## **CL-402: Chemical Process Technology**

July-November session, 2018

7<sup>th</sup> semester, Department of Chemical Engineering Indian Institute of Technology Guwahati, Guwahati

## **Tutorial 3**

**Use Aspen Plus V8.8 to solve all the problems.** 

## **Problem-1: Shortcut Distillation Calculation: DSTWU**

An equimolar mixture of benzene and toluene is to be separated by distillation to produce a distillate containing 90 mol% benzene and a bottom product that contains 89% toluene. The distillation column is to operate at 1 atm pressure and the feed to column is a saturated liquid. Use the DSTWU programme and the NRTL model to estimate:

a.the minimum reflux ration and the minimum number of stages to accomplish the separation. b. the actual number of stages and the location of the feed stage if the column is operated at 1.2 times the minimum reflux ratio.

## **Problem-2: Rigorous Distillation Calculations: RadFrac**

An equimolar mixture of benzene and toluene is to be separated by distillation to produce a distillate containing 90 mol% benzene and a bottom product that contains 98% toluene. The distillation column is to operate at 1 atm pressure and the feed to the column is a saturated liquid. Use the RADFRAC programme and the NRTL model to estimate **a.** the minimum reflux ratio and the minimum number of stages to accomplish the separation;

**b.** the actual number of stages and the location of the feed stage if the column is operated at 1.2 times the minimum reflux ratio.

**Problem 1** 

## **DSTWU**

- DSTWU performs *shortcut design calculations for single-feed, two-product distillation columns* with a partial or total condenser.
- DSTWU assumes constant molar overflow and constant relative volatilities.

DSTWU uses this	To estimate
method/correlation	
Winn	Minimum number of stages and optimum feed location at total reflux
Underwood	Minimum reflux ratio
Gilliland	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

For the specified recovery of light and heavy key components, DSTWU estimates:

•Minimum reflux ratio

•*Minimum number of theoretical stages* 

DSTWU then estimates one of the following:

Required reflux ratio for the specified number of theoretical stages
Required number of theoretical stages for the specified reflux ratio

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











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# **Problem 2**

## A Rigorous Distillation Calculation: RadFrac

## *RadFrac is a rigorous model for simulating all types of multistage vapour-liquid fractionation operations.* These operations include:

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

#### *RadFrac is suitable for:*

### •Two-phase systems

•Three-phase systems (only in equilibrium mode)

•Narrow and wide-boiling systems

•Systems exhibiting strong liquid phase nonideality

RadFrac can handle solids on every stage.

RadFrac can handle pumparounds leaving any stage & returning to the same stage or to a different stage.

RadFrac can model columns in which chemical reactions are occurring. Reactions can have fixed conversions, or they can be:

- •Equilibrium
- •Rate-controlled
- •Electrolytic

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 you can specify either Murphree or vaporization efficiencies. You can manipulate Murphree efficiencies 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).

You can use RadFrac to size and rate columns consisting of trays and/or packings. RadFrac can model both random and structured packings.











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Notestanding   Image: Statestanding   Image	Dynamics	Material Heat Load Work Vol.% Curv	ves   Wt. % Curves   Petroleum   Polymers   Soli	ds	
By Fordie   By Fordie <tr< td=""><td>Results</td><td></td><td></td><td></td><td>×</td></tr<>	Results				×
Stream Reules   Stream Reules   Summay   Summay   Substream   Occurspansion   Reules   Substream   Operating Costs   Stream Reules   Departing Costs   Stream Reules   Totulf-01   Operating Costs   Stream   Cutoregrener   Operating Costs   Stream Reules   Totulf-01   Operating Costs   Stream Reules   Totulf-01   Stream   Stream   Stream   Stream   Stream   Stream   Stream   Cutoregrener   Operating Costs   Stream   Stream </td <td>Profiles</td> <td>Display Streams + Format FULL</td> <td>Stream Table     Copy All</td> <td></td> <td></td>	Profiles	Display Streams + Format FULL	Stream Table     Copy All		
Summary   Summary   Summary   Summary   Substream: MUED   Note Free   Streams   Streams<	Stream Results	FEED	▼ DIST ▼ BOTTOM ▼		
• Mole Row kmol/nr       • Mole Row kmol/nr         • Mole Row kmol/nr       • States Massiss         • Mole Row kmol/nr       • States Massiss         • Reuting States       • Mole Row kmol/nr         • States Massiss       • States States         • Operations       • States States         • States Massiss       • TOLUE-01         • States Massiss       • States States         • States Massiss       • Total Row kmol/nr         • Total Row kmol/nr       1         • States Massiss       • Total Row kmol/nr         • Total Row kmol/nr       1         • States Massiss       • Total Row kmol/nr         • Total Row kmol/nr       1         • States Massiss       • Mole Row kmol/nr         • Charge Massiss       • Mole Row kmol/nr         • Interview Massiss       • Mole Row kmol/nr         • Katus Status       • Mole Row kmol/nr         • States Massiss       • Mole Row kmol/nr         • Charge Katus/sis       • Mole Row kmol/nr         • Katus Status       • Mole Row kmol/nr         • States Massis <t< td=""><td>Summary</td><td>Substream: MIXED</td><td></td><td>Stream Results</td><td></td></t<>	Summary	Substream: MIXED		Stream Results	
Sections Convergance Fowsheeting Options Sections	📜 Utilities	Mole Flow kmol/hr			
Image: Construction       Image: Construction         Image: Construction       Image: Construction <td>Reactions</td> <td>* BENZE-01 0.5</td> <td>0.489132 0.0108684</td> <td></td> <td></td>	Reactions	* BENZE-01 0.5	0.489132 0.0108684		
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Image: Streams   Image: Convergence   Image: Conv	Run Status	> TOLUE-01 0.5	0.0942007 0.976373		la de la companya de
Convergence   Convergence <	Streams	Mass Flow kg/hr			
CO2 Emissions   Streams (Custom)   Models   Streams (Custom)   Models   BENZE-01   0.458806   0.890732   0.001024   TOLUE-01   0.541134   0.109268   0.979898   Total Flow kmol/hr   1   0.54   0.46   Total Flow kmol/hr   1   0.54   0.6     Model Palette     Model Palette<	Convergence	> BENZE-01 39.0568	38.2079 0.848971		
Streams (Custom)   Madels   Models   Dynamic Configuration   Total Flow kmol/hr   1   0.54   0.458   Simulation     Model Palette     Material     Distle   Material     Check Status     Neture Check Status	CO2 Emissions	* TOLUE-01 46.0703	4.68704 41.3832		
Image: Nodels   Equipment   Dynamic Configuration   Total Flow kg/hr   1   0.54   0.46     Total Flow kg/hr   85.1271   42.8949   42.2322     Model Palette     Model Palette     Model Palette     Image: Column Reactors Pressure Changers Manipulators Solids Separators User Models     Model Palette     Model Palette     Image: Column Reactors Pressure Changers Manipulators Solids Separators User Models     Image: Column Reactors Pressure Changers Manipulators Solids Separators User Models     Image: Column Reactors Pressure Changers Manipulators Solids Separators User Models     Image: Column Reactors Pressure Changers Manipulators Solids Solids Separators User Models     Image: Column Reactors Pressure Changers Manipulators Solids Solids Separators User Models     Image: Column Reactors Pressure Changers Manipulators Solids Solids Separators User Models     Image: Column Reactors Pressure Changers Manipulators Solids Solids Separators User Models     Image: Column Reactors Pressure Changers Reac	Streams (Custom)	Mass Frac			
Image: Simulation   Image: Simulation <td>Z Equipment</td> <td>BENZE-01 0.458806</td> <td>0.890732 0.0201024</td> <td></td> <td></td>	Z Equipment	BENZE-01 0.458806	0.890732 0.0201024		
Image: Simulation     Image: Simulation     Image: Simulation     Image: Safety Analysis     Image: Safety Analysis <t< td=""><td>Dynamic Configuration</td><td>* TOLUE-01 0.541194</td><td>0.109268 0.979898</td><td></td><td></td></t<>	Dynamic Configuration	* TOLUE-01 0.541194	0.109268 0.979898		
Image: Simulation     Model Palette     Model Palette     Image: Stafety Analysis     Image: Stafety Analysis </td <td>&lt;[] →</td> <td>Total Flow kmol/hr 1</td> <td>0.54 0.46</td> <td></td> <td></td>	<[] →	Total Flow kmol/hr 1	0.54 0.46		
Simulation     Model Palette     Model Palette     Image: Columns     Mixers/Splitters     Separators     Exchangers     Columns     Reactors     Pressure Changers     Maipulators     Solids	Properties	> Total Flow kg/hr 85.1271	42.8949 42.2322		
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Safety Analysis       Mixers/Splitters       Separators       Exchangers       Columns       Reactors       Pressure Changers       Manipulators       Solids       Solids       Separators       User Models         Image: Separators		Model Palette			* 1 ×
Image: Second	Safety Analysis	Mixers/Splitters Separato	ors Exchangers Columns Reactors I	Pressure Changers Manipulators Solids Solids Separators User Mod	els
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A Cut METCBAR → Copy→ Paste Clipboard METCBAR → Next Next	Nun       Step       Stop       Reset       Control Panel       Model Summary       Input © Stream Summary       Stream Analysis       Heat Exchanger       Pressure Relief       Pressure Relief       Temperature       Temperature <th></th> <th></th>		
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Rate-Based Modelin Analysis	EU Model components		
Convergence     Dynamics	Calculated molar reflux ratio     1.14       Calculated bottoms rate [kmol/hr]     0.46		
🕨 🔯 EO Modeling 🦷	Calculated boilup rate [kmol/hr] 1.09295 For a flow of 1 kmol/hr		
Results	Calculated distillate rate [kmol/hr] 0.54		
Stream Results	Condenser / top stage temperature [C] 81.014/		
🕎 Stream Results (Cus 🗉	Condenser / top stage pressure [bar]		
🛃 Summary	$\frac{\text{Condenser / top stage field duty [Carsec]}}{\text{Condenser / top stage field duty }} = 2393 \text{ cal/sec,}$		z
Utilities	Condenser / top stage subcolica daty		
Convergence	$\frac{condenser/top stage free water reflux ratio}{condenser/top stage free water reflux ratio} = 2414 cal/sec.$		
Flowsheeting Options	Rehoiler pressure [har] 1		
🕨 🚞 Model Analysis Tools	Reboiler temperature [C] 109 138		
EO Configuration	Rebailer best duty [cs]/sec] 2414.48		
A Results Summary	Total feed stream (O2e flow [kg/kr] 0		
• [	Total needust stream CO2e flow [kg/m]		
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🛃 EO Variables	Т	FO CO	mnositions   K	-Values Hydr	aulics   Reaction	ns Efficiencies P	roperties Key Comr	ionents   Then	mal Analysis	lydraulic Analys	is   Rubble Dew	Points					
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locks	Vie	w All	- Ba	isis Mole	-												
Specifications		Stage	Temperature	Pressure	Heat duty	Liquid from (Mole)	Vapor from (Mole)	Liquid feed (Mole)	Vapor feed (Mole)	Mixed feed (Mole)	Liquid product (Mole)	Vapor product (Mole)	Liquid enthalpy	Vapor enthalpy	Liquid flow (Mole)	Vapor flow (Mole)	
Sizing and Rating		4	<u>с</u> -	bar 🔫	cal/sec 🝷	kmol/hr 🔹	kmol/hr +	kmol/hr 🝷	kmol/hr 🝷	kmol/hr 👻	kmol/hr 🔫	kmol/hr 🝷	cal/mol 🝷	cal/mol 🔫	kmol/hr 🝷	kmol/hr 🔫	
Rate-Based Modelin	\$	1	81.6147	1	-2393.74	1.1556	0	0	0	0	0.54	0	12927.1	20734.3	0.6156	0	
Convergence	*	2	84.1283	1	0	0.605712	1.1556	0	0	0	0	0	12068.9	20384.3	0.605712	1.1556	
Dynamics	•	3	86.6995	1	0	0.597632	1.14571	0	0	0	0	0	11270.9	19995	0.597632	1.14571	
EO Modeling	>	4	88.9143	1	0	0.592036	1.13763	0	0	0	0	0	10642.6	19632.1	0.592036	1.13763	
Profiles	*	5	90.5595	1	Tom	0.588565	1.13204	ition	<sup>o</sup> nrofi	lo in	the co		10208.1	19344.8	0.588565	1.13204	
Stream Results	3	6	91.6537	1		1.586537	1.12856		0.00272021				9933.25	19145	0.586537	1.12856	
🔂 Stream Results (Cus	ļ.	7	92.3314	1	0	1.58072	1.12382	0.99728	0	0	0	0	9768.38	19017.6	1.58072	1.12382	
Summary ities	3	8	93.4127	1	0	1.5763	1.12072	0	0	0	0	0	9513.39	18808.4	1.5763	1.12072	
actions	\$	9	95.0173	1	0	1.57076	1.1163	0	0	0	0	0	9152.32	18484.2	1.57076	1.1163	
ivergence	*	10	97.1849	1	0	1.56471	1.11076	0	0	0	0	0	8694.75	18018.5	1.56471	1.11076	
Arsheeting Options		11	99.775	1	0	1.55957	1.10471	0	0	0	0	0	8188.58	17418.1	1.55957	1.10471	
Canfinantian *	>	12	102.463	1	0	1.55607	1.09957	0	0	0	0	0	7703.9	16740.8	1.55607	1.09957	
mellis oj 🔸	*	13	104.883	1	0	1.55416	1.09607	0	0	0	0	0	7297.68	16080	1.55416	1.09607	
erties	*	14	106.808	1	0	1.5533	1.09416	0	0	0	0	0	6992.08	15517.8	1.5533	1.09416	
lation	4	15	108.199	1	0	1.55295	1.0933	0	0	0	0	0	6779.7	15090.3	1.55295	1.0933	
nocom	1	16	109.138	1	2414.48	0.46	1.09295	0	0	0	0.46	0	6639.89	14791.2	0.46	1.09295	
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Stream Results	> From			COLUMN	COLUMN				
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Utilities	Substream: MIXED								155
Reactions	Phase:		Mixed	Liquid	Liquid	04			
Convergence Elowsbeeting Options	Component Mole Flow					Stre	eam results		
Model Analysis Tools	> BENZE-01	KMOL/HR	0.5	0.488129	0.0118706				
EO Configuration	> TOLUE-01	KMOL/HR	0.5	0.0518706	0.448129				
Results Summary	Component Mole Fraction								
Streams	BENZE-01		0.5	0.903943	0.0258057				
Convergence	> TOLUE-01		0.5	0.0960567	0.974194				
Operating Costs	Component Mass Flow								
Streams (Custom)	BENZE-01	KG/HR	39.0568	38.1296	0.92726				
🧭 Models	> TOLUE-01	KG/HR	46.0703	4.77939	41.2909				
Equipment	> Component Mass Fraction								
	BENZE-01		0.458806	0.888616	0.0219635				
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Properties	LA L PL	KHOLSID.		0.54	0.40				
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6 )	Mixers/Splitt	ers Separators	Exchangers Co	lumns Reacto	ors Pressure Cha	ingers Manipulators S	Solids Solids Separators User Model	•	
Safety Analysis		69	6		a 62		a La		
🚯 Energy Analysis	I ─── - ( U	• U •	Ų, -	Ŭ - U₅	₹ - 18				
	Material	Disti	RadFrac Ext	tract Multi	Frac SCFrac	PetroFrac Cont	Sep BatchSep		4
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Summary	Calculated boilup rate [kmol/hr]	1.12358		
Reactions	Calculated distillate rate [kmol/hr]	0.54		
🛛 🔯 Convergence	Condenser / top stage temperature [C]	81.6536	Condenser and reboiler heat duty.	
Flowsheeting Options	Condenser / top stage pressure [bar]	2461.54		
EO Configuration	Condenser / top stage reat duty [car/sec]	-2401.34		E
Results Summary	Condenser / top stage reflux rate [kmol/hr]	0.648		
Run Status	Condenser / top stage free water reflux ratio			
Convergence	Reboiler pressure [bar]	1		I
Operating Costs	Reboiler temperature [C]	109.039		
CO2 Emissions	Reboiler heat duty [cal/sec]	2482.05		
Streams (Custom)	Total feed stream CO2e flow [kg/hr]	0		
Z Equipment	Total product stream CO2e flow [kg/hr]	0		
Dynamic Configuration	Net stream CO2e production [kg/hr]	0		
• [	Utility CO2e production [kg/hr]	0	1	
Properties				Change grid orientatio
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imulation <	Capital: USD Utilities: USD/Year 🜑 Energy Savings: MW ( %) 💽 Exchangers - Unknown: 0 OK: 0 Risk: 0 🚱	♡					
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Stream Results (Custor	Product streams						
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COLUMN	DIST 1 Liquid Mole kmol/hr Feed basis						
Setup	BOTTOM 11 Liquid Mole kmol/hr Feed basis	E					
<ul> <li>Specification Sumn</li> <li>Design Specification</li> <li>Vary</li> <li>Efficiencies</li> <li>Properties</li> <li>Reactions</li> <li>Block Options</li> <li>User Subroutines</li> <li>Configuration</li> </ul>	Pseudo streams       Name       Pseudo Stream       Stage       Internal Phase       Reboiler Phase       Reboiler       Pumparound       Flow       Units         Type       Stage       Internal Phase       Reboiler Phase       Reboiler       Pumparound       ID       Conditions       Flow       Units						
Properties	m I						
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sults Available Check Status	Tutorial 3 - PowerPoint 100%						
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Reactions	Phase:		Liquid	Liquid	Mixed			E.		
Convergence	> Component Mole Flow		The second							
Model Analysis Tools	> BENZE-01	KMOL/HR	0.00647735	0.493523	0.5					
EO Configuration	> TOLUE-01	KMOL/HR	0.453523	0.0464773	0.5	Stream results				
Results Summary	Component Mole Fraction		4							
Streams	BENZE-01		0.0140811	0.913931	0.5					
Convergence	> TOLUE-01		0.985919	0.0860691	0.5					
Operating Costs	Component Mass Flow									
Streams (Custom)	BENZE-01	KG/HR	0.505969	38.5509	39.0568					
🛃 Models	> TOLUE-01	KG/HR	41.7878	4.28245	46.0703					
Equipment	Component Mass Fraction									
	BENZE-01		0.0119632	0.900021	0.458806					
T Proportion	> TOLUE-01		0.988037	0.0999793	0.541194					
roperues	J. L. M. L. M.	KLOLAID	0.10	0.64						
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S Energy Analysis		- ( -	Į -	V - U	f - M					
	Material	Distl	RadFrac	tract Multi	iFrac SCFrac	PetroFrac ConSep BatchSep		L		
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Summary	Calculated boilup rate [kmol/hr]	2.03258	_	
Reactions	Calculated distillate rate [kmol/hr]	0.54		
Convergence	Condenser / top stage temperature [C]	81.4447	Condenser and reboiler heat duty.	
Flowsheeting Options	Condenser / top stage pressure [bar]	1		
EO Configuration	Condenser / top stage neat duty [cal/sec]	-4408.84		
Results Summary	Condenser / top stage subcooled duty	1.62		
😡 Run Status	Condenser / top stage free water reflux ratio	1.02		
Streams	Reboiler pressure [bar]	1		2
Operating Costs	Reboiler temperature [C]	109.571		
CO2 Emissions	Reboiler heat duty [cal/sec]	4490,59		
Streams (Custom)	Total feed stream CO2e flow [kg/hr]	0		
Models	Total product stream CO2e flow [kg/hr]	0		
Dynamic Configuration	Net stream CO2e production [kg/hr]	0		
() +	Utility CO2e production [kg/hr]	0		·
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### We have found three column designs that meet the required composition specifications.

Their parameters are shown in the following table:

Reflux ratio	1.14	1.2	3
No. of stages	16	15	11
Feed stage	7	7	5
Reboiler heat duty (cal/sec)	2414	2482	4490
condenser heat duty (cal/sec)	2393	2461	4468

#### **Summary**

In a similar fashion, we can find other choices of column parameters that would meet the composition specifications. So the question is which one of the many possible configurations should be used. To answer that question, one has to bring other factors. If costs were the only consideration, then there would be a trade-off between capital costs and operating (heat and cooling) costs.

From the table above, we can see that as the reflux ratio increases, the number of stages (and therefore column height) decreases, thereby reducing that part of the capital cost. However, the vapor and liquid flow rates increase, so a larger diameter column is needed, which increases the capital cost. Also as the reflux ratio increases, the amount of liquid per unit of product that needs to be boiled in the reboiler increases, as does the amount of vapor that needs to be condensed. These increase the capital costs of these two heat exchangers, and more importantly the ongoing energy costs of both units. [Note that increasing the reflux ratio to 3 from 1.25 almost doubled the energy requirements.]

# In next Tutorial, we will Perform the steady-state economic optimization of the distillation column based on total annual cost (TAC).

THE END