenser is partial and all the distillate is vapour. The pressure at the condenser and reboiler is atmospheric pressure.

The customer requirement specifies that the toluene obtained should be of 99.9% and the plant profitability requires the flow rate of toluene at the outlet should not be less than 96 kmol/h. (HINT: Perform Optimization for distillation column, minimize mole flow of toluene in distillate of column, vary the "Recovery of light component in distillate" and put constraints on mole flow and mole fraction of toluene in the bottom of the column.)

PROBLEM 2

A hydro-dealkylation reaction for the production of benzene takes place with the following available composition of the feed initially from some other plant at standard conditions:

COMPOSITION	FLOW RATE (lbmol/h)
Hydrogen	2045.9
Methane	3020.8
Benzene	46.2
Toluene	362

The feed has to be compressed to 494 psi and heated to 1200 F and sent into a reactor. The main reaction is as follows:

$$C_7H_8 + H_2 \rightarrow CH_4 + C_6H_6$$

Consider a stoichiometric reactor with conversion as 76.5% of toluene.

The reactant has to be cooled to 77 F before flashing. The gas from the flash is split and part of it recycled in the ratio of 0.25 purge. The liquid is sent for distillation to extract benzene. The toluene recovered from the column is split and part of it is sent back and mixed with the feed (Purge: 0.1).

In the distillation column take initial guess for number of stages as 10. The light key is benzene with recovery of 0.999 and heavy key is toluene with recovery of 0.001. The condenser is partial and all the distillate is vapour. The pressure at the condenser and reboiler is atmospheric pressure.

Take compressor as isentropic

The requirement of the plant is the maximum production of benzene possible from the plant. (HINT: Perform Optimization to maximize flow rate of benzene, vary the split fraction of toluene splitter)

LITERATURE CITED:

- 3. Turton, Bailie, Whiting, and Shaeiwitz, 2012, Analysis, Synthesis, and Design of Chemical Processes, Prentice Hall, Fourth Edition.
- 4. ASPEN HELP
Experiment 12: Chemical Process Simulation using Aspen Hysys

1. Objectives:

After the completion of this module, the students will have:

- III. Apply Aspen HYSYS simulation-building techniques to build a turbo expander/fractionation plant model
- IV. Learn to add and define components, properties, equipment and streams in ApsenHysys.

2. Prerequisite Engineering & Science Skills

- 12. Knowledge of chemical process flow-sheeting, distillation design .
- 13. Knowledge of Aspen Plus.
- 3. **Workshop:** Construct a comprehensive Turbo Expander/Fractionation Plant model for NGL plant



In this workshop, LNG processing plant flowsheet will be built and simulated in Aspen Hysys. The liquid condensate has to be removed from the feed natural gas and then the lighter hydrocarbons have to be separated in de-methanizer and de-ethanizer columns to obtain rich natural gas, which needs to be further compressed to supply LNG to the market. The LNG exchanger will be used in the process which has the capacity to handle multiple streams in one exchanger.

CLASS PROBLEM

Regenerate the part of LNG processing plant flowsheet as shown below with the given data.



COMPONENT	INLET Conditions
Total flow	5000 kmol/h
Temperature	22°C
Pressure	3500 kPa
C1	0.5
C2	0.15
C3	0.1
i-C4	0.05
n-C4	0.05
N_2	0.05
H ₂ O	0.1

3-PHASE SEPARATOR SPECIIFCATIONS



Ð	3 F	hase Separator: V	V-100			×
Design Reacti	ons Rating Worksheet Dynamics					
Worksheet	Name	Inlet	L1	V1	L2	
Conditions	Vapour	0.8132	0.0000	1.0000	0.0000	
Properties	Temperature [C]	22.00	22.00	22.00	22.00	
Composition	Pressure [kPa]	3500	3500	3500	3500	
PF Specs	Molar Flow [kgmole/h]	5000	437.7	4066	496.3	
	Mass Flow [kg/h]	1.298e+005	1.938e+004	1.015e+005	8940	
	Std Ideal Liq Vol Flow [m3/h]	309.4	38.59	261.8	8.958	
	Molar Enthalpy [kJ/kgmole]	-1.048e+005	-1.240e+005	-8.062e+004	-2.864e+005	
	Molar Entropy [kJ/kgmole-C]	140.8	103.0	155.6	52.88	
	Heat Flow [kJ/h]	-5.242e+008	-5.426e+007	<empty></empty>	-1.421e+008	
D		3 Phase Separat	or: V-100			- 0

3 Phase Separator: V-100

Design Reacti	ons Rating Worksheet	Dynamics				
Worksheet			Inlet	L1	V1	L2
Conditions	Methane		0.5000	0.1393	0.5999	0.0000
Properties	Ethane		0.1500	0.1548	0.1678	0.0000
Composition	Propane		0.1000	0.2468	0.0964	0.0000
PF Specs	i-Butane		0.0500	0.2076	0.0391	0.0000
	n-Butane		0.0500	0.2454	0.0351	0.0000
	Nitrogen		0.0500	0.0056	0.0609	0.0000
	H2O		0.1000	0.0004	0.0009	1.0000

COOLER SPECIFICATIONS



isign prating	Worksheet Performance Dynamics				
Worksheet	Name	L1	L3	Q-100	
Conditions	Vapour	0.0000	0.0000	<empty></empty>	
Properties	Temperature [C]	22.00	-85.00	<empty></empty>	
Composition	Pressure [kPa]	3500	2790	<empty></empty>	
PF Specs	Molar Flow [kgmole/h]	437.7	437.7	<empty></empty>	
	Mass Flow [kg/h]	1.938e+004	1.938e+004	<empty></empty>	
	Std Ideal Liq Vol Flow [m3/h]	38.59	38.59	<empty></empty>	
	Molar Enthalpy [kJ/kgmole]	-1.240e+005	-1.348e+005	<empty></empty>	
	Molar Entropy [kJ/kgmole-C]	103.0	58.38	<empty></empty>	
	Heat Flow [kJ/h]	-5.426e+007	-5.899e+007	4.730e+006	

DE-METHANIZER SPECIFICATIONS

Design (Column Name DEMETH	ANIZER Sub-Flowsheet	Tag COL1					
ections tor					O <u>v</u> hd Vapo	ur Outlet		
s					L4		•	
s Summary						,		
s r	op Stage Inlet							
	<u>13</u>							
c	Optional Inlet Streams	Num of		Optional Side	e Dr <u>a</u> ws			
	Stream Inlet Sta	age Stages	2765 kPa	Stream	Туре	Draw Stage	e	
	<< Stream >>	n = 10		<< Stre	am >>			
			P reb					
		n-1	2800 KPa		Reboiler	Ener <u>gy</u> Stream		
		n			Q-102		•	
			+1 (S) Delta	a P	Bottoms	Liguid Outlet		
			0.00	000 kPa	L5		•	
			T				>	
		lume: DEMETHANIZER / C	Ol 1 Eluid Pka: F	Basis-1 / Peng-	Robinson		_	
sign Paramete	rs Side Ops Internals Ra	lumn: DEMETHANIZER / C	COL1 Fluid Pkg: E	Basis-1 / Peng-	Robinson		-	
sign Paramete Design	Co rs Side Ops Internals Ra Optional Checks	lumn: DEMETHANIZER / C ating Worksheet Performanc	COL1 Fluid Pkg: E e Flowsheet Read	Basis-1 / Peng-	Robinson	ray Positic	-	
sign Paramete Design nnections onitor	rs Side Ops Internals Ra Optional Checks Input Summary	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates	COL1 Fluid Pkg: E e Flowsheet Read	Basis-1 / Peng- ctions Dynamics Tempera	Robinson	ray Positic	- on from T	□ I
sign Paramete Design nnections onitor ecs ecs Summary	rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates brium Heat / Spec	OL1 Fluid Pkg: E e Flowsheet Read Profile © Temp © Press	Basis-1 / Peng- ctions Dynamics	Robinson	ray Positic	- on from T	□ ■ Fop
sign Paramete Design nnections nnitor ecs ecs Summary bcooling	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates brium Heat / Spec 0.012533 0.018476	CDL1 Fluid Pkg: E Flowsheet Read Profile Temp Press Flows	Basis-1 / Peng- ctions Dynamics	Robinson	ray Positic	- on from T	Гор
sign Paramete Design nnections onitor ecs ecs Summary bcooling ites	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates brium Heat / Spec 0.012533 0.018476 0.005377 0.010534 0.002174 0.007890	COL1 Fluid Pkg: E Flowsheet Read Profile Temp Press Flows	Basis-1 / Peng- ctions Dynamics Temperat	Robinson ture vs. T	ray Positic	- on from T	Image: constraint of the second secon
sign Paramete Design nnections onitor ecs ecs Summary bccoling tes	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000 5 1.0000 6 1.0000	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates Performanc brium Heat / Spec 0.012533 0.012533 0.018476 0.005377 0.002174 0.007890 0.000849	COL1 Fluid Pkg: E e Flowsheet Read Profile © Temp © Press © Flows	Basis-1 / Peng- tions Dynamics	Robinson ture vs. T	ray Positic	- on from T	Fop
ign Paramete Design nnections onitor ecs ecs Summary occoling tes	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000 5 1.0000 6 1.0000 7 1.0000	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates Performanc brium Heat / Spec 0.012533 0.012533 0.018476 0.005377 0.001274 0.007890 0.005246 0.000849 0.005246 0.003310	COL1 Fluid Pkg: E Flowsheet Read Profile Temp Press Flows	Basis-1 / Peng- ctions Dynamics	Robinson ture vs. T	ray Positic	on from T	Image: Cope of the second s
sign Paramete Design nnections onitor ecs ecs Summary bcooling ttes	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000 5 1.0000 6 1.0000 7 1.0000 5 Specifications	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates Performanc brium Heat / Spec 0.012533 0.012533 0.018476 0.005377 0.00174 0.007890 0.005246 0.000849 0.005246 0.003310	COL1 Fluid Pkg: E Flowsheet Reac Profile Temp Press Flows	Basis-1 / Peng- ctions Dynamics	Robinson ture vs. T	ray Positic	on from T	Image: Control of the second s
sign Paramete Design nnections onitor ecs ecs Summary bcooling ites	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000 5 1.0000 6 1.0000 5 Specifications Optid Dead Bate	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates Distribution Heat / Spec 0.012533 0.018476 0.005377 0.002174 0.007890 0.002246 0.000849 0.005246 0.003340 Specified Value 260.0 Inservat/6	COL1 Fluid Pkg: E Flowsheet Read Profile Temp Press Flows Current Value	Basis-1 / Peng- tions Dynamics Temperat 0.000 40.00 40.00 -40.00 0 0 0 0 0 0 0 0 0 0 0 0	-Robinson ture vs. To emperature 2 Active Estimat	ray Positic	on from T	
sign Paramete Design nnections onitor ecs ecs Summary bcooling tes	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000 5 1.0000 6 1.0000 6 1.0000 7 1.0000 5 Specifications	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates brium Heat / Spec 0.012533 0.018476 0.005377 0.010534 0.002174 0.007890 0.002174 0.007890 0.002174 0.007890 0.00246 0.00230 0.005246 0.00230 0.005246	COL1 Fluid Pkg: E Flowsheet Read Profile Temp Press Flows Current Value 64.99 372.7	Basis-1 / Peng- tions Dynamics Temperal 40.00 40.00 -40.00 -40.00 0 Wt. Error -0.8143 <empty></empty>	Active Estimat	ray Positic	on from T	Fop 10
sign Paramete Design nnections onitor ecs ecs Summary bcooling ites	Co rs Side Ops Internals Rz Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000 5 1.0000 6 1.0000 6 1.0000 5 5 1.0000 6 1.0000 5 5 1.0000 6 1.0000 7 1.0000 5 5 1.0000 6 1.0000 7 1.0000 8 5 1.0000 7 1.0000 8 5 1.0000 8 5 1.0000 9 5 1.0000 9 6 1.0000 9 7 1.0000 9 6 1.0000 9 7 1.0000 9 6 1.0000 9 7 1.00000 9 7 1.00000 9 7 1.00000 9 7 1.00000 9 7 1.00000000000000000000000000000000000	lumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates brium Heat / Spec 0.012533 0.018476 0.005377 0.010534 0.002174 0.007890 0.000849 0.005246 0.000249 0.005246 0.000210 Specified Value 350.0 kgmole/h <empty></empty>	Current Value 64.99 372.7 1.539	Basis-1 / Peng- tions Dynamics Temperat 40.00 -40 -40.00 -	Active Estima	ray Positic	on from T	
sign Paramete Design nnections onitor ecs ecs ecs summary bcooling ites	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000 5 1.0000 6 1.0000 6 1.0000 7 1.0000 6 1.0000 7 1.0000 7 1.0000 8 Specifications Ovhd Prod Rate Btms Prod Rate Boilup Ratio Comp Recovery Comp Eraction	lumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates brium Heat / Spec 0.012533 0.018476 0.005377 0.010534 0.000549 0.005246 0.000849 0.005246 0.000320 Specified Value 350.0 kgmole/h <empty> 0.9500 0.0280</empty>	Current Value 64.99 372.7 0.9891 0.9280	Basis-1 / Peng- ctions Dynamics Temperal 80.00 40.00 40.00 -40.00 0 Wt. Error -0.8143 <empty> <empty> 0.0197 -0.001</empty></empty>	Active Estima	ray Positic	on from T	Fop
sign Paramete Design nnections anitor ecs ecs Summary bcooling ites	Co rs Side Ops Internals Ra Optional Checks Input Summary Iter Step Equili 3 1.0000 4 1.0000 5 1.0000 6 1.0000 5 1.0000 5 Specifications Specifications Ovhd Prod Rate Btms Prod Rate Boilup Ratio Comp Recovery Comp Fraction	Iumn: DEMETHANIZER / C ating Worksheet Performanc View Initial Estimates brium Heat / Spec 0.012533 0.018476 0.005377 0.010534 0.002174 0.007890 0.002174 0.007890 0.002174 0.007890 0.002164 0.00220 0.00246 0.00220	Current Value 64.99 372.7 1.539 0.9280	Basis-1 / Peng- ctions Dynamics Temperal 0.000 40.00 0 -40.00 0 -40.00 0 -40.00 0 -40.00 0 -40.00 0 -40.00 0 -40.00 0 -40.00 0 -0.8143 <empty> <empty> 0.0197 -0.0001 -0.0001</empty></empty>	Active Estimate	ray Positic	on from T	

Component Recovery: Percentage of component in feed recovered in output stream **Component fraction:** Mole fraction of component in the stream.

DE-ETHANIZER SPECIFICATIONS





Calculate flow rates and compositions of Stream V1, L2, L4, L6 and L7. Also, calculate heat duty of Q-100, Q-102, Q-103 and Q-104.

	Object	Variable	Value	Units	Tag	Access Mode
1	L1	Total Component Mole Flows	437.7010	kgmole/h	No Tag	No Transfer
	L2	Total Component Mole Flows	496.2527	kgmole/h	No Tag	No Transfer
	L3	Total Component Mole Flows	437.7010	kgmole/h	No Tag	No Transfer
1	L4	Total Component Mole Flows	64.9961	kgmole/h	No Tag	No Transfer
5	L5	Total Component Mole Flows	372.7049	kgmole/h	No Tag	No Transfer
j	L6	Total Component Mole Flows	72.4931	kgmole/h	No Tag	No Transfer
7	L7	Total Component Mole Flows	300.2118	kgmole/h	No Tag	No Transfer
3	E-100	Duty	4.730e+006	kJ/h	No Tag	No Transfer
)	Q-100	Heat Flow	4.730e+006	kJ/h	No Tag	No Transfer
10	Q-102	Heat Flow	7.801e+006	kJ/h	No Tag	No Transfer
11	Q103	Heat Flow	5.189e+006	kJ/h	No Tag	No Transfer
12	Q104	Heat Flow	6.712e+006	kJ/h	No Tag	No Transfer
13	v1	Total Component Mole Flows	4066.0463	kgmole/h	No Tag	No Transfer
4	V-100	Duty	0.0000	kJ/h	No Tag	No Transfer

LITERATURE CITED:

- 7. Aspen Help
- 8. Aspen HysysSOlutions

APPENDIX

Module A1: Cost Estimation and Analysis of process flow-sheet using ASPEN Plus

1. **Objectives:**

After the completion of this module, the students will have:

- VI. Reviewed and expanded knowledge of cost estimation and analysis of process plant.
- VII. Learned to use Aspen Plus to perform cost estimation of process plant.

2. Prerequisite Engineering & Science Skills

- VII. Knowledge of chemical process flow-sheeting.
- VIII. Knowledge of Aspen Plus.

CLASS PROBLEM

The ammonia synthesis process has to be performed in the Ammonia production plant using the feed at 27 atm and 280° C with following composition:

COMPONENT	MOLE FLOW (kmol/h)
Hydrogen	5160
Nitrogen	1732
Methane	72
Argon	19
Carbon monoxide	17

Customer requirement specifies that the liquid ammonia purity should not be less than 96 mole %. Moreover, the plant should produce at least 3250 kmol/hr of liquid ammonia for profitable operation. A purge stream is used in this process to create an exit for the impurities or by-products contained in the process.

Reaction Involved:

$N_2 + 3H_2 \rightarrow 2NH_3$

The reactor is RStoic with a fractional conversion of 40% of nitrogen and operates at 270 atm and 481.85° C. The compressors used are isentropic and their outlet pressure is 271 atm. The product from the reactor is cooled to 27° C before entering the flash column. The heat duty flash column is zero. The splitter purges 10% of the effluent and recycles the rest in to the system.

SIMULATION OF AMMONIA SYNTHESIS PROCESS FLOW-SHEET

This is the same problem of ammonia synthesis process that was simulated in Class Problem of Module 12. The flow-sheet is shown in Figure 1. The same steps as in the Class Problem of Module 12 has to be followed and simulation has to be run.

Estimation of Operating Cost of ammonia synthesis process flow-sheet

Step 1:Add all the required inputs and Run the Simulation for ammonia synthesis process flow-sheet.

EQUIPMENT	UTILITY
Compressor (C101)	Electricity
Compressor (C102)	Electricity
Heater (H101)	Furnace
Cooler(E101)	Cooling water

Step 2: Basically there are four equipment where utilities are required.

- Step 3:Select Setup of equipment "Compressor C100" and select the Utility tab. Select New and name 'U-1' and select 'Electricity' as shown in Fig. 2. The Utility tab will get blue. Repeat the same for "Compressor C102". Add 'U-1' for C102.
- **Step 4:** Select Setup of equipment "Heater H100". In the Utility tab create a new utility 'U-2' and select type as 'Fired Heat 1000' as required.
- **Step 5:** Select Setup of equipment "Cooler E100" and create a new utility 'U-2' and select type as 'Cooling water' as required. This may ask to add 'Water' in the Components List in 'Properties' and update the Binary Parameters.
- Step 6: Click the 'Economics' tab at the top and click 'Stream Price' tab. Select the raw material streams (In this case 'FEED' i.e. synthesis gas) and then select the product streams (In this case 'LIQ-NH3' i.e. liquid ammonia) as shown in Fig. 3. The approximate price of liquid ammonia is \$ 500/tonne and synthesis gas is \$ 0.2/kg. The current prices can be viewed in http://www.icis.com.
- **Step 7:** The cost of Process Utilities can be changed if needed by clicking the 'Process Utilities' tab. Since the required utilities are complete, Run the Simulation.

The Results can be seen in the Result Summary in 'Operating Cost' as shown in Fig. 4.





Specifications	Calculation Options	Power Loss	Convergence	Integration Parameters	Utility	Information
Select utility for th	is block					
Utility ID:	<new></new>	-				
			8	New Utility		×
			Create a new ut	tility:		
			U-1			
			Copy from:			
			<blank></blank>			•
			< Blanks			
			SUIdTIKZ			

Fig 2: Required input for Utilities (Electricity) of compressor.

Main	Flowsheet × Stream Price × +					
Ølr	nput Information					
- Spe	cify stream price for material streams					
	Stream ID	Source	Destination	Basis	Price	Unit
	FEED		C101	Mass	0.2	\$/kg
	LIQ-NH3	V101		Mass	500	\$/tonne
A	Add Feed Streams Add Product Streams	s				

Fig 3: Required input for Stream price of raw materials and products.

Op	perating Cost Summary Utility Cost Summary		
	Utility		
	Total heating duty:	cal/sec	1.5602e+07
	Total cooling duty:	cal/sec	1.78346e+07
	Net duty (Total heating duty - Total cooling duty):	cal/sec	-2.23254e+06
	Total heating cost flow:	\$/hr	2451.24
	Total cooling cost flow:	\$/hr	56.988
	Net cost (Total heating cost + Total cooling cost):	\$/hr	2508.22
	Stream cost		
	Net cost flow of feeds:	\$/hr	12262.3
	Net cost flow of products:	\$/hr	25371.9
	Overall net cost flow:	\$/hr	13109.6

Fig 4: Result Summary of Operating cost.

Estimation of Capital Cost of ammonia synthesis process flow-sheet

Step 1:In the Economics click the Economics Active tab to activate the economics.

- **Step 2: Mapping:** In this step, the unit operations is mapped from the simulation to real equipment models. This can be seen in Fig. 5. Click the Map button at the top and click OK with default values. Map Preview will appear as shown in Fig. 6. The Aspen has chosen a default equipment defined in the data banks for each equipment. For example, for C101 the default equipment as 'Centrifugal horizontal compressor'. To change the equipment type click the suggested equipment type and anew window will open as shown in Fig. 7. Similarly other equipment have to be mapped. The default equipment is selected after rigorous analysis and gives good match of the equipment. Some equipment like mixer and splitter are T-junction in most plants and does not carry an equipment cost. These unit operations do not correlate with actual equipment and can be mapped as Quoted equipment i.e. 'C' units.
- **Step 3: Sizing:** Click 'Size' to size the mapped equipment. Equipment sizes are determined from the available simulation data. Missing data is estimated by the system. If Aspen cannot estimate the size of the equipment it will skip the equipment and perform calculations for other equipment which will later appear as error in the Results.
- Step 4: Click 'Evaluate' to conduct the economic analysis.
- **Step 5**: Click 'View Equipment' to view the overall results of the evaluation. Relative estimates of the total capital cost, operating cost, and utility cost can be found in the 'Summary' tab. In the 'Equipment' tab the errors occurred on the Sizing of the equipment are marked as red. The description of the error can be seen by clicking the equipment.
- **Step 7:** The detailed Cost Analysis can be obtained by clicking 'Investment Analysis' at the top which will generate a detailed Excel file



Fig 5: Mapping Radfrac column from Simulation unit to equipment model.

Unit Operations			
C101(COMPR)	Equipment Tag	Equipment Type	Description
C102(COMPR) E101(HEATER) H101(HEATER) M101(MIXER) R101(RSTOIC) SP101(FSPLIT) V101(FLASH2)	C101 Add Delete Configuration	DGC CENTRIF ~	Centrifugal compressor - horizontal

Fig 6: Map preview for equipment.

	
2	۱.
а	
•••	/

E	quipment Selection
Project Equipment Name	C101
Project Componen	nts
Process equipment	
Plant bulks	
Site development	
Buildings	
Quoted equipment	
Unit cost library	
Equipment model library	

b)

	Equipment	Selection	
Pr	oject Equipment Name C101		
	Project Components Process equipment		
A	gitators- mix, react, knead	(AG AT BL K MX)	^
C	ompressors and blowers	(AC GC FN)	
D	rivers	(MOT TUR)	
H	eat exchangers, heaters	(HE RB FU)	
	ackings, linings	(PAK LIN)	
Pa		(171122111)	
Pa Pu	umps	(CP GP P)	
Pa Pu To	umps owers, columns- trayed/packed	(CP GP P) (DDT TW)	
Pa Pu To Va	umps owers, columns- trayed/packed acuum system equipment	(CP GP P) (DDT TW) (C EJ VP)	
Pa Pu To Va Va	umps owers, columns- trayed/packed acuum system equipment essels- pressure, storage	(CP GP P) (DDT TW) (C EJ VP) (HT VT)	ļ
Pa Pu To Va Ci	umps owers, columns- trayed/packed acuum system equipment essels- pressure, storage rushers,flakers,mills,stock	(CP GP P) (DDT TW) (C EJ VP) (HT VT) (CR FL M ST)	
Pa Pu To Va Ci Ev	umps owers, columns- trayed/packed acuum system equipment essels- pressure, storage rushers,flakers,mills,stock raporators, dryers, cryst.	(CP GP P) (DDT TW) (C EJ VP) (HT VT) (CR FL M ST) (CRY E WFE AD D DD RD TDS)) _

l	Equipment Selection	>
	Project Equipment Name C101	
	Project Components Process equipment Compressors and blowers (AC GC FN) Compressor - gas	
	Centrifugal compressor - horizontal Centrifugal - integral gear	
	Reciprocating compressor	
	Keciprocating compr integral gas engine	
	OK Cancel	

Fig. 7: Equipment selection window.

c)

LITERATURE CITED:

- 7. Aspen Tutorial"Jump Start: Integrated Economics in Aspen Plus V 7.3.2".
- **8.** ASPEN Help.