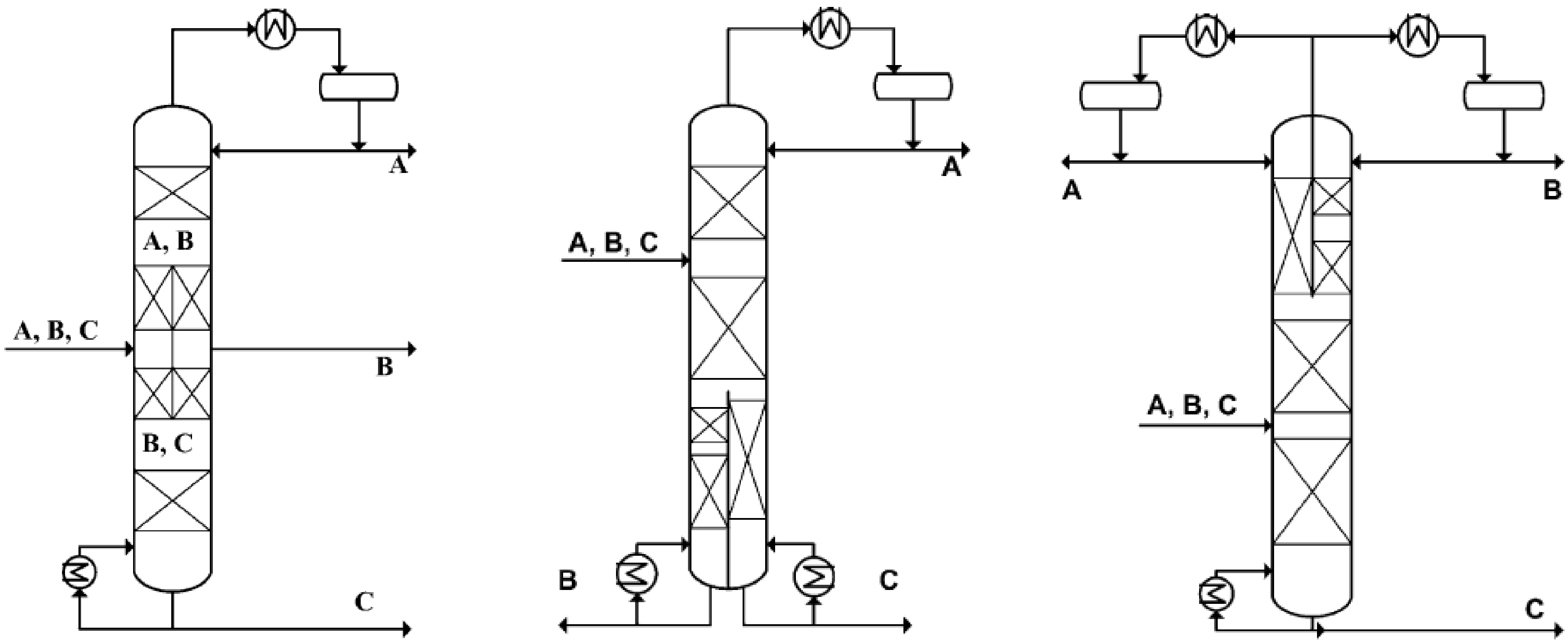
An Equation-Based Parallel Column Model

Jingsong Zhou, Harry Kooijman, and Ross Taylor

Department of Chemical and Biomolecular Engineering
Clarkson University
Potsdam, NY 13699

Dividing Wall Columns: Not New Anymore

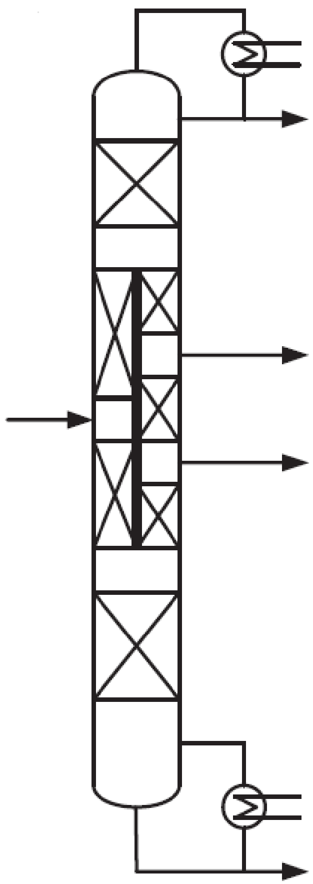
- DWCs with three products

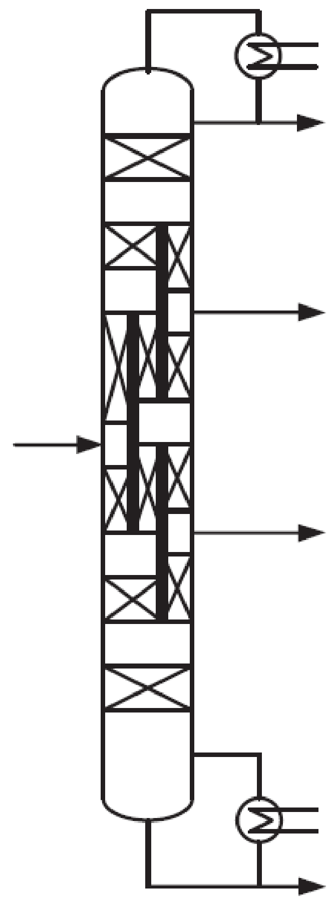


Dejanović, I., Matijašević, L., & Olujić, Ž. (2010). Dividing wall column—a breakthrough towards sustainable distilling. *Chemical Engineering and Processing: Process Intensification*, ***49***(6), 559-580.

Dividing Wall Columns: Not New Anymore

- DWCs with more than three products





Kaibel, B. Dividing-Wall Columns, in *Distillation: Equipment and Processes* pp 183–199, Academic Press, 2014

Dividing Wall Columns: Not New Anymore

- Dejanović, I., Matijašević, L. & Olujić, Ž. Dividing wall column—a breakthrough towards sustainable distilling. *Chem. Eng. Process. Process Intensif.* 49, 5 pp 59–580, 2010
- Yildirim, Ö, Kiss, A.A., Kenig, E.Y., Dividing wall columns in chemical process industry: A review on current activities, *Separation and Purification Technology*, 80, pp 403-417, 2011
- Kiss, Anton A. *Advanced distillation technologies: design, control and applications*. John Wiley & Sons, 2013.
- Kaibel, B. Dividing-Wall Columns, in *Distillation: Equipment and Processes* pp 183–199, Academic Press, 2014

Dividing Wall Columns: What They Said

Dejanović et al. (2010) wrote:

*Carrying out DWC performance simulations **requires great experience** and these are more or less computationally very demanding. … well established commercial software packages still do not contain a DWC as a standard model. This however will occur sooner or later, most probably as a **simultaneous, equation based model**.*

Kaibel (2014) wrote:

*Due to the potential variability of complex internal configurations, there is no dedicated software package for this purpose. … As there are strong interactions between the parameters, a rather stiff system of equations has to be solved. The convergence behavior of programs with sequential operation is sometimes problematic. **Equation-based programs normally show better convergence characteristics**.*

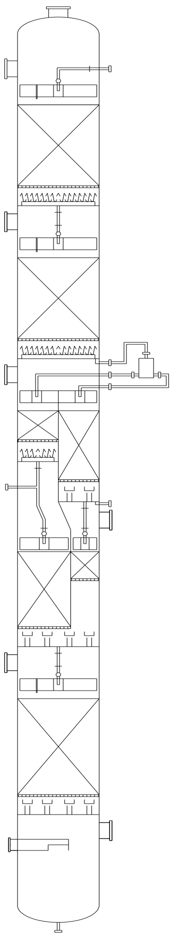
But, so far, nobody has provided any evidence that that is true!

Outline

- Introduction
- Existing simulation strategies and challenges
- An equation-based parallel column model
- Examples
- Validation with Pilot DWC Data
- Conclusions
- Coming soon…

Existing Simulation Strategy

- Dejanović et al. Aromatics DWC



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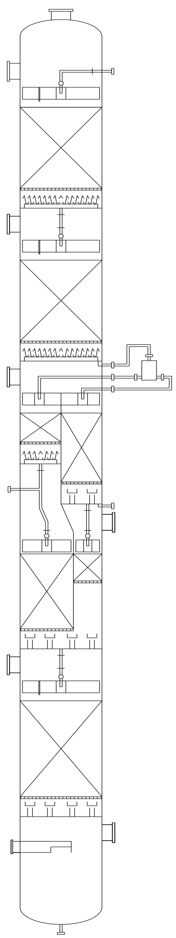

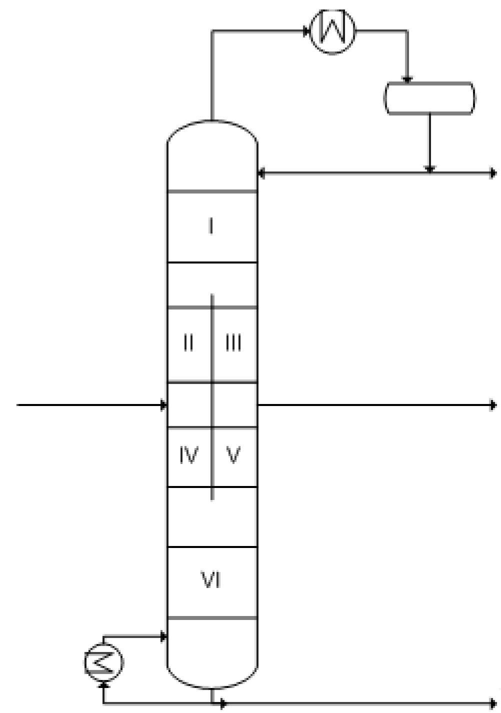

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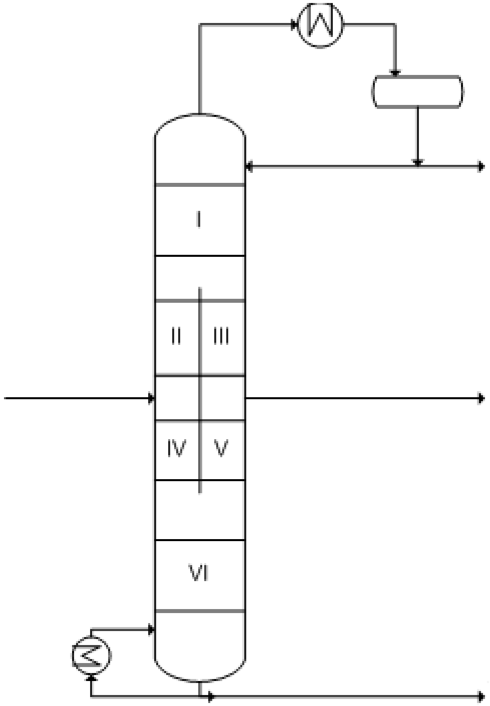
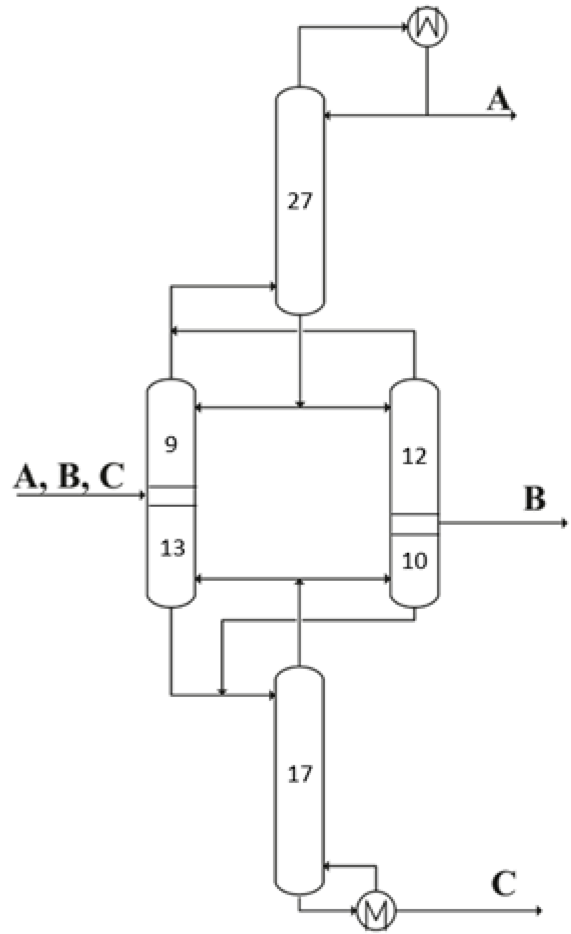
Existing Simulation Strategy

- Generally modeled as multi-column systems

Dejanović et al. Aromatics DWC



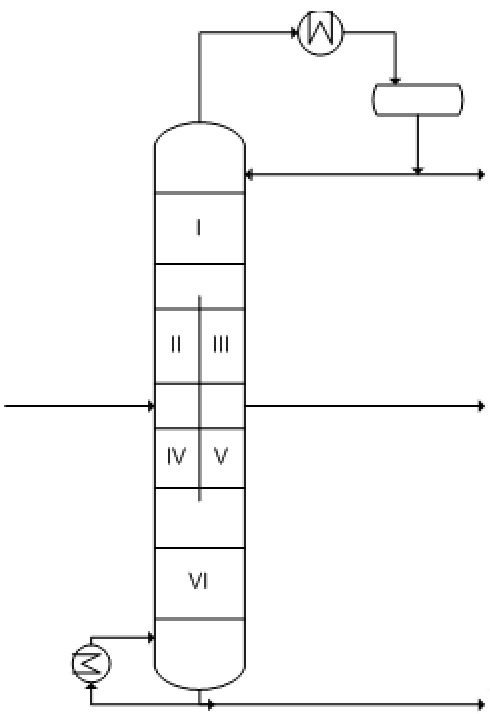
Four-column model



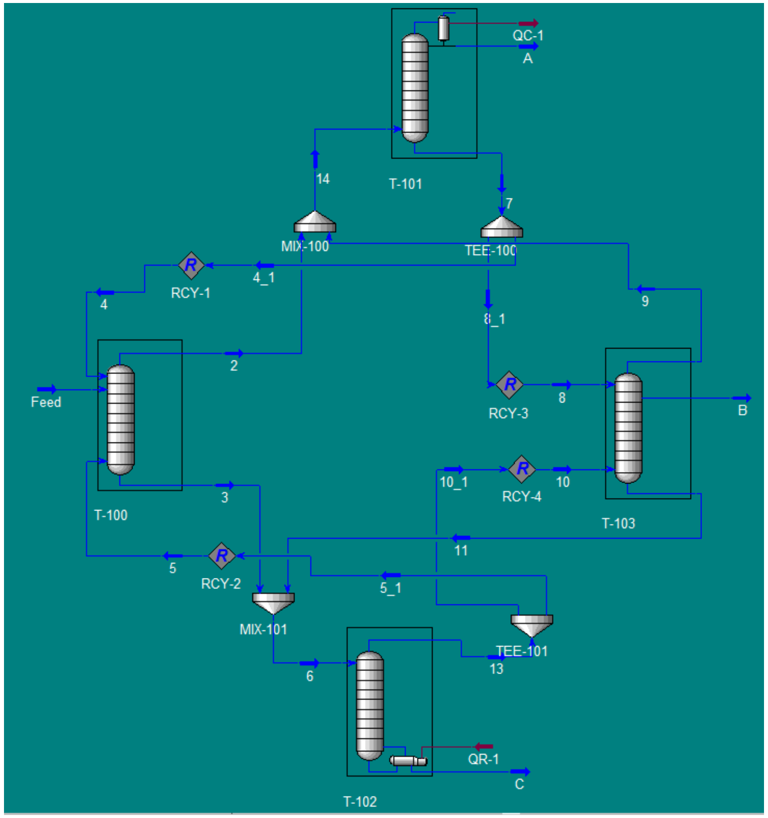
Existing Simulation Strategy

- Generally modeled as multi-column systems

Dejanović et al. Aromatics DWC



Four-column model in UNISIM Design



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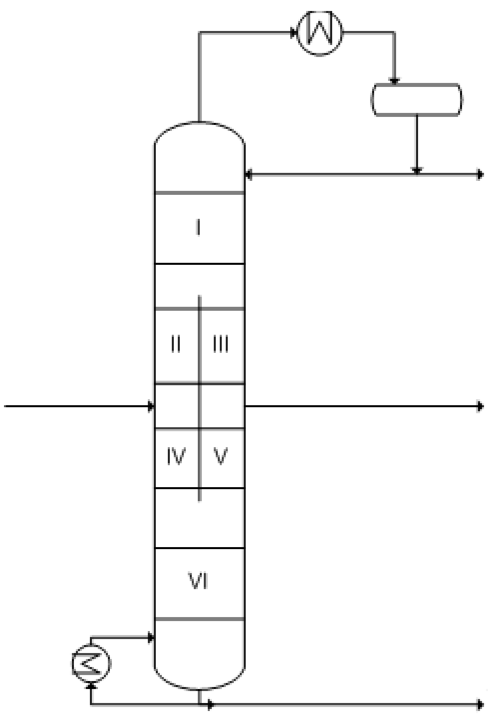
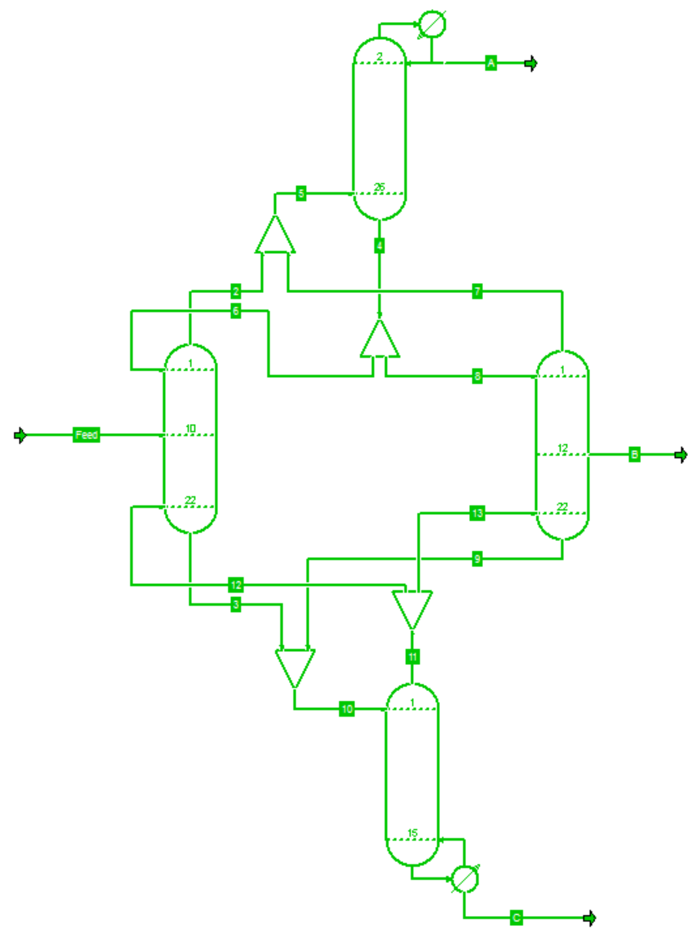


Four-column model in COCO



Existing Simulation Strategy

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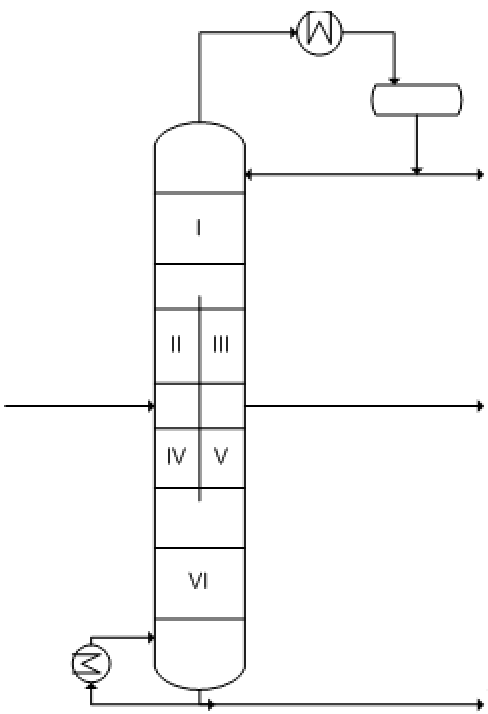
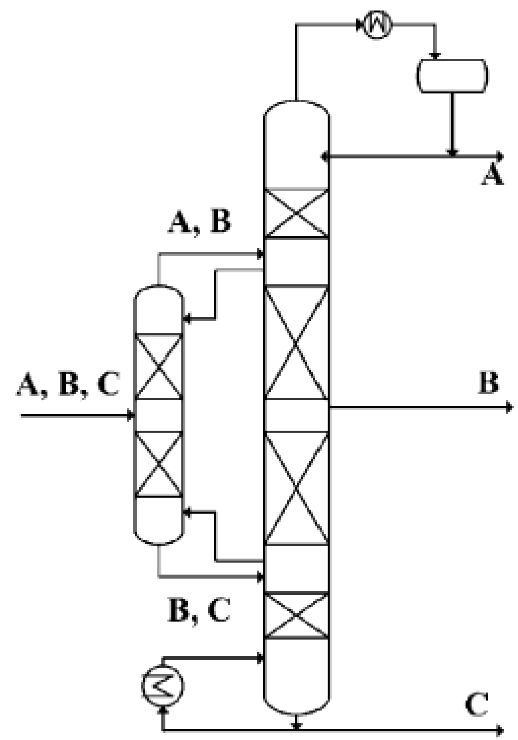
Dejanović et al. Aromatics DWC



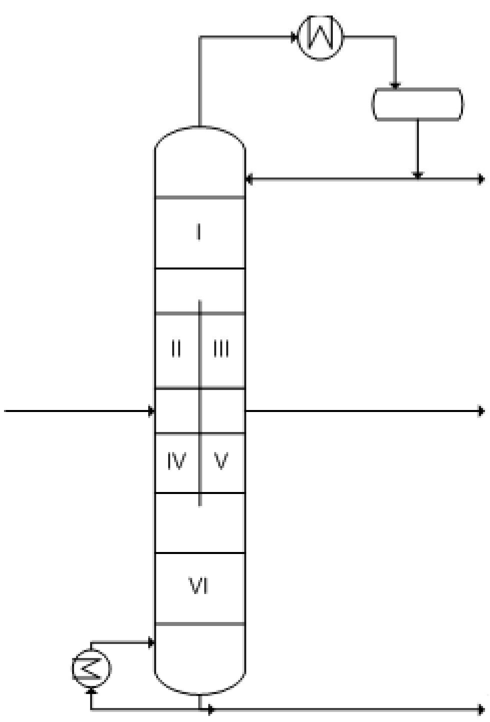
Two-column model



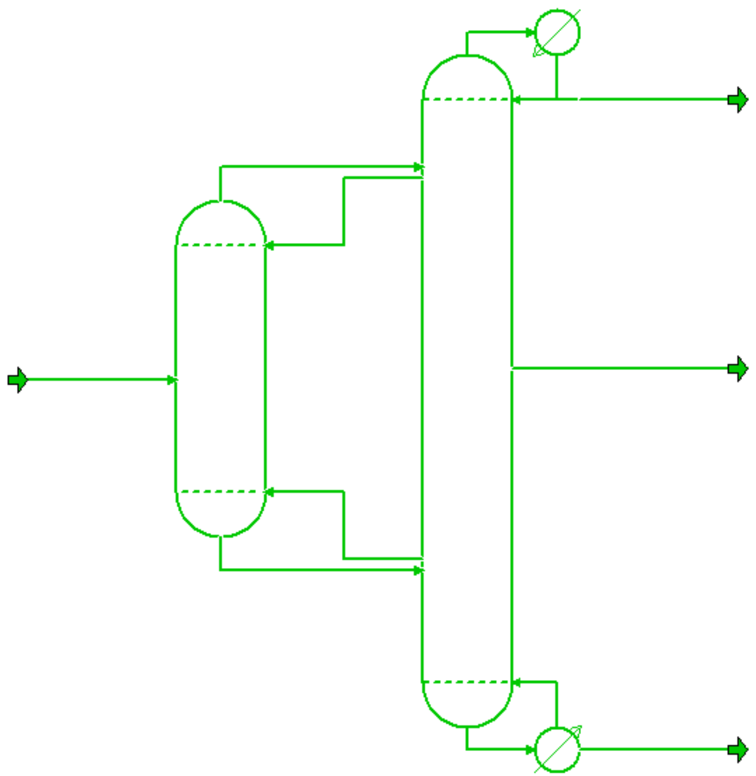
Existing Simulation Strategy

- Generally modeled as multi-column systems

Dejanović et al. Aromatics DWC

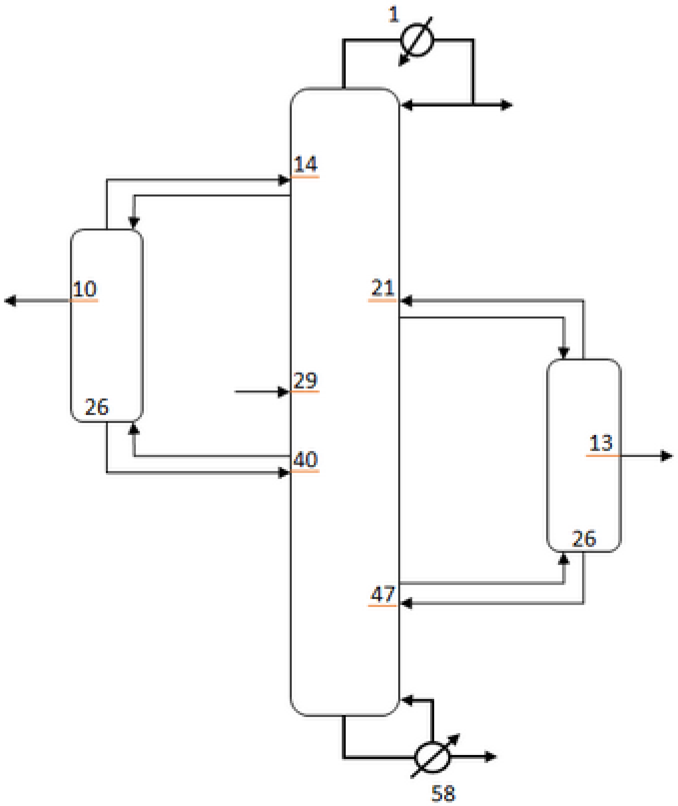


Two-column model in COCO



Satellite Column System

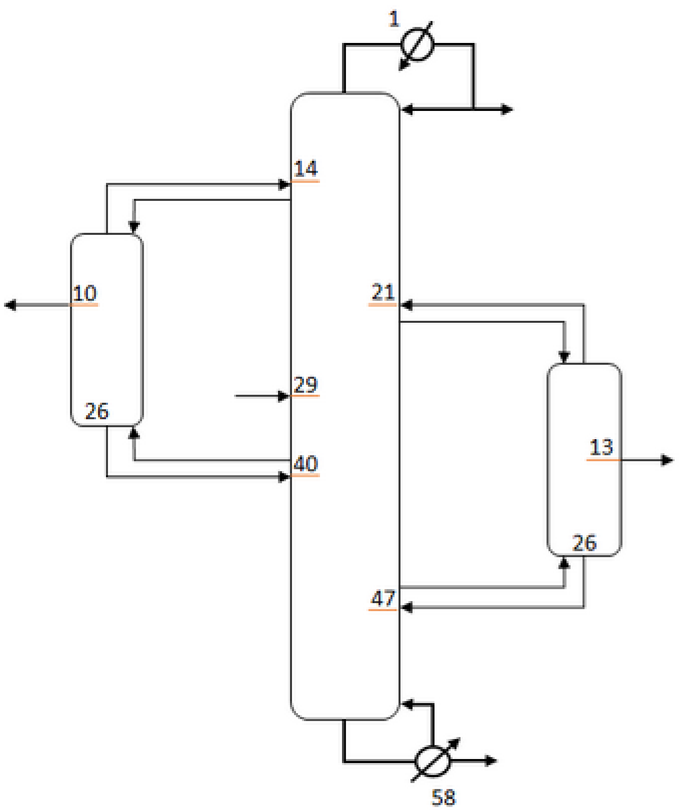
Satellite Column Schematic



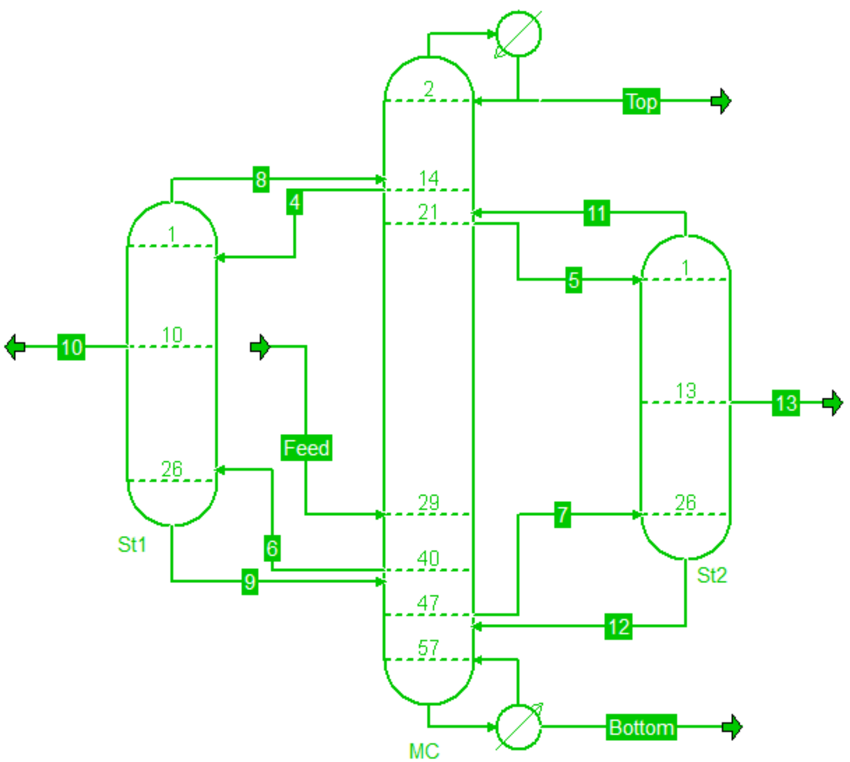
Tututi-Avila, S., Domínguez-Díaz, L. A., Medina-Herrera, N., Jiménez-Gutiérrez, A., & Hahn, J. (2017). Dividing-wall columns: Design and control of a kaibel and a satellite distillation column for BTX separation. *Chemical Engineering and Processing: Process Intensification*, ***114***, 1-15.

Satellite Column System

Satellite Column Schematic

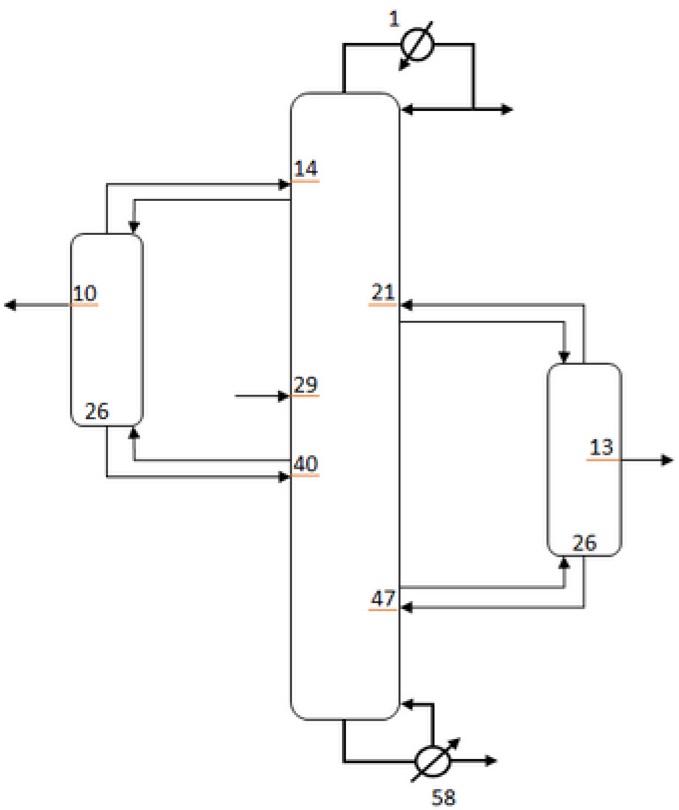


Satellite Column System in COCO (easy to converge)

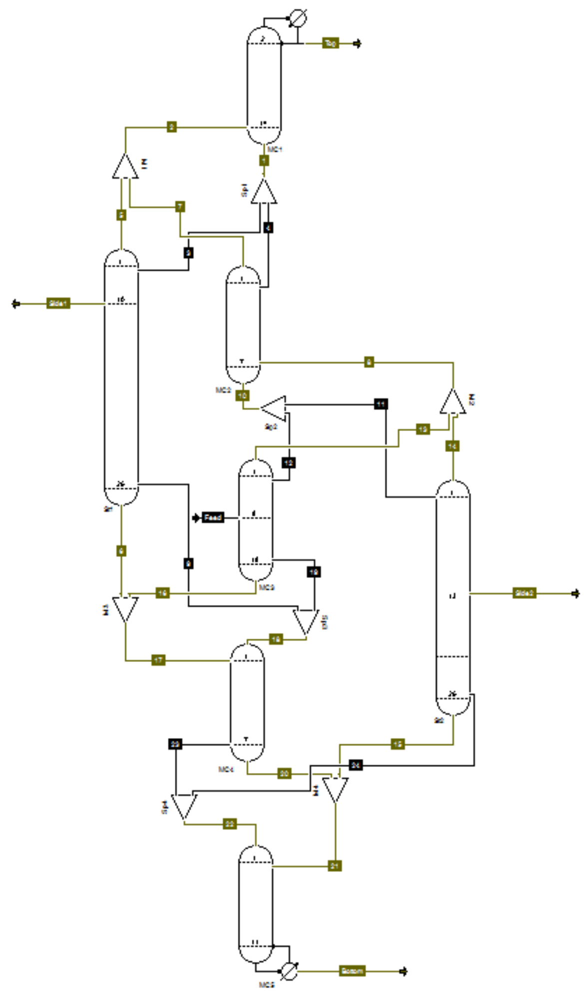


Satellite Column System

Satellite Column Schematic

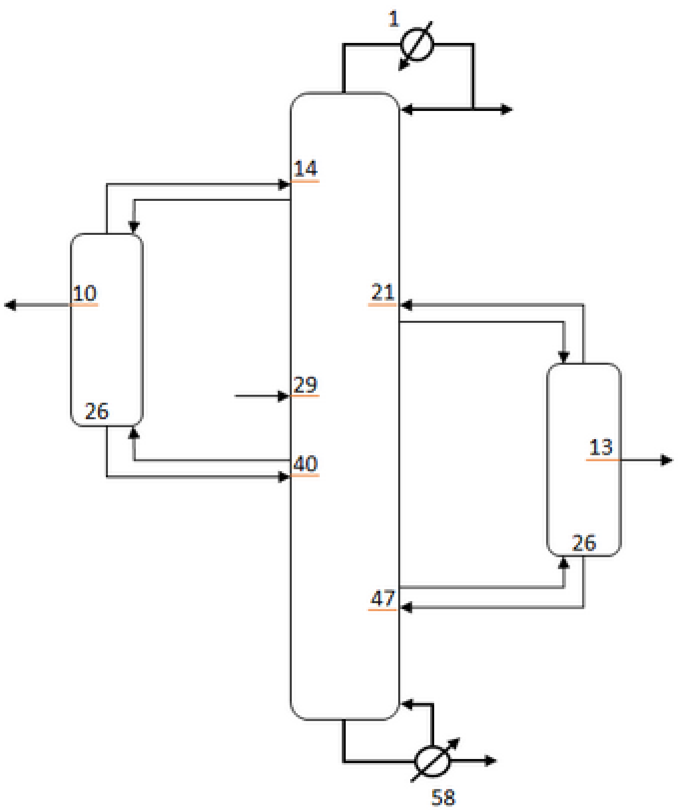


Satellite Column System in COCO (no convergence)

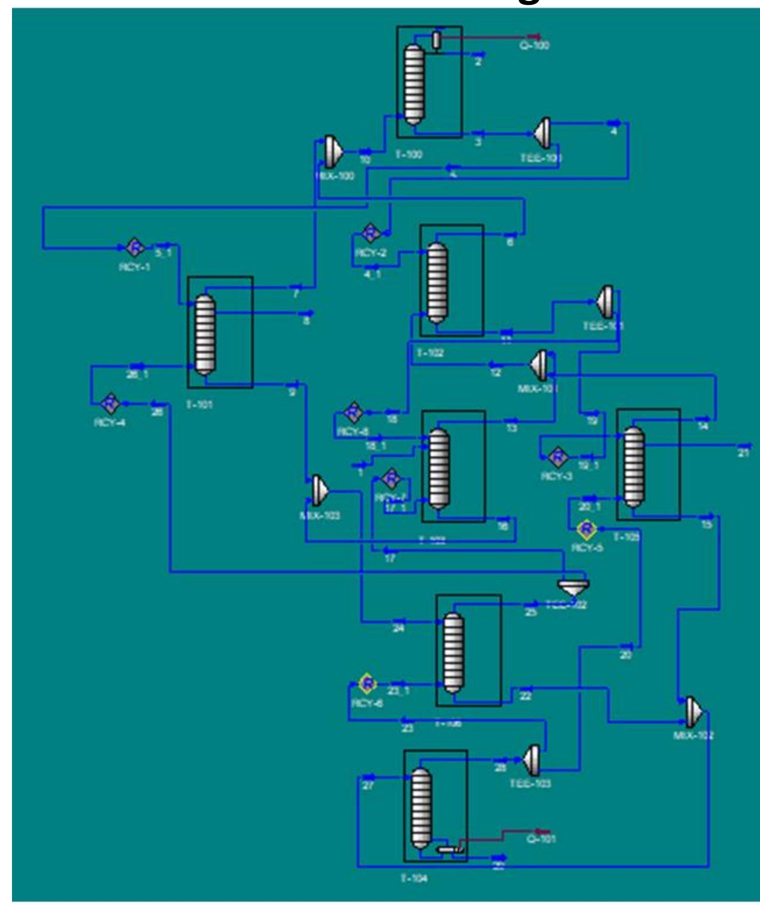


Satellite Column System

Satellite Column Schematic

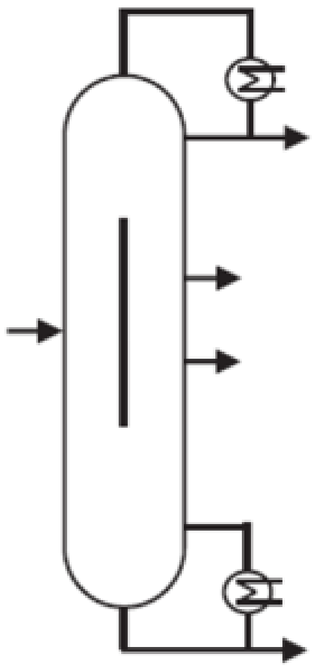


Satellite Column System in UNISIM Design

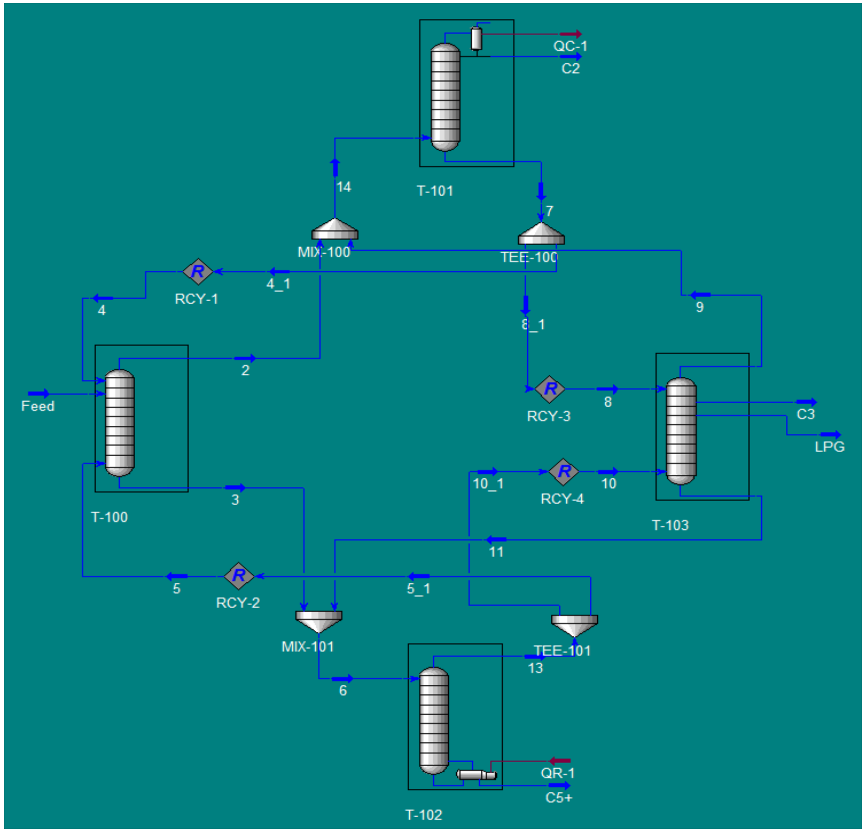


Kaibel Column

Kaibel Column



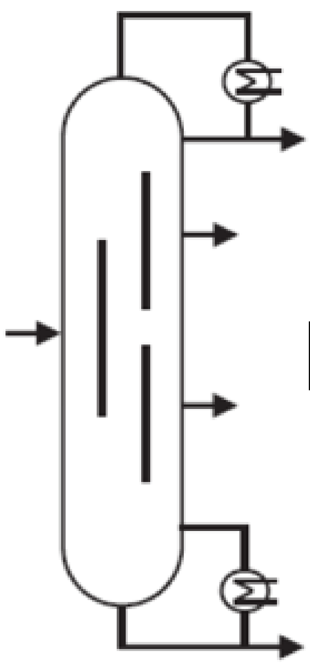
Kaibel Column
in UNISIM Design



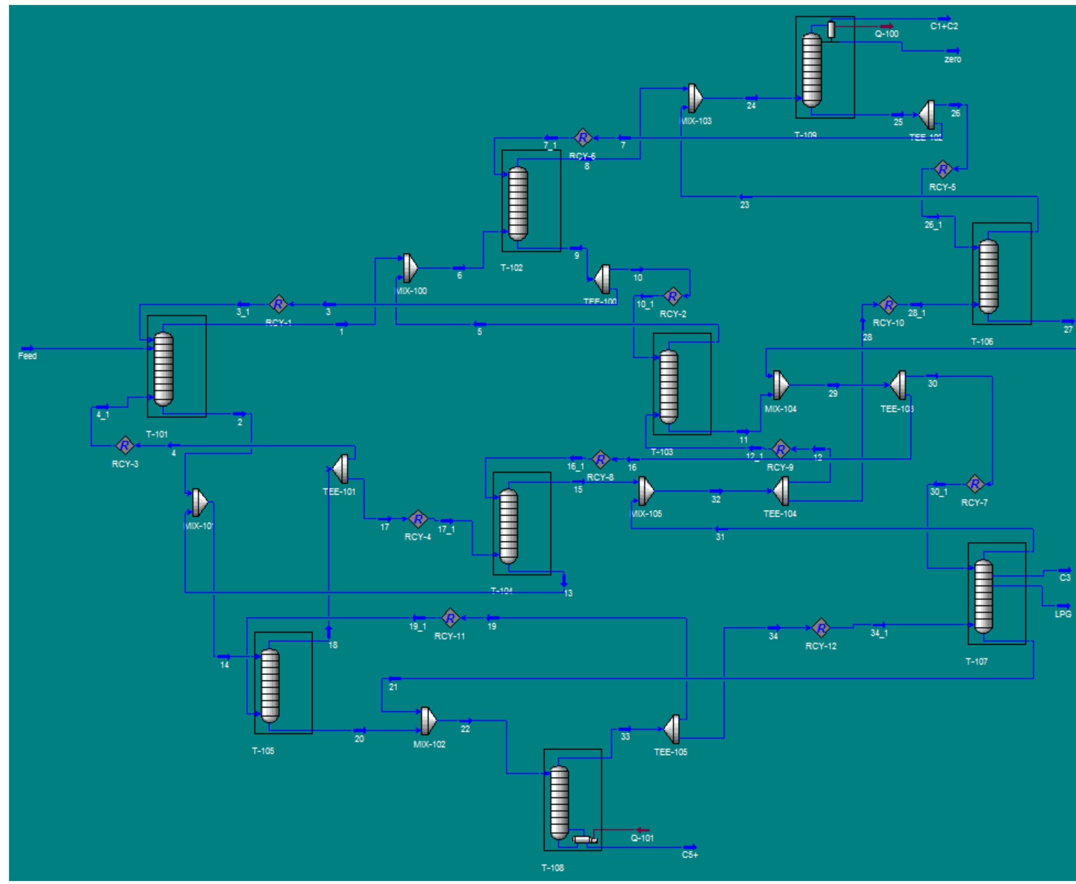
Ashrafian, R. (2014). *Using Dividing Wall Columns (DWC) in LNG Production: deviding wall column, double dividing wall column, prefractionator arrangement, Petlyuk column, NGL recovery, distillation* (Master's thesis, Institutt for energi-og prosessteknikk).

Multiple Wall Column

Multiple Wall Column



Multiple Wall Column in UNISIM Design



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Divided Top Column

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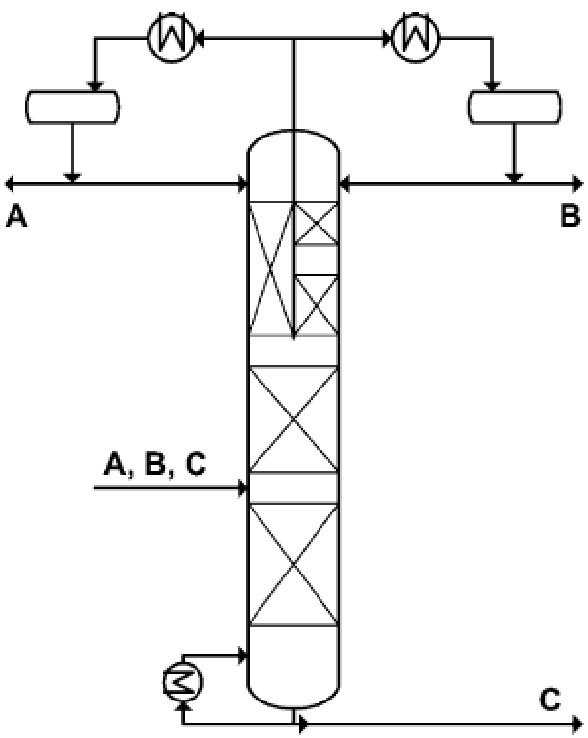
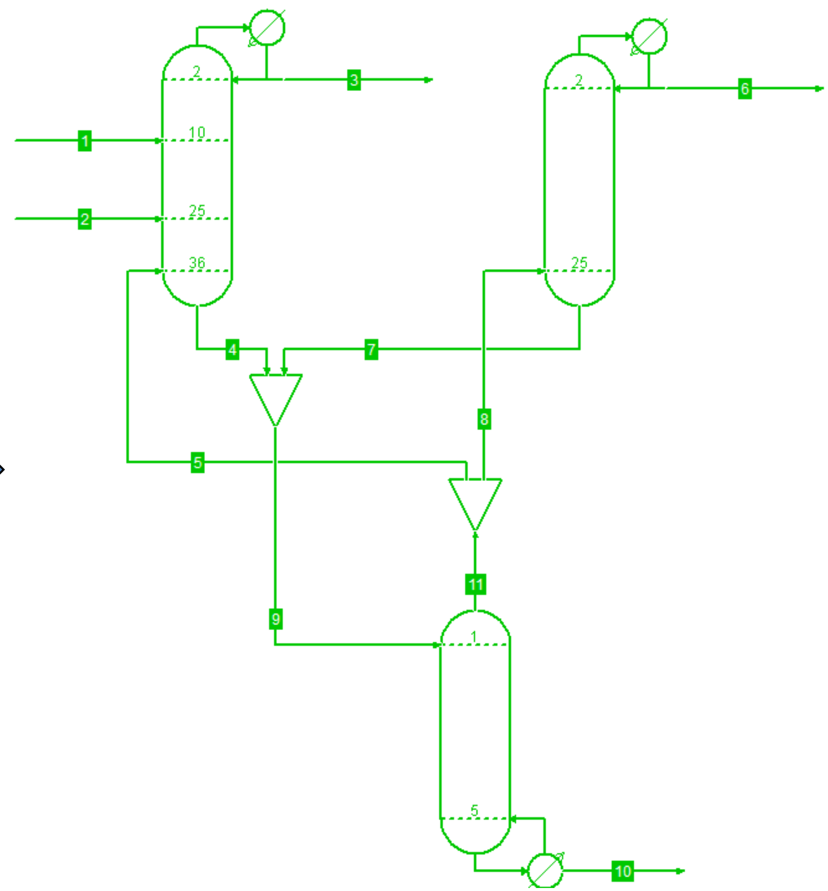
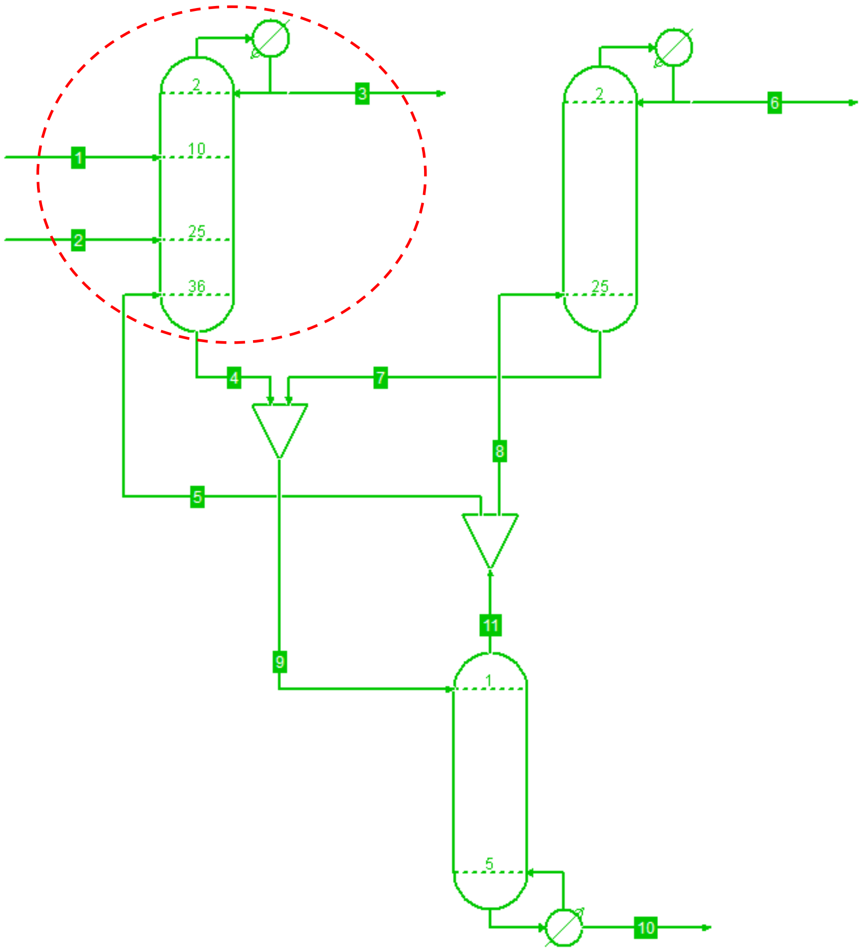


Divided Top Column in COCO

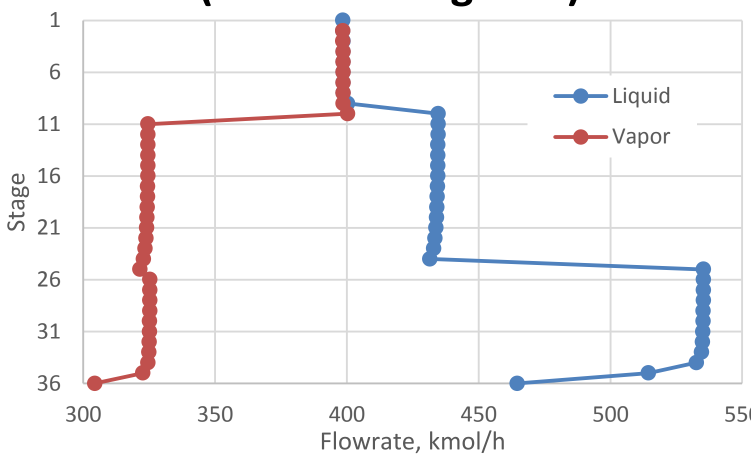


Dai, X., Ye, Q., Qin, J., Yu, H., Suo, X., & Li, R. (2016). Energy-saving dividing-wall column design and control for benzene extraction distillation via mixed entrainer. *Chemical Engineering and Processing: Process Intensification*, ***100***, 49-64.

Divided Top Column



Divided Top Column in COCO (false convergence)



Divided Top Column

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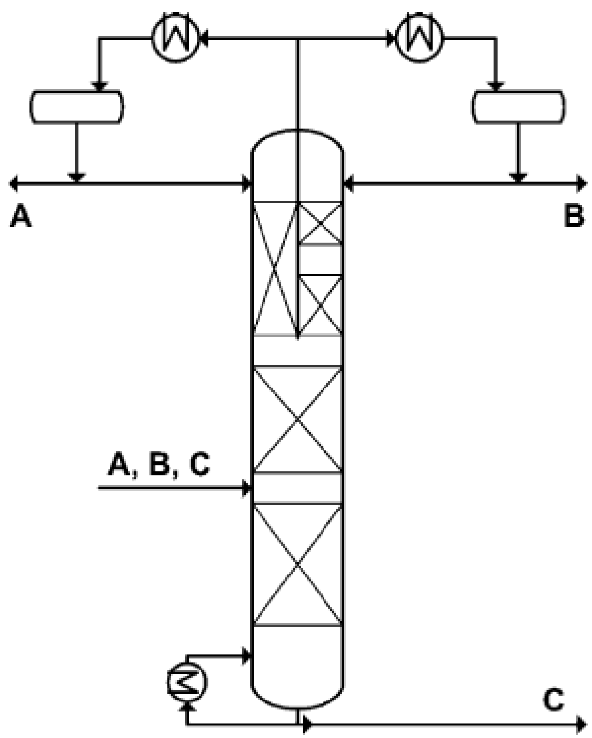
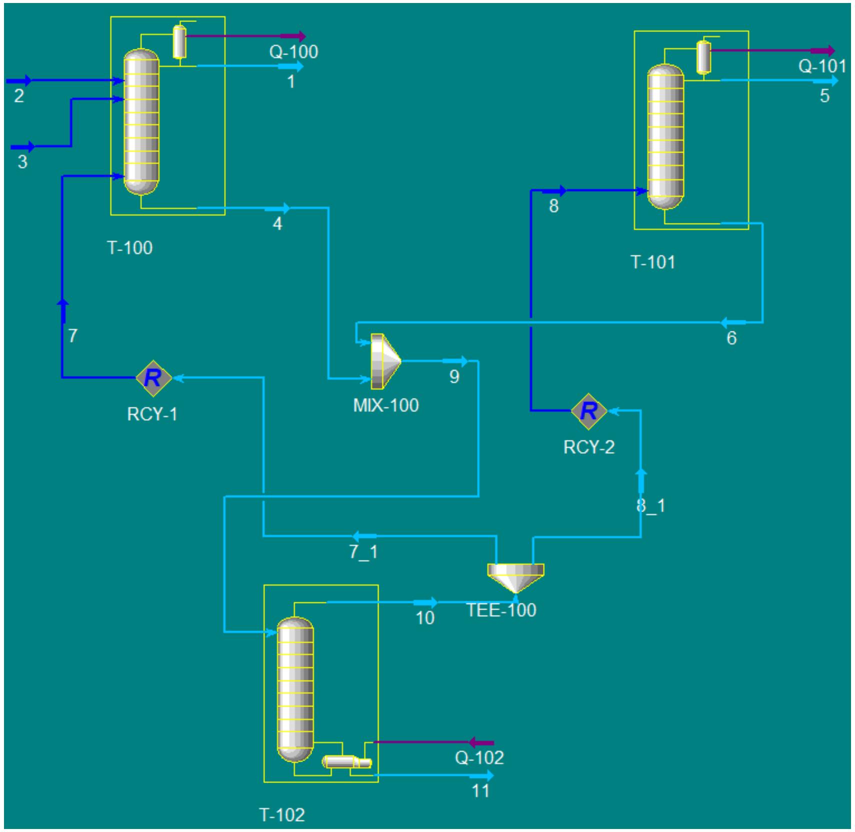


Divided Top Column in UNISIM Design (No convergence)



The Challenges

- Considerable effort needed to set up a multi-column model
- Difficult to provide adequate initial guesses of linking streams
- Slow, no, or false convergence
- Some desirable specifications cannot be used (e.g. recovery)

Equation-Based Parallel Column Model

MESH equations:

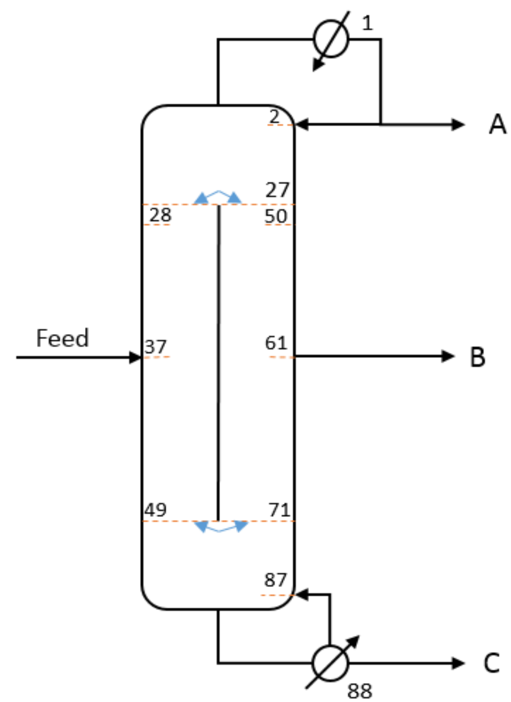
- M: Material balance

$$M_{ij} \equiv L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} + F_j z_{ij} - (L_j + U_j)x_{ij} - (V_j + W_j)y_{ij} = 0$$

- H: Energy balance

$$H_j \equiv L_{j-1}H_{j-1}^L + V_{j+1}H_{j+1}^V + F_j H_j^F - (V_j + W_j)H_j^V - (L_j + U_j)H_j^L - Q_j = 0$$

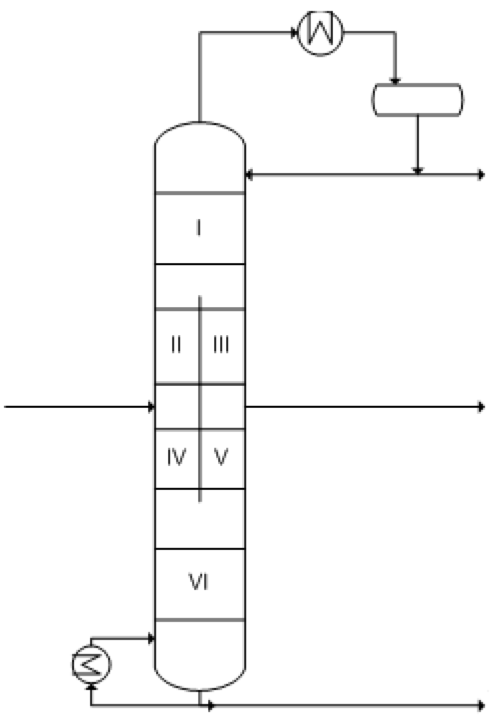
Phase	From Stage	To Stage	Split Ratio
Liquid	27	28	0.5
		50	0.5
	49	50	0
		72	1.0
Vapor	72	49	0.5
		71	0.5
	50	49	0
		27	1.0



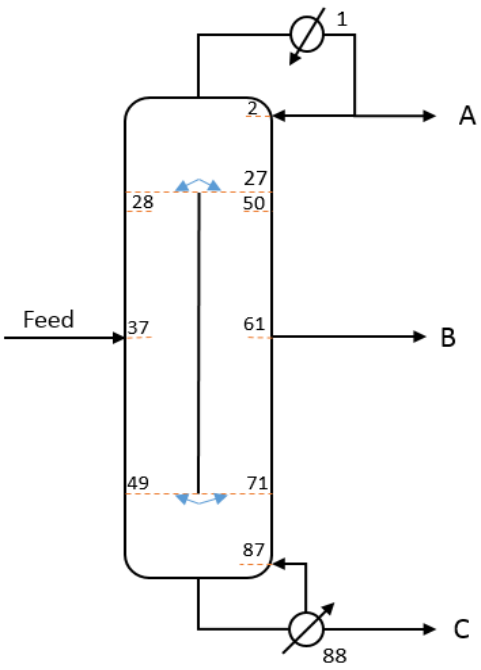
Equation-Based Parallel Column Model

- All equations for all stages solved simultaneously

Dejanović et al. Aromatics DWC

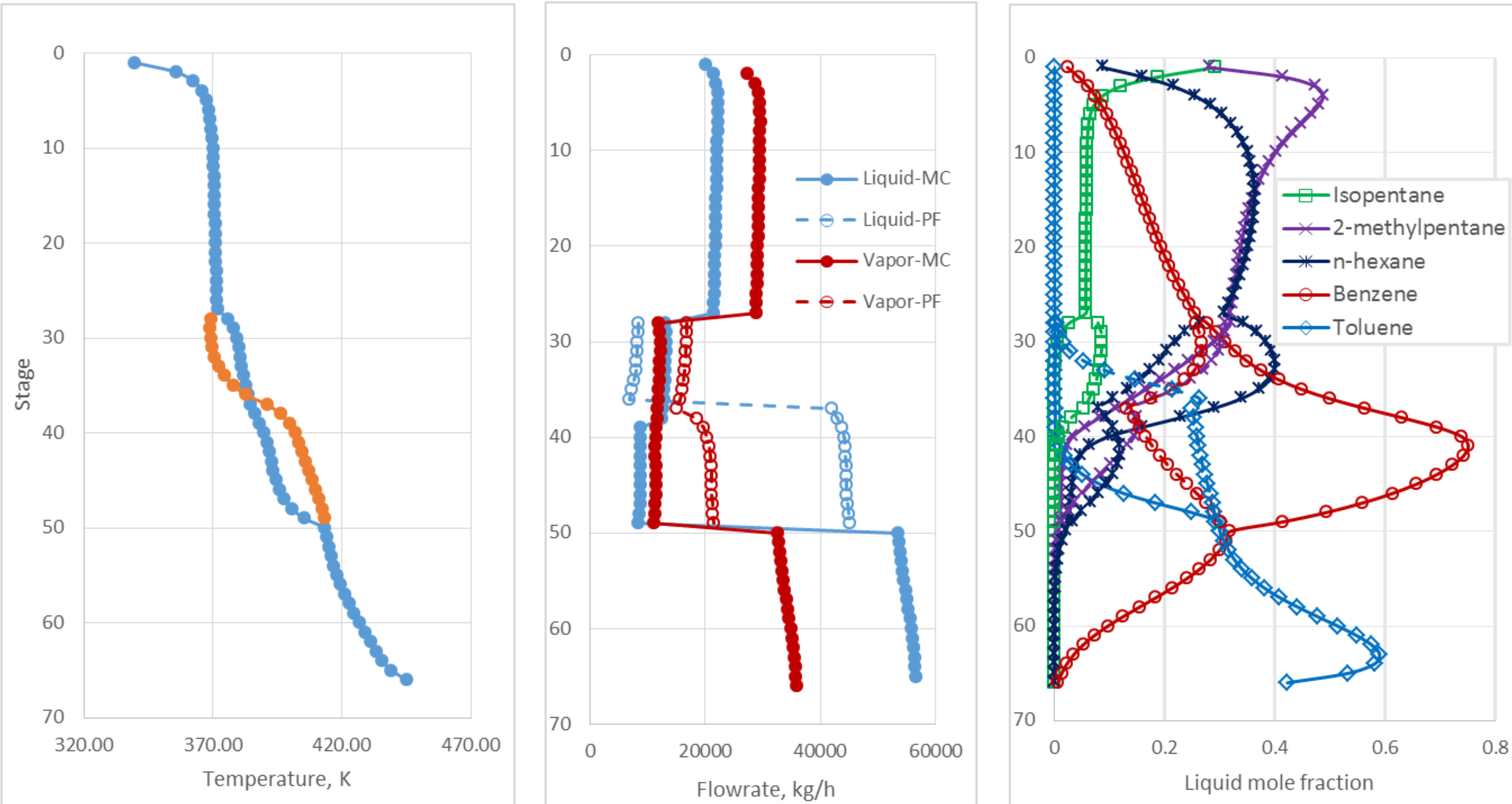


Equation-based ChemSep PCM



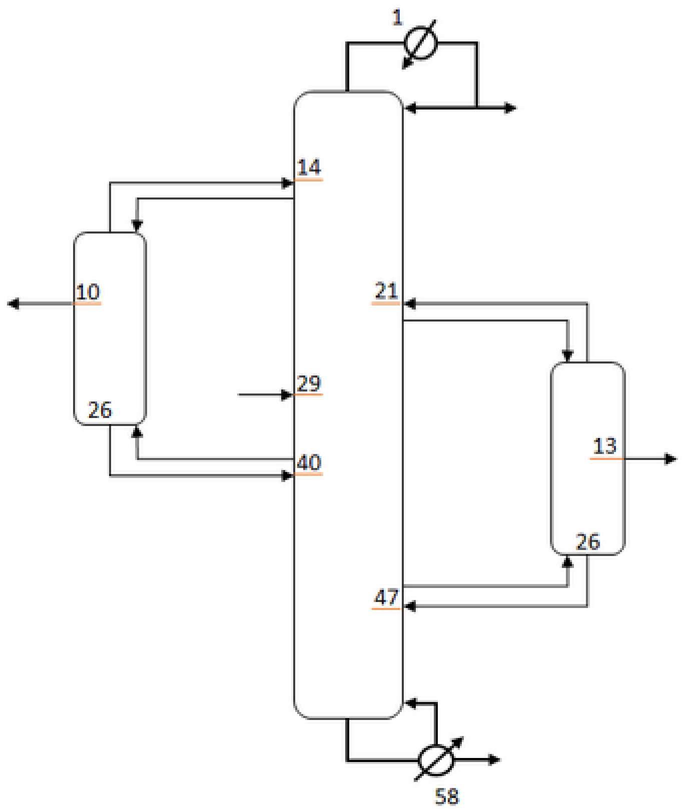
Equation-Based Model

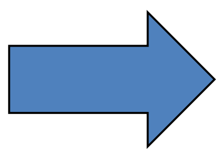
- Dejanović et al. Aromatics DWC Modelled Using ChemSep PCM



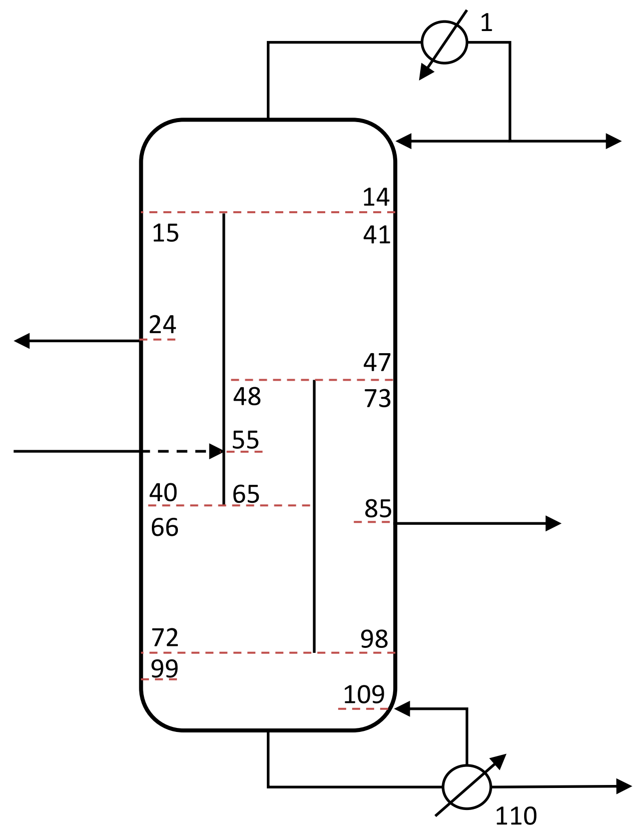
Satellite Column System

Satellite Column Schematic



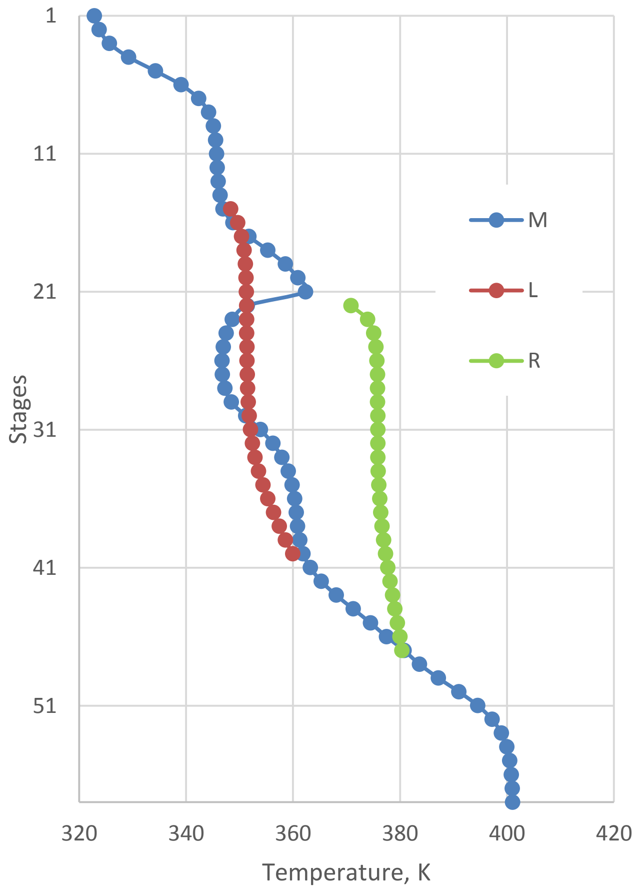


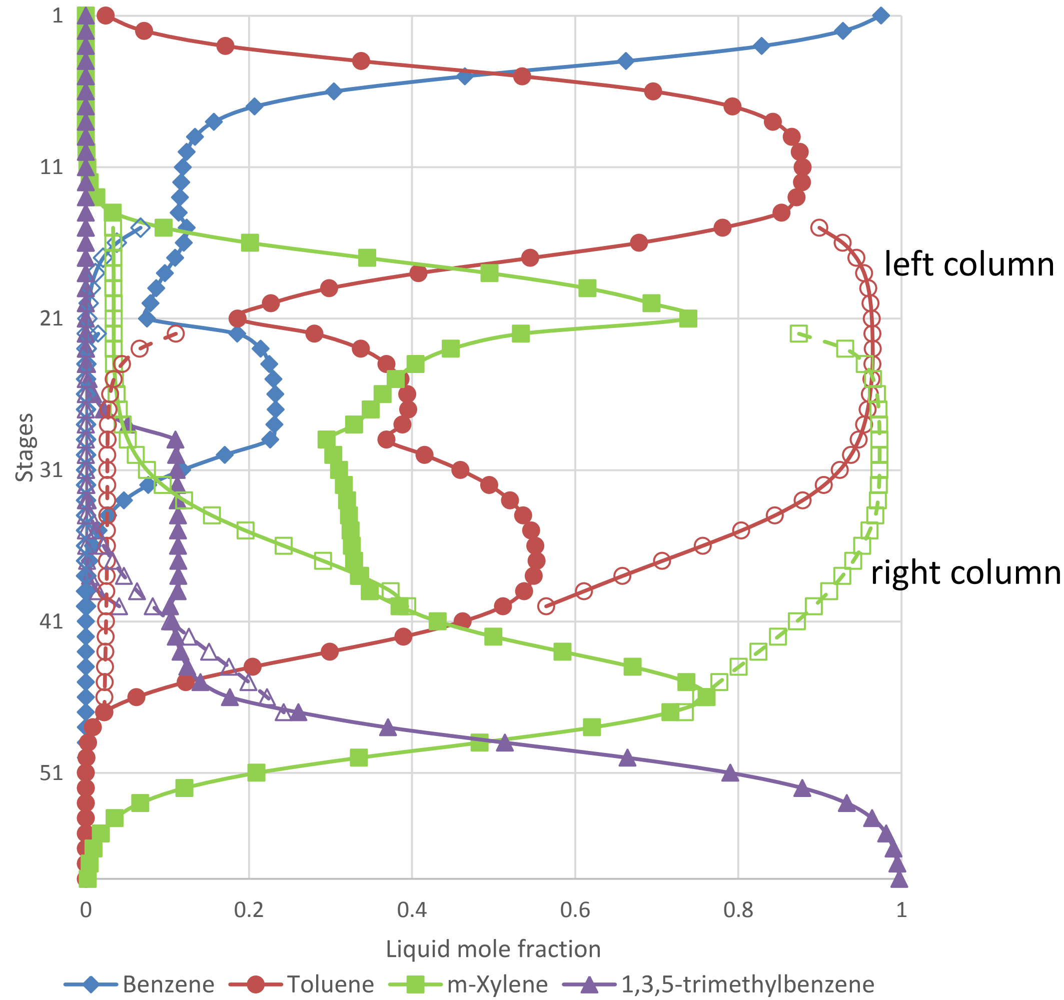
Equation-based ChemSep PCM
(very easy to converge)



(Agrawal arrangement)

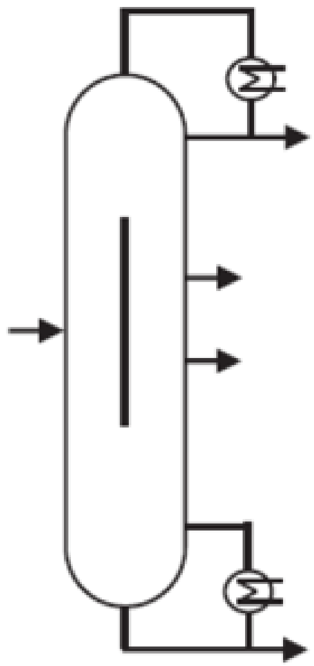
Satellite Column System



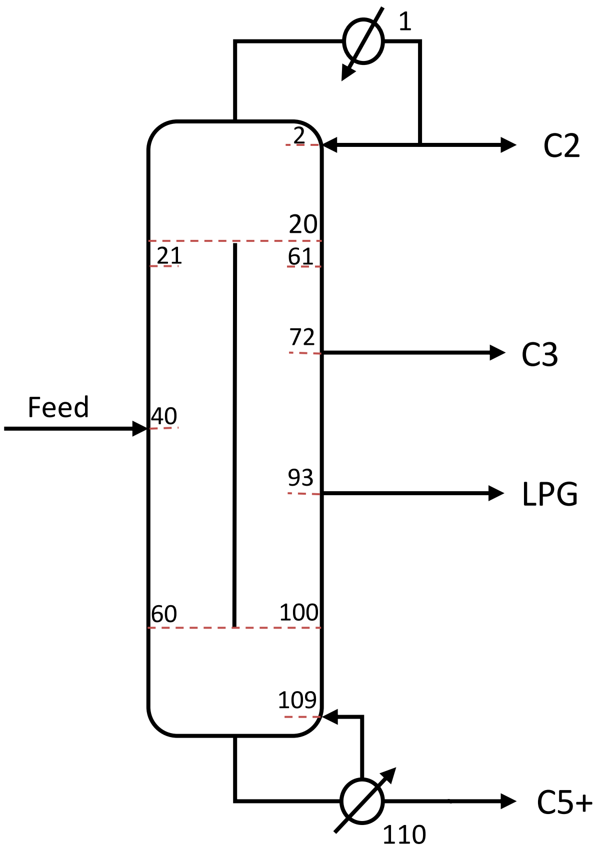


Kaibel Column

Kaibel Column



Equation-based ChemSep PCM



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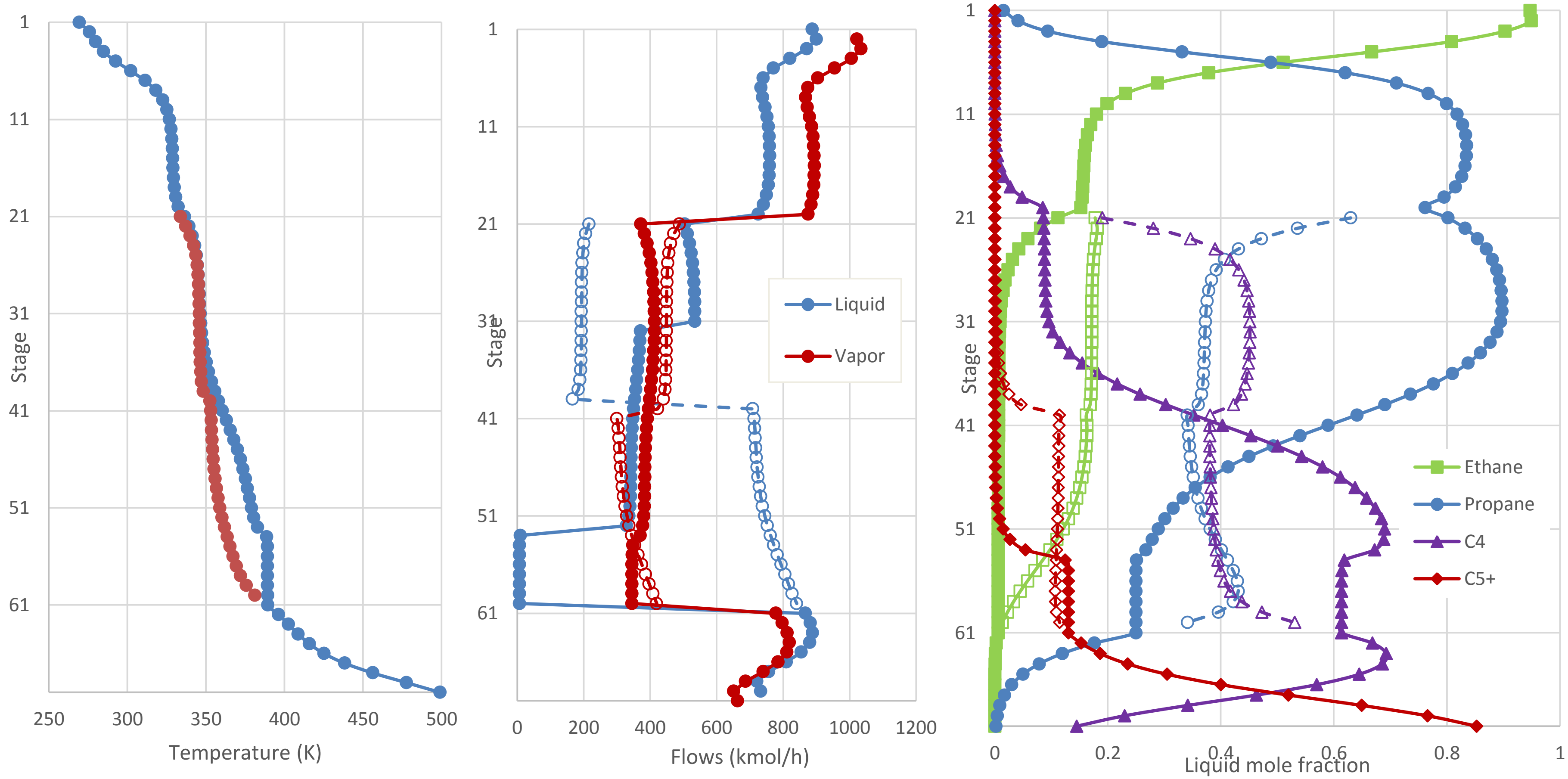
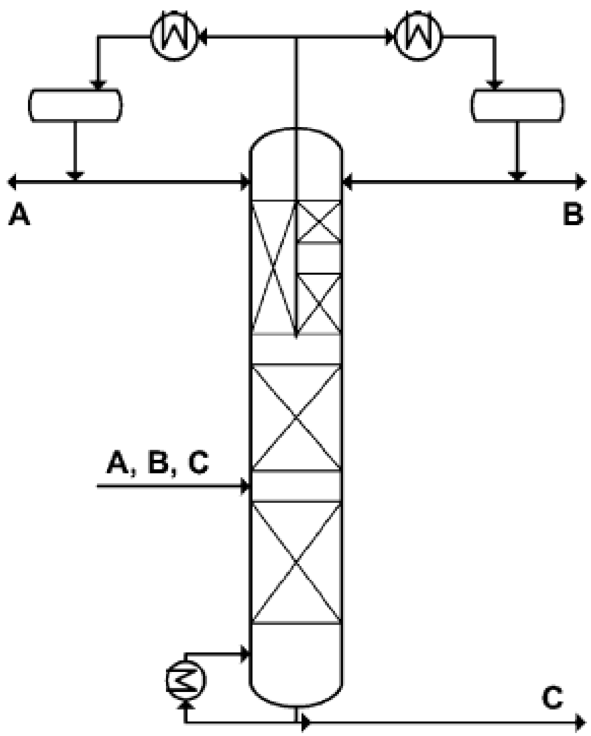
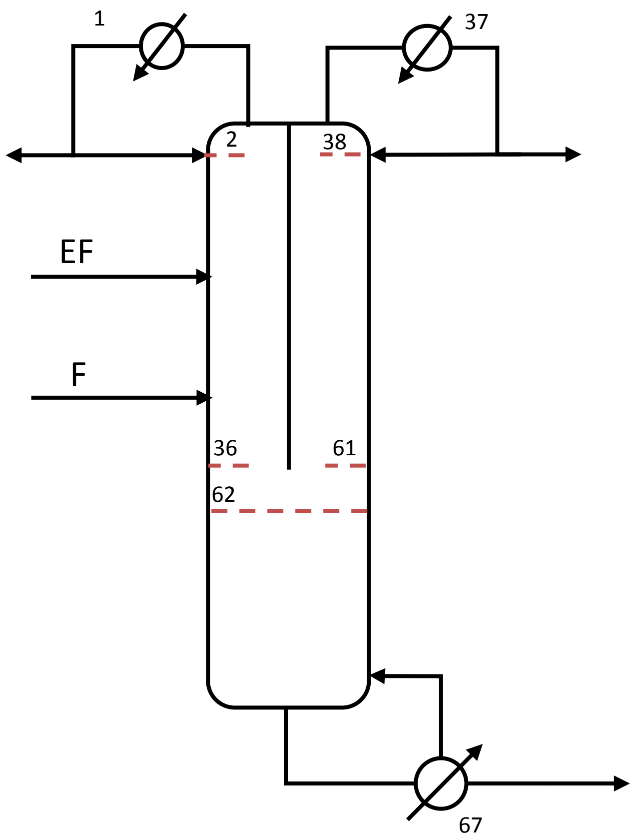


Divided Top Column

Divided Top Column



Equation-based ChemSep PCM



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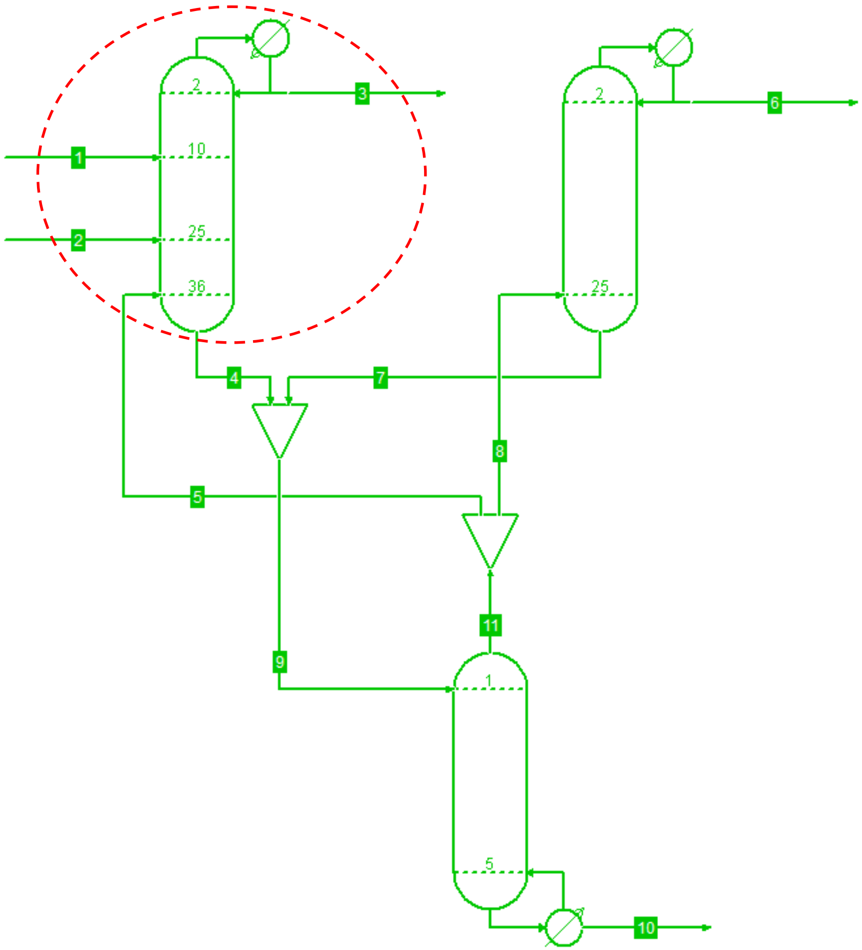
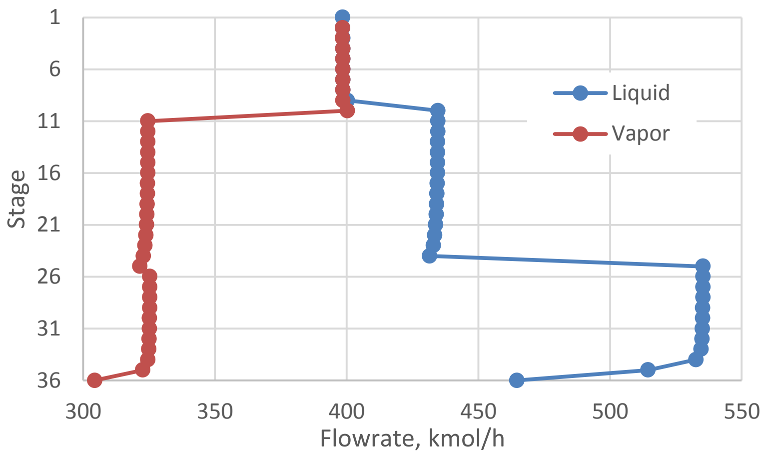
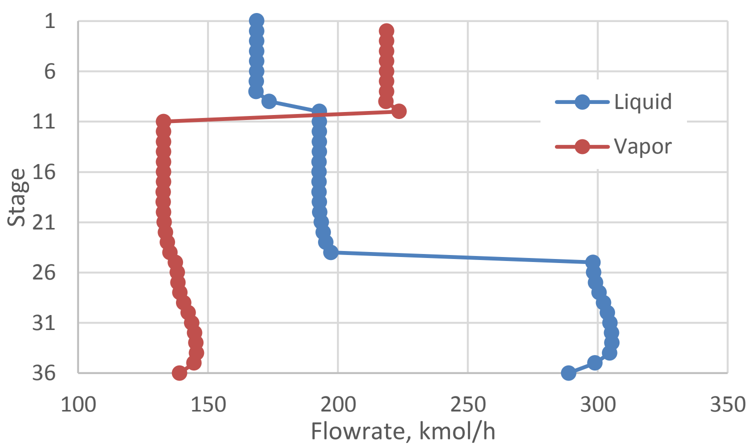


COCO (false solution)



ChemSep PCM (correct solution)



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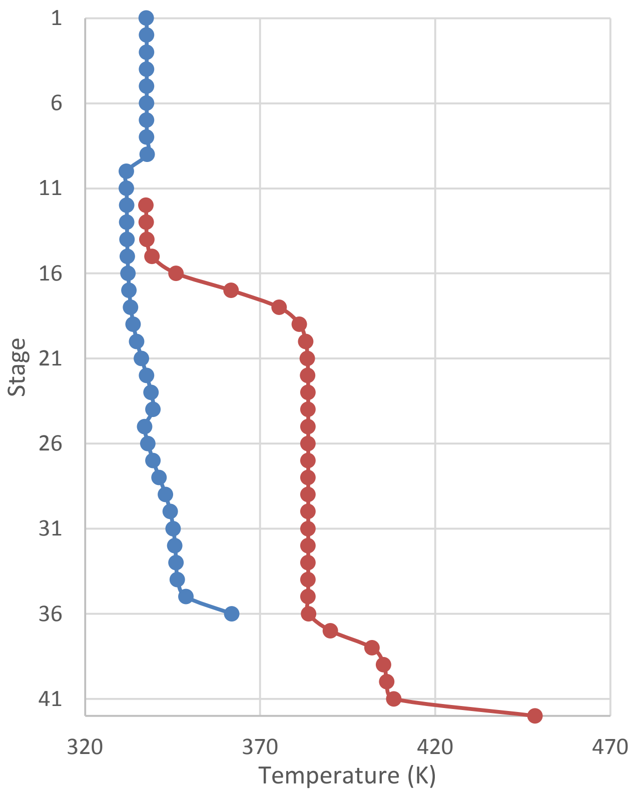

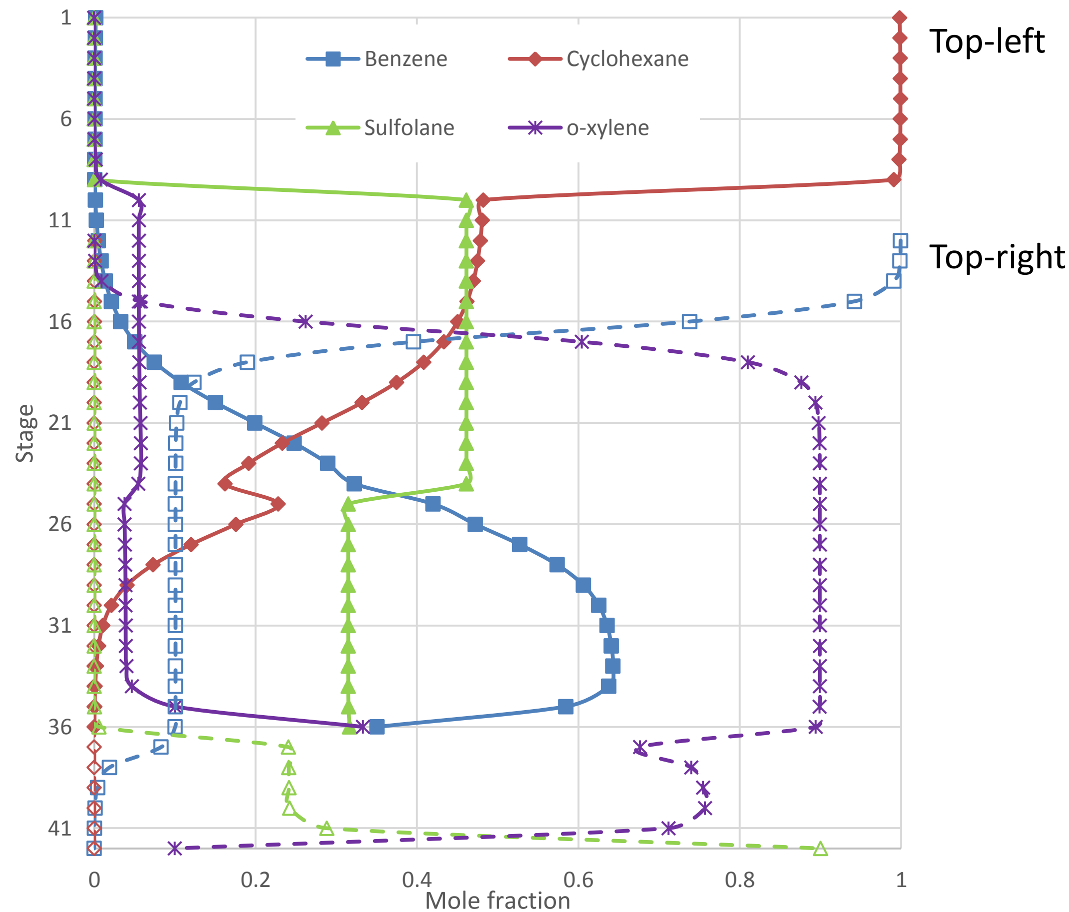

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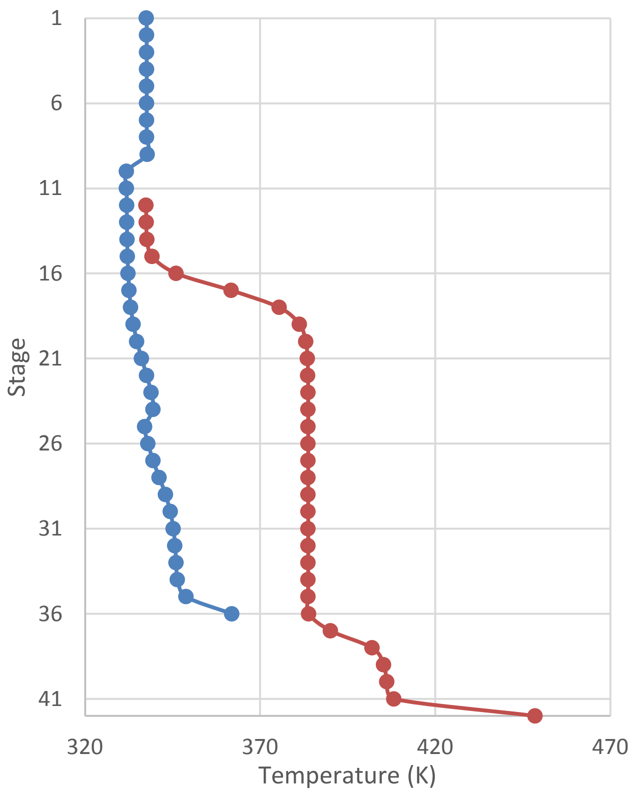
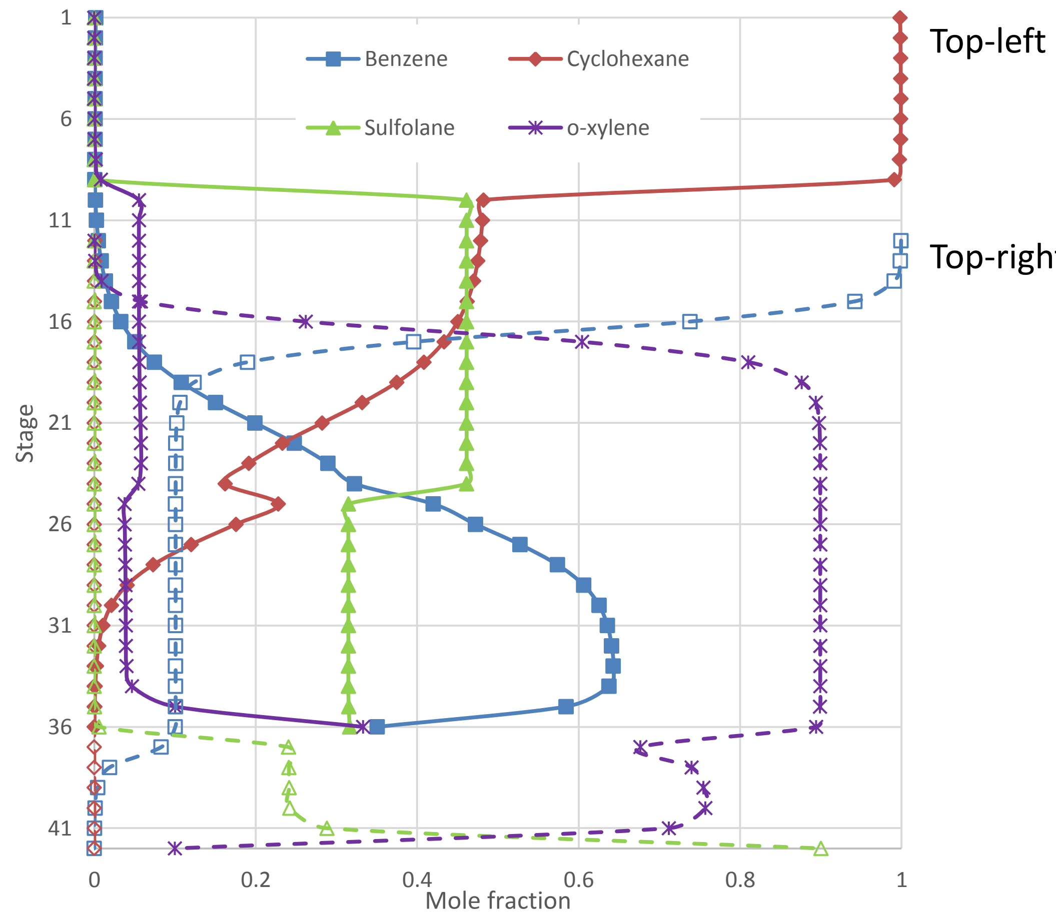
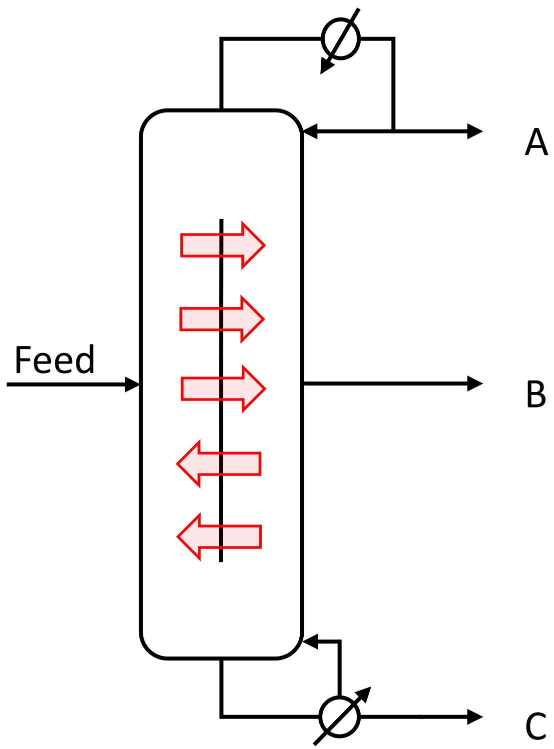




Temperature gradient across wall can be significant

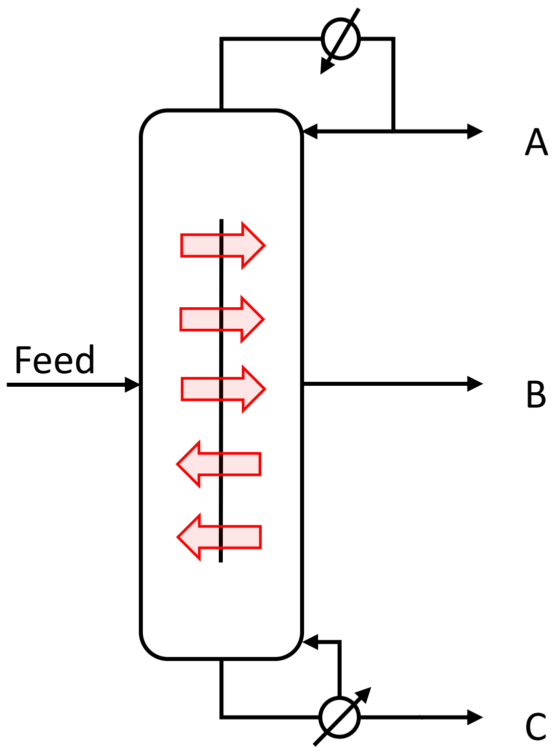
Heat Transfer

- Dividing walls are not insulators



Heat Transfer

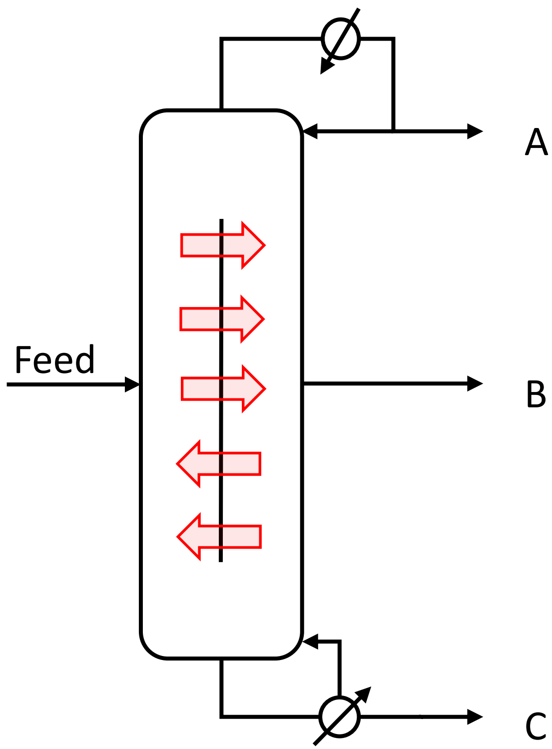
- Dividing walls are not insulators
- Extremely difficult to include heat transfer in multi-column models



Requires many energy interlinks

Heat Transfer

- Dividing walls are not insulators
- Extremely difficult to include heat transfer in multi-column models
- Very easy to include heat transfer in Parallel Column Model



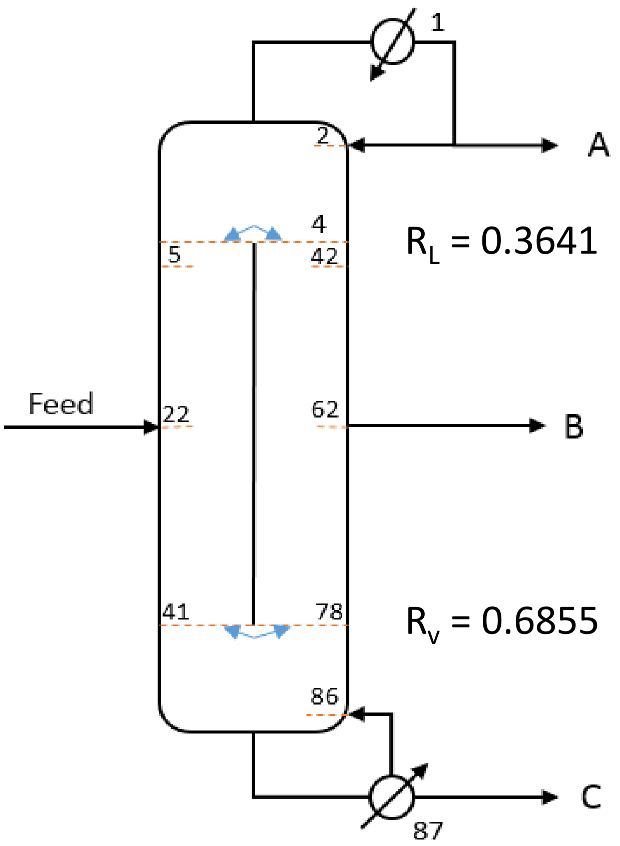
Terms added to energy balance

$$Q_j = U \cdot A_j \cdot \Delta T_j$$

U – Overall heat transfer coefficient
A_j – Heat transfer area on stage j
ΔT_j – Temperature difference

Heat Transfer

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

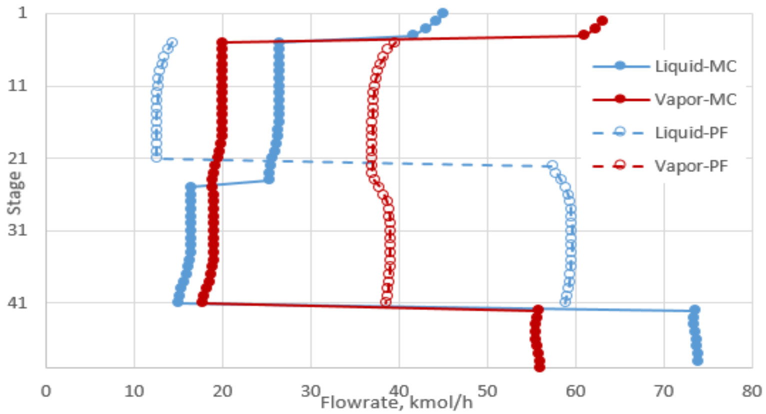


$R_L = 0.3641$

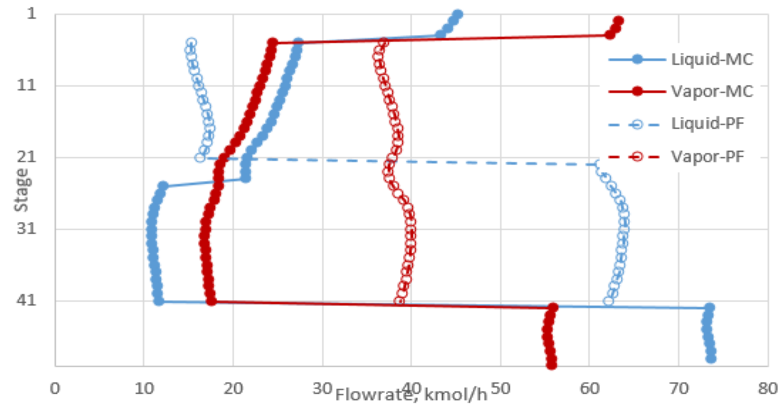
$R_V = 0.6855$

$U_{wall} = 800\ W/m^2K$

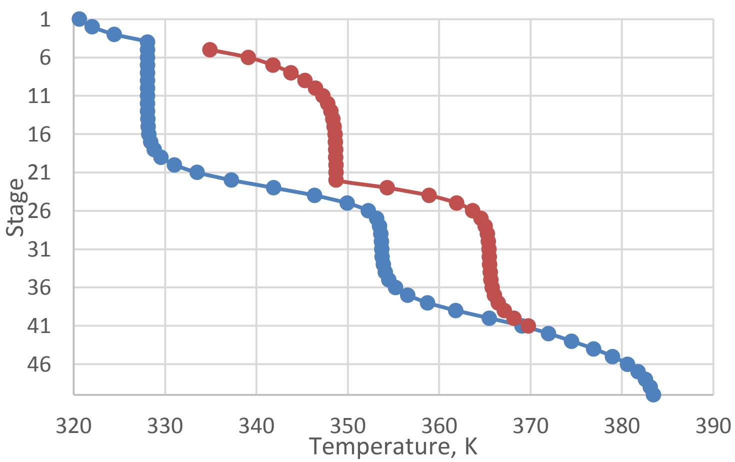
Heat Transfer



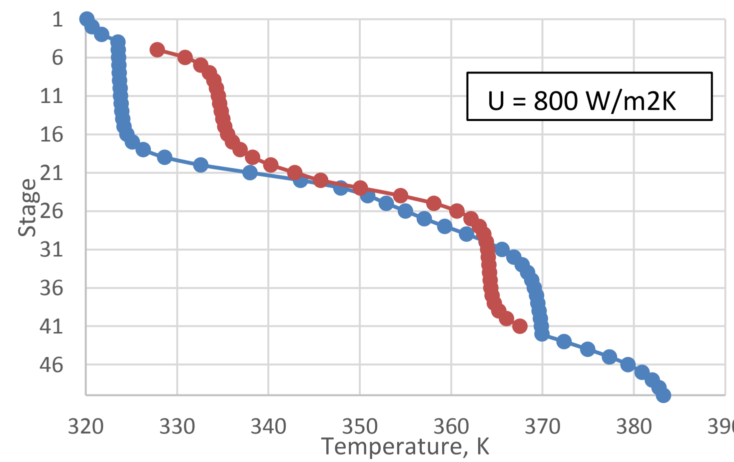
(a) Without heat transfer



(b) With heat transfer

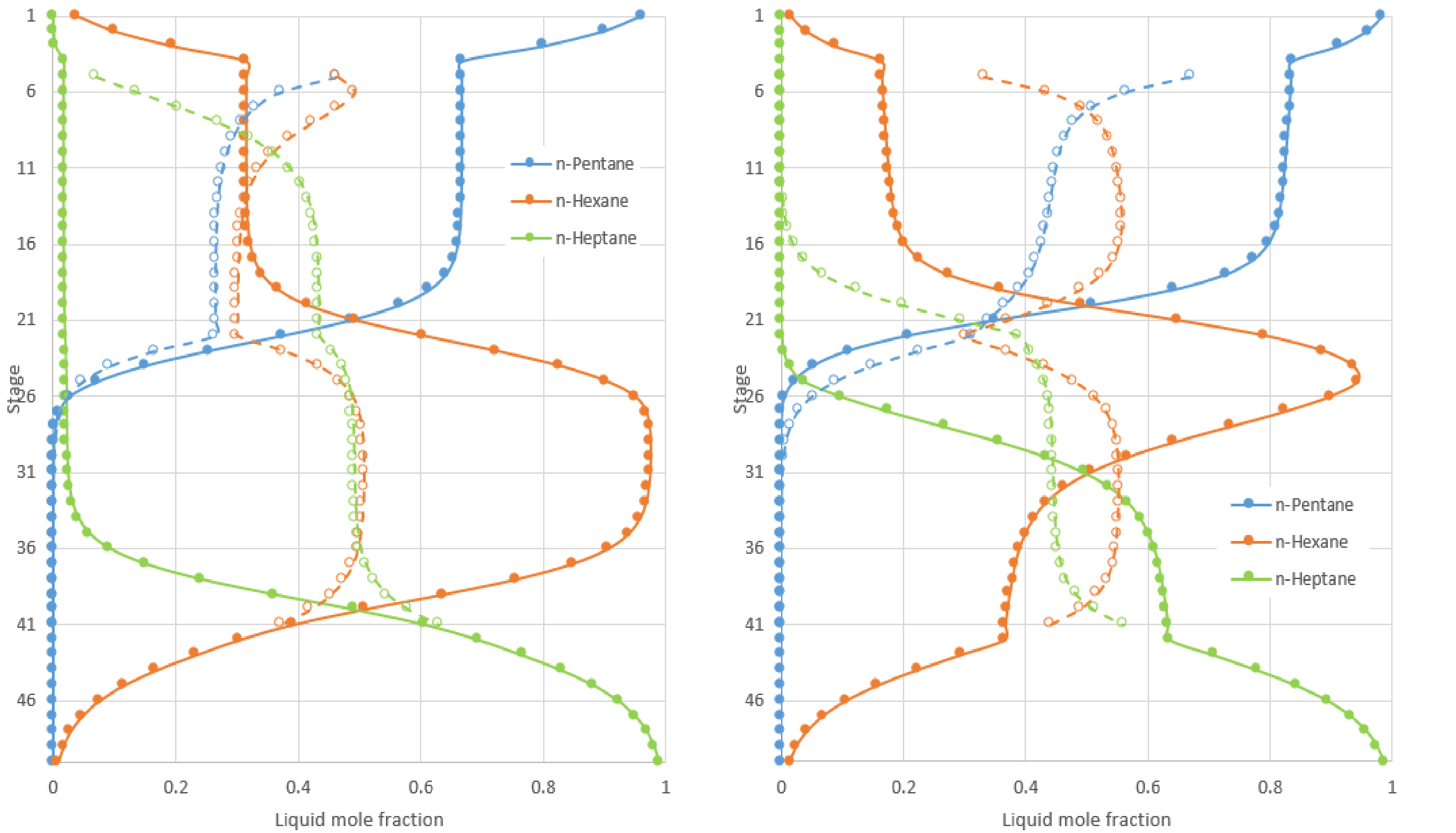


(a) Without heat transfer



(b) With heat transfer

Heat Transfer



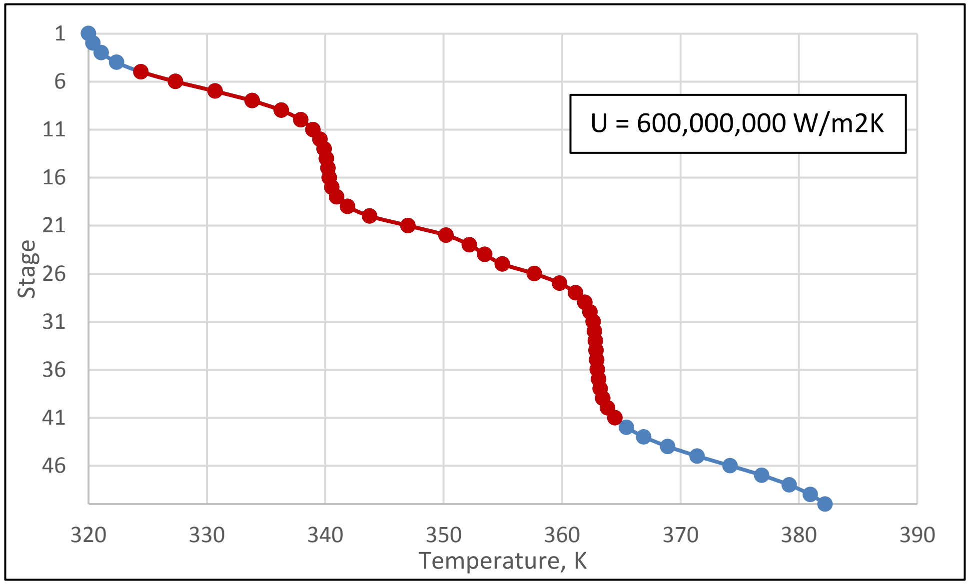
(a) Without heat transfer

(b) With heat transfer

Heat transfer affects product purity

Heat Transfer

What if U_{wall} goes to infinity…?



Conclusions

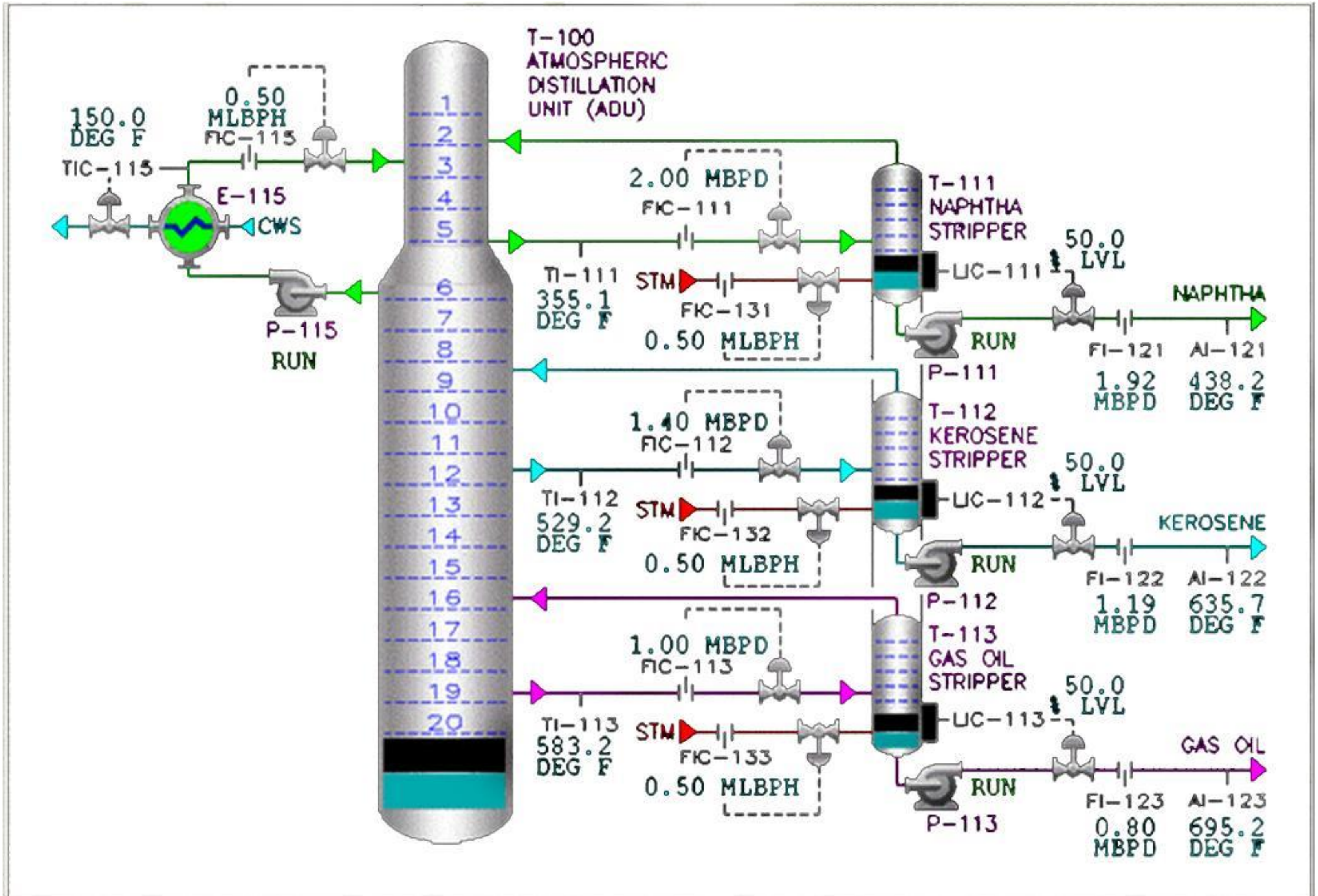
Compared to multi-column models, the ChemSep PCM

- Takes very little effort to set up
- Requires no initial guesses from engineer
- Converges much quicker
- Converges to the correct solution when other simulators fail
- Makes it easy to model heat transfer across the wall

Coming Soon…

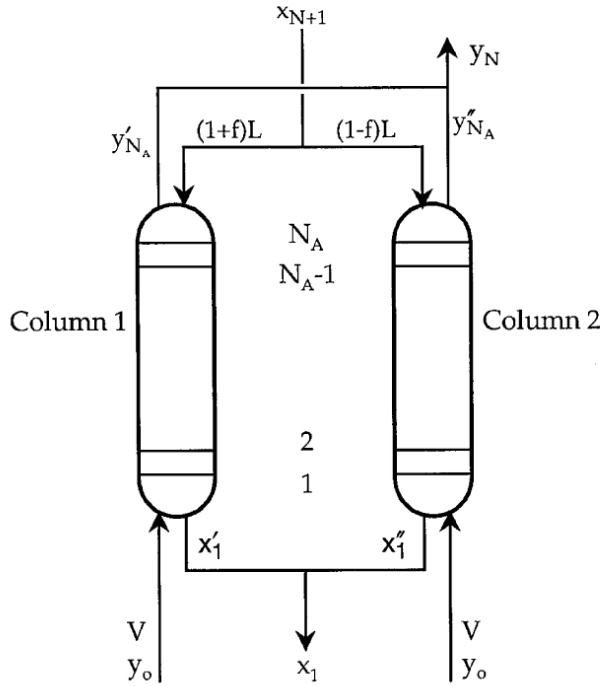
- Rate-based Parallel Column Model
- Other Uses for a PCM…

Crude Column Systems

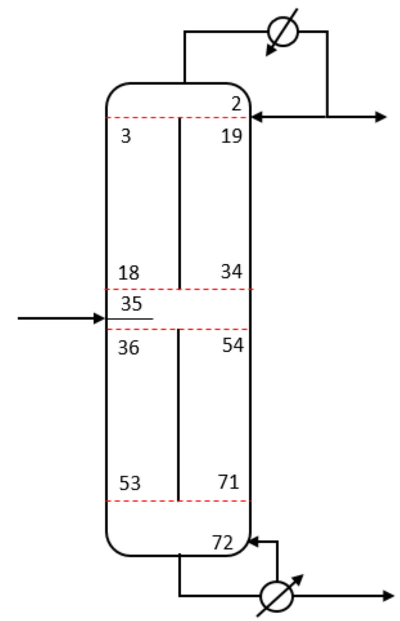


PCM for Maldistribution

Billingham and Lockett Maldistribution Model



Equivalent PCM Structure



- Redistributors modeled as stages with no mass transfer