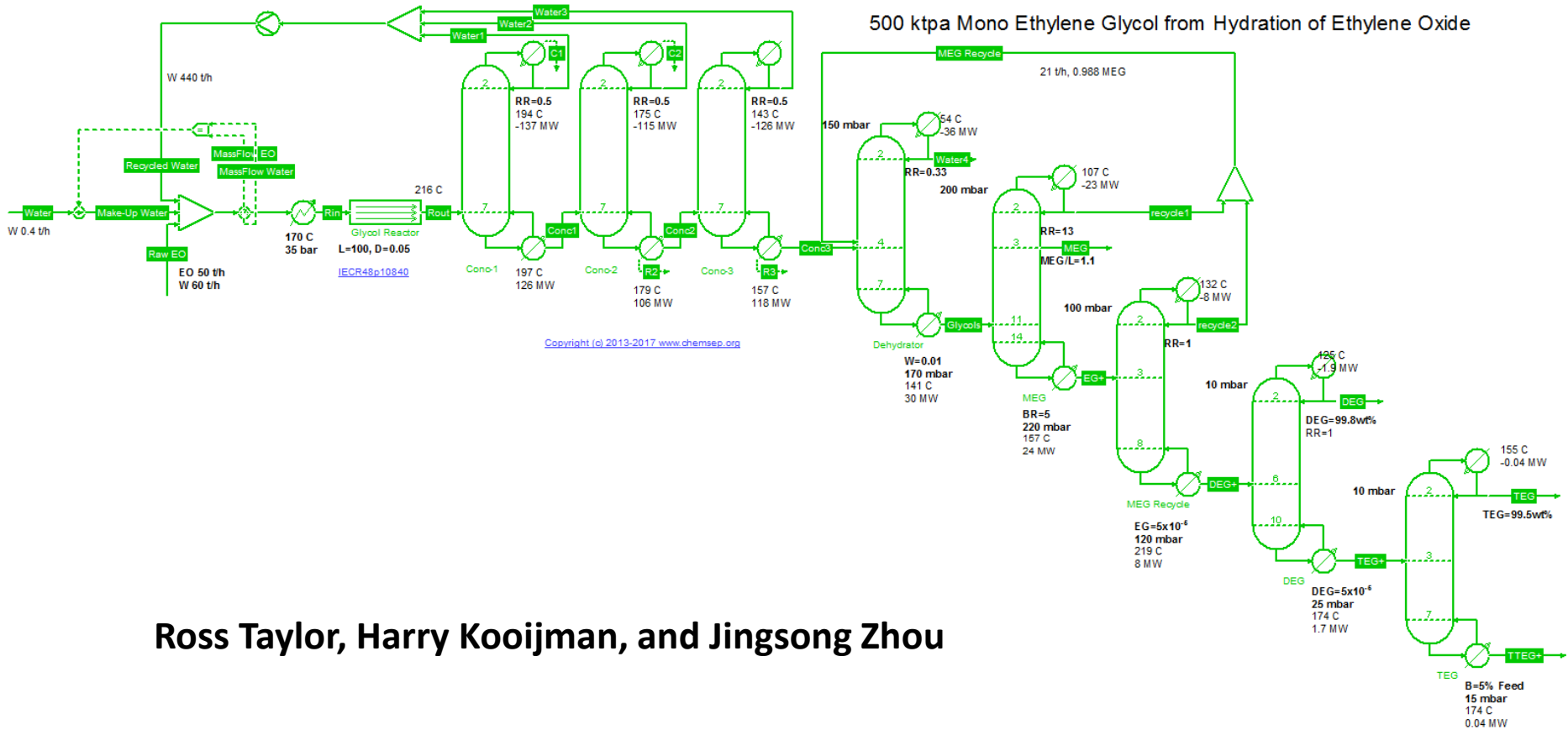


# Process Optimization using CAPE-OPEN Tools



Ross Taylor, Harry Kooijman, and Jingsong Zhou

# Outline

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- Rating and Cost Estimation
- Export to Column Vendor Tools
- Faster Rate-Based Column Simulations
- Iconography
- Equation-Oriented (and Rate-Based) Parallel Column Model
- Other Topics

# Column Rating and Cost Estimation in ChemSep

**Pointer hovers over column icon to display summary which includes cost estimates**

name: Dehydrator  
type: ChemSep  
status: solved

Solved in 7 iterations to 0.000001  
 Reflux ratio = 0.33 (-)  
 Qcondenser[1]=-35.9989 (MW) RR=0.33 (molar)  
 Water mole fraction = 0.01 (-)  
 Qreboiler[8]=30.567 (MW) BR=1.211989 (molar)  
 Recoveries: Water / Ethylene glycol  
 T[1]=52.35 (C) p[1]=0.14 (bar) Top: 0.993741 / 0.0000141436  
 T[4]=64.37 (C) p[4]=0.146667 (bar) Feed1: 0.994066 / 0.753131 Feed2: 0.00593413 / 0.246869  
 T[8]=138.53 (C) p[8]=0.16 (bar) Bottom: 0.00625885 / 0.999986  
 Section 1: M25Y D=3.99 (m) H=4.2 (m)  
 Section 2: M250Y D=4.24 (m) H=3.57 (m)  
 Total height=10.38 (m)  
 Total Annual.Cost (k\$/yr)=6098

Stream	Raw EO	Rin	Rout	Conc1	Conc2	Conc3	Conc4	Conc5	Conc6	Conc7	Conc8	Conc9	Conc10
Pressure	35	30	20.9997	14	9	9	9	9	9	9	9	9	9
Temperature	25	170	211.951	197.46	179.	179.	179.	179.	179.	179.	179.	179.	179.
Flow rate	110	551.009	551.009	385.825	251.	251.	251.	251.	251.	251.	251.	251.	251.
Mass frac Water	0.545455	0.909017	0.873899	0.819872	0.	0.	0.	0.	0.	0.	0.	0.	0.
Mass frac Monoethylene glycol	0	6.82976e-08	0.115729	0.185356	0.253983	0.577509	0.934283	0.99979	2.84036e-05	1.18991e-13	1.01506e-22	1.01506e-22	1.01506e-22
Mass frac Diethylene glycol	0	6.35044e-13	0.00982756	0.0140424	0.0215419	0.0490441	0.0597892	1.01572e-11	0.99808	0.00105985	4.76897e-08	4.76897e-08	4.76897e-08
Mass frac Triethylene glycol	0	1.98987e-13	0.000482241	0.000703351	0.00107899	0.00246851	0.00299508	3.51574e-11	0.00191137	0.994417	0.440281	0.440281	0.440281
Mass frac Tetraethylene glycol	0	7.77372e-15	1.77356e-05	2.5342e-05	3.88763e-05	8.86091e-05	0.000107842	7.37472e-19	1.14083e-08	0.00452354	0.559719	0.559719	0.559719
Mass frac Ethylene oxide	0.454545	0.0009785	0.000233998	1.79989e-08	5.40778e-09	1.58481e-12	1.11989e-24	0	0	0	0	0	0
MolecularWeight				18.3079	18.4245	19.147	53.4274	61.381	108.112	148.857	157.344	157.344	157.344
				Liquid phase									
MolecularWeight	24.8329	19.0389	19.816	20.8989	22.488	32.9251	63.3141	82.036	108.177	150.261	172.01	172.01	172.01

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TEG

Document Explorer | Watch | Log | Solved | 30 warnings

Overlaid images not to same scale

# Column Rating and Cost Estimation in ChemSep

The screenshot displays the ChemSep (TM) (CAPE-OPEN) - Dehydrator interface. The top part shows a process flow diagram with a Glycol Reactor, a Dehydrator, and several distillation columns. The bottom part shows the 'Rating' panel for the dehydrator column, which includes various input parameters and two data tables.

**Rating Panel Inputs:**

- Reference: ChemSep CO Unit 0
- Default internals: Sieve Zlt
- Default system factor: 1
- Default fraction of flood: 0.75
- Default efficiency: 1
- Default height liq. feed (m): 0.8
- Sump residence times (s): 20
- Reboil: 200
- Product: 200
- System factors: Koch (selected), Norton, Specified
- Efficiencies: Duss-Taylor, Traditional (selected)

**Table 1: Column Rating Data**

Section	1	2
Start stage	2	4
End stage	3	7
Internal type	M252Y	M250Y
System factor	1	1
Flood fraction	0.75	0.75
Method slope equilibrium	Ethylene glycol	Water
Efficiency estimated	0.21	0.44
HETS estimated (m)	2.068	0.916
Flow parameter	0.002	0.042
Capacity factor (m/s)	0.126	0.088
Diameter section (m)	3.99	4.24
Design stage	2	7
Height section (m)	4.2	3.57
Diameter (m)	4.24	
Height (m)	10.38	

**Table 2: Simple column costing**

ACCR (1/year)	0.32	Shell TIC (k\$)	461
Uptime (hrs/year)	8160	Internals TIC (k\$)	338
Materials	1	Condenser TIC (k\$)	1643
M&S Index (\$)	1400	Reboiler TIC (k\$)	1477
Fuel price (\$/GJ)	8	Condenser OPEX (k\$/yr)	74
	(1 bbl oil = 6.1 GJ)	Reboiler OPEX (k\$/yr)	4770
		Total Annual Cost (k\$/yr)	6098

**Table 3: Process Stream Data**

MEG	DEG	TEG	TTEG+	Unit
0.201538	0.01	0.01	0.015	bar
15.296	117.058	150.914	170.887	°C
3.7782	5.47049	0.255513	0.0153945	ton / h
0.00020978	0	0	0	
0.99979	2.84036e-05	1.18991e-13	1.01506e-22	
1.01572e-11	0.99898	0.00105985	4.768897e-08	
3.51574e-11	0.00181137	0.994417	0.440281	
7.37472e-19	1.14083e-08	0.00452354	0.559719	
0	0	0	0	
1.381	108.112	149.857	157.344	
2.038	108.177	150.281	172.01	

Open ChemSep GUI to see new rating panel with cost estimation

# Column Rating and Cost Estimation in ChemSep

- **Desire to compare process lineups on economic basis**
  - Need for basic cost information in PME
  - Actual cost calculations performed in UO
  
- **Simple cost functions in ChemSep**
  - Sum costs of vessel, internals, and heat exchangers
  - Add energy cost (but pumping costs ignored here)
  - To be documented

Simple column costing

ACCR (1/year)	<input type="text" value="0.32"/>	<input type="button" value="Copy"/>	Shell TIC (k\$)	461
Uptime (hrs/year)	<input type="text" value="8160"/>		Internals TIC (k\$)	338
Materials	<input type="text" value="1"/> <input type="text" value="Carbon Steel"/>		Condenser TIC (k\$)	1643
M&S Index (\$)	<input type="text" value="1400"/>		Reboiler TIC (k\$)	1477
Fuel price (\$/GJ)	<input type="text" value="8"/> (1 bbl oil = 6.1 GJ)		Condenser OPEX (k\$/yr)	74
			Reboiler OPEX (k\$/yr)	4770
			<b>Total Annual Cost (k\$/yr)</b>	<b>6098</b>

# Export to Vendor Tools

The screenshot displays the ChemSep (TM) (CAPE-OPEN) - Dehydrator interface. The main window shows a process flow diagram with various units including a Glycol Reactor, a Dehydrator, and several distillation columns. A McCabe-Thiele tray design window is open in the foreground, showing design parameters and a tray cost table. A red arrow points to the 'Vendor Tools' button in the McCabe-Thiele window.

**McCabe-Thiele Tray Design Parameters:**

Section	1	2
Start stage	2	4
End stage	3	7
Internal type	M252Y	M250Y
System factor	1	1
Flood fraction	0.75	0.75
Method slope equilibrium	Ethylene glycol	Water
Efficiency estimated	0.21	0.44
HETS estimated (m)	2.068	0.916
Flow parameter	0.002	0.042
Capacity factor (m/s)	0.126	0.088
Diameter section (m)	3.99	4.24
Design stage	2	7
Height section (m)	4.2	3.57
Diameter (m)	4.24	
Height (m)	10.38	

**Simple column costing:**

ACCR (1/year)	0.32	Copy	Shell TIC (k\$)	461
Uptime (hrs/year)	8160		Internals TIC (k\$)	338
Materials	1	Carbon Steel	Condenser TIC (k\$)	1643
M&S Index (\$)	1400		Reboiler TIC (k\$)	1477
Fuel price (\$/GJ)	8	(1 bbl oil = 6.1 GJ)	Condenser OPEX (k\$/yr)	74
			Reboiler OPEX (k\$/yr)	4770
			Total Annual Cost (k\$/yr)	6098

**Process Flow Diagram Labels:** Water, Water1, Water2, Water3, Recycled Water, Make-Up Water, Raw EO, MassFlow EO, MassFlow Water, Rin, Glycol Reactor, Route, Conco1, Conco2, Conco3, MEG Recycle, Dehydrator, Glycol, MEG, recycle1, recycle2, DEG, TEG, TTEG+.

**Click on Vendor Tools  
Save file in desired format Open  
vendor tool**

## KG Tower from Koch Glitsch

**LOADINGS**

Project Name: ChemSep CO Unit Operation "Dehydrator" in COFE Flo  
 Tower Name: Tower  
 Case Name: Case

	Load 1	Load 2
Zone	S1	S2
Description	Max.load	Max.load
Tray or Bed Number	2	4

**Vapor**

	Load 1	Load 2
Mass Rate	kg/hr 54450.14	40340.64
Density	kg/m3 0.093344	Calc 0.095963
Std. Actual Vol.Flow	m3/s 162.04	116.77
Viscosity	cP 0.010563	0.011024
Min. Rate	% 0.00	0.00
Max. Rate	% 0.00	0.00

**Liquid**

	Load 1	Load 2
Mass Rate	kg/hr 13489.81	129584.9
Density	kg/m3 986.2022	981.1357
Volume Rate	m3/hr 13.679	132.076
Surface Tension	dyne/cm 67.58926	57.03806
Viscosity	cP 0.526234	2.319535
Min. Rate	% 0.00	0.00
Max. Rate	% 0.00	0.00

System Factor: 1.00    Load OK    Load OK

Min Design Max

Select Design :    TRAYS    **PACKINGS**    DEMIST

**PACKED TOWER DESIGN**

Project Name: ChemSep CO Unit Operation "Dehydrator" in COFE Flowsheet  
 Tower Name: Tower  
 Case Name: Case

	Load 1	Load 2
Zone	S1	S2
Description	Max.load	Max.load
Bed Number	2	4

**Packing Type**

	Load 1	Load 2
Packing Type	FLEXIPAC® (Metal)	FLEXIPAC® (Metal)
Packing Size	250Y	250Y
	Effic.	Effic.

**Tower Diameter** mm: 4190.00    3950.00

**Number of Layers**: 0.0    0.0

**Packing height** mm: 0.00    0.00

**Capacity, Const. L/V** %: 73.08    82.31

**System Limit** %: 58.49    49.59

**Fs** m/s\*(kg/m3)^0.5: 3.59    2.95

**Cv** m/s: 0.114    0.094

**Liquid Load** m3/hr/m2: 0.99    10.78

**Pressure Drop** mbar/m: 3.598    2.976

## SulCol from Sulzer ChemTech

SULCOL 3.2.20

File Edit Project Window Help

Unit Type: SI Material: AISI No NTS/HETP

Loadings - C:\Users\Harry.Kooijman\AppData\Local\Temp\test.sulcol

**Sec. 1**

Packing

Diam [mm] Fluid Data Packing Design Packing-Type Height [m] NTS req. HETP [mm]

4190 S1 stages 2(max)/' Packing1 M250.Y 3.990 0.0 0

Flows

	G [kg/h]	L [kg/h]	$\rho_G$ [kg/m <sup>3</sup> ]	$\rho_L$ [kg/m <sup>3</sup> ]	$\sigma$ [mN/m]	$\eta_L$ [cP]	$\eta_G$ [cP]	Cap [%]	F-F [Pa <sup>0.5</sup> ]	Liq. load [m <sup>3</sup> /m <sup>2</sup> h]	$\Delta p / \Delta z$ [mbar/m]	hl [%]	dp [mbar]
Top	54450.1	13489.8	0.093	986.20	67.59	0.526	0.0106	62.1	3.59	0.99	4.04	1.6	12.76
Btm	40939.1	13509.9	0.093	986.21	67.62	0.522	0.0106	48.4	2.70	0.99	2.35		

Text Section 1 System factor 1.00  Geom. Details

**Sec. 2**

Packing

Diam [mm] Fluid Data Packing Design Packing-Type Height [m] NTS req. HETP [mm]

3950 S2 stages 4(max)/' Packing2 M250.Y 2.940 2.0 1470

Flows

	G [kg/h]	L [kg/h]	$\rho_G$ [kg/m <sup>3</sup> ]	$\rho_L$ [kg/m <sup>3</sup> ]	$\sigma$ [mN/m]	$\eta_L$ [cP]	$\eta_G$ [cP]	Cap [%]	F-F [Pa <sup>0.5</sup> ]	Liq. load [m <sup>3</sup> /m <sup>2</sup> h]	$\Delta p / \Delta z$ [mbar/m]	hl [%]	dp [mbar]
Top	40340.6	129584.9	0.096	981.14	57.04	2.320	0.0110	84.0	2.95	10.78	3.88	4.6	9.59
Btm	38965.3	65074.3	0.098	980.71	56.86	2.304	0.0110	68.6	2.82	5.41	2.64		

Text Section 2 System factor 1.00  Geom. Details

Total sections Column data

**2** p top [mbar] 146.70  $\Delta p$  total [mbar] 22.35

Current Section: 1

Sulzer Num Off Caps Off



# New: Export to Vendor Tools

## WinSorp from Raschig GmbH

WINSORP - Raschig Tower Design Program

Process File Warnings Info.. Help End Warning Message

Fluid Dynamics 1.1.3

Units:  SI Units  US Units

**Input values**

**Bed Position**

Column diameter mm  
Flood factor %  
Bed height mm

**Liquid**

Flow rate kg/h  
Density kg/m<sup>3</sup>  
Viscosity mPa.s  
Surface tension mN/m

**Gas**

Flow rate kg/h  
Density kg/m<sup>3</sup>  
Viscosity mPa.s  
Turn up/down %  
System factor / Foam factor  Calculate

**Packing**

Active  Active  Active  Active

**Section 1 - Input**

S 1  
Stage 2  
4190  
3990  
13489.81  
986.2022  
0.526234  
67.58926  
133.3333  
54450.14  
0.0933436  
0.0105633  
100  
1  
Raschig Pak 250 Y Metal

**Section 2 - Input**

S 2  
Stage 4  
3950  
2940  
129584.9  
981.1357  
2.319535  
57.03806  
133.3333  
40340.64  
0.0959631  
0.0110238  
100  
1  
Raschig Pak 250 Y Metal

**Section 3 - Input**

Picture

**Section 4 - Input**

Picture

**Section 1**

Column ChemSep CO Unit Operation "[I  
Remark Section #0

**Section 2**

Column ChemSep CO Unit Operation "[I  
Remark Section #1

**Section 3**

Column  
Remark

**Section 4**

Column  
Remark

Copy data from  
Delete data from

**Packing Details**

Packing for Packing type

Sec 1 Raschig Pak 250 Y Metal  
 Sec 2 Raschig Pak 250 Y Metal  
 Sec 3  
 Sec 4

Calculate Print  
Exit

**Output**

	Section 1 Output	Section 2 Output	Section 3 Output	Section 4 Output
Calculation according to Billet/Schultes				
F - Factor	3.59	2.95		
Liquid load	1.32	14.37		
Flood factor	62.3	89.7		
Hold-Up	0.009	0.065		
Dry Pressure drop	3.37	2.34		
Spec. Pressure drop	3.6	4.28		
Pressure drop	14.37	12.57		
Working range from	32	22		
Working range to	128	89		
System limit	59.6	50.5		
Pressure drop for high pressure distillation	3.6	4.28		
aph / a	55.6	82		

## Faster Rate-Based Models

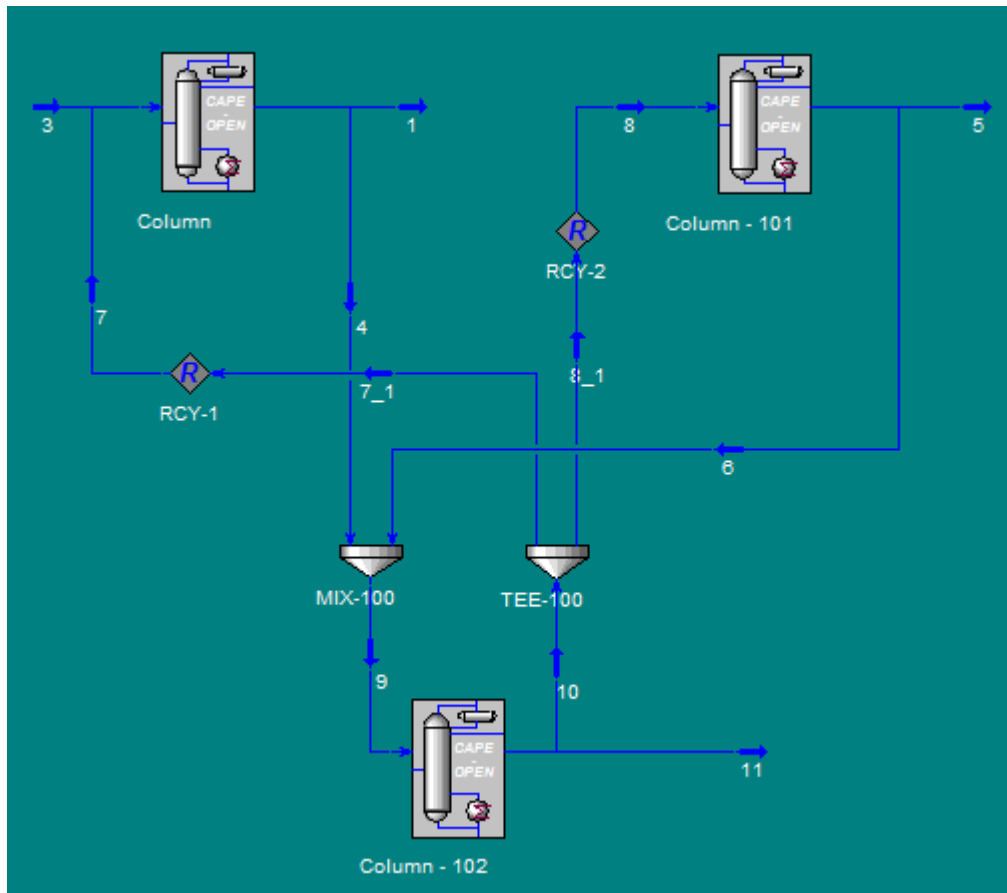
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- **Rate-based models inevitably slower than equilibrium stages**
  - Actual number of stages (not some hypothetical lower number)
  - Flow models other than *mixed* require extensive matrix computations
- **New rate-calculation procedures speed up these models**
  - Speed increase depends on number of components
  - Nearly 20 times faster for 50 stage debutanizer with 42 compounds
- **COSE compounds**
  - Require frequent calls to PME for basic property information
  - ChemSep now writes same to local databank
  - Calculation time decrease when used with ChemSep thermo
  - Significant aid when troubleshooting – reduces need for PME

# Iconography

- CAPE-OPEN icon in some PME's do not adequately represent UO

## Multiple ChemSep UOs in UNISIM Design

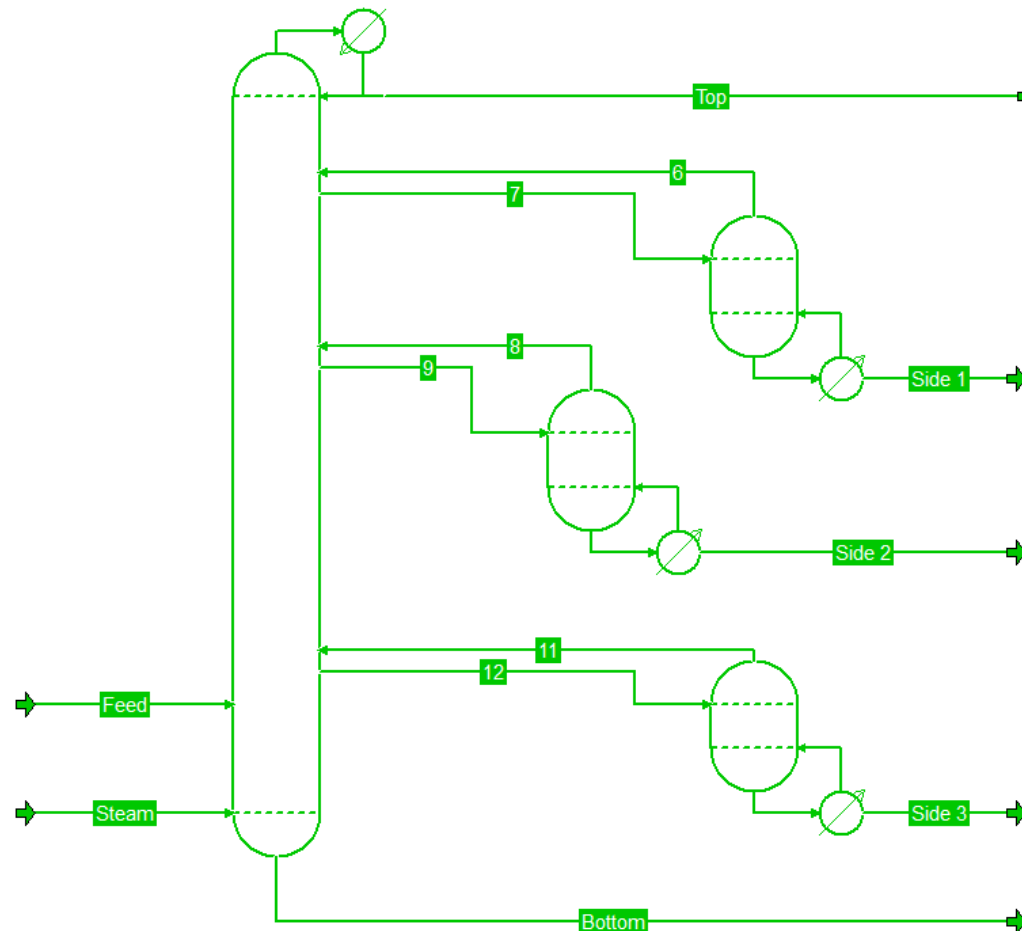


- Icons not representative
- Only one has a condenser
- Only one has reboiler
- Multiple products appear as one
- Multiple feeds appear as one

# Iconography

## ■ Adaptive icons in COCO

- Reflect actual configuration
- Automatically change when configuration changes



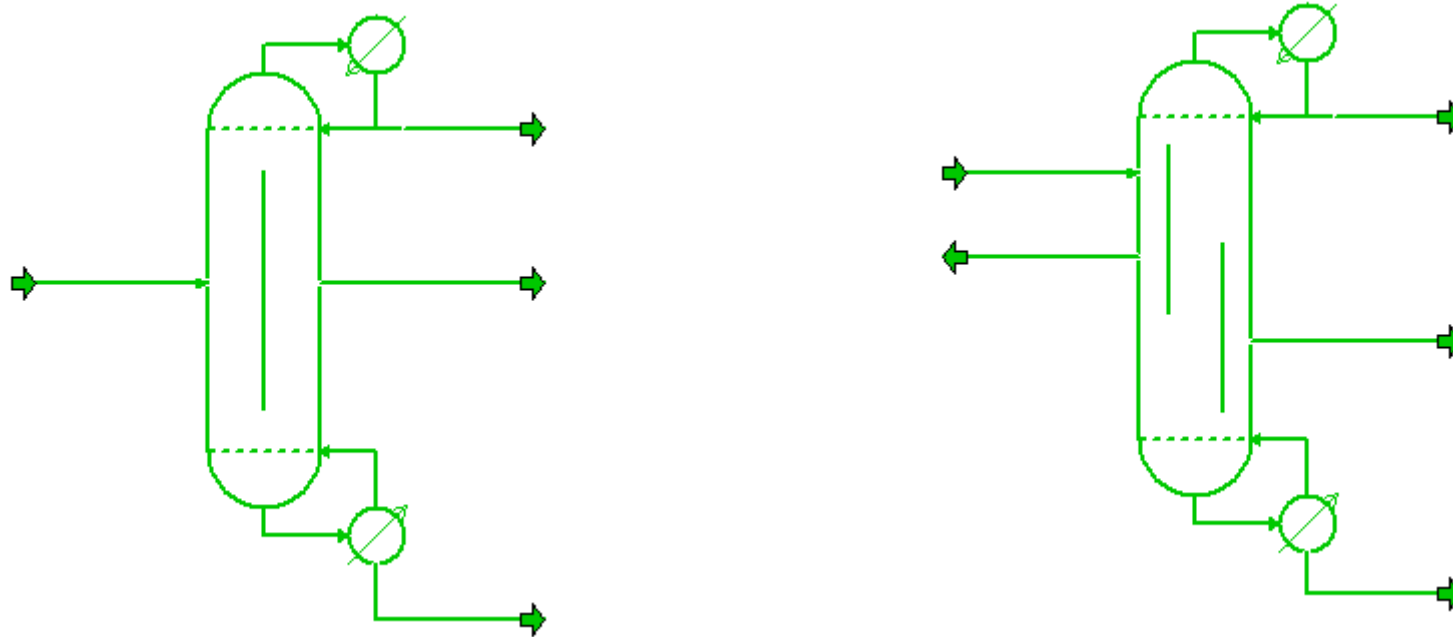
## Iconography

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- ChemSep writes icon structure to sep file in COCO format
- COCO reads sep file, checks if icon has been changed
- If new icon, COCO asks to update icon
  
- UO could write icon as SVG image
- PME reads UO output, determines from checksum if icon changed
- PME displays new icon

# Iconography

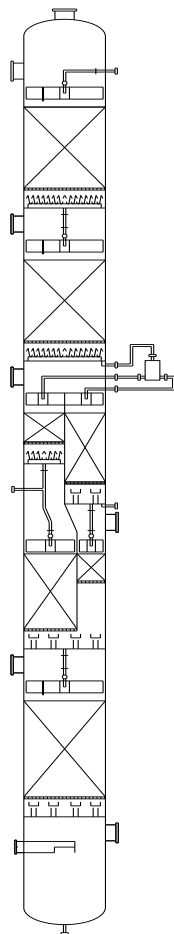
- Is COCO the only PME that permits newly designed icons?



**Dividing Wall Column (DWC) icons for COCO**

# Dividing Wall Columns

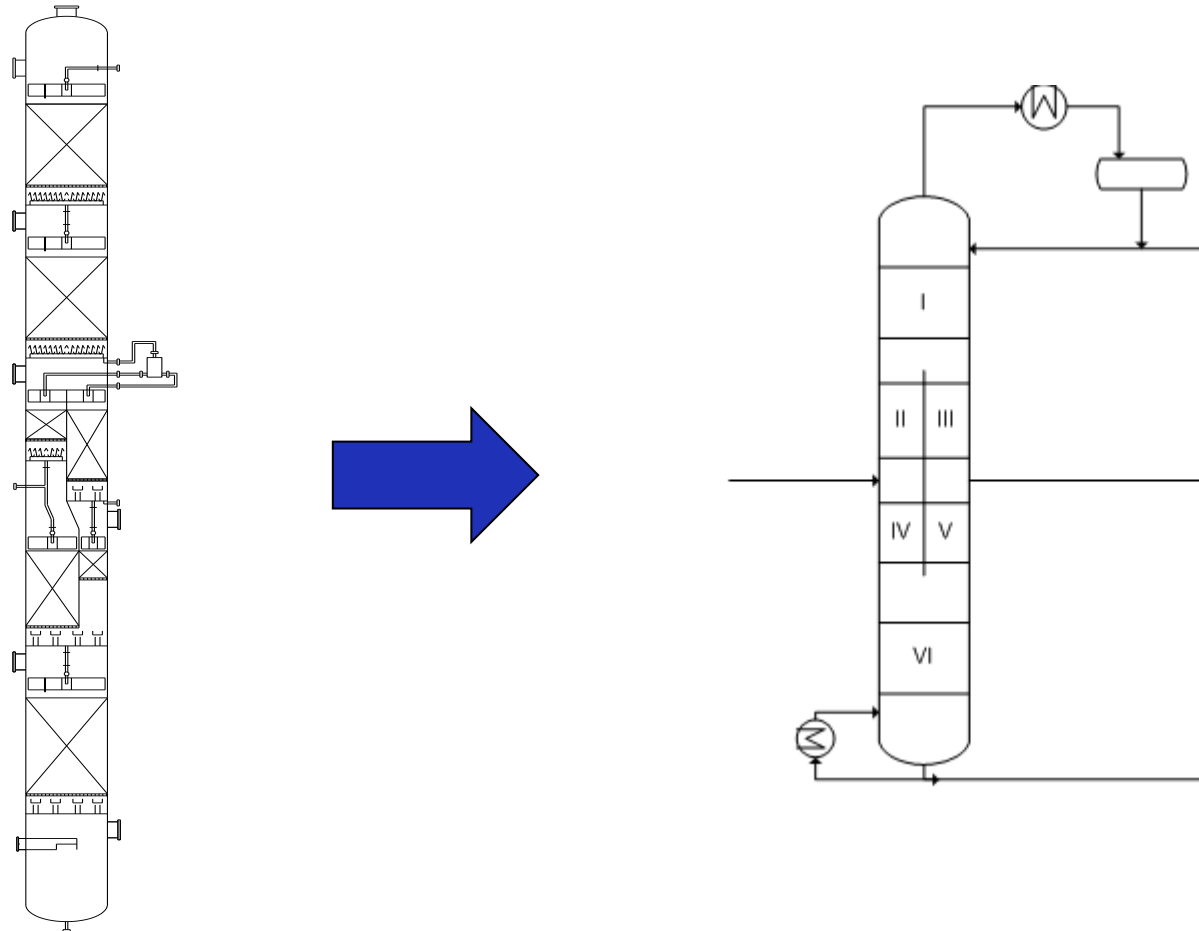
## ■ Dejanović et al. Aromatics DWC



Dejanovic, I., Matijašević, L., Jansen, H., & Olujic, Z. (2011). Designing a packed dividing wall column for an aromatics processing plant. *Industrial & Engineering Chemistry Research*, **50**(9), 5680-5692.

# Dividing Wall Columns

## ■ Dejanović et al. Aromatics DWC



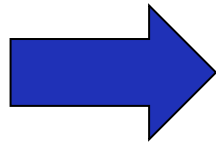
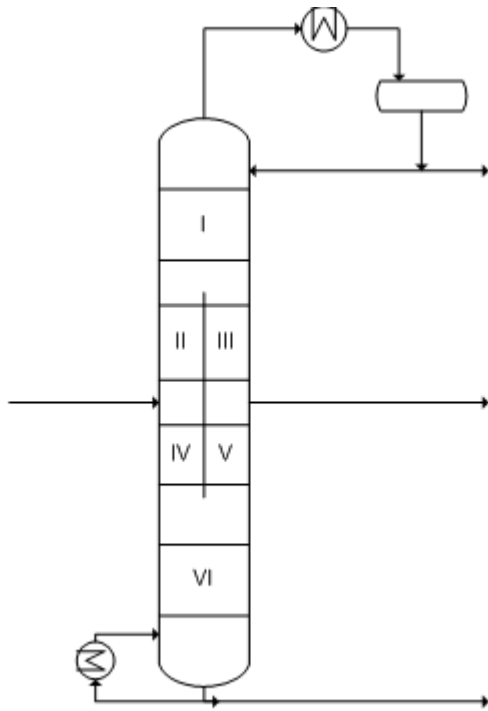
Dejanovic, I., Matijašević, L., Jansen, H., & Olujic, Z. (2011). Designing a packed dividing wall column for an aromatics processing plant. *Industrial & Engineering Chemistry Research*, **50**(9), 5680-5692.



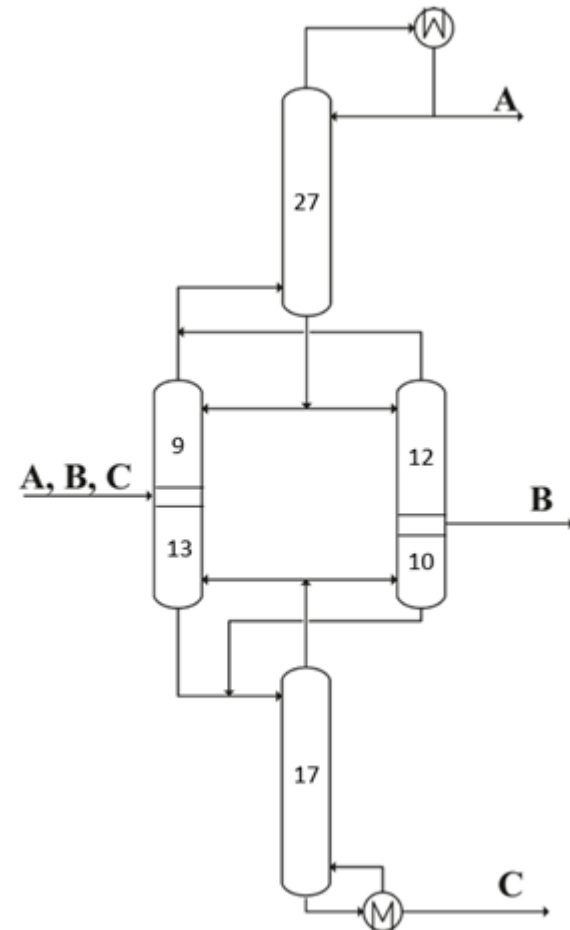
# Dividing Wall Columns

- Generally modeled as multi-column systems

## Dejanović et al. Aromatics DWC



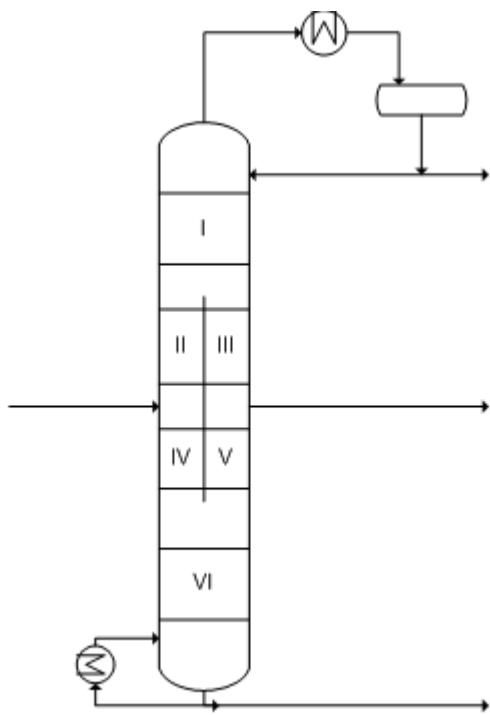
## Multi-column model



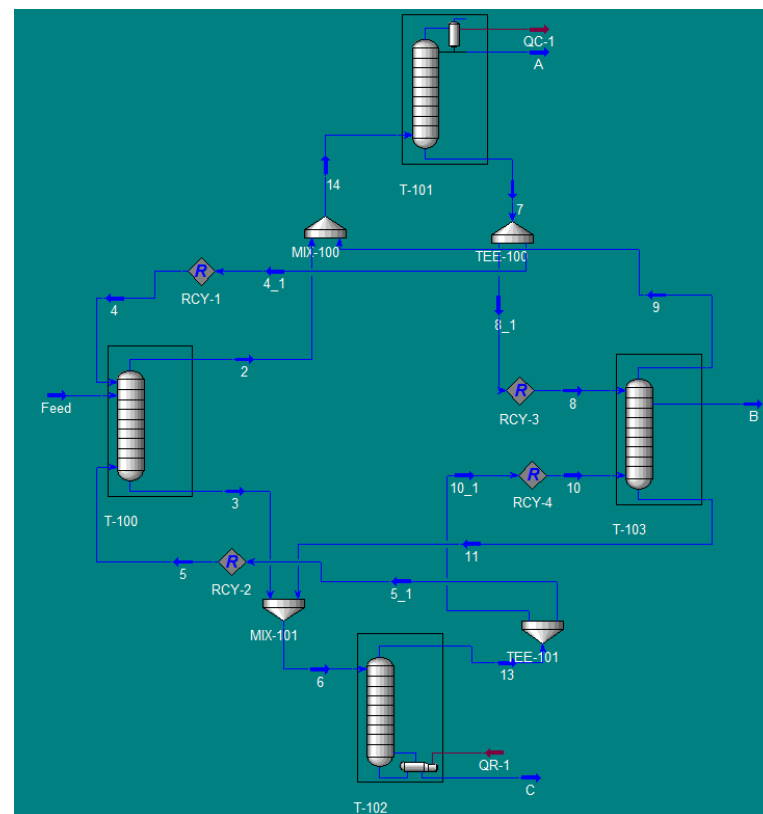
# Dividing Wall Columns

- Generally modeled as multi-column systems

## Dejanović et al. Aromatics DWC



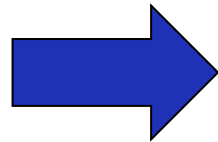
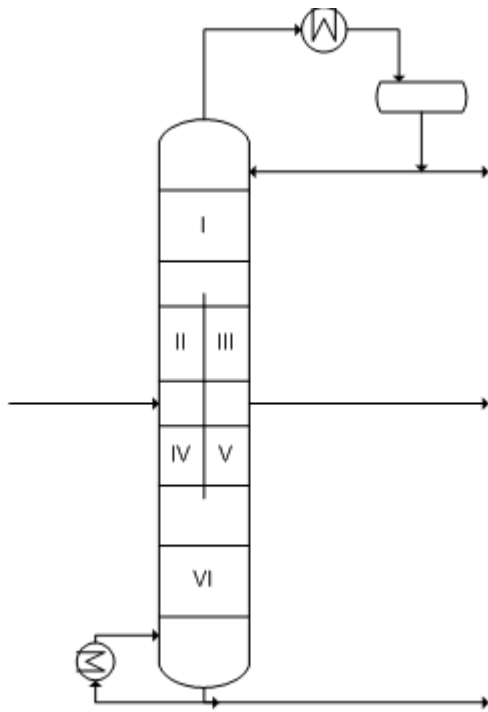
## Multi-column model in UNISIM Design



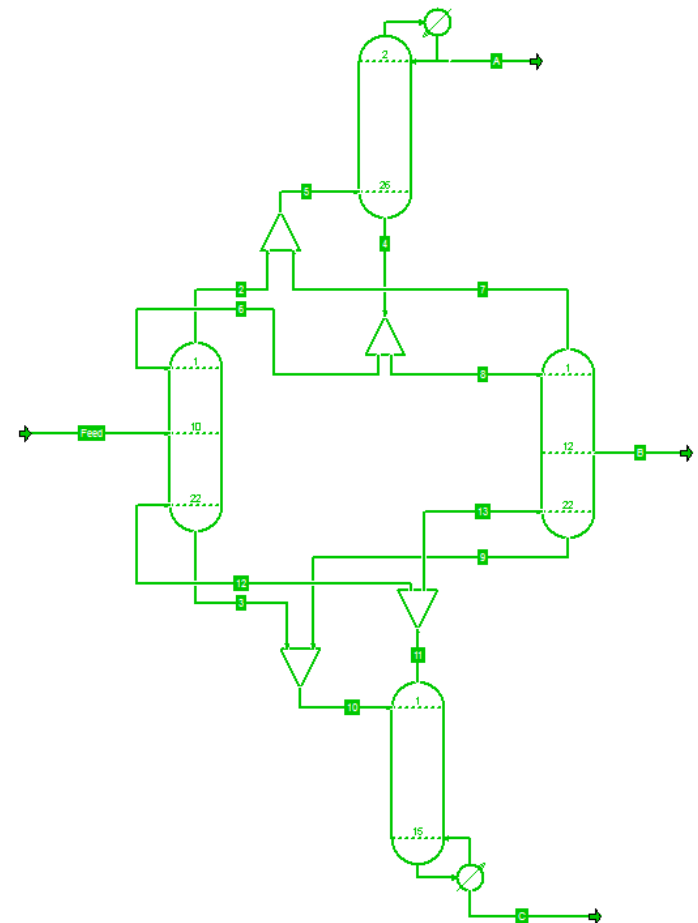
# Dividing Wall Columns

- Generally modeled as multi-column systems

Dejanović et al. Aromatics DWC



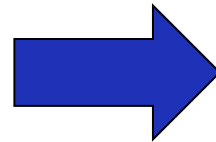
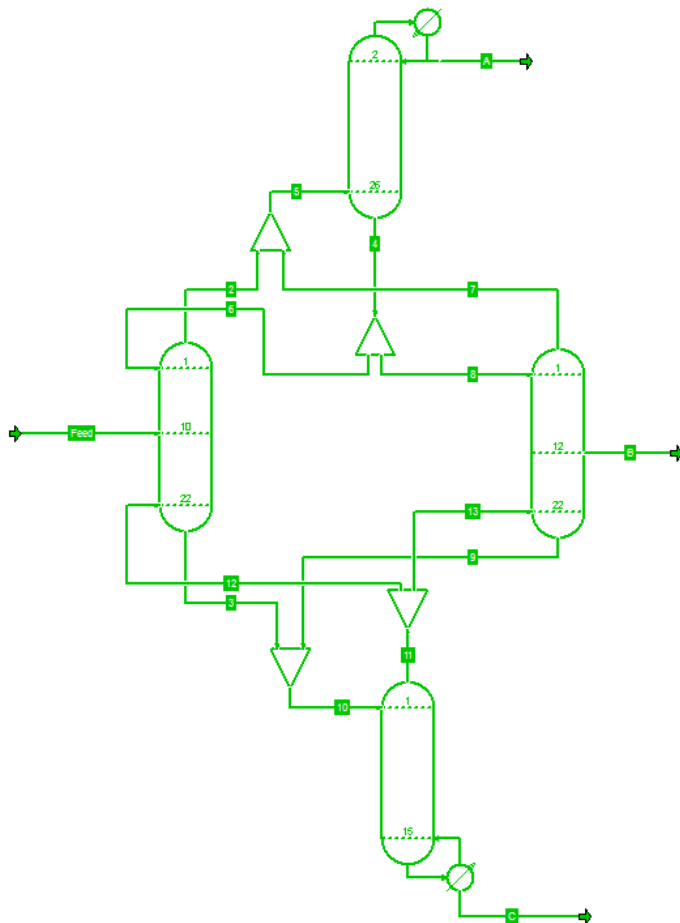
Multi-column model in COCO



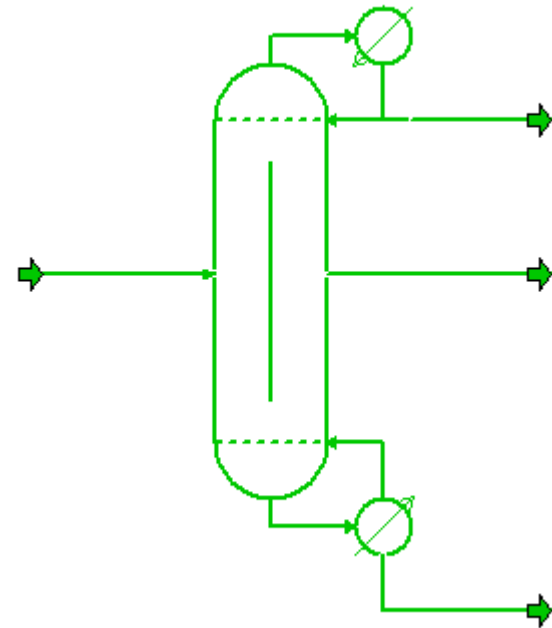
# Dividing Wall Columns

- Generally modeled as multi-column systems

Multi-column model in COCO



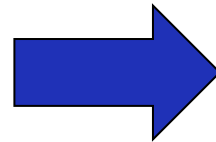
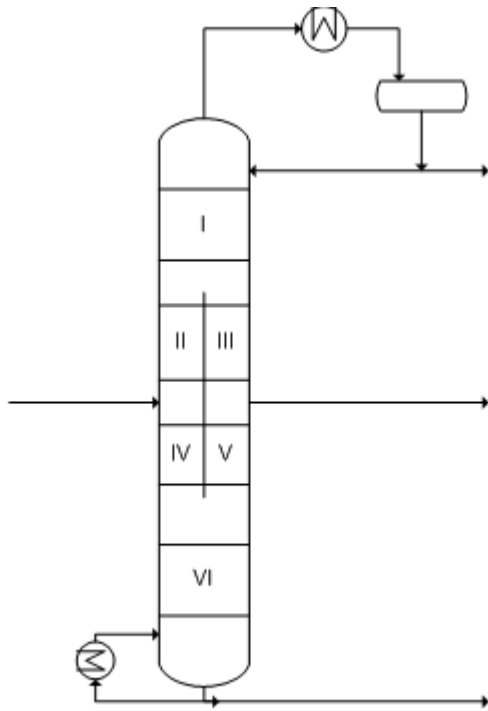
DWC icon hides subflowsheet



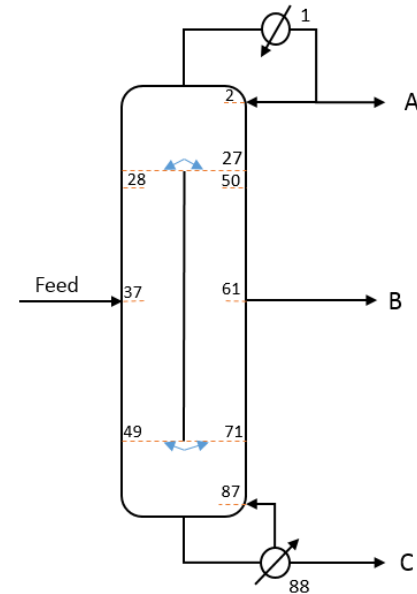
# Dividing Wall Columns

## ■ ChemSep Parallel Column Model (PCM)

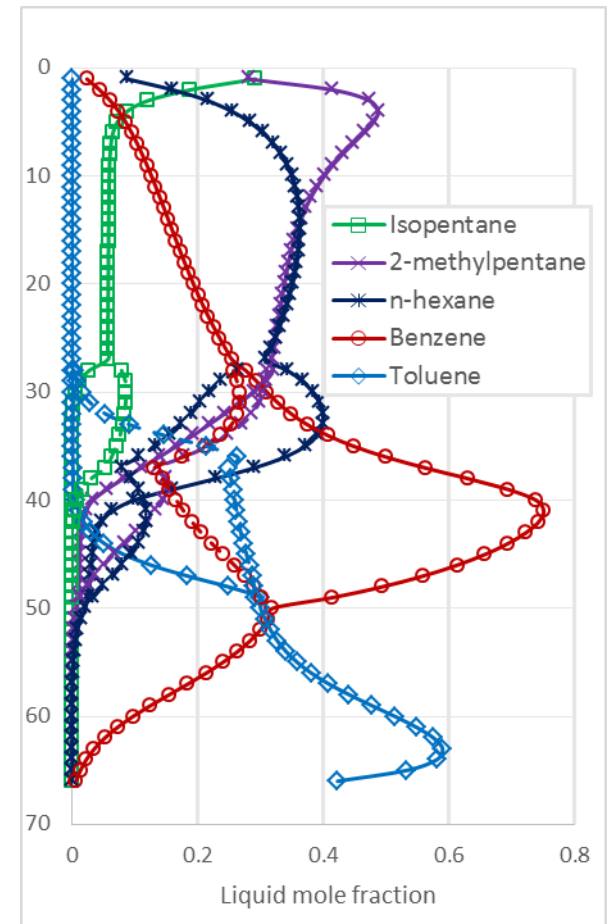
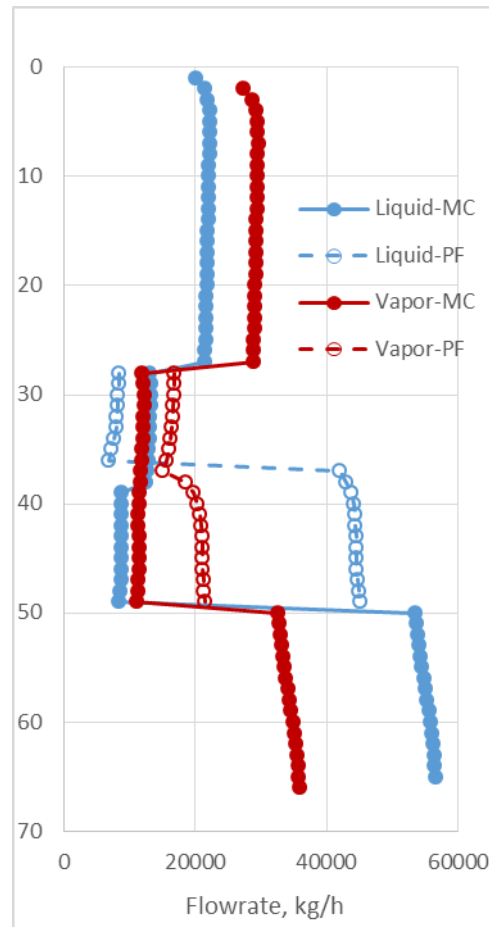
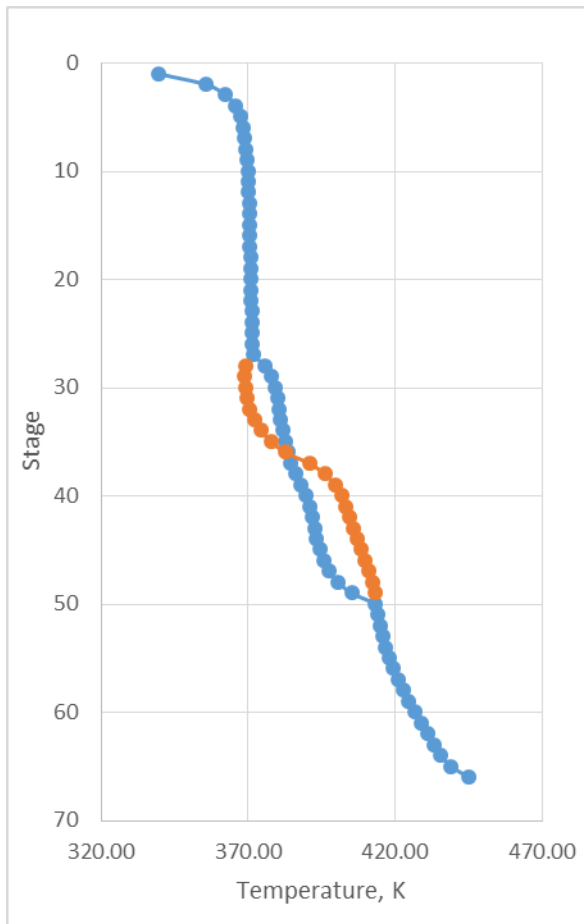
Dejanović et al. Aromatics DWC



Equation-based ChemSep PCM



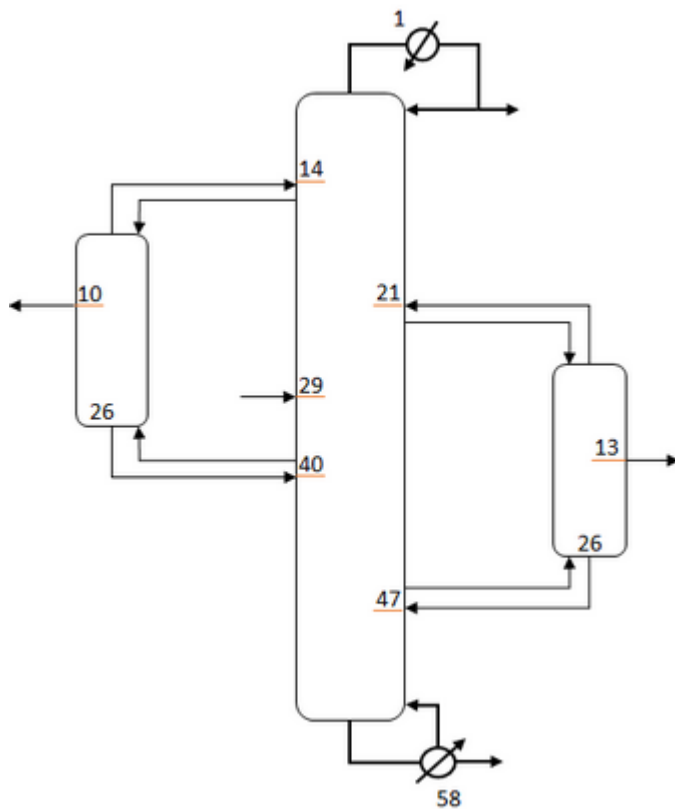
## Dejanović et al. Aromatics DWC Modelled Using ChemSep PCM



# Dividing Wall Columns

- Generally modeled as multi-column systems

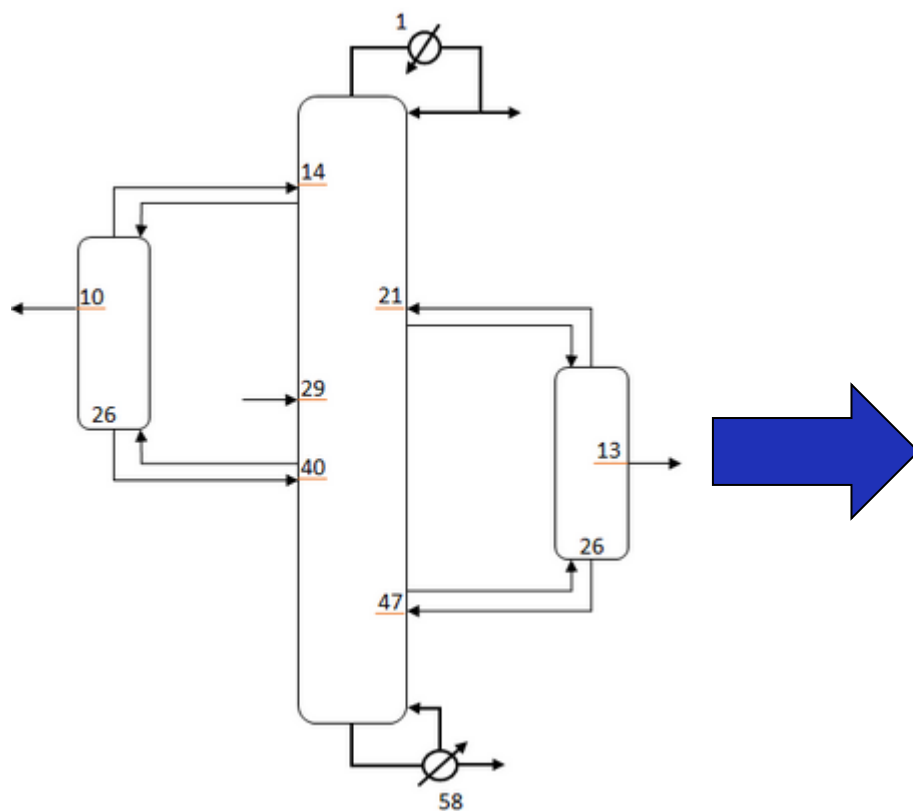
## Satellite Column System



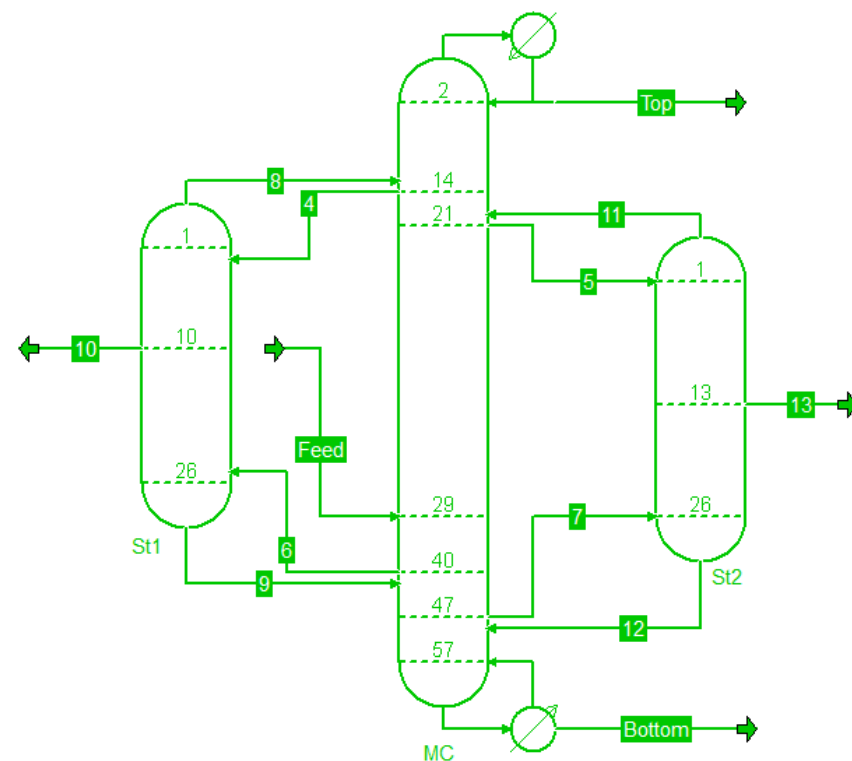
# Dividing Wall Columns

- Generally modeled as multi-column systems

**Satellite Column System**



**Satellite Column System in COCO  
(easy to converge)**

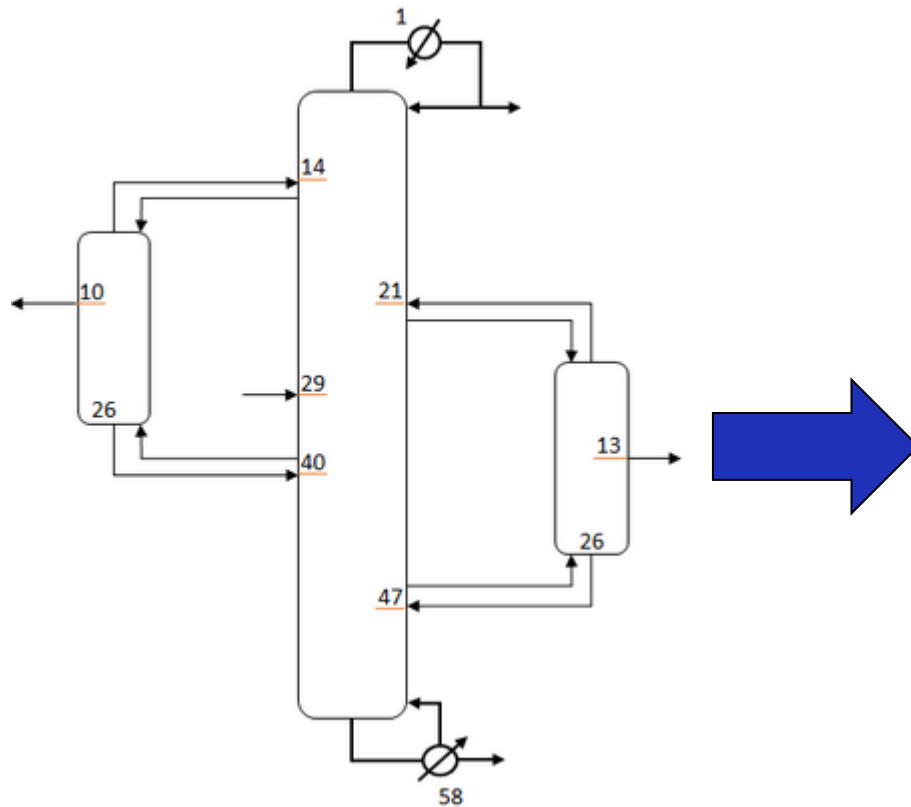




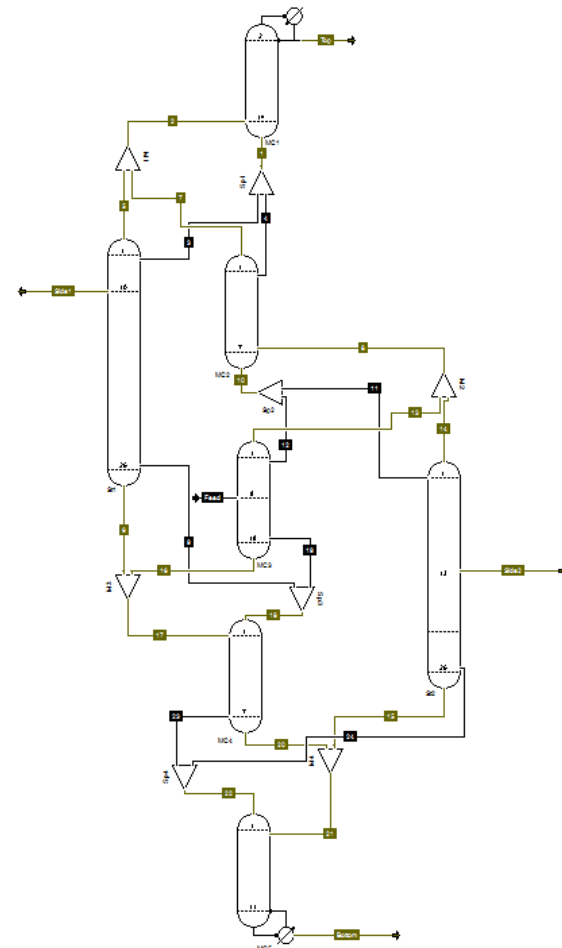
# Dividing Wall Columns

- Generally modeled as multi-column systems

**Satellite Column System**



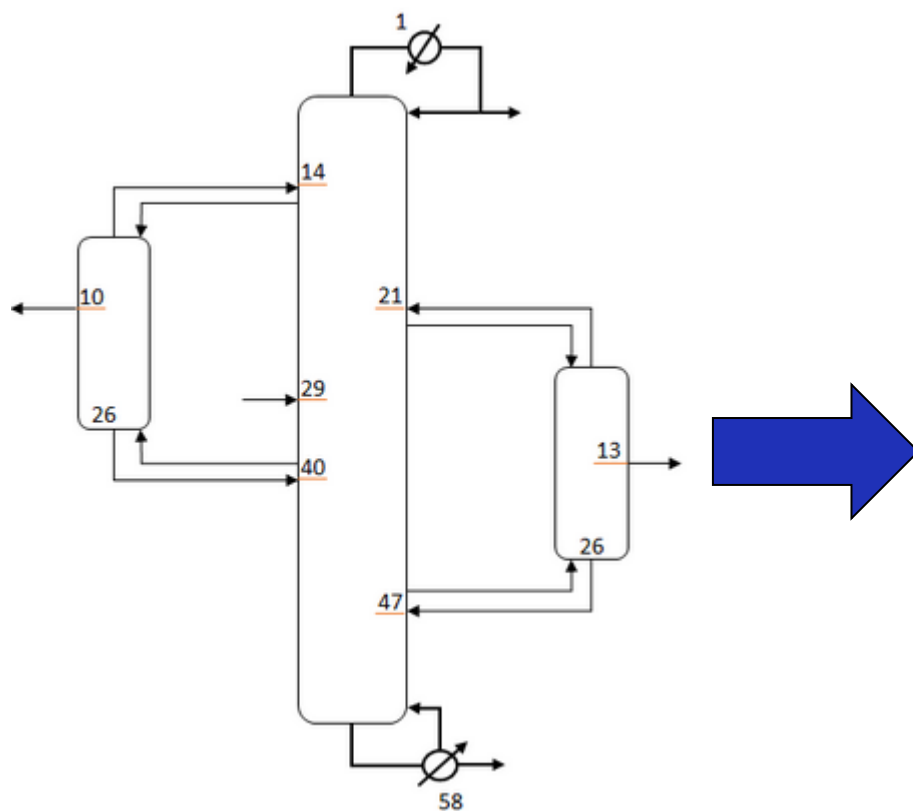
**Satellite Column System in COCO  
(hard to converge)**



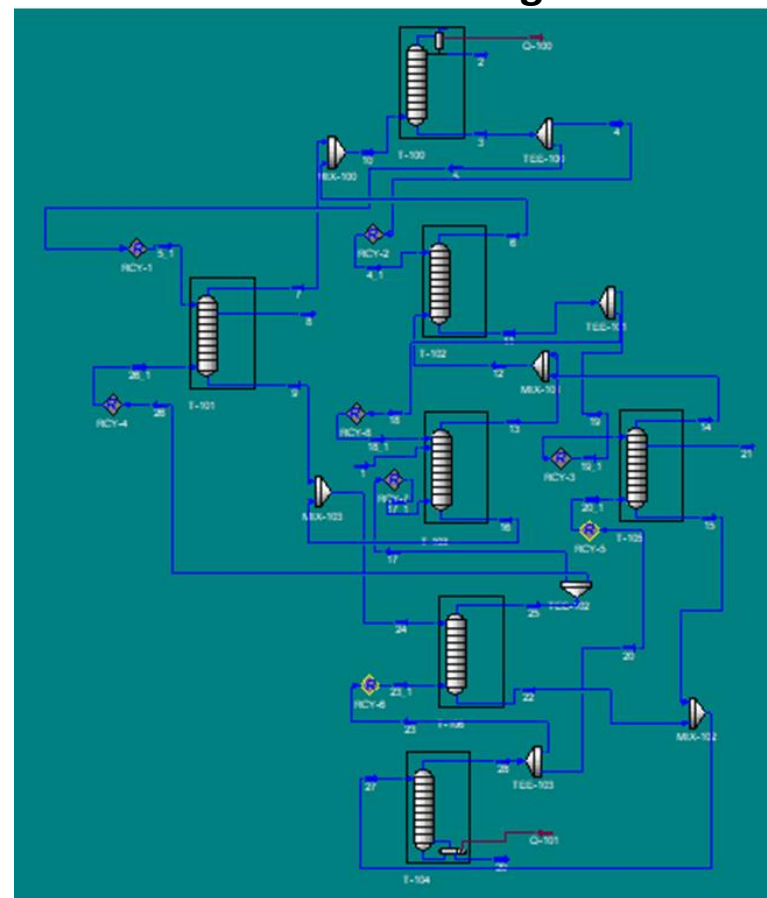
# Dividing Wall Columns

- Generally modeled as multi-column systems

**Satellite Column System**



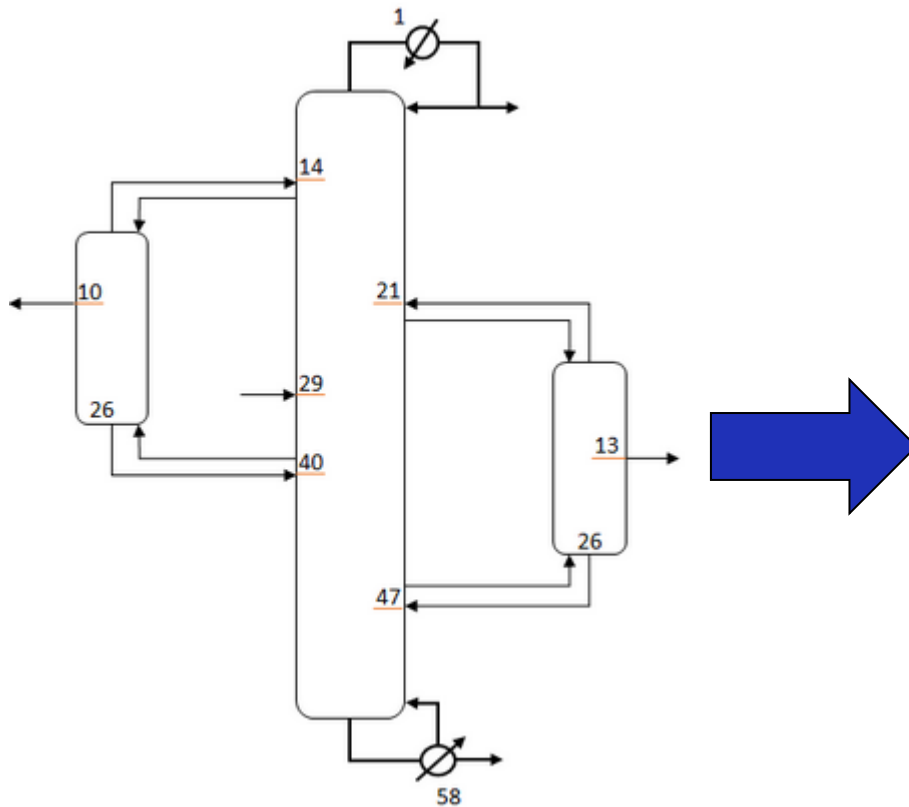
**Satellite Column System  
in UNISIM Design**



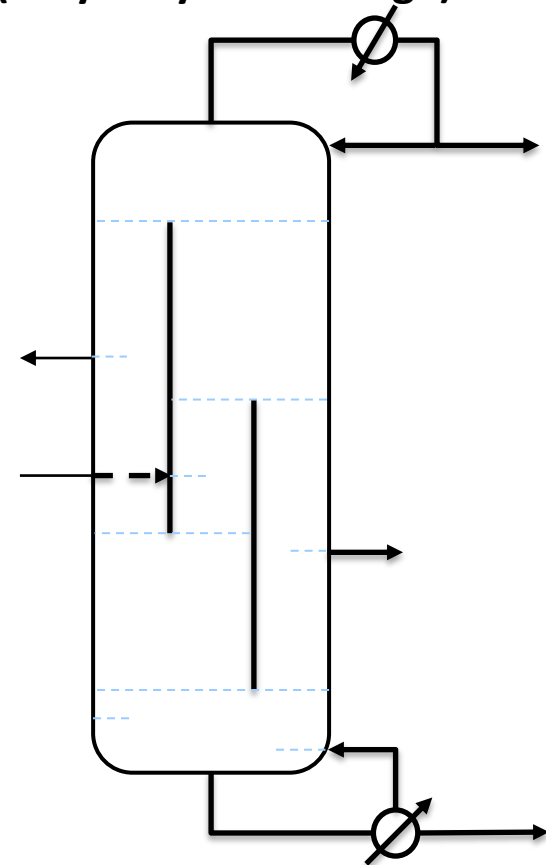
# Dividing Wall Columns

## ■ ChemSep Parallel Column Model (PCM)

Satellite Column System



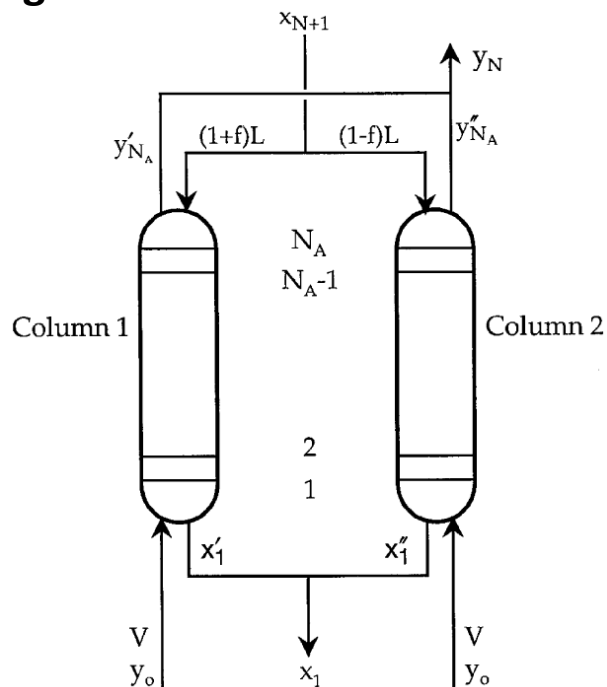
Equation-based ChemSep PCM  
(very easy to converge)



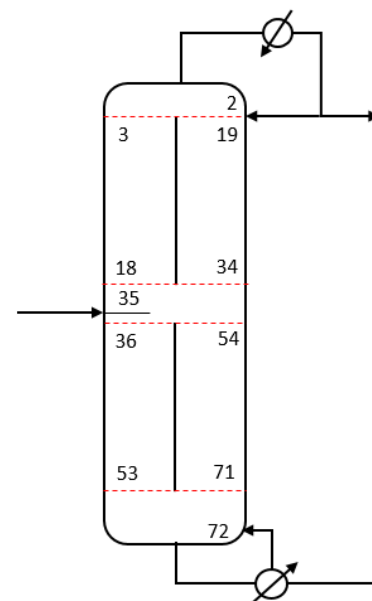
# Maldistribution Models

- ChemSep PCM can be used to model maldistribution

## Billingham and Lockett Maldistribution Model



## Equivalent PCM Structure

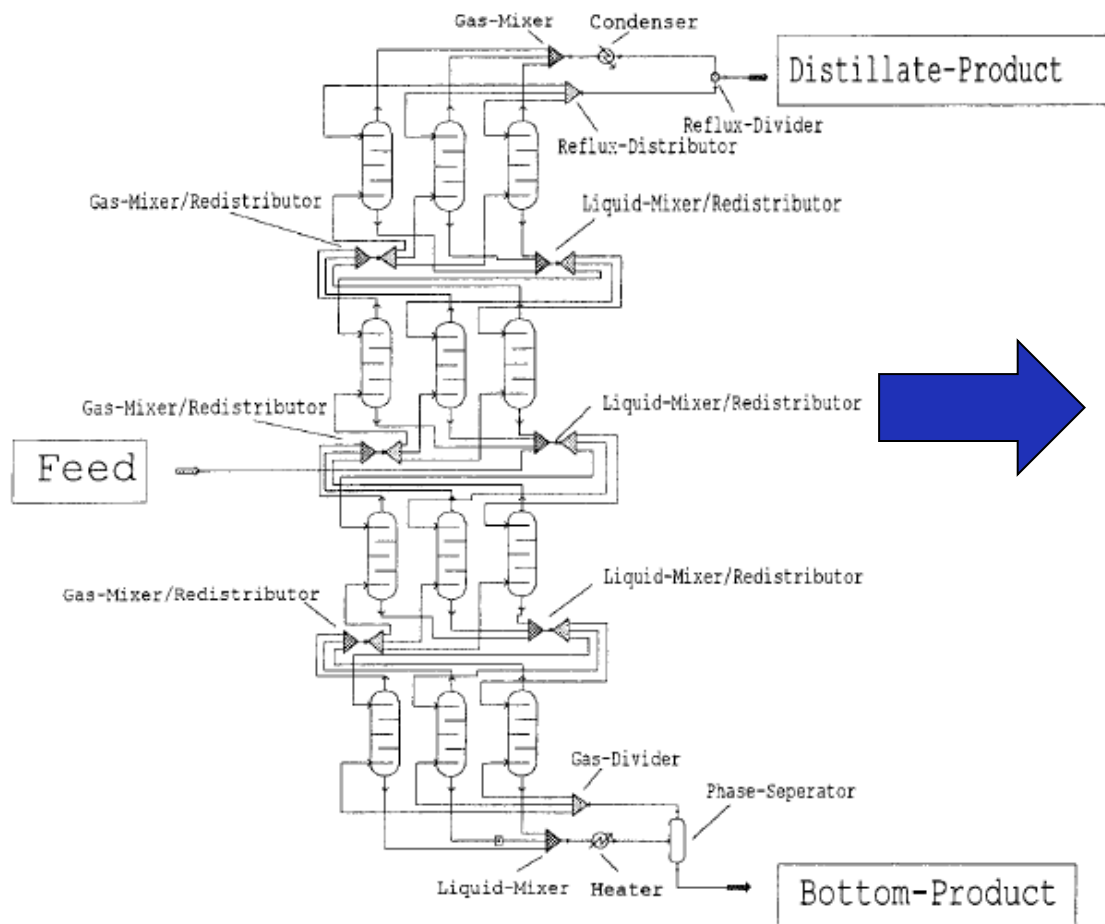


- Redistributors modeled as stages with no mass transfer

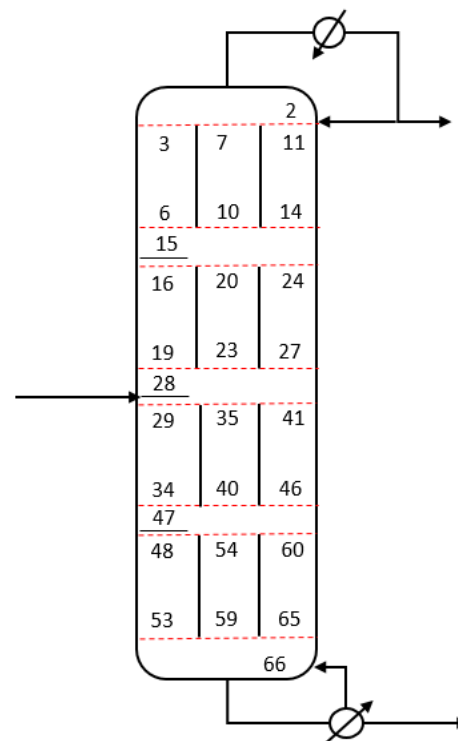
# Maldistribution Models

- ChemSep PCM can be used to model maldistribution

## Schultes Maldistribution Model

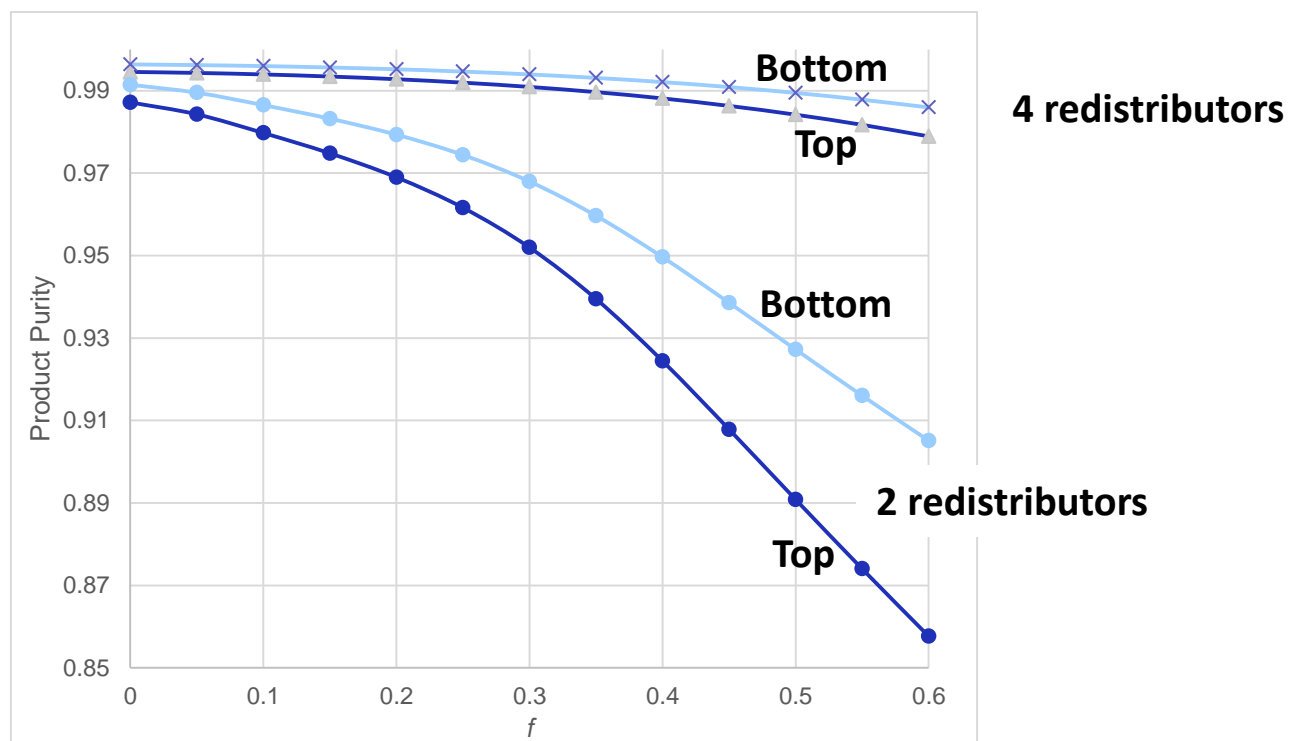


## Equivalent PCM Structure



# Maldistribution Models

- ChemSep PCM can be used to model maldistribution



**Significant influence of the number of redistributors**

## Other Matters

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- **Thermo 1.0 vs Thermo 1.1**
  - Some ChemSep users unable to use Thermo 1.1
  - ChemSep NOT in favor of deprecating 1.0 while this state continues
- **Specific gravity at 60 F as property constant**

# Conclusion

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- **New in ChemSep Version 7.2**
  - Fitting of Group Contribution Model (e.g. UNIFAC) Parameters
  - Rapid rating and costing
  - Export to column vendor tools
- **Faster rate-based simulation (much faster in some cases)**
- **Wish List**
  - Adaptable and editable icons in all but COCO (which already has them)
  - Pointing at a UO displays simulation summary for that UO (possible in COCO)
  - Do not deprecate Thermo 1.0 until all users can easily use Thermo 1.1
  - Specific gravity at 60 F as property constant
- **Propose CAPE-OPEN Cost Library (COCL) of basic callable functions**
  - Cost of metal
  - Cost of steam at different levels
  - Cost of pressure vessel
  - M+S index + Energy cost functions imply currency (basis should be US dollar)

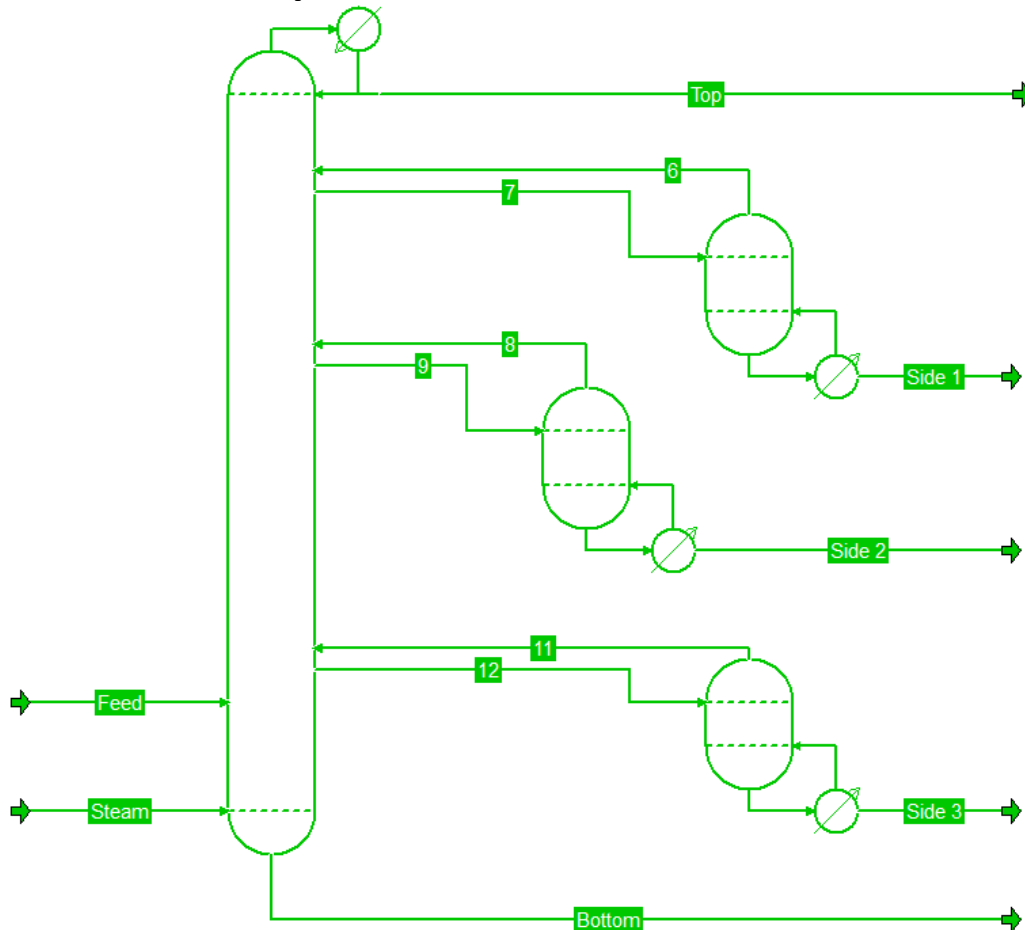


# Coming Soon to ChemSep Version 8

## Parallel Column Model

- Dividing Wall Columns, Maldistribution, Multi-column Systems

Multiple column model in COCO



One equation-based model  
ChemSep Version 8

