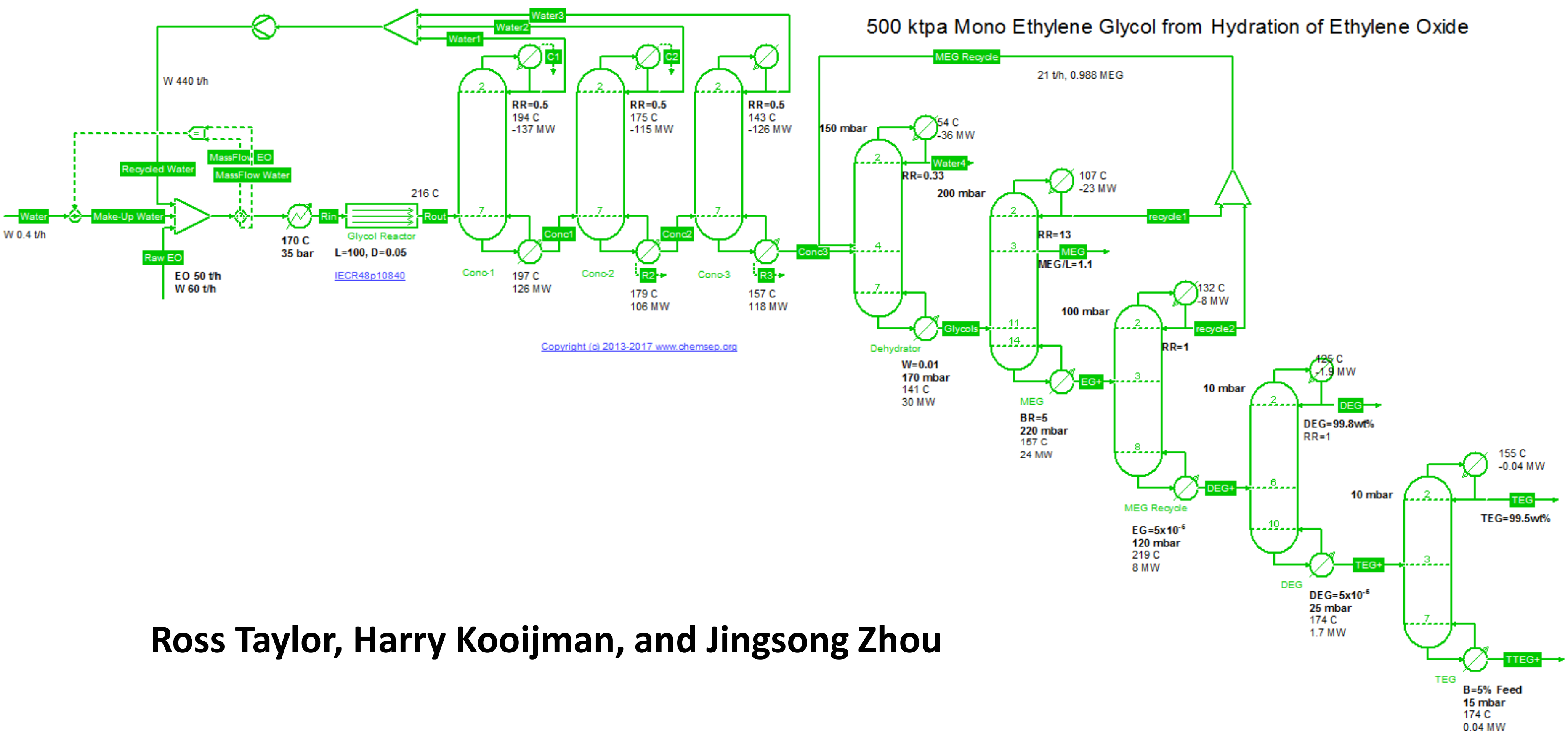
Process Optimization using CAPE-OPEN Tools

ChemSep
Modeling Separation Processes

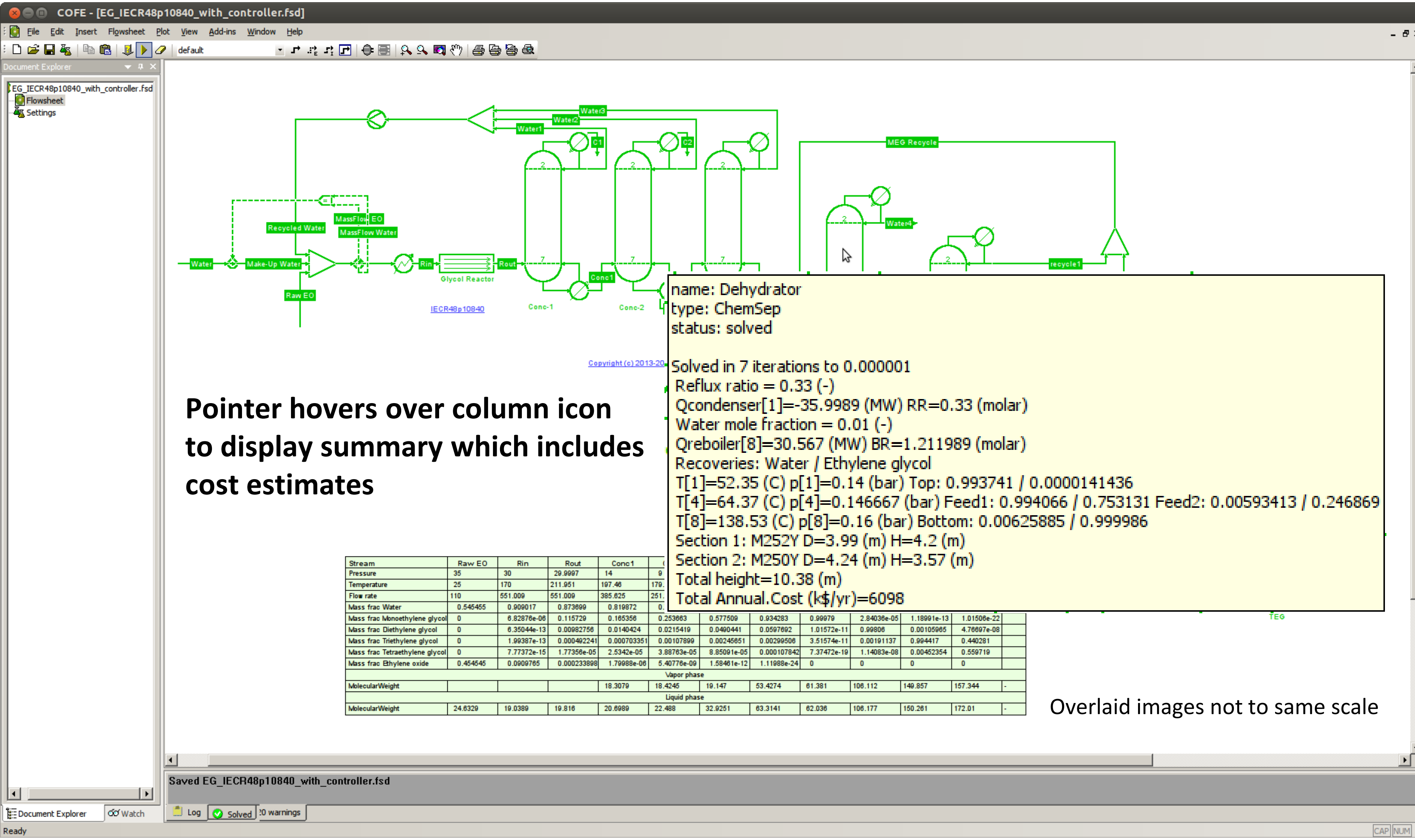


Ross Taylor, Harry Kooijman, and Jingsong Zhou

Outline

- 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



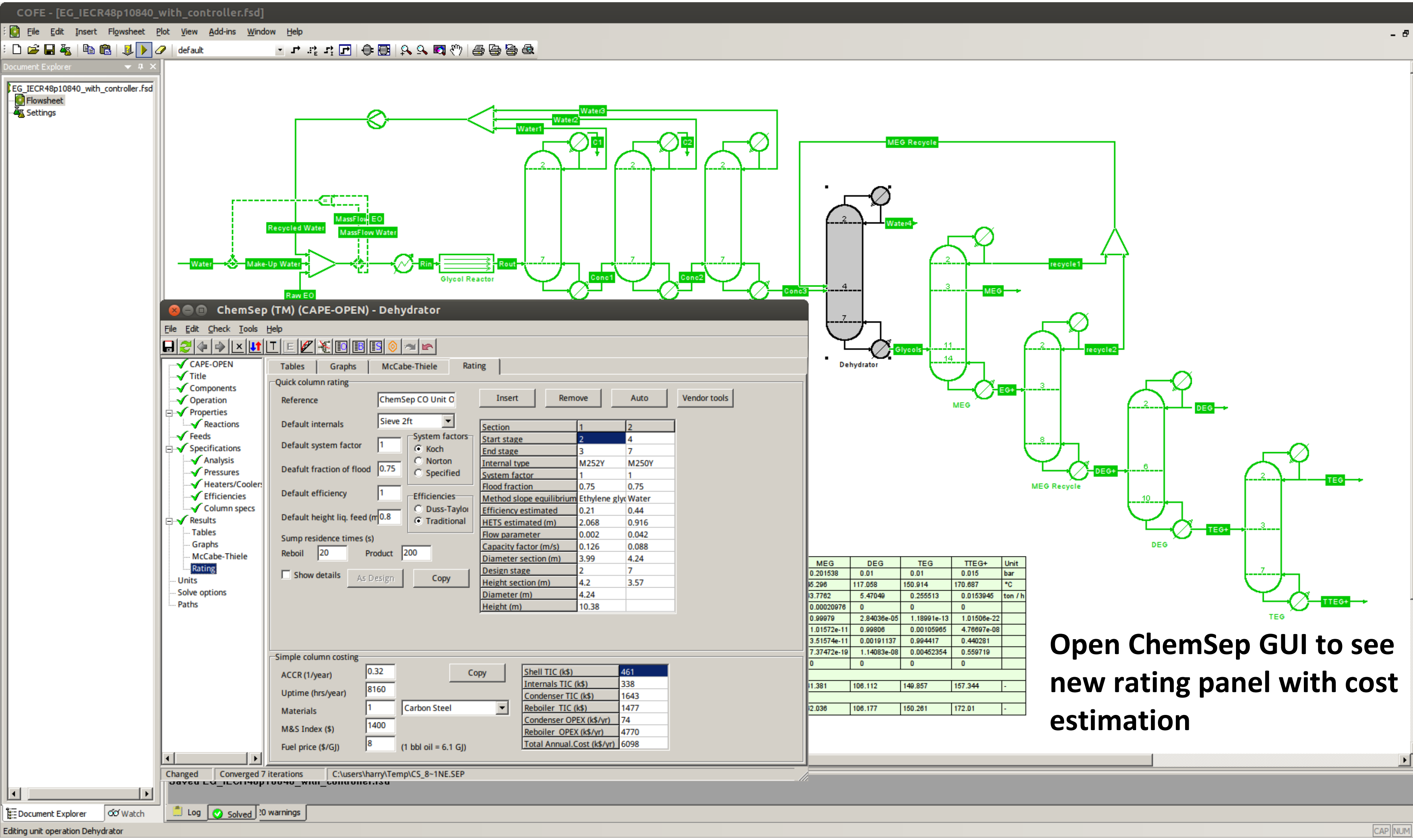
Stream	Raw EO	Rin	Rout	Conc1								
Pressure	35	30	29.9997	14	9							
Temperature	25	170	211.951	197.46	179.							
Flow rate	110	551.009	551.009	385.625	251.							
Mass frac Water	0.545455	0.909017	0.873699	0.819872	0.							
Mass frac Monoethylene glycol	0	6.82876e-06	0.115729	0.165356	0.253663	0.577509	0.934283	0.99979	2.84036e-05	1.18991e-13	1.01506e-22	
Mass frac Diethylene glycol	0	6.35044e-13	0.00982756	0.0140424	0.0215419	0.0490441	0.0597692	1.01572e-11	0.99806	0.00105965	4.76697e-08	
Mass frac Triethylene glycol	0	1.99387e-13	0.000492241	0.000703351	0.00107899	0.00245651	0.00299506	3.51574e-11	0.00191137	0.994417	0.440281	
Mass frac Tetraethylene glycol	0	7.77372e-15	1.77356e-05	2.5342e-05	3.88763e-05	8.85091e-05	0.000107842	7.37472e-19	1.14083e-08	0.00452354	0.559719	
Mass frac Ethylene oxide	0.454545	0.0909765	0.000233898	1.79988e-06	5.40776e-09	1.58461e-12	1.11988e-24	0	0	0	0	
Vapor phase												
MolecularWeight				18.3079	18.4245	19.147	53.4274	61.381	106.112	149.857	157.344	-
Liquid phase												
MolecularWeight	24.6329	19.0389	19.816	20.6989	22.488	32.9251	63.3141	62.036	106.177	150.261	172.01	-

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

Overlaid images not to same scale

Column Rating and Cost Estimation in ChemSep

ChemSep
Modeling Separation Processes



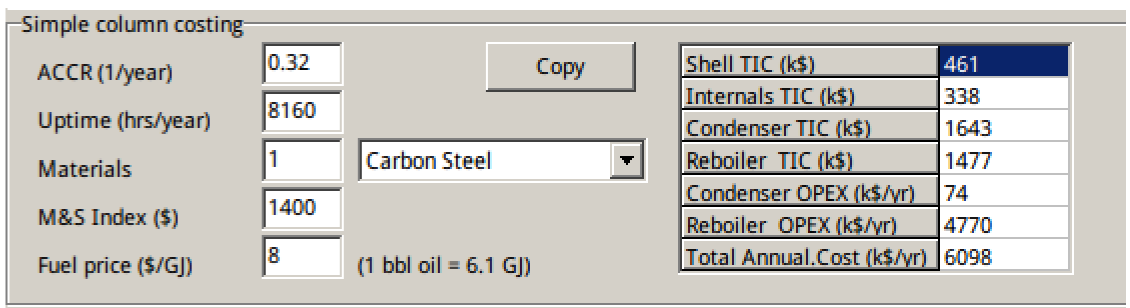
Open ChemSep GUI to see new rating panel with cost estimation

Column Rating and Cost Estimation in ChemSep

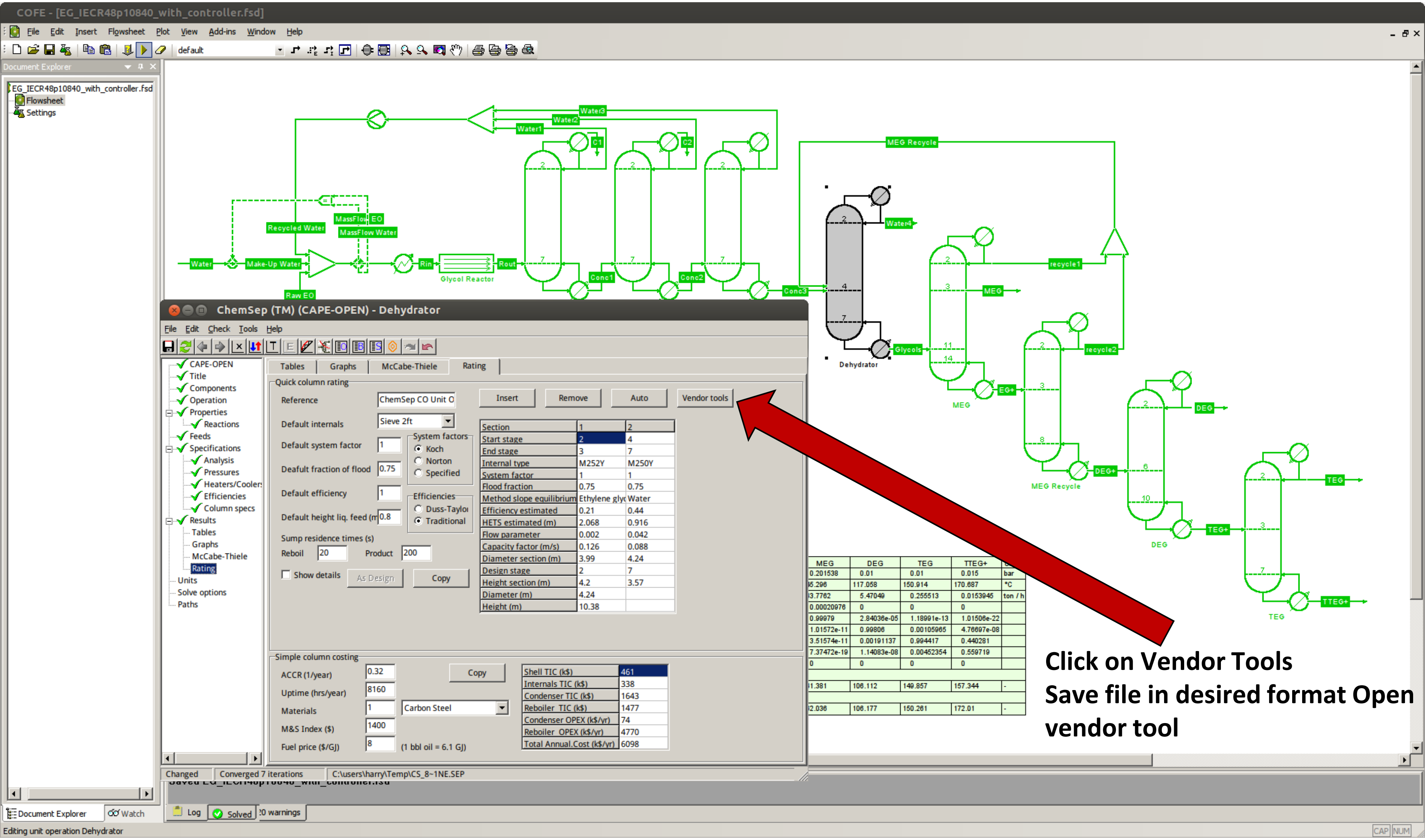
ChemSep Modeling Separation Processes

- **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



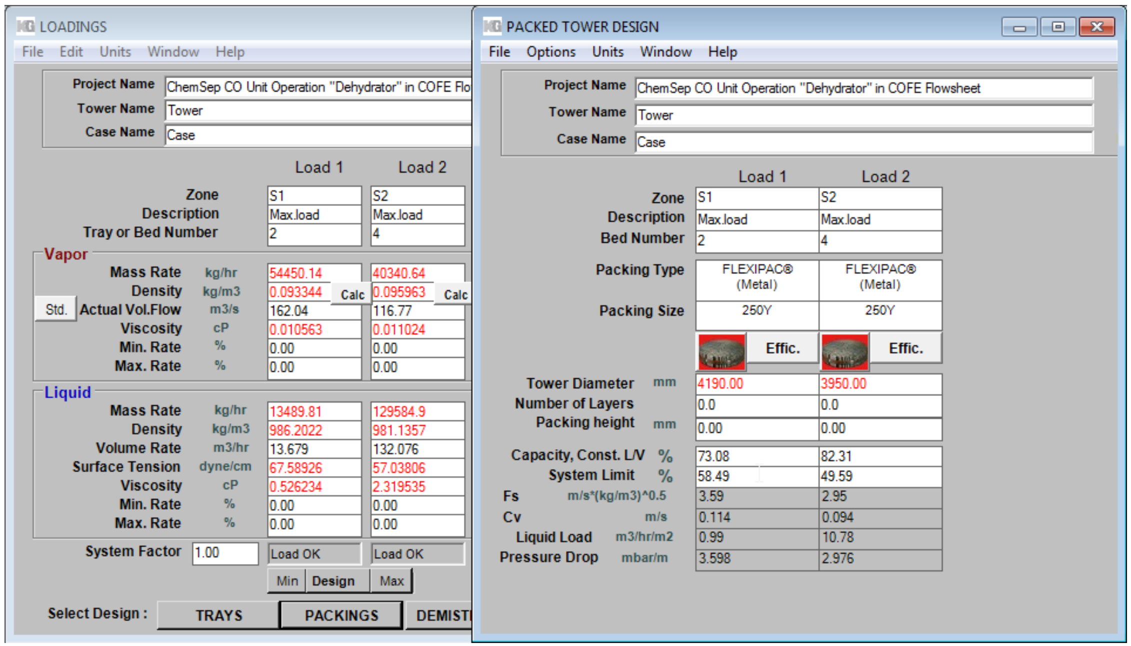
Export to Vendor Tools



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

Export to Vendor Tools

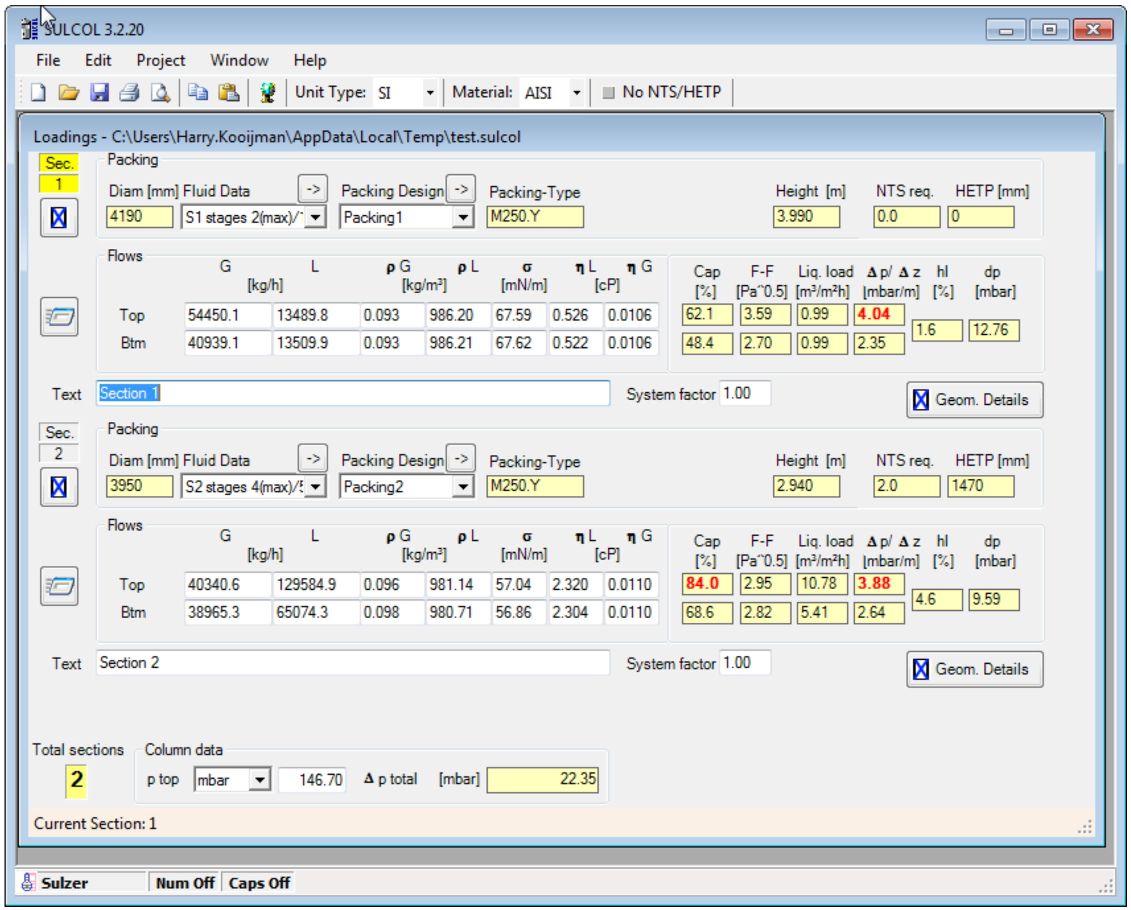
KGTower from Koch Glitsch



Export to Vendor Tools

ChemSep
Modeling Separation Processes

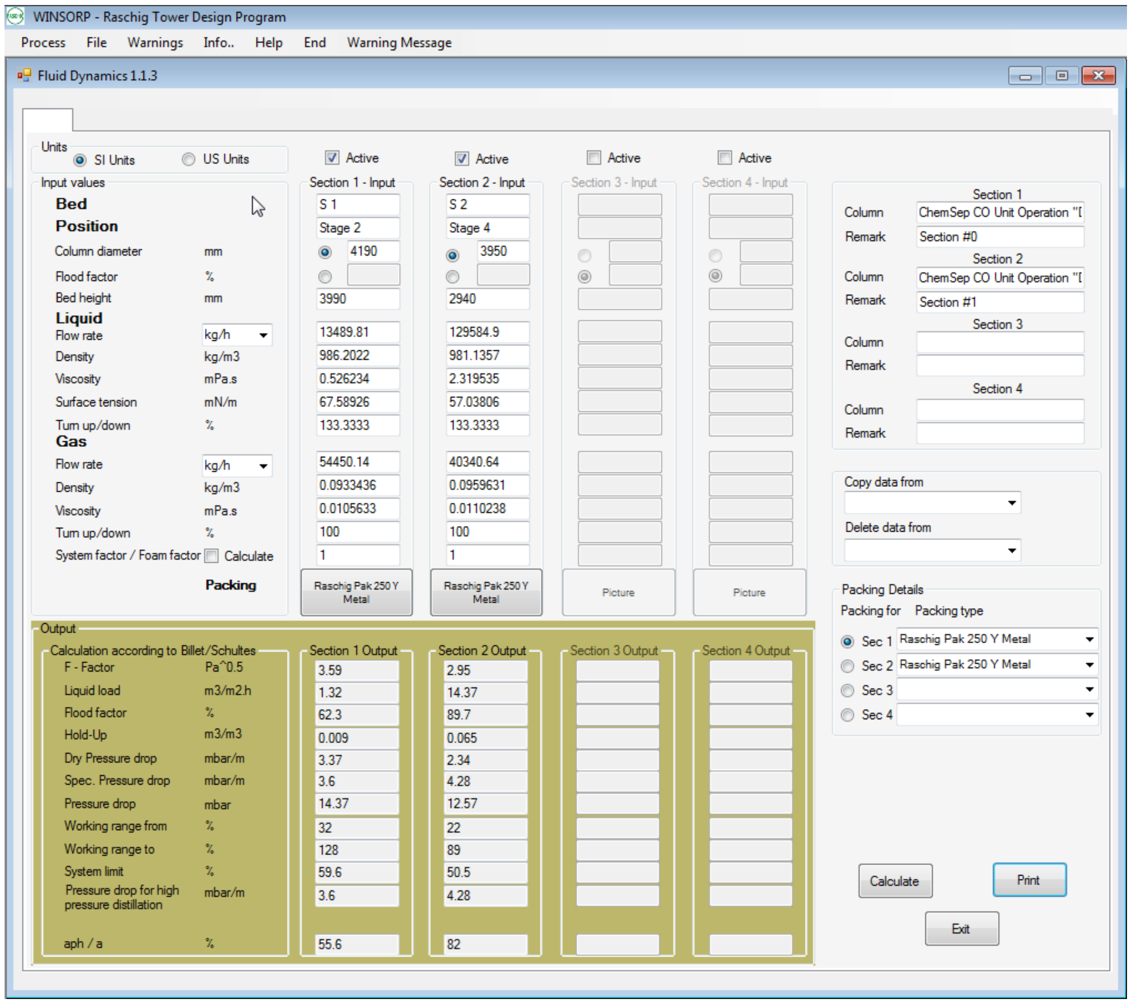
SulCol from Sulzer ChemTech



New: Export to Vendor Tools

ChemSep
Modeling Separation Processes

WinSorp from Raschig GmbH



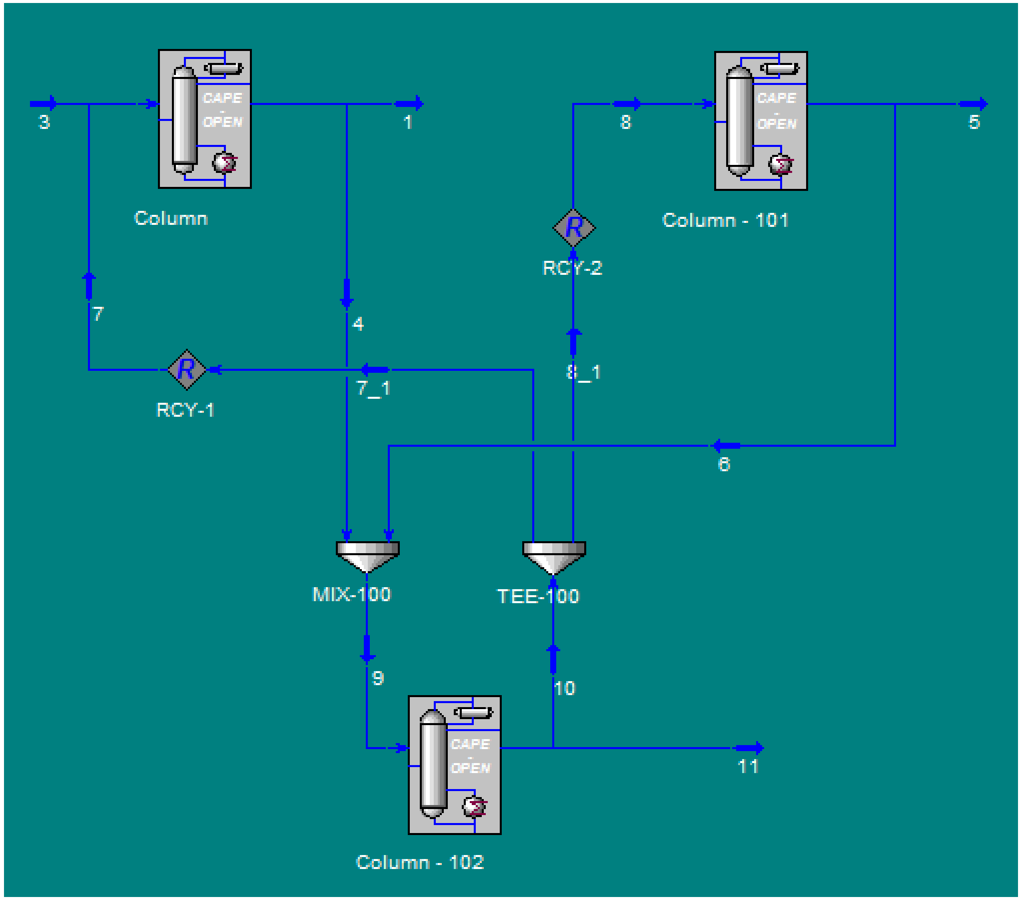
Faster Rate-Based Models

- **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 PMEs do not adequately represent UO

Multiple ChemSep UOs in UNISIM Design

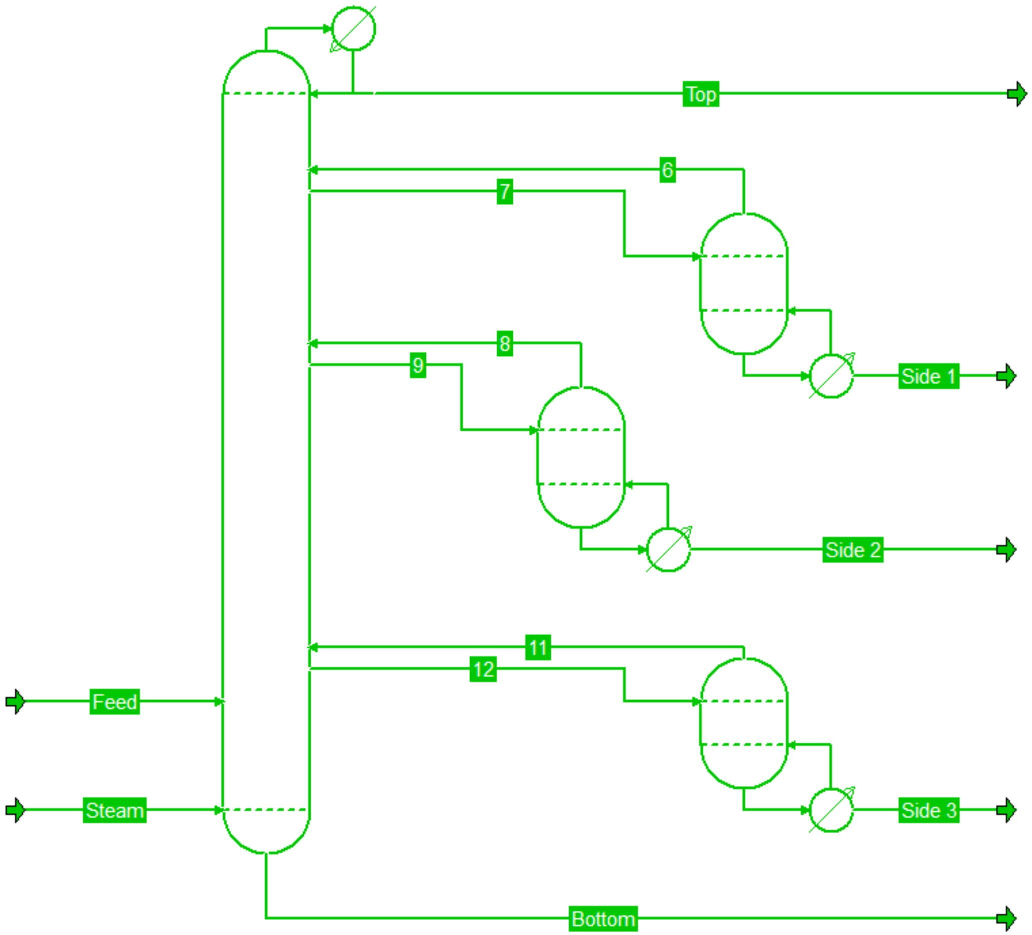


- Icons not representative
- Only one has a condenser
- Only one has reboiler
- Multiple products appear as one
- Multiple feeds appear as one

Iconography

ChemSep Modeling Separation Processes

- **Adaptive icons in COCO**
  - Reflect actual configuration
  - Automatically change when configuration changes



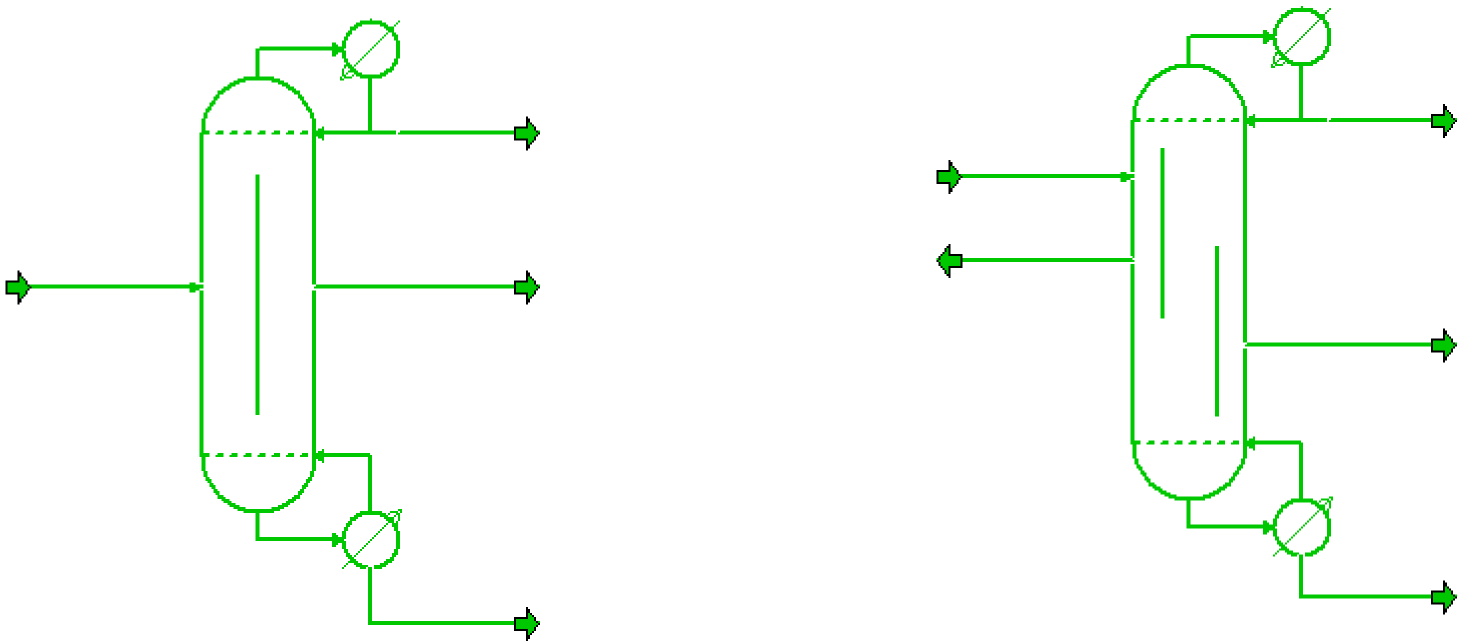
Iconography

- 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

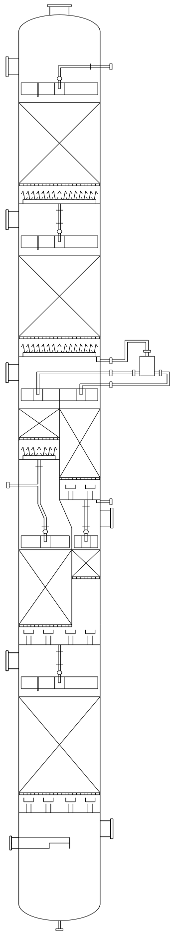
- Is COCO the only PME that permits newly designed icons?



Dividing Wall Column (DWC) icons for COCO

Dividing Wall Columns

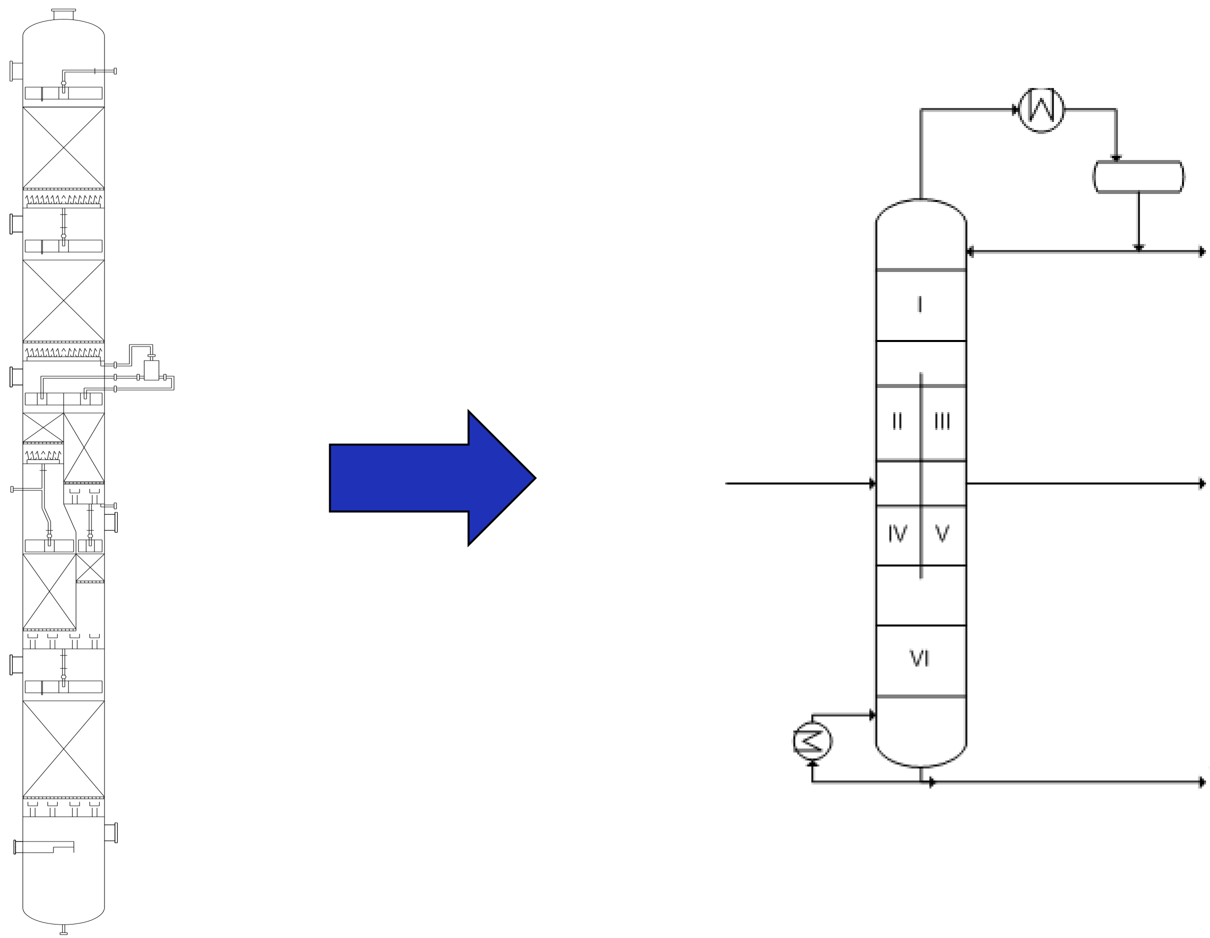
- **Dejanović et al. Aromatics DWC**



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



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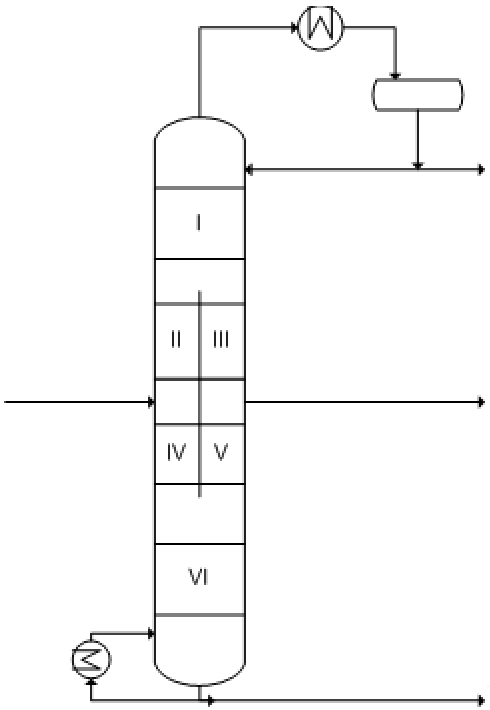
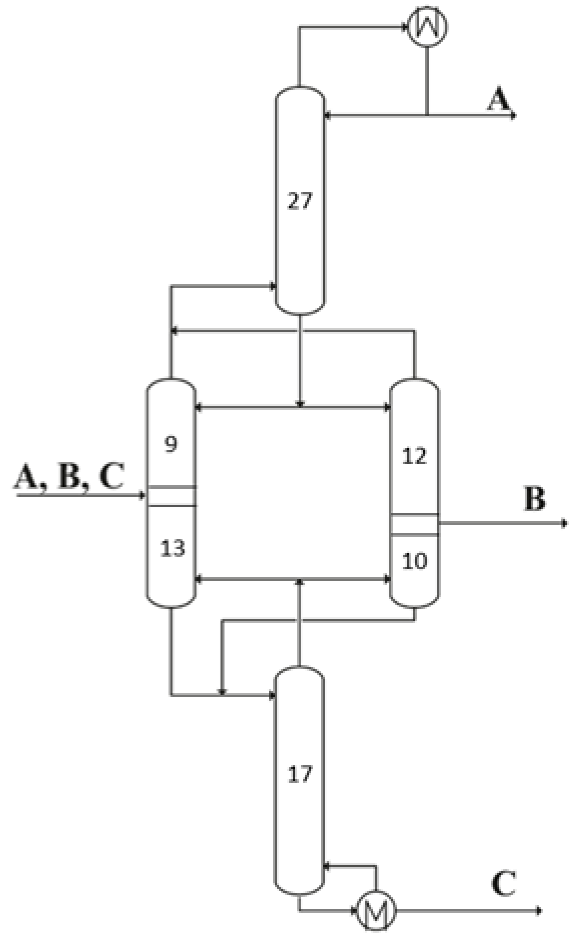
Dividing Wall Columns

- Generally modeled as multi-column systems

Dejanović et al. Aromatics DWC



Multi-column model



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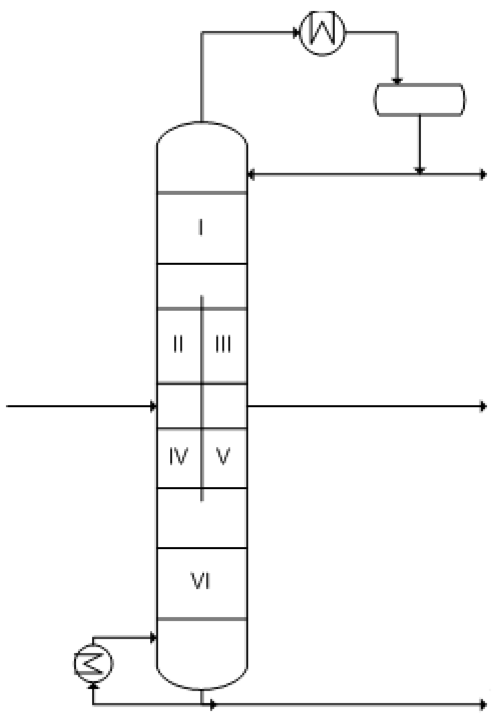
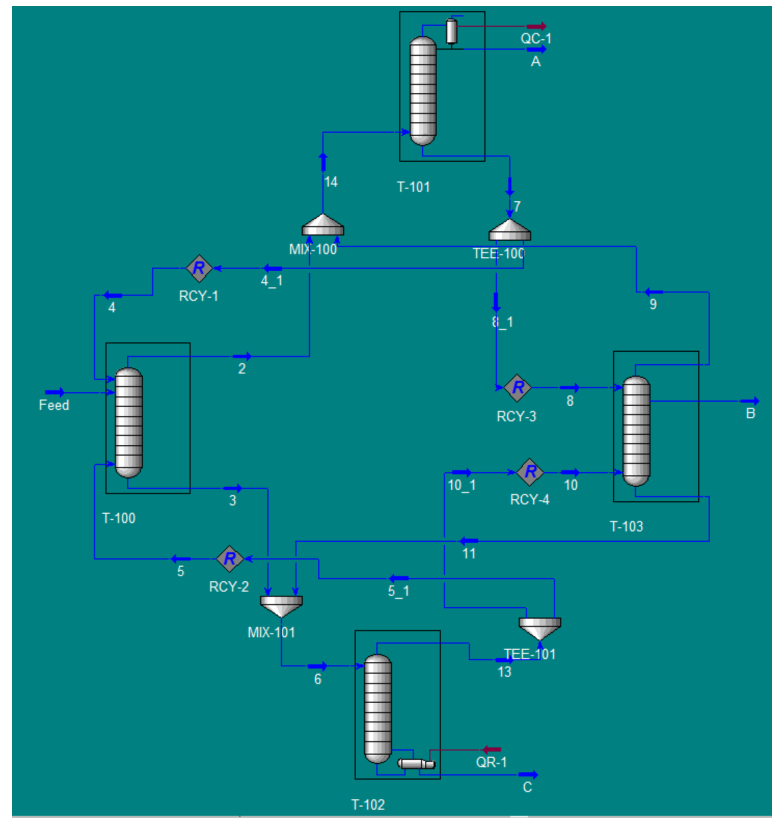


Multi-column model in UNISIM Design



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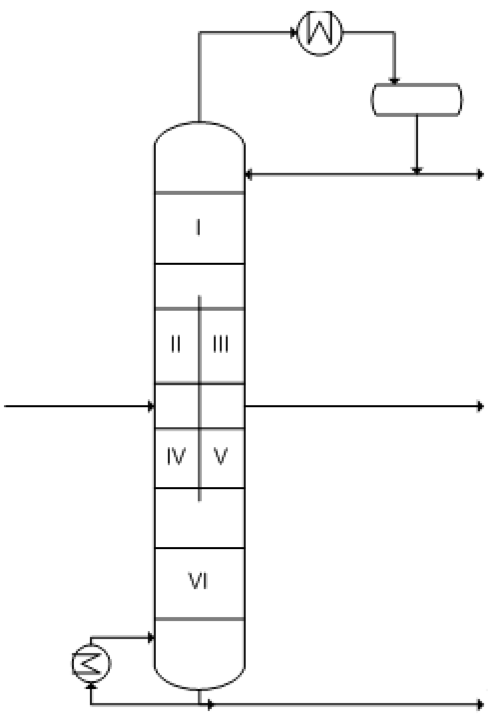
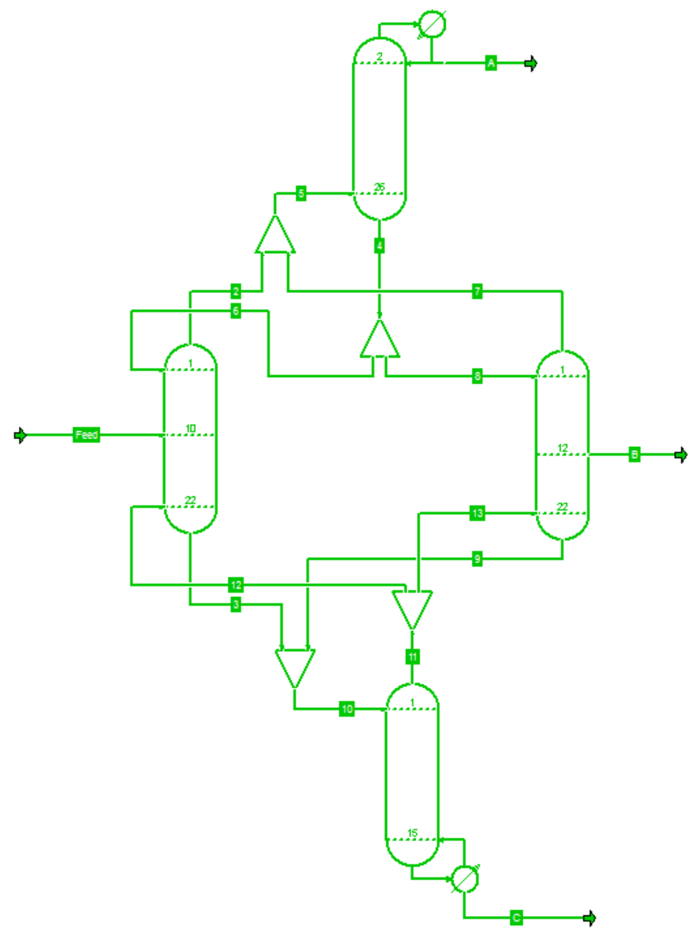


Multi-column model in COCO



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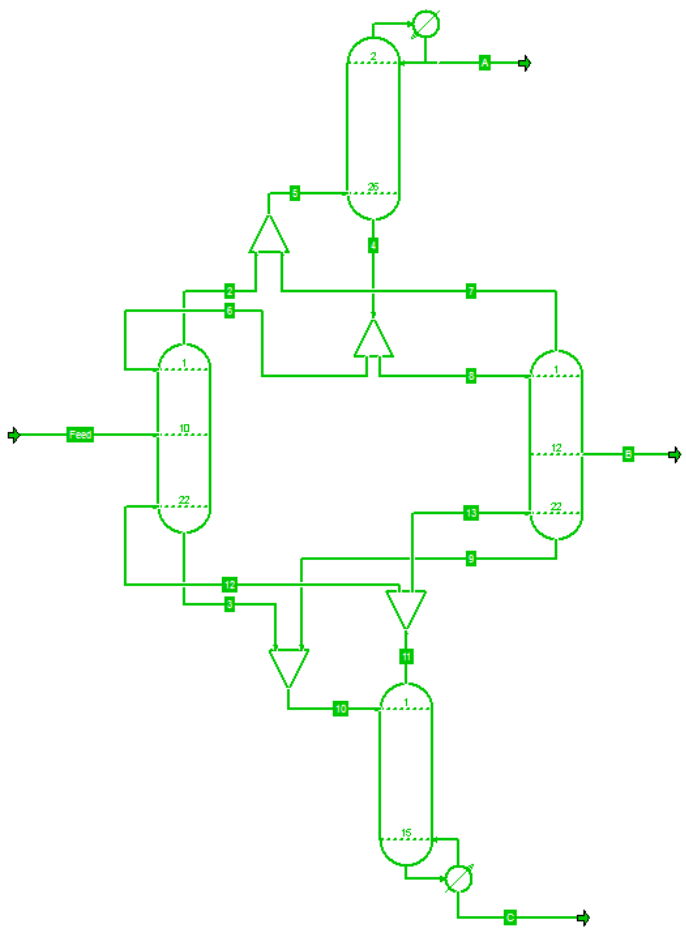
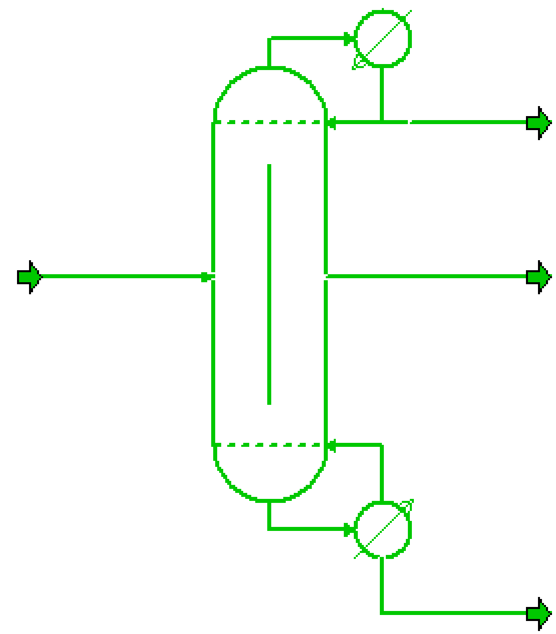
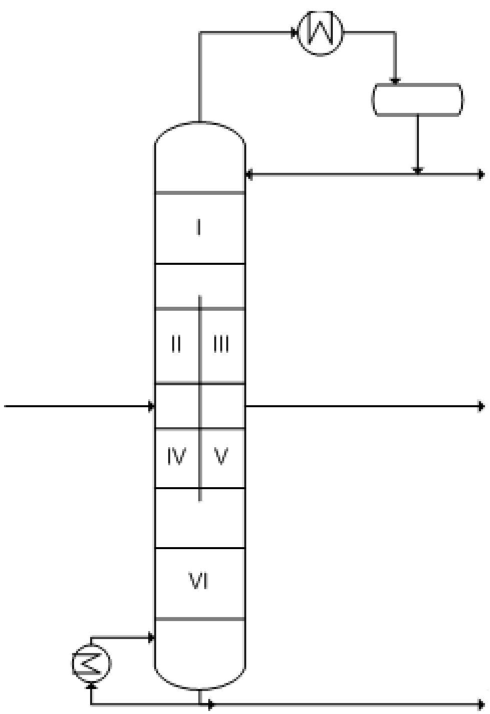


DWC icon hides subflowsheet

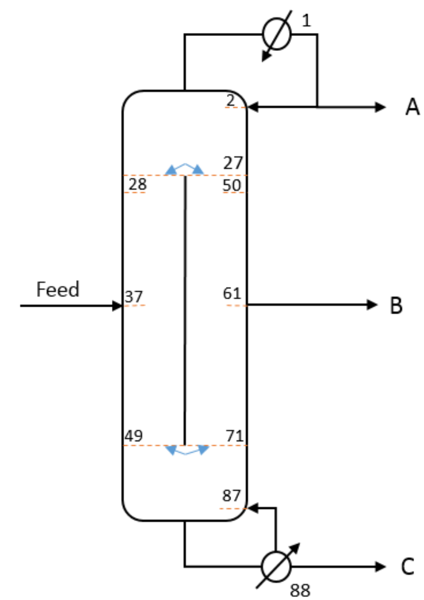


ChemSep Parallel Column Model (PCM)

Dejanović et al. Aromatics DWC

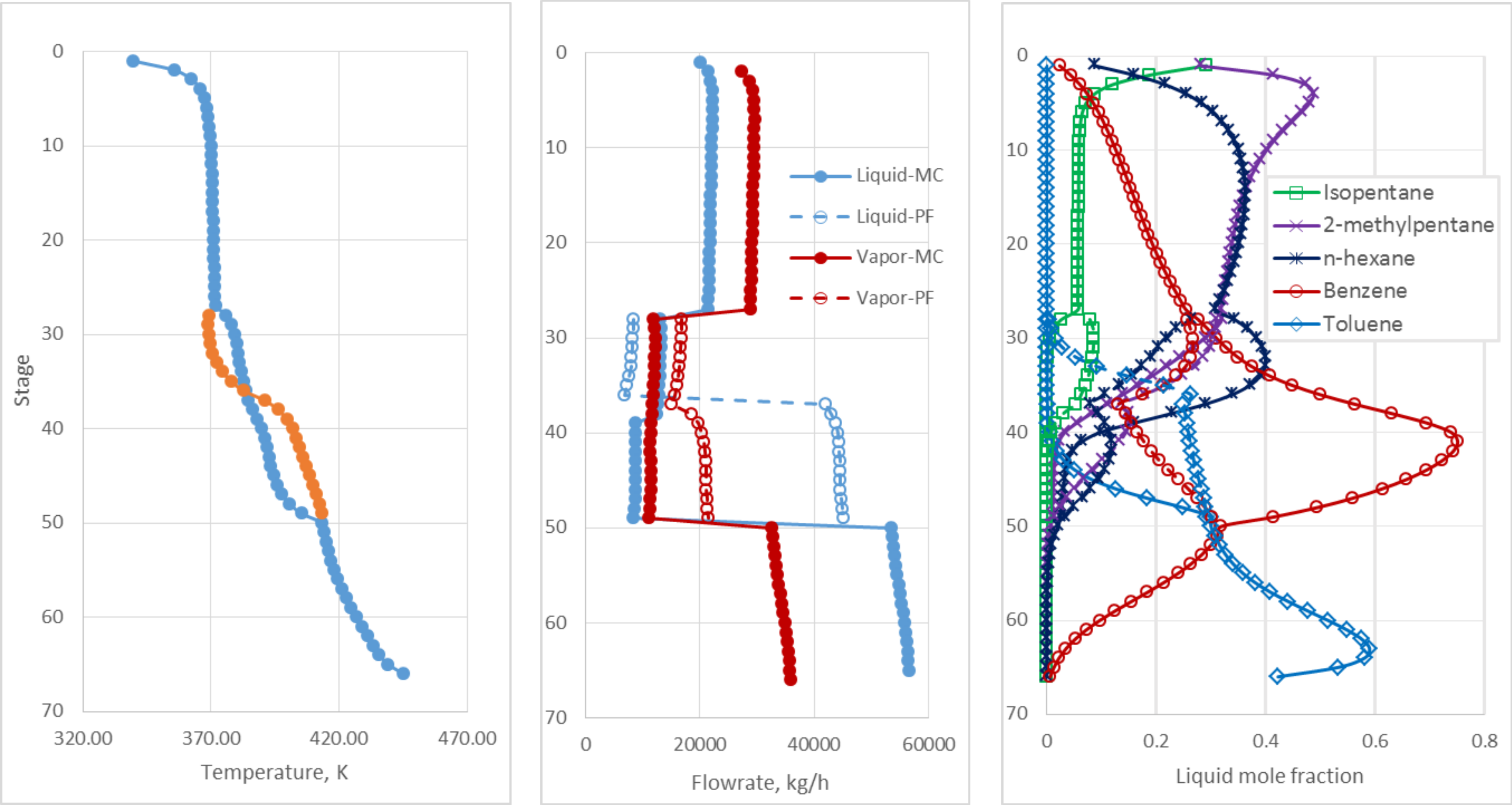


Equation-based ChemSep PCM



ChemSep Modeling Separation Processes

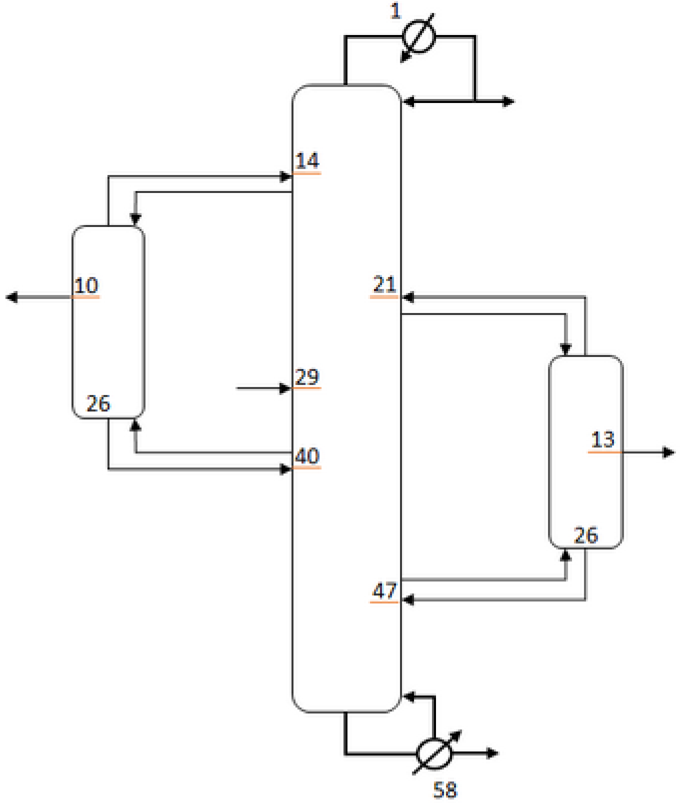
- **Dejanović et al. Aromatics DWC Modelled Using ChemSep PCM**



Dividing Wall Columns

- Generally modeled as multi-column systems

Satellite Column System



Dividing Wall Columns

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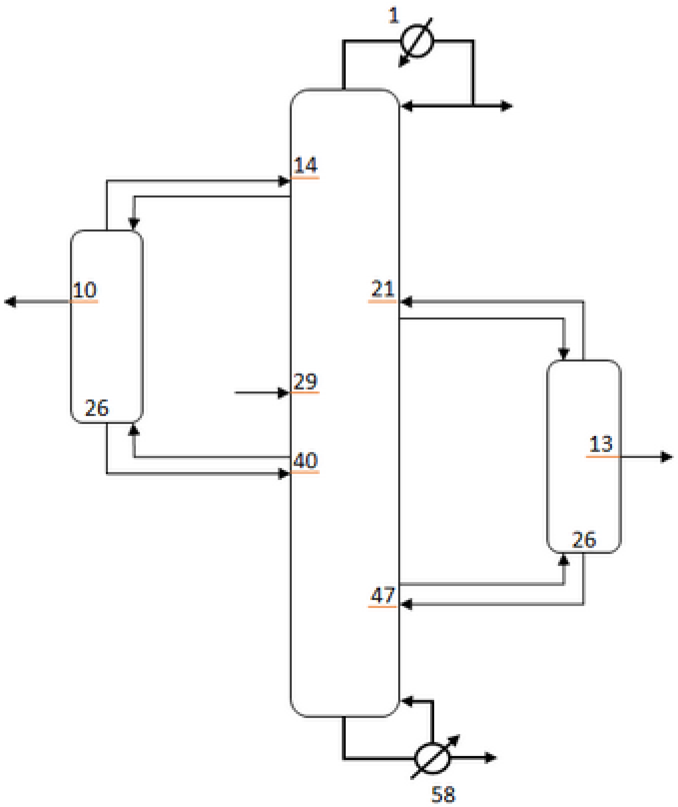
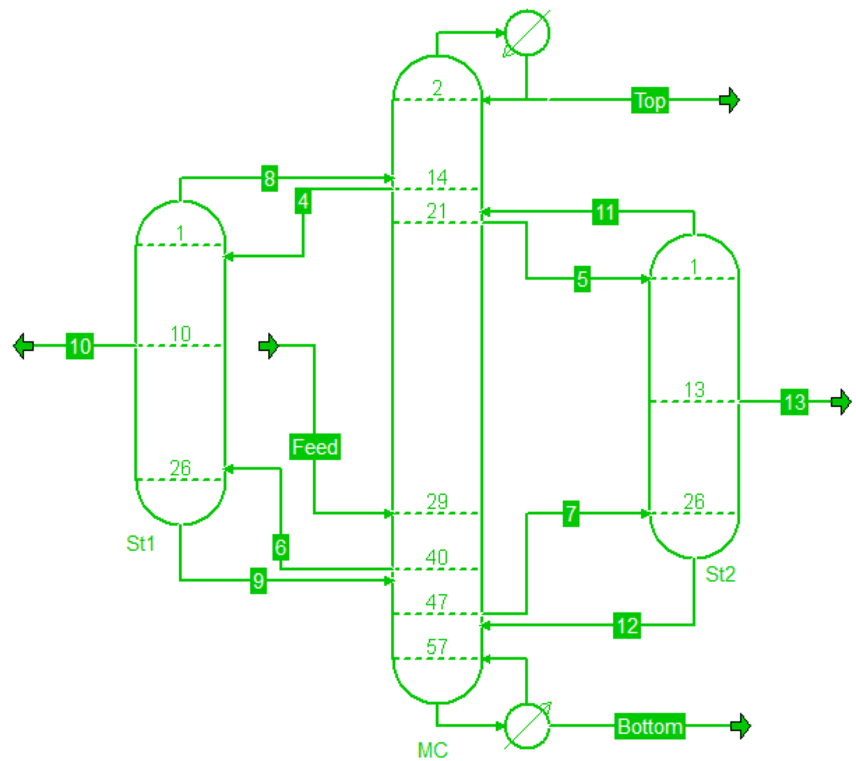


Satellite Column System in COCO (easy to converge)



Dividing Wall Columns

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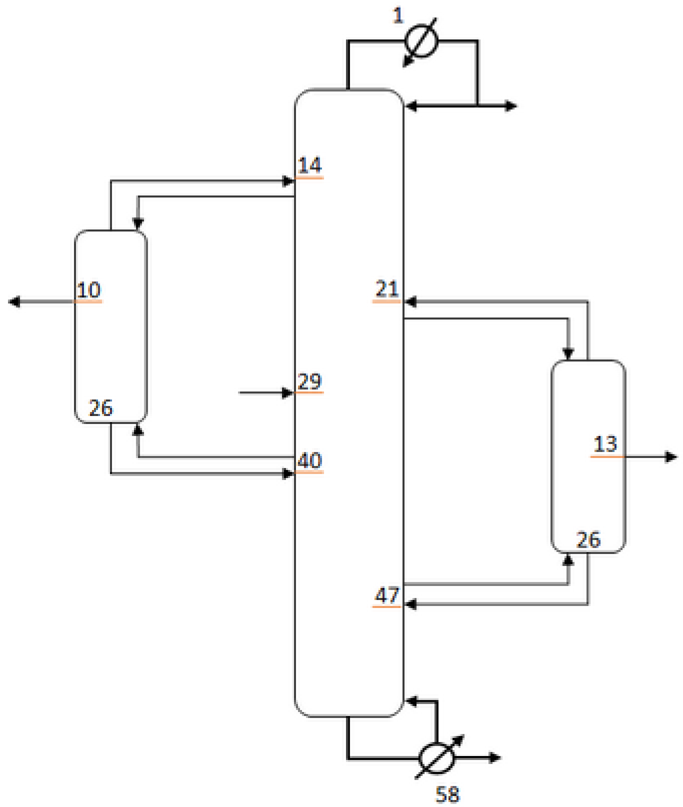
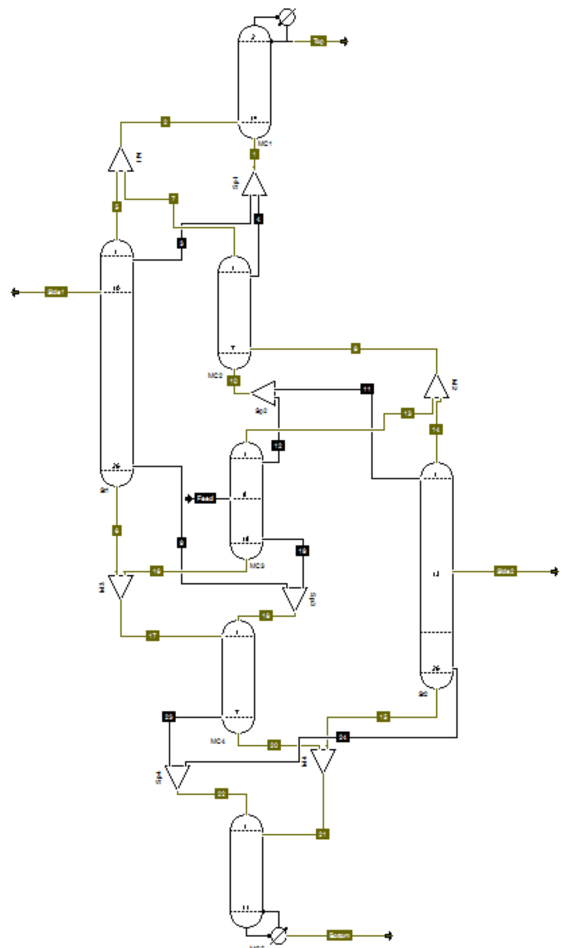


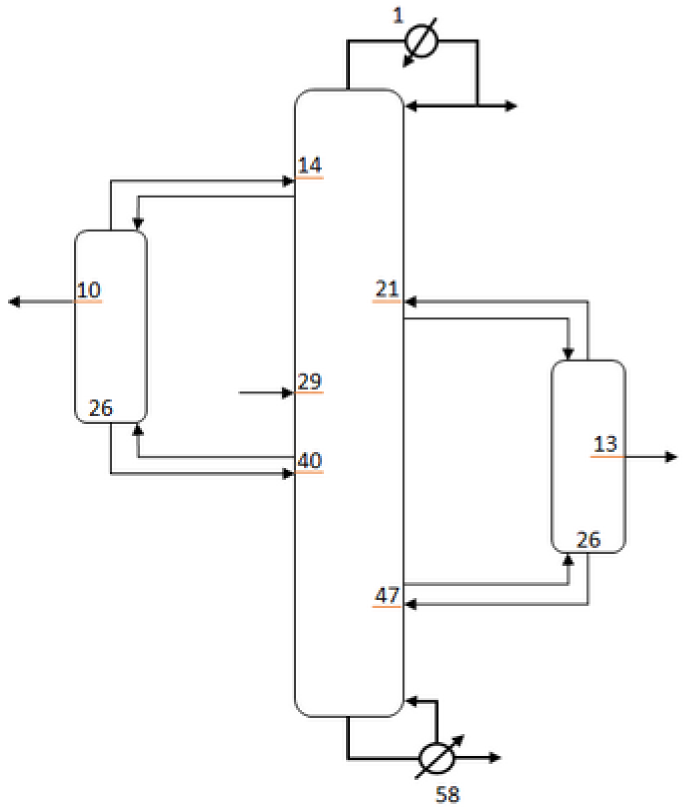
Satellite Column System in COCO (hard to converge)



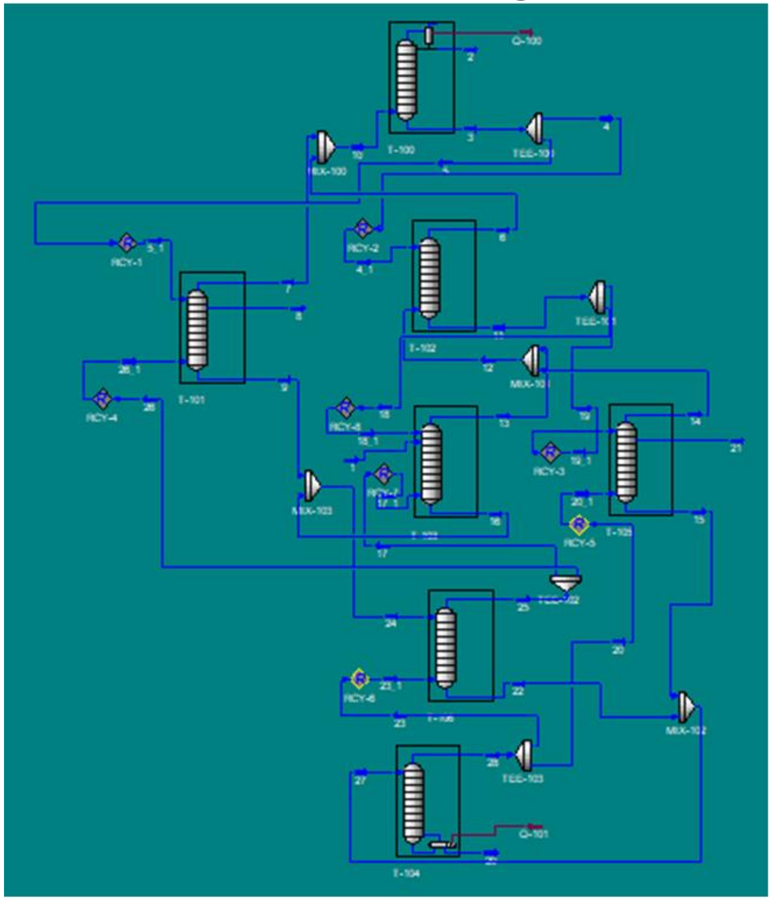
Dividing Wall Columns

- Generally modeled as multi-column systems

Satellite Column System



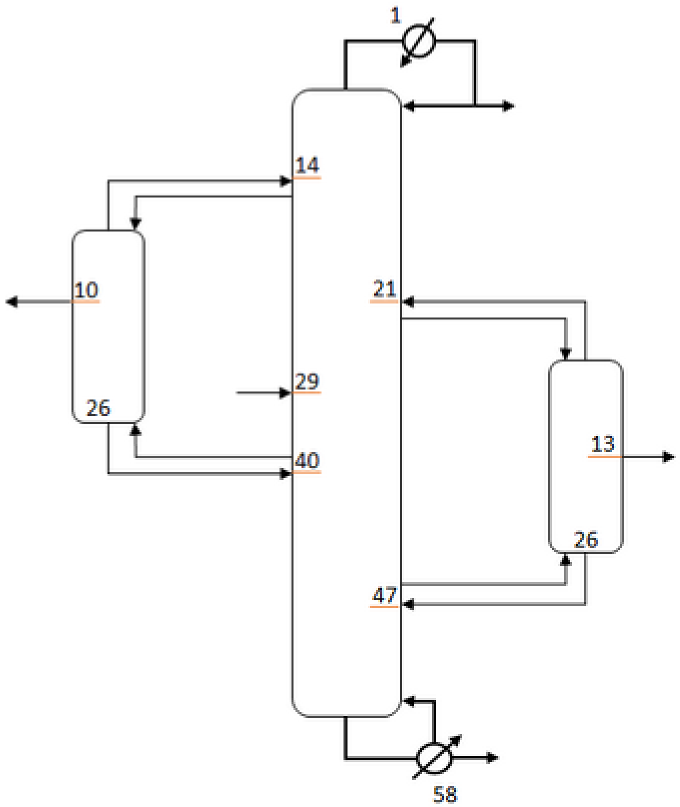
Satellite Column System in UNISIM Design



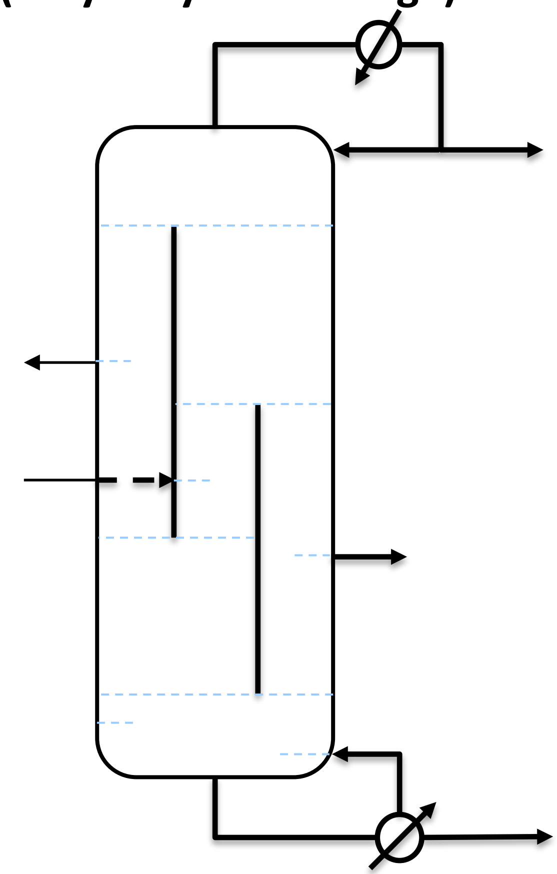
Dividing Wall Columns

ChemSep Parallel Column Model (PCM)

Satellite Column System



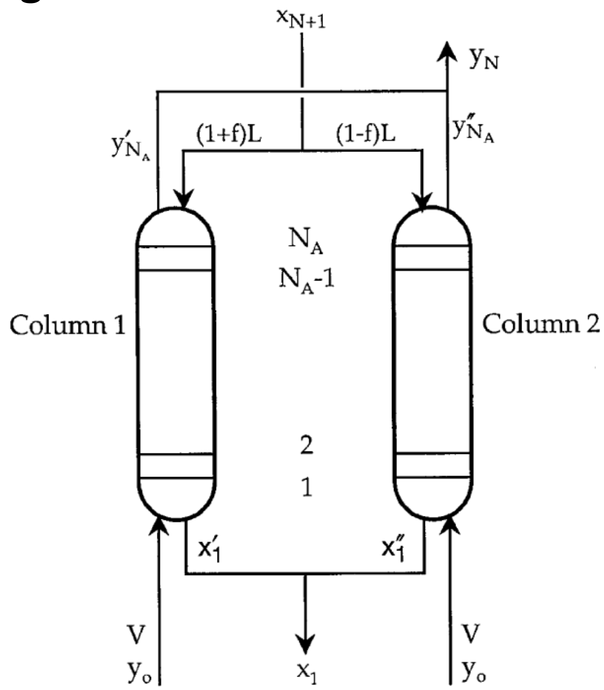
Equation-based ChemSep PCM (very easy to converge)



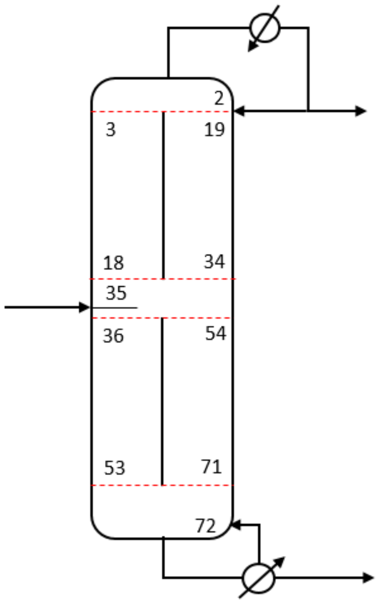
Maldistribution Models

- **ChemSep PCM can be used to model maldistribution**

Billingham and Lockett Maldistribution Model



Equivalent PCM Structure

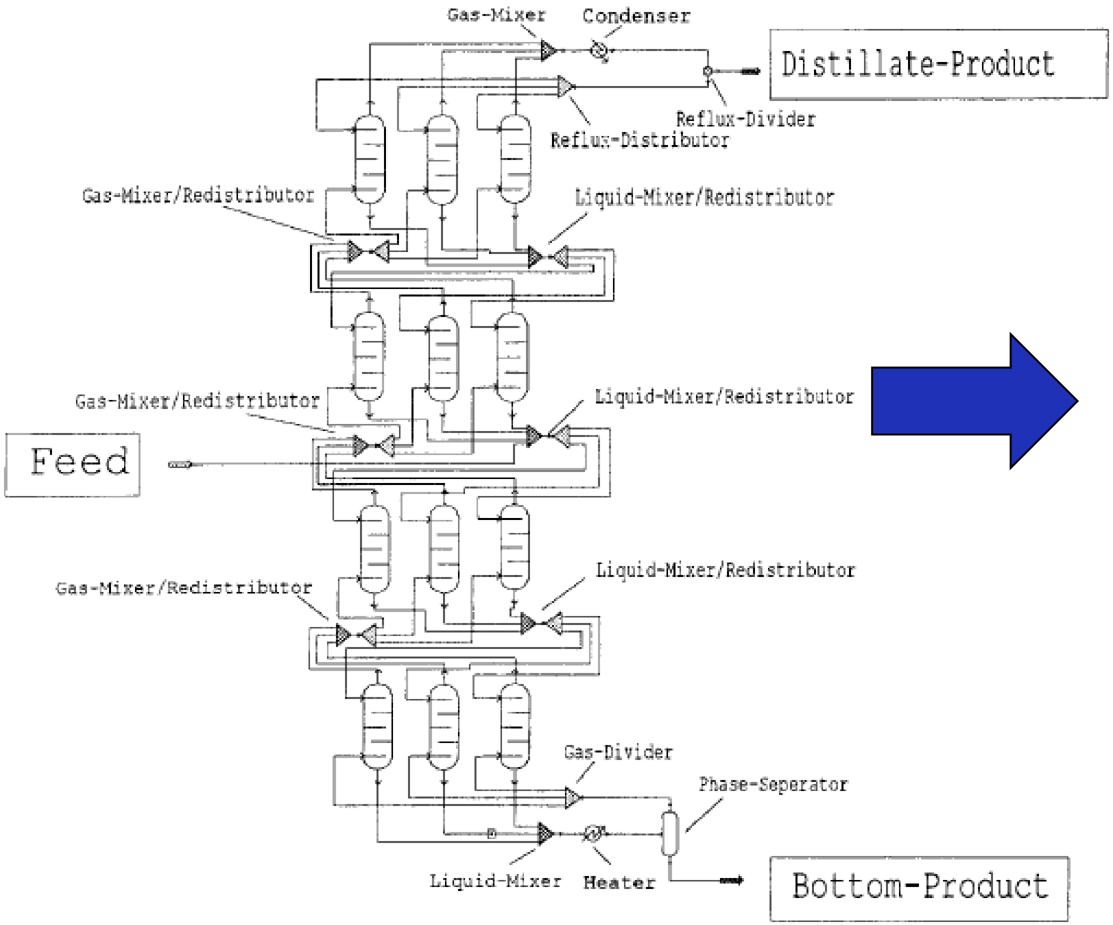


- Redistributors modeled as stages with no mass transfer

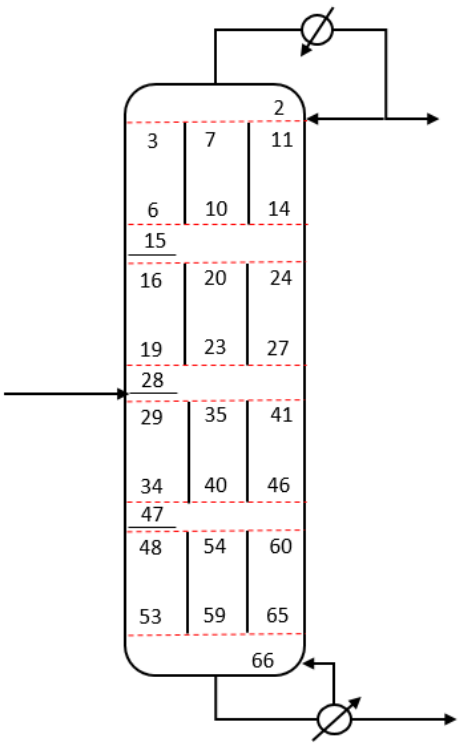
Maldistribution Models

- ChemSep PCM can be used to model maldistribution

Schultes Maldistribution Model

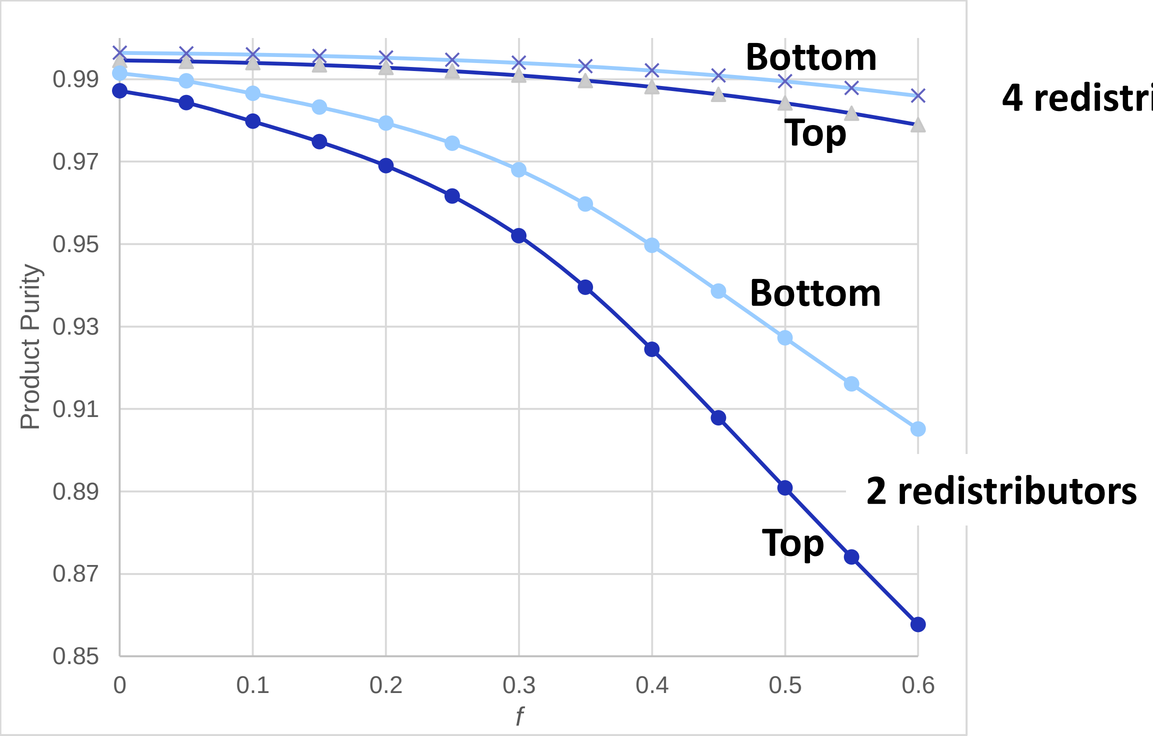


Equivalent PCM Structure



Maldistribution Models

- ChemSep PCM can be used to model maldistribution



Significant influence of the number of redistributors

Other Matters

- **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

- **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)

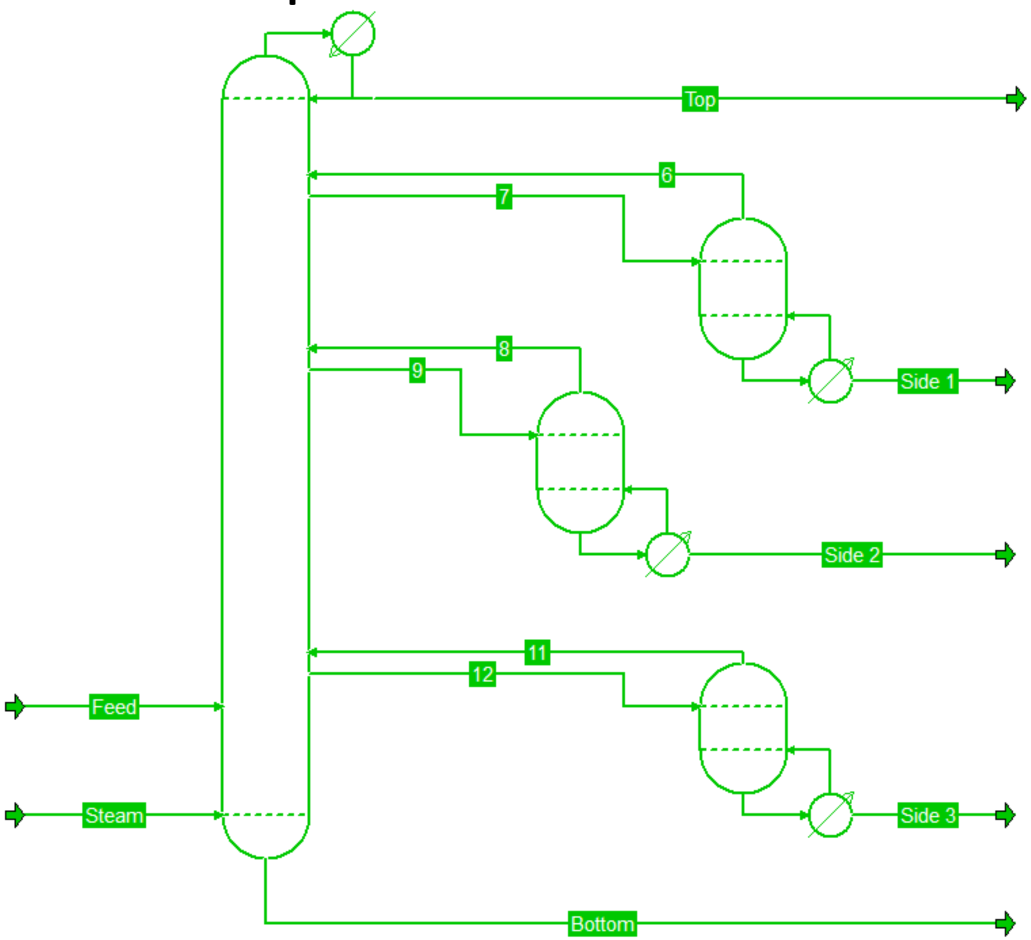
Coming Soon to ChemSep Version 8

ChemSep
Modeling Separation Processes

Parallel Column Model

- Dividing Wall Columns, Maldistribution, Multi-column Systems

Multiple column model in COCO



One equation-based model ChemSep Version 8