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PROCESS SIMULATION USING DWSIM:

A Free and Open Source Chemical Process Simulator

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> Level: Basic Version: v02 December 2017

This manual uses DWSIM ver 5.1 (Class UI)

PREFACE

The manual "Process Simulation Using DWSIM" presents a set of eleven basic exercises using a free and open source chemical process simulator "DWSIM" and can be utilized to establish process simulation laboratory as part of undergraduate chemical engineering degree or in allied degree curriculum. Simulation covers topics across the broad spectrum of chemical engineering courses covering mixing, reaction, phase equilibrium, heat and mass transfer operations. The problem statements are rightly placed at the beginner's level with each exercise complete in terms of sufficient instructions that enable the learner to perform the exercise with ease on their own. Supplementary self-learning exercises are also provided for simulation experiments to further aid a curious learner. This manual is the second version brought out by the SASTRA FOSSEE Centre, a partner with FOSSEE, IIT-B. At this juncture, I thank Prof Kannan M. Moudgalya, Professor, IIT-B for initiating me into FOSSEE tools and helping to establish the FOSSEE at SASTRA. I also owe my sincere thanks to my earlier students G. Jayaram and A. S. Ragul, who interned at FOSSEE and developed the version 1 of this manual. I believe the manual is helpful and can meet its intended objective. Care is taken to ensure the manual is free from factual and typological errors. However, I request the users to debug the exercises given in the manual and if you find any errors or discrepancy in using the manual, you can feel free to bring to my notice.

Thanks

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PROCESS SIMULATION USING DWSIM: A FREE AND OPEN SOURCE CHEMICAL PROCESS SIMULATOR

PREAMBLE

DWSIM is an open-source CAPE-OPEN compliant chemical process simulator. It features a Graphical User Interface (GUI), advanced thermodynamics calculations, reactions support and petroleum characterization / hypothetical component generation tools. DWSIM can simulate steady-state, vapor–liquid, vapor–liquid-liquid, solid–liquid and aqueous electrolyte equilibrium processes and has built-in thermodynamic models and unit operations (https://en.wikipedia.org/wiki/DWSIM). It is available for Windows, Linux and Mac OS.

The objective of the course is to create awareness of the open source process simulator "DWSIM" among prospective graduates and practicing process engineers. The course will cover basic aspects of create flow sheet in DWSIM and simulation of simple units such as Mixer, Heat Exchanger, Equilibrium reactor, CSTR, Distillation column.

Target Audience

- III / Final year B. Tech. Chemical Engineering students
- M. Tech. Chemical Engineering students
- Practicing Process Engineers

Prerequisites

• Participants should have pursued the following courses as part of their degree program / have good working knowledge in (i) Fluid mechanics (ii) Chemical Reaction Engineering (iii) Chemical Engineering Thermodynamics (iv) Heat and Mass Transfer (v) Numerical analysis

INSTALLATION GUIDELINES FOR WINDOWS OS

System Requirements for DWSIM on Windows Platform

OS:	Windows: 64-bit x86 XP/Vista/7/8/10
	Linux: 64-bit x86 Ubuntu 12.04 or newer / 32-bit armhf Raspbian/Ubuntu MATE
	macOS: 10.7 (OS X Lion) or newer
Software:	Microsoft .NET Framework 4.5 or newer (Windows)
	Mono Framework 5.0.0 or newer (Linux/macOS)

CPU: 1.0 GHz dual-core processor (minimum)

Memory: 1 GB RAM

Graphics Card: 128 MB with OpenGL hardware acceleration

Display: a 1280x800 display resolution is recommended as a minimum.

Disk space: 300 MB for program files

Steps to be followed for installing DWSIM Version 5.1 (Windows)

- 1. Download the latest version of DWSIM (DWSIM version 5.1) from http://dwsim.inforside.com.br/wiki/index.php?title=Downloads
- 2. Once downloaded the executable file "DWSIM_bin_v51u6_setup", right-click the file and select "**Run as Administrator**" option.
- 3. Once you click it, you will be alerted with a dialog box asking for installer language. Choose **English**
- 4. Then **DWSIM 5.1 Setup** wizard appears. Click **Next** to continue.
- 5. Then click **I Agree** followed by **Next**. Now you will be asked to choose components to be installed by showing a list of 5 components [DWSIM, ChemSep 7.15, CAPE-OPEN type libraries for 32-bit and 64-bit Windows, Register type libraries]. Make sure that you check all the checkboxes in the list (i.e, choose all 5 components) and click **Next** to continue.



- 6. To install in different folder, you can change the destination but please remember the location of the destination file.
- 7. Click **Next** to continue and click **Install** to begin the installation.
- 8. The installation begins and waits till you encounter a **ChemSep 7.15 LITE** Setup wizard. Now just click **I Agree** button [retain the default installation option: "Install for anyone using this computer"] and click **Next** till you see **Install** button and then click it to begin the installation of Chemsep. Follow the screen instructions till you finish the installation.
- 9. Once ChemSep 7.15 installation is complete setup wizard for CAPE-OPEN type libraries will show up. Follow the instructions on screen and complete the same.
- 10. Once installation is completed without error, click **Next** and click **Finish** to close the wizard. You will notice two icons in the desktop titled "DWSIM (Classic UI)" and "DWSIM"

Additional Guidelines to enable updates in DWSIM

- 1. Locate DWSIM file from installed location and open DWSIM v5.1 (Classic UI) in your computer (Right click the DWSIM icon and run as administrator).
- 2. Close the welcome screen
- 3. Locate Edit in the menu bar at the top and click on it.
- 4. Under Edit menu, select General Settings
- 5. A wizard appears. Select Other tab (last tab in the top) in the wizard
- 6. At the bottom, one can see an option called **Check for updates on startup.** Click it or enable it.
- 7. Similarly, one can see an option called Enable automatic updates. Click it or enable it.



Note:

DWSIM requires Microsoft .NET framework and Visual C++ 2015 Redistributable. If it is not installed in your system, you can download the same and install <u>https://www.microsoft.com/net/download/windows</u> https://www.microsoft.com/en-us/download/details.aspx?id=52685

DWSIM INSTALLATION FOR OTHER PLATFORMS

DWSIM is also available for other platforms such as Linux, mac OS and Raspberry pi. Instructions for the same are available at <u>http://dwsim.inforside.com.br/wiki/index.php?title=Downloads</u>

OBJECTIVE

• To enable students to simulate different process units using a process simulator tool and there by facilitate performance analysis of different units.

LIST OF SIMULATION EXPERIMENTS/ TUTORIALS

- 1. Mixing of ideal liquid streams
- 2. Determination of thermo-physical properties of pure components
- 3. Generation of VLE data of binary component system
- 4. Determination of equilibrium conversion of reversible reactions
- 5. Material balance on reactor based on yield/conversion data
- 6. Simulation of an CSTR for liquid phase reaction
- 7. Simulation of a flash column
- 8. Simulation of a distillation column
- 9. Determination of heat duty
- 10. Shortcut Simulation of heat exchanger to determine outlet stream temperature
- 11. Detailed Simulation of heat exchanger

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- S. I. Sandler. Using Aspen Plus in thermodynamics instruction A step-by-step guide. New Jersey: John Wiley Sons, Inc., 2015.
- Schefflan, R. Teach yourself The basics of Aspen Plus. New Jersey: John Wiley & Sons, Inc., 2011.
- Seider, W. D., J. D. Seader, J. D. and D. R. Lewin, D. R. Product and process design Principles, 2/e. New York: John Wiley and Sons, Inc., 2008

USEFUL LINKS

- <u>http://dwsim.inforside.com.br/</u>
- <u>http://dwsim.fossee.in/</u>
- <u>http://spoken-tutorial.org/</u>
- <u>http://forums.fossee.in/</u>
- <u>https://sourceforge.net/p/dwsim/discussion/</u>
- <u>http://dwsim.inforside.com.br/wiki/index.php?title=Category:Tutorials</u>
- <u>https://sites.google.com/site/prnarenportal/dwsim</u>

Expt.	Title	Page no.
No.		
1.	Mixing of ideal liquid streams	1
2.	Determination of thermo-physical properties of pure components	5
3.	Generation of VLE data of binary component system	9
4.	Determination of equilibrium conversion of reversible reactions	13
5.	Material balance on reactor based on yield/conversion data	17
6.	Simulation of an CSTR for liquid phase reaction	21
7.	Simulation of a flash column	25
8.	Simulation of a distillation column	29
9.	Determination of heat duty	33
10.	Shortcut Simulation of heat exchanger to determine outlet stream temperature	37
11.	Detailed Simulation of heat exchanger	41

TABLE OF CONTENTS

This manual uses DWSIM ver 5.1 (Class UI)

Mixing of Ideal Liquid Streams

Objective

Develop a simple process sheet to mix two liquid streams and estimate the flow rate and composition of outlet stream.

Data

Inlet stream 1: 10 mol % Methanol solution flowing at 20 kmol/h Inlet stream 2: 80 mol % Methanol solution flowing at 10 kmol/h Both the streams are at 30 °C and at 1 bar pressure The liquid streams can be considered as ideal

DWSIM Blocks Used

Mixer

- 1. Start a new DWSIM Simulation (DWSIM VER 5.1 CLASSIC UI). Click on "New steady state Simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. It shows a specification page. Add components required to solve the problem statement. In the present case, add Water and Methanol. Ensure all components are added from the same property database. For instance, in this case, both components are added from "ChemSep" database.
- 3. Specify the thermodynamic package as Raoult's law.
- 4. Customize the system of units for the simulation and click "Next".
- 5. The flowsheeting section of simulation window will be opened. First, let provide input and output streams for the unit operation to be performed. Drag and drop two Material streams available at the right, in the object palette. Rename them stream as "Inlet-Stream-1" and "Inlet-Stream-2". These serve as input streams.
- 6. On clicking the "Inlet-Stream-1" and "Inlet-Stream-2" stream, general information about the stream will be displayed on the left side of screen. Specify the feed compositions, temperature and pressure for the inlet streams. Once credentials are specified for the inlet streams, the color of stream turns blue.

Stream	Molar Flowrate (kmol/hr)	Mol fraction MeOH	Mol fraction Water	Temperature °C	Pressure bar
		(-)	(-)		
Inlet Stream1	20	0.1	0.9	30	1
Inlet Stream 2	10	0.8	0.2	30	1

Specification for the inlet streams

- 7. Add one more Material stream i.e. Drag and drop it into the flow sheet. Rename the stream as "Outlet Stream". This serves as output stream.
- 8. Below the Unit Operation tab on left, locate the Stream Mixer block. Drag and drop into the flow sheet. Rename it as "Mixer".



- 9. No separate specification is required for the "Mixer" block.
- 10. Now, all necessary credentials required for simulation are added. It should be connected in a proper sequence. Click on "Mixer" block, the general information about the block is displayed on the right. Under "connections" tab, for all streams click the dropdown button and select the necessary connections. If all the connections are given correctly, all the blocks will turn blue.
- 11. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen.

12. To analyze/display the results, select on "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

Results

Stream Results

Simulation-Results				
Object	Inlet-Stream-1	Inlet-Stream-2	Outlet-Stream	
Temperature	30.000000	30.000000	30.000000	С
Pressure	1.000000	1.000000	1.000000	bar
Mass Flow	388.354000	292.366000	680.720000	kg/h
Molar Flow	20.000000	10.000000	30.000000	kmol/h
Volumetric Flow	0.351959	0.313660	0.603321	m3/h
Molar Fraction (Overall Liquid Phase) / Methanol	0.100000	0.800000	0.333333	
Molar Flow (Overall Liquid Phase) / Methanol	2.000000	8.000000	10.000000	kmol/h
Molar Fraction (Overall Liquid Phase) / Water	0.900000	0.200000	0.666667	
Molar Flow (Overall Liquid Phase) / Water	18.000000	2.000000	20.000000	kmol/h

Self-Learning Exercises

1. How to modify the simulation, if pure methanol is mixed with water to form solution?

2. What if enthalpy of mixing is not negligible?

Determination of Thermo-physical Properties of Pure Component

Objective

Determine the thermo-physical properties of pure component as function of temperature and pressure. For instance, determine the specific heat capacity of liquid water at 1 bar from 30 $^{\circ}$ C to 90 $^{\circ}$ C

Data

Fluid: Water Thermodynamic model: Ideal

DWSIM Block

No blocks required

- 1. Start a new DWSIM simulation (DWSIM VER 5.1 CLASSIC UI). Click on "New steady state simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. The specification page will appear. Select the component required for the simulation. In this case Water is added.
- 3. Select and add the property package (Raoult's law) and click "Next". Add the default flash algorithm for the simulation. Click "Next".
- 4. Choose the desired system of units for the simulation and click "Next".
- 5. The flow sheeting section will be opened.
- 6. In the top menu, under the "Tools" tab, click on "Pure component property viewer" to generate thermo-physical property data.
- 7. On clicking the tab, pure component property window will appear. Select the component for which the thermo-physical data has to be generated. In this case it is water.
- 8. Once you selected the component, the appearance of window will be changed as shown in figure.

omponent	Water		\sim	Original Data		Enable Constant Property Editing	Restore Defaults
Molecular	Constants	Liquid Phase	Vapor Phase	Solid Phase	Comments		Ŧ
Molecular S	tructure						
Formula		НОН					
UNIFAC	Groups	H2O 1					
MODFAC	-Do Groups	H2O 1					
MODFAC	-NIST Groups	H2O 1					
SMILES S	tring	0					
InChI Str	ing	InChI=1S/H2O/h	1H2				
2D Render							
20 Hender			_	_		-	
					_		
				- 4			

9. Below the component tab, identify a tab named "Liquid-phase". On clicking this tab, a graph for temperature versus specific heat capacity of water will be generated.



10. To view the results in tabulated form, click on "Data-table" option where, all the thermo-physical properties are tabulated.

Results

View									
Component	Water		✓ Original Direction	ata	E	Enable Consta	nt Property Editin	g Rest	ore Defaults
Molecular	Constants Liquid F	hase Vapo	r Phase Solid Phas	e Commen	ts				Ŧ
Heat Capac	ty Vaporization Entl	halpy Vapor	Pressure Surface	Tension Vi	scosity Densit	ty Thermal	Conductivity	Data Table	
Temp C	Heat Capacity kJ/[kg.K]	Temp C	Vaporization Enthalpy kJ/kg	Temp C	Vapor Pressure bar	Temp C	Surface Tension N/m	Temp C	Viscosity (Liquid) Pa.:
0.050000	4.193125	0.000000	2,497.607501	-10.000000	0.002852	-8.050000	0.077288	115.134000	0.000241
5.151000	4.193133	7.482600	2,480.726973	-2.317200	0.005144	-0.410000	0.076072	120.311120	0.000230
10.352000	4.193148	14.965200	2,463.827651	5.365600	0.008943	7.230000	0.074867	125.488240	0.000220
15.553000	4.193175	22.447800	2,446.883424	13.048400	0.015031	14.870000	0.073665	130.665360	0.000211
20.754000	4.193222	29.930400	2,429.867599	20.731200	0.024496	22.510000	0.072460	135.842480	0.000203
25.955000	4.193298	37.413000	2,412.752850	28.414000	0.038804	30.150000	0.071245	141.019600	0.000196
31.156000	4.193421	44.895600	2,395.511159	36.096800	0.059885	37.790000	0.070015	146.196720	0.000189
6.357000	4.193609	52.378200	2,378.113746	43.779600	0.090226	45.430000	0.068766	151.373840	0.000182
41.558000	4.193890	59.860800	2,360.531011	51.462400	0.132954	53.070000	0.067495	156.550960	0.000176
46.759000	4.194296	67.343400	2,342.732452	59.145200	0.191939	60.710000	0.066199	161.728080	0.000171
51.960000	4.194868	74.826000	2,324.686590	66.828000	0.271878	68.350000	0.064875	166.905200	0.000165
57.161000	4.195652	82.308600	2,306.360885	74.510800	0.378383	75.990000	0.063523	172.082320	0.000160
52.362000	4.196702	89.791200	2,287.721635	82.193600	0.518064	83.630000	0.062139	177.259440	0.000155
57.563000	4.198077	97.273800	2,268.733881	89.876400	0.698595	91.270000	0.060725	182.436560	0.000151

Self-Learning Exercise

1. Determine the thermal conductivity and viscosity of liquid water and in vapour phase.

Generation of VLE Data of Binary Component System

Objective

Generate vapour-liquid equilibrium data (VLE) for a binary component system

Data

Fluid components: Benzene - Toluene

Pressure = 1 atm

Thermodynamic model: Ideal

DWSIM Block

Material Stream

- 1. Start a new DWSIM simulation (DWSIM VER 5.1 CLASSIC UI). Click on "New steady state simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. The specification page will appear. Select the components required for the simulation, namely "Benzene" and "Toluene". Ensure, components are added from same property database. In this illustration, both components are added from "ChemSep" database.
- 3. Select and add the property package (Raoult's law) and click "Next". Add the default flash algorithm for the simulation. Click "Next".
- 4. Choose the desired system of units for the simulation and click "Next".
- 5. The flowsheeting section will be opened.
- 6. To generate binary VLE, at least one material stream is required in the flowsheeting section. Hence, click on material stream object at the object palette and drag it to the flowsheet section.
- 7. Click the "material stream" to open its specification window. Next to the object name, you will find an icon, click it to attach utility and under utility add an "Binary Envelope" as shown in the figure below

laterial Stream: I	MSTR-000	џ	×	Flowsheet			Material Streams	Spreadshe	et
General Info			^						
Object	MSTR-000)	Attach Utility	•	÷	Phase Envelope		٦
Status	Inactive	1	Π			्रि	Binary Envelope (VLE/	VLLE/SLE)	٦ſ
Linked to						÷	Ternary Envelope (LLE))	1
Connections						÷	Petroleum Properties		
Upstream		¥ 🍠					Natural Gas Hydrates		ľ
Downstream		✓			Ľ	;;;	True Critical Point		

8. A new window opens. Enlarge it. Use the different pull down menus available in the window to generate the Txy and VLE plot for Benzene and Toluene at given pressure. Provide settings as shown below and click at "Calculate" to see the Txy plot

Settings to generate '	Fxy at given pressure
Compound 1	Benzene
Compound 2	Toluene
Envelope type	Тху
Txy diagram options	VLE
X axis basis	Mole fraction
Pressure	1 atm
Property package	PP_1 (Raoult's Law)



Settings to genera	ate xy (VLE plot) at given pressure
Compound 1	Benzene
Compound 2	Toluene

Envelope type	(T)xy
Txy diagram	VLE
options	
X axis basis	Mole fraction
Pressure	1 atm
Property package	PP_1 (Raoult's Law)



Self-Learning Exercises

- 1. Generate P-x-y data at T = 120 °C for benzene toluene system.
- 2. Generate T-x-y at P = 5 bar and compare your results with 1 bar to make suitable observations
- 3. Generate the T-x-y data for Water-Ethanol system at 1 bar using "Ideal" and "NRTL" or "Peng Robinson" method. What differences are observed?

Determination of Equilibrium Composition

Objective

Develop a simple process flow sheet to determine the equilibrium composition for the given reaction stoichiometry at specified reaction temperature and pressure

Data

Reaction: Water-gas shift reaction

 $CO_{(g)} + H_2O_{(g)} \rightleftharpoons CO_{2(g)} + H_{2(g)}$ Inlet stream: 20 kmol/h of stoichiometric ratio of CO and H₂O. The inlet stream and the reactor is at 800 K and 1 bar pressure CO_2 and H₂ not present in the inlet stream

DWSIM Blocks Used

Equilibrium reactor

- 1. Start a new DWSIM Simulation (DWSIM VER 5.1 CLASSIC UI). Click on "New steady state Simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. Add 4 components required for the simulation- Carbon monoxide, Carbon dioxide, Hydrogen and Water
- 3. Ensure that all the components are added from same property package. Example: All the components are selected from Chemsep database. Click "Next" button.
- 4. Select and add the property package and click "Next". Add the default flash algorithm for the simulation. Click "Next".
- 5. The flowsheeting section of simulation window will be opened. Drag and drop the Material stream from the object palette. Rename the stream as "Feed". This serves as input.
- 6. On clicking the "Feed" stream, general information about the block will be displayed on left of the screen.
- 7. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams. Choose "Temperature and Pressure" as the flash specification method for the inlet material stream. Once composition and flow rate are specified for the inlet streams, the color of stream turns blue.

Quantity	Value
Temperature, (K)	800
Pressure, (bar)	1
Molar Flowrate (kmol/h)	20
Composition (mol fraction)	CO: 0.5
	CO ₂ : 0
	H ₂ : 0
	H ₂ O: 0.5

Specification for the inlet stream

- 8. Add two more Material streams i.e. Drag and drop it into the flow sheet. Rename them as "Vapor" and "Liquid". These serves as output streams.
- 9. Add an energy stream from the object palette
- 10. Locate the Equilibrium reactor block. Drag and drop into the flow sheet. Rename it as "EQ-React".
- 11. Under "Tools" tab in select "Reaction Manager" tab. choose the type of reaction i.e. "Equilibrium reaction" for this problem. A dialogue box will appear. Give an appropriate name and description about the reaction. Select the checkboxes adjacent to the component names, which has to be included in the reaction. Give the stoichiometry of the reaction and choose appropriate base component. In this case the base component is "Carbon Monoxide". Once base component is chosen and stoichiometry is specified, a text "OK" appears in the stoichiometry tab. By default, the basis is activity and liquid phase. Change it to partial pressure and specify the phase as "vapour" and click "OK"
- 12. Click on "EQ-React" block. The general information about the block is displayed on the left. Under "connections" tab, click the dropdown button and select the necessary connections. If all the connections are given correctly, all the blocks will turn blue.



- 13. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen.
- 14. To analyze/display the results, select on "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

Results

Stream Results

Results				
Object	Feed	Liquid	Vapour	
Temperature	526.850000	526.850000	526.850000	С
Pressure	1.000000	1.000000	1.000000	bar
Mass Flow	460.250000	0.000000	460.252559	kg/h
Molar Flow	20.000000	NaN	20.000000	kmol/h
Molar Fraction (Mixture) / Carbon monoxide	0.500000	0.000000	0.163336	
Molar Flow (Mixture) / Carbon monoxide	10.000000	NaN	3.266727	kmol/h
Molar Fraction (Mixture) / Carbon dioxide	0.000000	0.000000	0.336664	
Molar Flow (Mixture) / Carbon dioxide	0.000000	NaN	6.733273	kmol/h
Molar Fraction (Mixture) / Water	0.500000	0.000000	0.163336	
Molar Flow (Mixture) / Water	10.000000	NaN	3.266727	kmol/h
Molar Fraction (Mixture) / Hydrogen	0.000000	0.000000	0.336664	
Molar Flow (Mixture) / Hydrogen	0.000000	NaN	6.733273	kmol/h

Self-Learning Exercises

1. How to run the simulation to obtain equilibrium conversion at 1000 K and 2 bar pressure?

2. Modify the simulation to compute equilibrium composition involving multiple reactions, say for instance, methane steam reforming along with water-gas shift.

Material Balance on Reactor Based on Yield - Conversion Data

Objective

Develop a simple process sheet to determine the exit composition from a reactor based on conversion (or yield) data and given stoichiometry

Data

Reaction: Ammonia Formation

 $N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$

100 kmol/h of gaseous stream containing 25 mol% N_2 and rest H_2 at 25°C and 1 atm enters a reactor operating at 25°C, 1 atm. Conversion of nitrogen to ammonia is 20%. Determine the composition of exit stream from the reactor.

DWSIM Blocks Used

Conversion Reactor

- 1. Start a new DWSIM Simulation (DWSIM ver 5.1 Classic UI). Click on "New steady state Simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. It shows a specification page. Add the three components for Ammonia formation reaction, namely, Nitrogen, Hydrogen and Ammonia. Ensure that all the components are added from same property package. Example: All the 3 components are selected from Chemsep database. Click "Next" button.
- 3. Specify the thermodynamic package as Raoult's law.
- 4. Customize the system of units in which the simulation has to be carried out and click "Next".
- 5. The flowsheeting section of simulation window will be opened. It is necessary to provide input and output streams for the unit operation to be performed. Drag and drop the Material stream available at the right, in the object palette. Rename the stream as "Feed". This serves as input stream.
- 6. Double click the "Feed" stream. The general information about the stream will be displayed on the right side of screen. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams once composition and flow rate are specified for the inlet streams, the color of stream turns blue.

- 7. Add two more Material streams i.e. Drag and drop it into the flow sheet. Rename those streams as "Vapour-Outlet" and "Liquid-Outlet". These serves as output streams.
- 8. Add an energy stream from the object palette to the flowsheet section.
- 9. Below the Unit Operation tab on left, locate the "Conversion Reactor" block. Drag and drop into the flowsheet.



Specification for the inlet stream

Quantity	Value
Temperature, (°C)	25
Pressure, (atm)	1
Molar Flowrate (kmol/hr)	100
Composition	Nitrogen: 0.25
(Mol fraction)	Hydrogen: 0.75
	Ammonia: 0

10. Under "Tools" tab in select "Reaction Manager" tab. Towards the left of the screen locate a green colored button to choose the type of reaction i.e. Conversion reaction for the given problem. A dialogue box will appear, in which name of the equation and description about the equation can be mentioned. Select the checkboxes adjacent to the component names, give the stoichiometry of the reaction and choose appropriate base component. In this case the base component is "Nitrogen". Once base component is selected, stoichiometry is properly specified, a text "OK" appears in the stoichiometry tab. Change the phase to vapor phase and specify the given value of conversion in percentage and click on OK.

			Edit Conversion Re	eaction		
Identification	n					
Name	Ammonia-Formation					
Description	N2 + 3H2	>>2NH3				
Components	s/Stoichiome	try				
Name			Molar Weight	Include	BC	Stoich. Coeff.
Nitrogen			28.014000	•	•	-1
Hydrogen			2.015880	•		-3
Ammonia			17.031000	-		2
oichiometry	· <u>OX</u>	Bal	ance Heat of Reacti	on (kJ/kmol_BC	C) (25 °C)	-91,796.000000
toichiometry quation	v V2 + 3H2 -> Reaction Pa	Bal 2NH3	ance Heat of Reacti	on (kJ/kmol_BC	C) (25 °C)	-91,796.000000
toichiometry quation N Conversion Base Comp	v 0X N2 + 3H2> Reaction Par Ntrogen	Bal 2NH3 rameters	ance Heat of React	on (kJ/kmol_BC	C) (25 °C) Phase V	-91,796.000000
toichiometry quation Conversion Base Comp Conversion	V2 + 3H2> Reaction Pai Ntrogen [%, f(T)] =	2NH3 rameters 20	Heat of React	on (kJ/kmol_BC	C) (25 °C) Phase V	-91,796.000000

11. Now, all necessary credentials required for simulation are added. It should be connected in a proper sequence. Click on "Conversion Reactor" block in the flowsheet section. The general information about the block is displayed on the right. Under "connections" tab, for all streams click the dropdown button and select the appropriate streams. Under "Calculation Parameters" choose the Reaction Set and set Calculation Mode to "Isothermic" If all the connections are given correctly, all the blocks will turn blue.

- 12. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen.
- 13. To analyze/display the results, select on "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

Results

Stream Results

Simulation-Results			
Object	Feed	Vapour-Outlet	
Temperature	25.000000	25.000000	С
Pressure	1.013250	1.013250	bar
Mass Flow	851.541000	851.541000	kg/h
Molar Flow	100.000000	89.999810	kmol/h
Molar Fraction (Vapor Phase) / Nitrogen	0.250000	0.222222	
Molar Flow (Vapor Phase) / Nitrogen	25.000000	19.999958	kmol/h
Molar Fraction (Vapor Phase) / Hydrogen	0.750000	0.666667	
Molar Flow (Vapor Phase) / Hydrogen	75.000000	59.999873	kmol/h
Molar Fraction (Vapor Phase) / Ammonia	0.000000	0.111111	
Molar Flow (Vapor Phase) / Ammonia	0.000000	9.999979	kmol/h

Self-Learning Exercises

1. Can you determine the heat duty for the reaction?

2. Check if the backward reaction can be included? If so, assume, 2% of Ammonia formed dissociates to form Nitrogen and Hydrogen and determine the exit composition

Simulation of a CSTR for Liquid Phase Reaction

Objective

Develop a simple process sheet to determine the exit composition from a Continous stirred tank reactor (CSTR)

Data

Reaction: Ethylene glycol production in CSTR: Ethylene oxide reacts with water to form Ethylene Glycol

$$C_2H_4O_{(1)} + H_2O_{(1)} \rightarrow C_2H_6O_{2(1)}$$

Inlet stream: 26 m³/h of aqueous solution of Ethylene oxide with a mol fraction of 15% and rest water. Reaction carried out at 55 $^{\circ}$ C under atmospheric condition in CSTR of 2 m³

Reaction rate: $-r = kC_{EO}$

Where C_{EO} : Molarity of Ethylene oxide; k: rate constant = 0.005 1/s

DWSIM Blocks Used

Continous Stirred Tank Reactor (CSTR)

- 1. Start a new DWSIM Simulation (DWSIM VER 5.1 CLASSIC UI). Click on "New steady state Simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. Add 3 components for the simulation Ethylene oxide, Ethylene Glycol and Water
- 3. Ensure that all the components are added from same property package. Example: All the 3 components are selected from Chemsep database. Click "Next" button.
- 4. Select and add the property package and click "Next". Add the default flash algorithm for the simulation. Click "Next".
- 5. The flowsheeting section of simulation window will be opened. Drag and drop the Material stream from the object palette and rename the stream as "Feed". This serves as input.

- 6. On clicking the "Feed" block, general information about the block will be displayed on the left of the screen.
- 7. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams once composition and flow rate are specified for the inlet streams, the color of stream turns blue.

	X 7 1
Quantity	Value
Temperature, (°C)	55
Pressure, (bar)	1
Volumetric Flowrate (m ³ /h)	26
Composition	Ethylene oxide: 0.15
(mol fraction)	Ethylene glycol: 0
	Water: 0.85

Specification for the inlet stream

- 8. Add one more Material streams i.e. Drag and drop it into the flow sheet. Rename it as "Product". This serves as output stream.
- 9. Add an energy stream which is available in the object palette below the Material stream.
- 10. Below the Unit Operation tab, locate the "Continous Stirred Tank Reactor" CSTR block. Drag and drop into the flow sheet. Rename it as "CSTR".
- 11. Under "Tools" tab in select "Reaction Manager" tab. choose the type of reaction i.e. "Equilibrium reaction" for this problem. A dialogue box will appear. Give an appropriate name and description about the reaction.
- 12. Select the checkboxes adjacent to the component names, which has to be included in the reaction. Give the stoichiometry of the reaction and choose appropriate base component.
- 13. In this case the base component is "Ethylene Oxide". Once base component, stoichiometry is specified, a text "OK" appears in the stoichiometry tab. Specify the rate constant of the reaction.
- 14. By default, the basis is activity and liquid phase. In this case it has to be changed to Molar concentration and specify the phase as liquid.
- 15. Specify the rate constant of the reaction and click "OK".
- 16. Click on "CSTR-REC" block, the general information about the block is displayed on the right. Under "connections" tab, for all streams click the dropdown button

and select the necessary connections. If all the connections are given correctly, the blocks will turn blue.



- 17. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen.
- 18. To analyze/display the results, select on "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

23 | P a g e

Results

Stream Results

Results			
Object	Feed	Product	
Temperature	55.000000	55.000000	С
Pressure	1.000000	1.000000	bar
Mass Flow	30,089.868298	30,089.868298	kg/h
Molar Flow	1,372.672892	1,250.152614	kmol/h
Volumetric Flow	26.000000	24.497600	m3/h
Vapor Phase Volumetric Fraction	0.000000	0.000000	
Liquid Phase (Mixture) Density	1,157.302627	1,228.278229	kg/m3
Molar Flow (Mixture) / Ethylene oxide	205.900934	83.381606	kmol/h
Molar Flow (Mixture) / Ethylene glycol	0.000000	122.519160	kmol/h
Molar Flow (Mixture) / Water	1,166.771958	1,044.251848	kmol/h

Self-Learning Exercises

1. If the CSTR is replaced by PFR of same volume of 64 m length and 20 cm diameter, determine the exit composition

Simulation of a Flash Column

Objective

Develop a simple process flow sheet to estimate the liquid and vapour composition of multi-component mixture undergoing partial vaporization.

Data

Components: n-pentane, n-hexane, and n-heptane

Feed composition: 25 mol % n-pentane, 45 mol % n-hexane, and 30 mol % n-heptane

Basis: 100 kmol/h

Operating conditions

Temperature = $69 \,^{\circ}\text{C}$

Pressure = 1.013 bar

DWSIM Blocks Used

Gas-Liquid Separator

- 1. Start a new DWSIM Simulation (DWSIM ver 5.1 Classic UI). Click on "New steady state Simulation" as a template for new simulation.
- 2. The simulation configuration window will be opened. It shows a specification page. Add the three components n-pentane, n-hexane, and n-heptane. Ensure that all the components are added from same property package. Example: All the 3 components are selected from Chemsep database. Click "Next" button.
- 3. Specify the thermodynamic package as Raoult's law.
- 4. Customize the system of units for the present simulation and click "Next".
- 5. The flowsheeting section of simulation window will be opened. It is necessary to provide input and output streams for the unit operation to be performed. Drag and drop the Material stream available at the right, in the object palette. Rename the stream as "Feed-In". This serves as the input stream.
- 6. On clicking the "Feed-In" stream, general information about the stream will be displayed on the left side of screen. Specify the feed compositions, flow rate, temperature and pressure for the stream, once composition and flow rate are specified for the inlet stream, the color of stream turns blue.



- 7. Add two more Material streams i.e. Drag and drop it into the flowsheet. Rename those streams as "Vap-Out" and "Liq-Out". These serves as output streams.
- 8. Below the unit operation tab on left, locate the Gas-Liquid Separator block. Drag and drop into the flow sheet. Rename it as "Flash Column".

Quantity	Value
Temperature, (°C)	69
Pressure, (bar)	1.013
Molar Flowrate (kmol/h)	100
Composition (mole fraction)	n-pentane: 0.25
	n-hexane: 0.45
	n-heptane: 0.30

Specification for the inlet stream

- 9. Now, all necessary credentials required for simulation are added. It should be connected in a proper sequence. Click on "Flash Column" block, the general information about the block is displayed on the right. Under "connections" tab, for all streams click the dropdown button and select the necessary connections. If all the connections are given correctly, all the blocks will turn blue.
- 10. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen. It will be in the shape of Triangle.
- 11. To analyze/display the results, select on "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

Results

Stream Results

Simulation-Results				
Object	Feed-In	Liq-Out	Vap-Out	
Temperature	69.000000	69.000000	69.000000	С
Pressure	1.013000	1.013000	1.013000	bar
Mass Flow	8,687.835000	5,432.217763	3,255.617237	kg/h
Molar Flow	100.000000	60.565694	39.434306	kmol/h
Molar Fraction (Mixture) / N-pentane	0.250000	0.149588	0.404219	
Molar Flow (Mixture) / N-pentane	25.000000	9.059889	15.940111	kmol/h
Molar Fraction (Mixture) / N-hexane	0.450000	0.450284	0.449564	
Molar Flow (Mixture) / N-hexane	45.000000	27.271752	17.728248	kmol/h
Molar Fraction (Mixture) / N-heptane	0.300000	0.400128	0.146217	
Molar Flow (Mixture) / N-heptane	30.000000	24.234052	5.765948	kmol/h

Self-Learning Exercises

1. Re-run the simulation using SRK or PR thermodynamic model. Predict the percentage change in the vapour and liquid composition

2. Determine the following

a) Operating pressure at which the feed is completely vaporized at 69 $^{\circ}$ C

b) Operating temperature at which the feed is completely vaporized at 1.013 bar

3. Is a flash column object really necessitated to perform a flash operation in DWSIM? Explore Material stream and answer

Simulation of a Distillation Column

Objective

Develop a simple process flow sheet to estimate distillate and bottom composition of a distillation column

Problem statement

100 kmol/h of an equimolar mixture of benzene and toluene at 70°C and 1 atm pressure is to be separated by staged distillation column. A reflux ratio of 3 is used. Composition of benzene in the distillate should be 99% (by mol) toluene in the bottom should be 99% (mol). A total condenser and reboiler, both at 1 atm pressure are used. Determine the actual no. of stages, minimum reflux ratio and the minimum no. of stages for the operation.

DWSIM Blocks Used

Shortcut Column

Procedure

- 1. Start a new DWSIM Simulation (DWSIM VER 5.1 CLASSIC UI). Click on "New steady state Simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. Add the two components required for simulation Benzene and Toluene. Ensure that all the components are added from same property package. Example: All the 2 components are selected from Chemsep database. Click "Next" button.
- 3. Select and add the property package and click "Next". Add the default flash algorithm for the simulation. Click "Next".
- 4. The flowsheeting section of simulation window will be opened. Drag and drop the Material stream from the object palette. Rename it as "Feed". This serves as input stream.
- 5. On clicking the "Feed" stream, general information about the block will be displayed on the left of the screen. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams. Once composition and flow rate are specified for the inlet streams, the color of stream turns blue.

Specification for the inlet stream

Quantity	Value
Temperature, (°C)	70
Pressure, (atm)	1
Molar Flow rate (kmol/h)	100
Composition (mole fraction)	Benzene: 0.5
	Toluene: 0.5

- 6. Add two more Material streams i.e. Drag and drop them into the flow sheet. Rename them as "Distillate" and "Bottoms". These serves as output streams.
- 7. Add two energy streams, one is for condenser duty (C-Duty) and the other is for re-boiler duty (R-Duty).
- 8. Below the Unit Operation tab, locate the "Shortcut Column" block. Drag and drop into the flow sheet. Rename it as "DC".



9. Click on "DC" block, the general information about the block is displayed on the left of the screen. Provide calculation parameters as shown in the screenshot given below

hortcut Column: DC		ņ
Status	Calculated (23-02-2017 02:02:54))
Linked to		_
Connections		
Feed Stream	Feed V	چ 💉
Distillate Stream	Top	چ 🔊
Bottoms Stream	Bottoms 🗸	چ 💉
Condenser Duty	C-Duty 🗸	چ 💉
Reboiler Duty	R-Duty V	چ 💉
Calculation Parameters		
Light Key Compound (LK)	Benzene	~
Heavy Key Compound (HK)	Toluene	~
LK Mole Fraction in Bottoms	0.010000	
HK Mole Fraction in Distillate	0.010000	
Reflux Ratio	3.000000	
Condenser Type	Total O Partial	
Condenser Pressure	1.000000 atm	\sim
Reboiler Pressure	1.000000 atm	\sim
Property Package Settings		
Property Package	PP_1	¥ 🔅
Flash Algorithm	Default	× 🔅

- 10. Under Column configuration select "connections" tab. Click the dropdown button and give appropriate connections. If all the connections are given correctly, the blocks will turn blue.
- 11. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen.
- 12. To analyze/display the results, select on "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

Result				
Object	Feed	Distilalte	Bottoms	
Temperature	70.000000	80.368919	109.936927	С
Pressure	1.000000	1.000000	1.000000	atm
Molar Flow	100.000000	50.000000	50.000000	kmol/h
Molar Fraction (Mixture) / Benzene	0.500000	0.990000	0.010000	
Molar Flow (Mixture) / Benzene	50.000000	49.500000	0.500000	kmol/h
Molar Fraction (Mixture) / Toluene	0.500000	0.010000	0.990000	
Molar Flow (Mixture) / Toluene	50.000000	0.500000	49.500000	kmol/h

Result				
Object	DC			
Reflux Ratio	3.000000			
Minimun Reflux Ratio	1.104760			
Minimum Stages	9.109130			
Optimal Feed Stage	6.320107			
Condenser Duty	1,712.122379	kW		
Reboiler Duty	1,838.194911	kW		

Results

Self-Learning Exercises

1. Simulate the column with feed given at (i) Stage 5 (ii) Stage 15 of the distillation column. Make inferences appropriately.

2. Simulate the column at reflux ratio of 2. Discuss your results

Determination of Heat Duty of Heater

Objective

Develop a simple process flow sheet to determine the heat duty required to heat a fluid to a desired temperature

Data

Fluid: Water Inlet mass flow rate: 50 kg/h Inlet temperature: 25°C Outlet temperature: 90°C Pressure: 1 bar

DWSIM Blocks Used

Heater

- 1. Start a new DWSIM Simulation (DWSIM ver 5.1 Classic UI). Click on "New steady state Simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. It shows a specification page. Add the component "Water"
- 3. Specify the thermodynamic package as Raoult's law.
- 4. Select the system of units for the simulation and click "Next".
- 5. The flow sheeting section of simulation window will be opened. Drag and drop the Material stream available at the right, in the object palette. Rename the stream as "Flow-In". This serves as input stream.
- 6. Double click the "Flow-In" stream. The general information about the stream will be displayed on the right side of screen. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams once composition and flow rate are specified for the inlet streams, the color of stream turns blue.
- 7. Add one more Material stream i.e. Drag and drop it into the flow sheet. Rename the stream as "Flow-Out". This serves as the output stream.

- 8. Add an energy stream from the object palette to the flowsheeting section.
- 9. Below the Unit Operation tab on left, locate the Heater block. Drag and drop into the flow sheet. Rename it as "HEATER".

Quantity	Flow-In
Temperature, (°C)	25
Pressure, (bar)	1
Mass Flowrate (kg/h)	50
Composition (mass fraction)	Water: 1

Specification for the inlet stream

10. Click on "HEATER" block, the general information about the block is displayed on the right. Under "connections" tab, for all streams click the dropdown button and select the necessary connections. Under calculation type choose "Outlet Temperature". If all the connections are given correctly, all the blocks will turn blue.



- 11. Run the simulation by clicking on "Solve flow sheet" icon / button on the top corner of the screen.
- 12. To analyze/display the results, select on "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

Results

Stream Results

Simulation-Results						
Object	Flow-In	Flow-Out				
Temperature	25.000000	90.000000	С			
Pressure	1.000000	1.000000	bar			
Vapor Phase Volumetric Fraction	0.000000	0.000000				

Self-Learning Exercises

1. Determine the heat duty required to completely vaporize the water entering the heater at 25°C and at 1 bar pressure? What is the temperature of the vapour generated?

2. Is it possible to use the same heater block to determine the heat rejected, when hot fluid stream is cooled, say water from 90° C is cooled to 25° C at 1 bar?

Simulation of Heat Exchanger Using "Heater" and "Cooler" Blocks

Objective

Develop a simple process flow sheet to simulate heat exchanger using "heater" and "cooler" blocks and determine the heat duty and exit temperature of a stream

Problem statement (Adapted from Example 13.7, Seider et. al., 2008)

Hot Stream Fluid: Styrene Molar Flow rate = 150000 lb/h Inlet Temperature = 300 °F Exit Temperature = 178 °F Pressure = 50 psia **Cold Stream** Fluid: Toluene Molar Flow rate = 125000 lb/h Inlet Temperature = 100 °F Pressure = 90 psia

DWSIM Blocks Used

Heater and Cooler

- 1. Start a new DWSIM Simulation (DWSIM VER 5.1 CLASSIC UI). Click on "New steady state Simulation" as a template for new simulation
- 2. The simulation configuration window will be opened. Add two components required for the simulation Toluene and Styrene. Ensure that all the components are added from same property package. Example: The 2 components are selected from Chemsep database. Click "Next" button.
- 3. Select and add the property package and click "Next". Add the default flash algorithm for the simulation. Click "Next".

- 4. The flowsheeting section of simulation window will be opened. Drag and drop the Material streams from the object palette. Rename them as "Hot-In", "Hot-Out", and "Cold-In", Cold-Out".
- 5. Insert an Energy stream from the object pallet and Rename it as "Q-Stream".
- 6. On clicking any of these streams, general information about the stream will be displayed on the left of the screen. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams. Once composition and flow rate are specified for the inlet streams, the color of stream turns blue.

Quantity	Hot-In	Cold-In
Temperature, (°F)	300	100
Pressure, (psia)	50	90
Molar Flowrate (lb/h)	150000	125000
Composition (mass fraction)	Styrene: 1	Styrene: 0
	Toluene: 0	Toluene: 1

S	pecific	ation	for	the	inlet	streams
	peenne	auon	101	une	miet	Streams

- 7. Below the Unit Operation tab, locate the "Cooler" block. Drag and drop into the flow sheet. Rename it as "Cooler".
- 8. On clicking the cooler block, the information about the block will be displayed. Under "connections" tab, click the dropdown button and select the necessary connections. In calculation parameter, specify the calculation as "Outlettemperature"



9. Now, locate the "Heater" block. Drag and drop into the flow sheet. Rename it as "Heater".

- 10. On clicking the Heater block, the information about the block will be displayed. Under "connections" tab, click the dropdown button and select the necessary connections. No need to give a separate energy stream for heater. The "Q-stream" itself serves as energy stream for this also. In calculation parameter, specify the calculation as "Energy stream"
- 11. Once all the connections are given correctly, the blocks will turn blue. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen.
- 12. To analyze/display the results, select on "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

Results

Results: Material Streams						
Object	Cold-In	Cold-Out	Hot-In	Hot-Out		
Temperature	100.000000	254.199180	300.000000	178.000000	F	
Pressure	90.000000	90.000000	50.000000	50.000000	psi	
Mass Flow	1,25,000.000000	1,25,000.000000	1,50,000.000000	1,50,000.000000	lbm/h	

sults: Heater			Results: Cooler		
bject	Heater		Object	Cooler	Γ
Outlet Temperature	254.199164	F	Outlet Temperature	178.000000	t
leat Added	2,670.533188	kW	Heat Removed	2,670.533188	t

Reference

Seider, W. D., Seader, J. D. and Lewin, D. R. (2008). Product and Process Design Principles, Second Edn., John Wiley and Sons, Inc., New York.

Self-Learning Exercises

1. Determine the exit temperature of hot (styrene) and cold (toluene) streams, if heat duty removed from hot stream is 3 MW

2. How to perform simulation for a counter-current heat exchanger using two heaters?

3. Find out the inlet temperature of toluene if toluene should be heated to 250 $^{\circ}$ F using the available styrene feed

Detailed Simulation of a Heat Exchanger

Objective

Develop a simple process flow sheet with a shell and tube heat exchanger. Given the configuration details of a shell and tube heat exchanger and operating conditions of inlet streams, perform detailed simulation of the heat exchanger to determine the outlet temperature of fluid streams, shell and tube side pressure drops and the heat duty

Problem statement (Adapted from Example 13.7, Seider et. al., 2008)

An existing 2-8 shell and tube heat exchanger in a single shell is to be used to transfer heat to a toluene feed stream from a styrene product stream. The toluene enters the exchanger on the tube side at a flow rate of 125000 lb/hr at 100°F and 90 psia. The styrene enters on the shell side at a flow rate of 150000 lb/hr at 300°F and 50 psia. The exchanger shell and tubes are carbon steel of thermal conductivity 31 BTU/h °F ft. The shell has an inside diameter of 39 in. and contains 1024 tubes of ³/₄ in., 14 BWG, 16 ft long on 1 in. square pitch. 38 segmental baffles are used with a baffle cut of 25%. Fouling factors are estimated to be 0.002 (hr ft² °F/BTU) on each side. Determine the exit temperatures of the two streams, the heat duty, and the pressure drops.

DWSIM Blocks Used

Rigorous Heat Exchanger

- 1. Start a new DWSIM Simulation (DWSIM ver 5.1 Classic UI). Click on "New steady state simulation" as a template for new simulation.
- 2. The simulation configuration window will be opened. It shows a specification page. Add two components namely "styrene" and "toluene". Ensure that all the components are added from same property package. Click "Next" button.
- 3. Specify the thermodynamic package as Raoult's law.
- 4. Customize the units for the present problem (mass flow rate in lbm/h, Pressure in psi and Temperature in °F and so on as per problem statement) and click "Next".

- 5. The flow sheeting section of simulation window will be opened. Provide input and output streams for the unit operation to be performed. For heat exchanger two inlet and two outlet streams are required to be drawn.
- 6. Drag and drop two Material streams available at the right, in the object palette. Rename the stream as "Styrene-In" and "Toluene-In". These serves as the input streams.



7. On clicking the "Feed" block, general information about the block will be displayed on the right side of screen. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams once composition and flow rate are specified for the inlet streams, the color of stream turns blue.

Quantity	STYRENE-IN	TOLUENE-IN
Temperature, (°F)	300	100
Pressure, (psia)	50	90
Molar Flowrate (lb/hr)	150000	125000
Composition (mass fraction)	Styrene: 1	Styrene: 0
	Toluene: 0	Toluene: 1

S	necifica	tion for	• the	inlet	stream
\mathbf{D}	peeniea	1011 101	unc	mici	Sucam

- 8. Add two more Material streams i.e. Drag and drop it into the flow sheet. Rename those streams as "Styrene-Out" and "Toluene-Out". These serve as the output streams.
- 9. Below the Unit Operation tab on left, locate the "Heat Exchanger" block. Drag and drop into the flow sheet.
- 10. Click at the "Heat Exchanger" block in the flow sheeting window and connect the inlet and outlet streams to the heat exchanger appropriately. Under calculation parameters change the calculation parameters to "Shell and Tube Exchanger Rating" and specify the specifications for the heat exchanger by clicking at "Edit Shell and Tube Exchanger Properties" as shown below:



- 11. Run the simulation by pressing "Solve flow sheet" button on the top left corner of the screen.
- 12. To analyze/display the results, select the "Master property table" icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click "OK". The property table will be opened showing all the results as shown in the figure below.

Reference

Seider, W. D., Seader, J. D. and Lewin, D. R. (2008). Product and Process Design

Principles, Second Edn., John Wiley and Sons, Inc., New York.

Results

Results from heat exchanger block

Simulation-Results						
Object	HE-001					
Global Heat Transfer Coefficient (U)	51.651140	BTU/[ft2.h.R]				
Heat Exchange Area (A)	3,191.853337	ft2				
Heat Load	87,43,507.579325	BTU/h				
Cold fluid outlet temperature	249.306278	F				
Hot fluid outlet temperature	184.164546	F				
Logarithmic mean temperature difference LMTD	66.014761	F.				
Thermal Efficiency	71.605024	%				