

A Rate-Based Equation-Oriented Parallel Column Model: Application to Dividing Wall Columns

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DWCs at BASF

- First industrial DWC (1985)
- First 4-product DWC (2002)
- Several dozen DWCs now operating (according to Kaibel, about 70 in 2014)
- Simulation using equation oriented models for many years (Benfer, 2018)

Asprion and Kaibel (2010): *Simulation of dividing wall column is a challenging issue. We recommend to use a simultaneous equation based solver which is better suited than the use of a sequential solver strategy.*

Kaibel (2014) wrote: *Due to the potential variability of complex internal configurations, there is no dedicated software package for this purpose.*

This, now, is about to become available.

Kaibel: *Equation-based programs normally show better convergence characteristics*

But, so far, nobody provided evidence to show that this is true.

Dividing Wall Columns: What Was Said

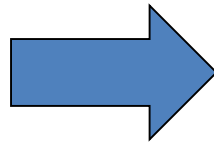
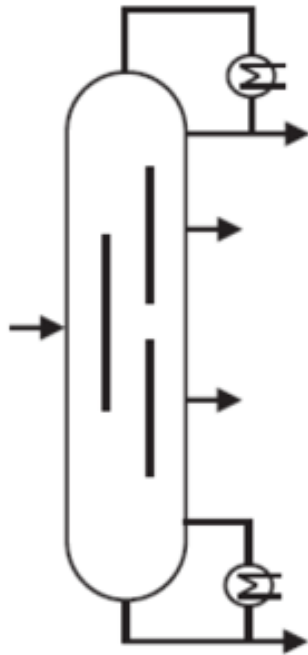
Dejanović et al. (2010) wrote:

*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.*

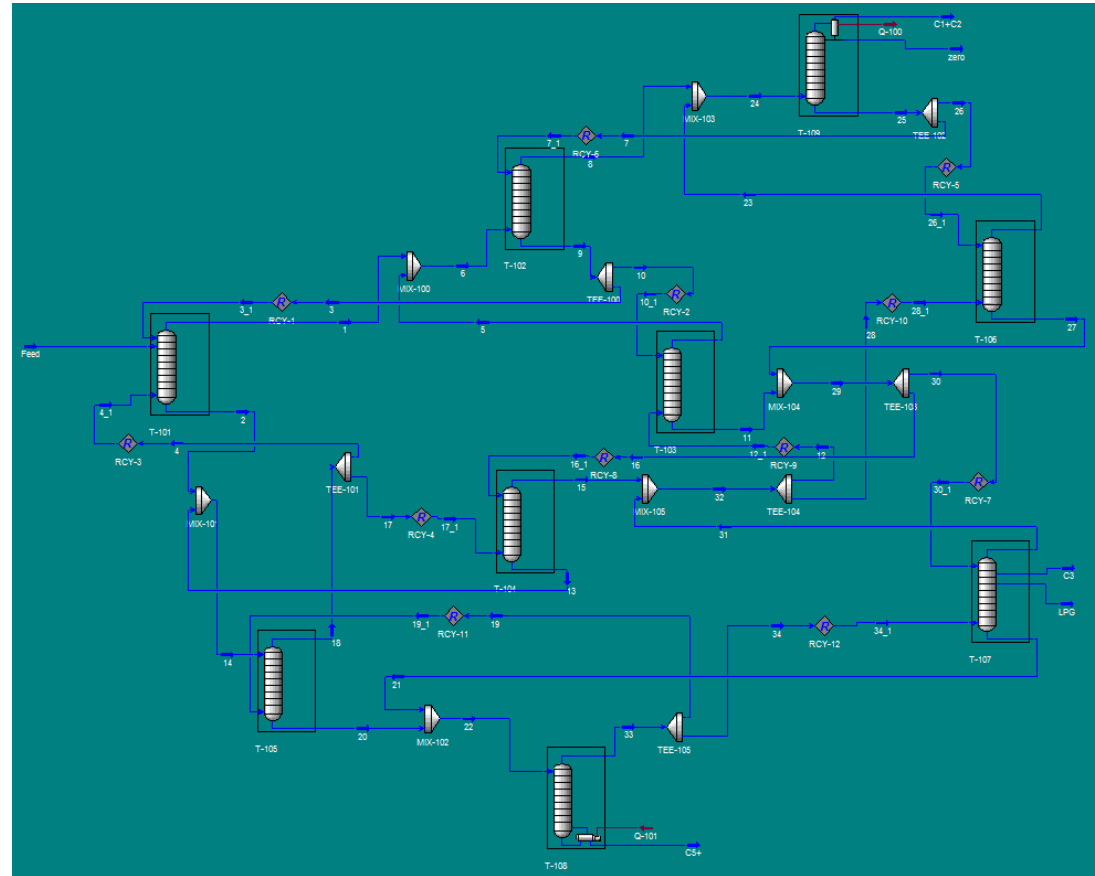
Engineers have, therefore, developed alternative approaches to model DWCs...

Dividing Wall Columns: What Was Done

Dividing Wall Column



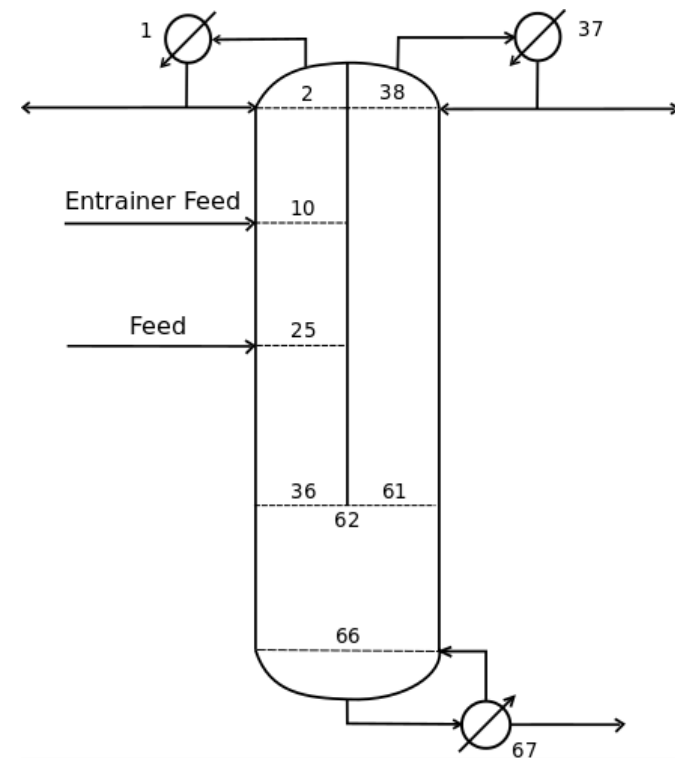
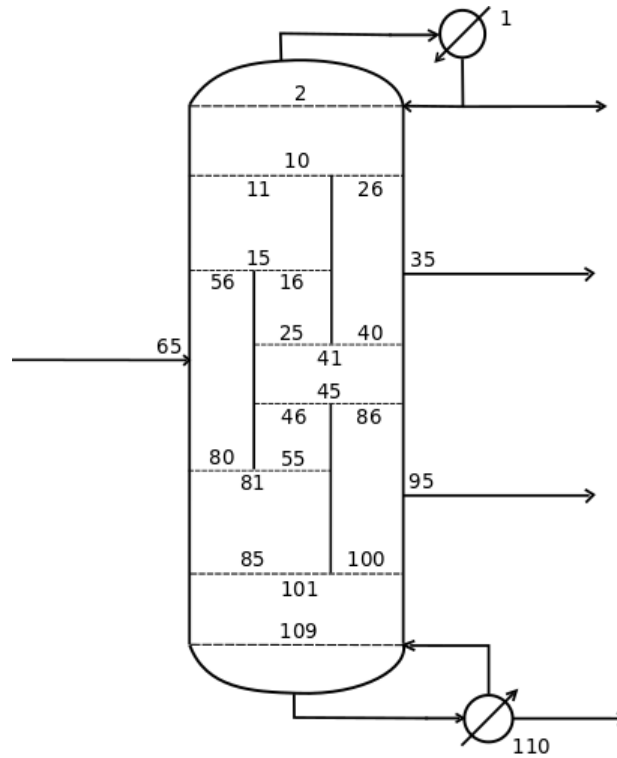
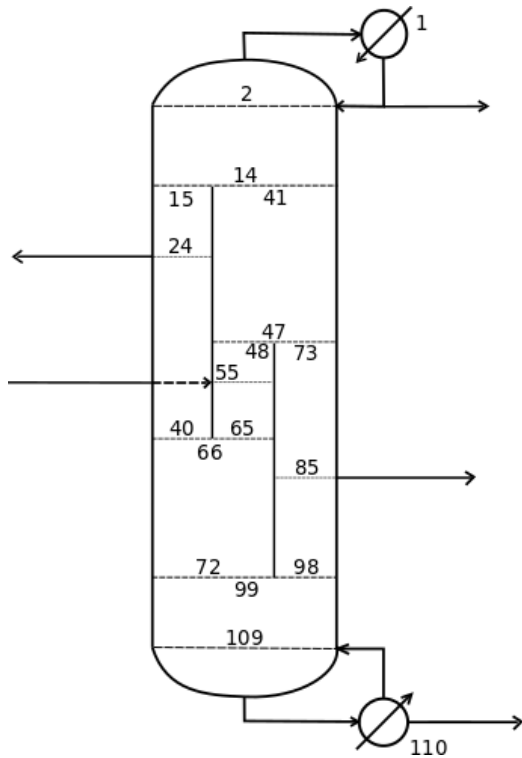
Simulated with a multi-column model, this example in UNISIM Design



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

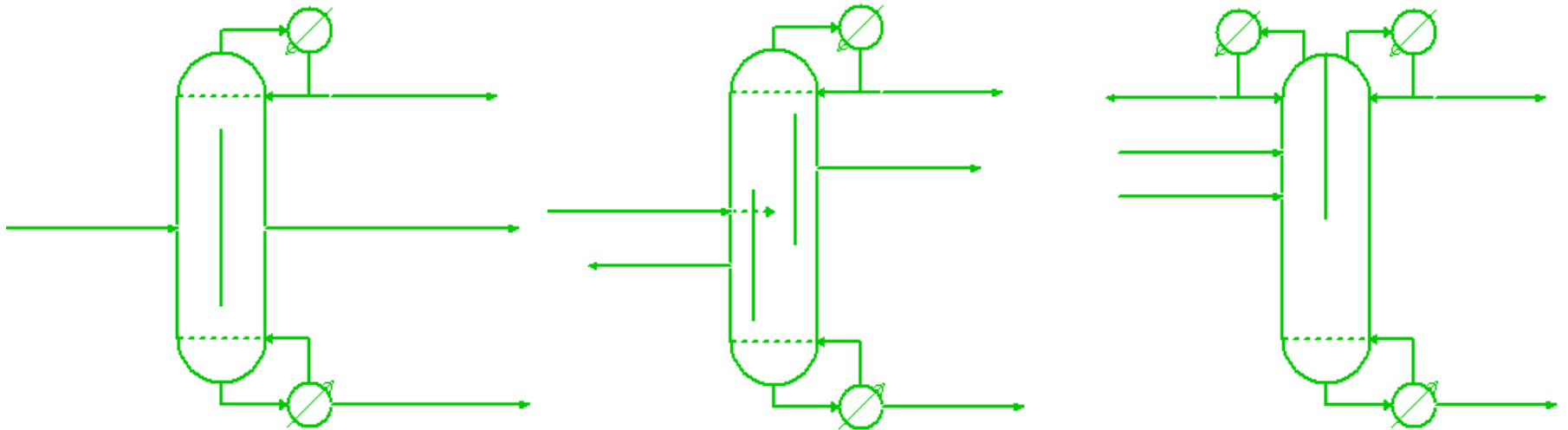
Dividing Wall Columns: What We Did

- Equation-oriented parallel column model (PCM)
 - Simulates dividing wall columns (DWCs) of arbitrary configuration



ChemSep Parallel Column Model: What's New

- Flowsheet simulation with CAPE-OPEN compliant PCM
- Rate-based Parallel Column Model
- Maldistribution model

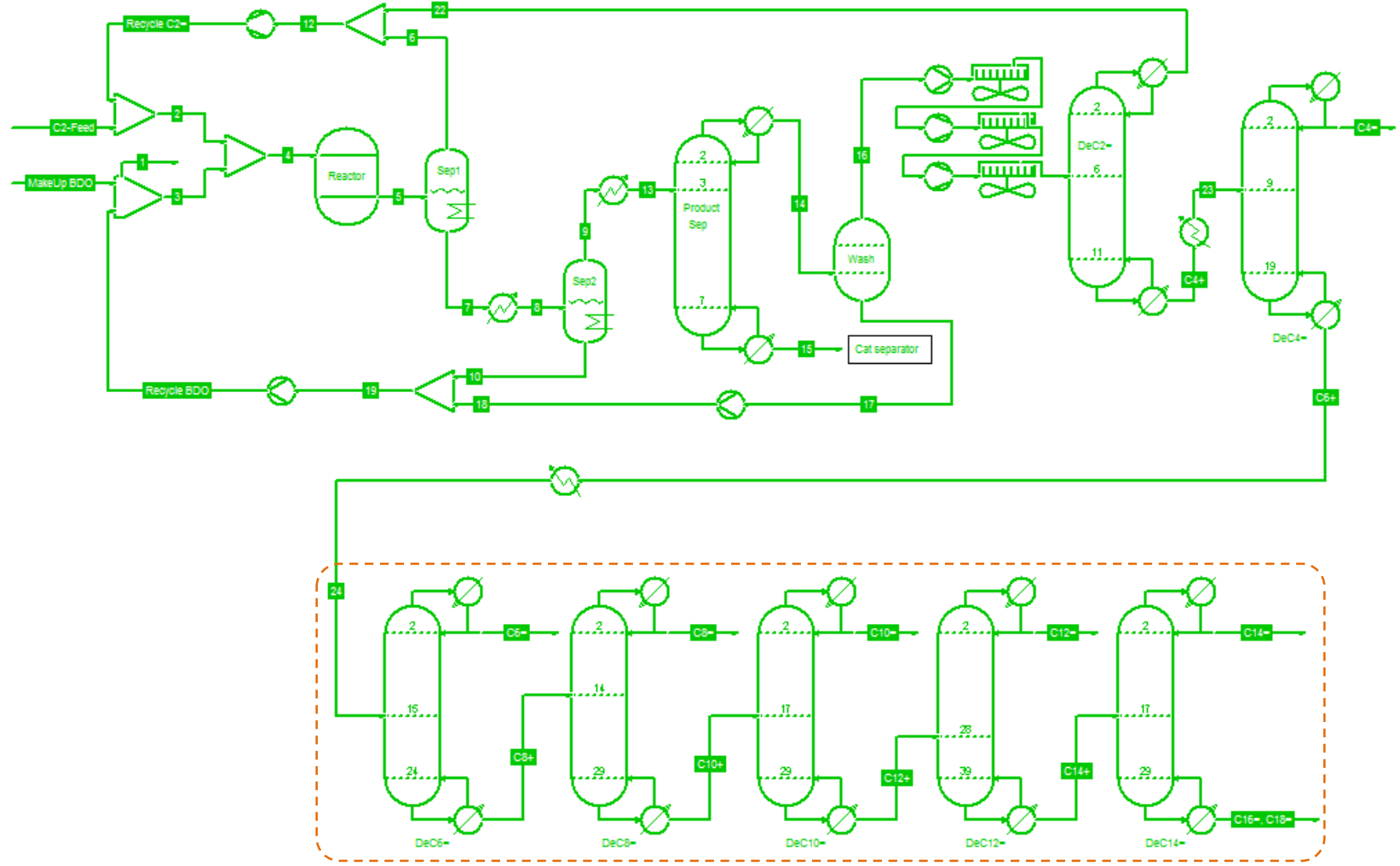


Icons show different DWCs in COCO (www.cocosimulator.com)

Flowsheet Simulation with CAPE-OPEN PCM

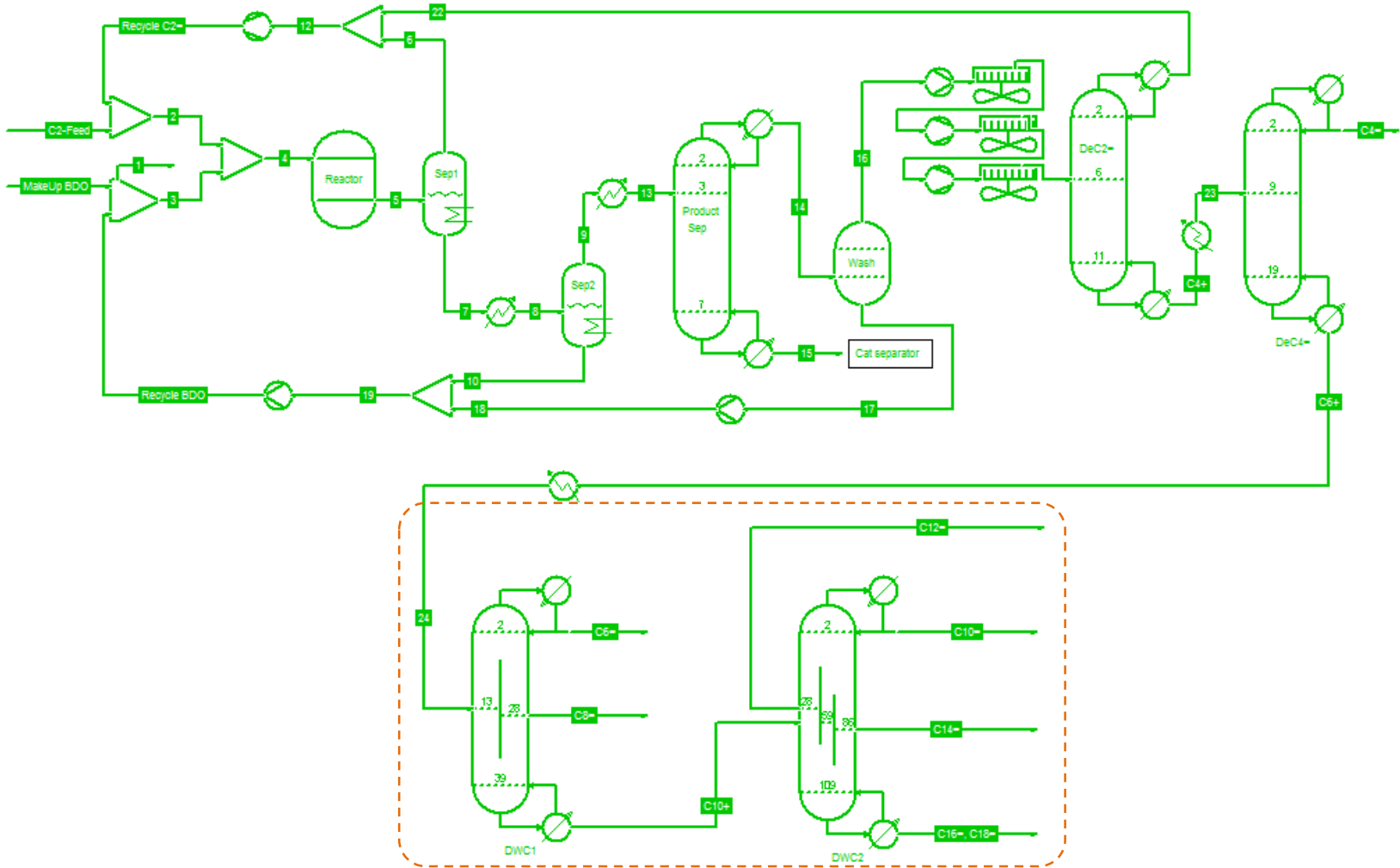
- Standard column model for CAPE-OPEN compliant systems
- Flowsheet intensification with DWCs
- Easy column configuration with multiple walls
- Icons immediately reflect actual configuration
- Connection to vendor tools for easy detailed rating
- Rapid tray/packing internals design of each column section, with selection of any modern type separations internals
- Overall column sizing including feed inlets and draw-off trays
- CAPEX & OPEX estimates enables Total Annual Cost comparison

Flowsheet Intensification with DWCs - I



Separation using *Direct Sequence of Distillation Columns*

Flowsheet Intensification with DWCs - II



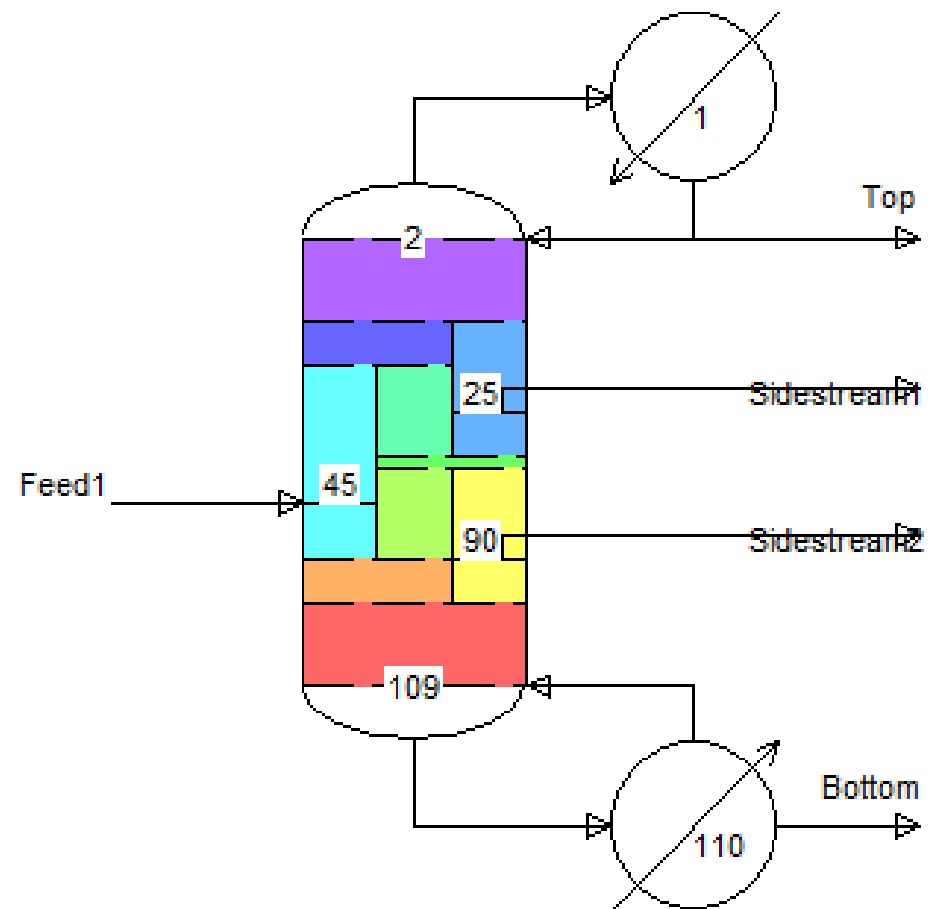
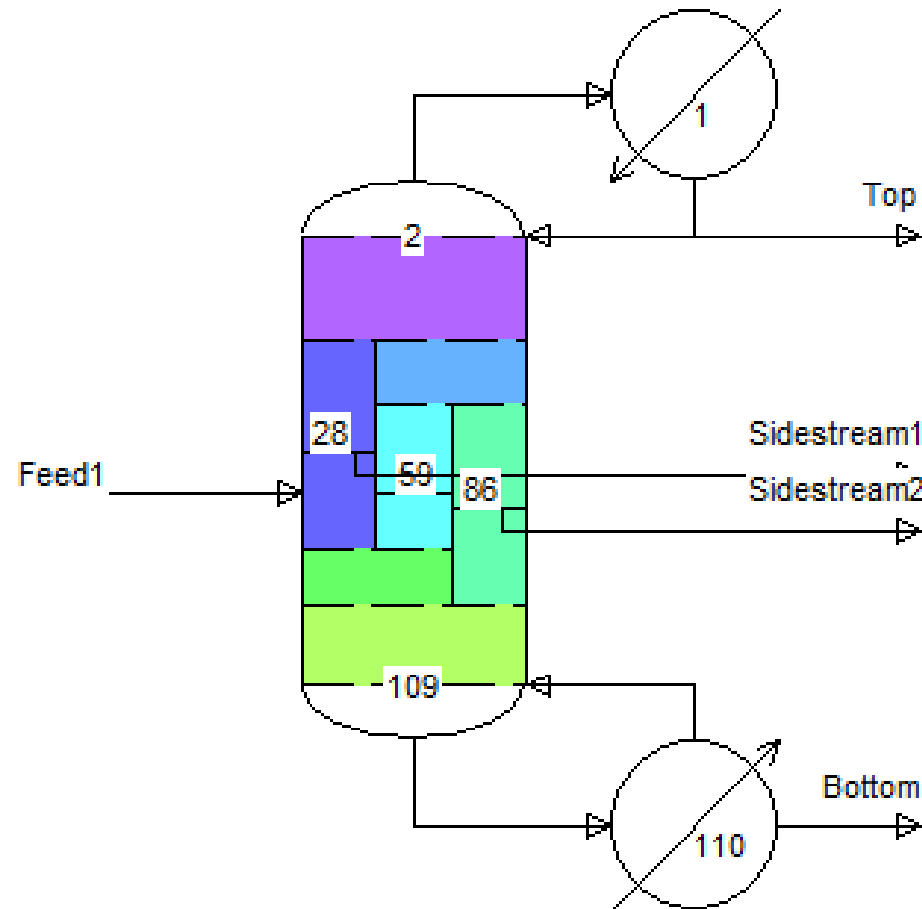
Separation using *Dividing Wall Columns*

Flowsheet Intensification with DWCs - III

Movie

Easy Configuration with Multiple Walls

- Clear identification of column sections to guide engineer



Rate-Based Models

- Real distillation operations do not reach equilibrium
- Details of column internals are not always considered
- Heat transfer usually not included in simulation
- Column hydraulics are oversimplified (or ignored)



Rate-Based Parallel Column Model

Rate-Based Models

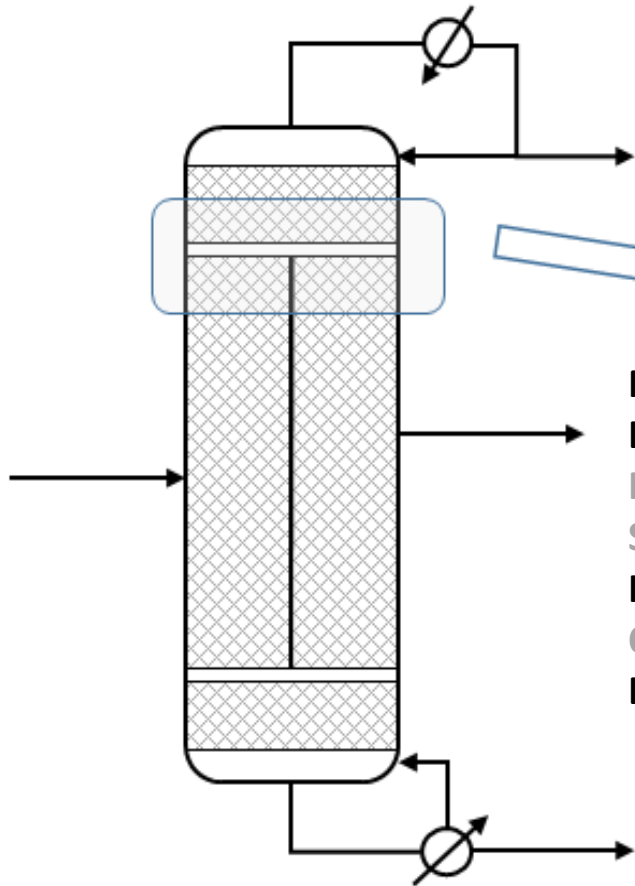
Aspen Custom Modeler (ACM) Based Models

- Mueller, I., & Kenig, E. Y. Reactive distillation in a dividing wall column: rate-based modeling and simulation. *Industrial & engineering chemistry research*. 46(11), pp3709-3719, 2007
- Hiller, C., Buck, C., Ehlers, C., & Fieg, G. Nonequilibrium stage modelling of dividing wall columns and experimental validation. *Heat and mass transfer*. 46(10), pp1209-1220, 2010

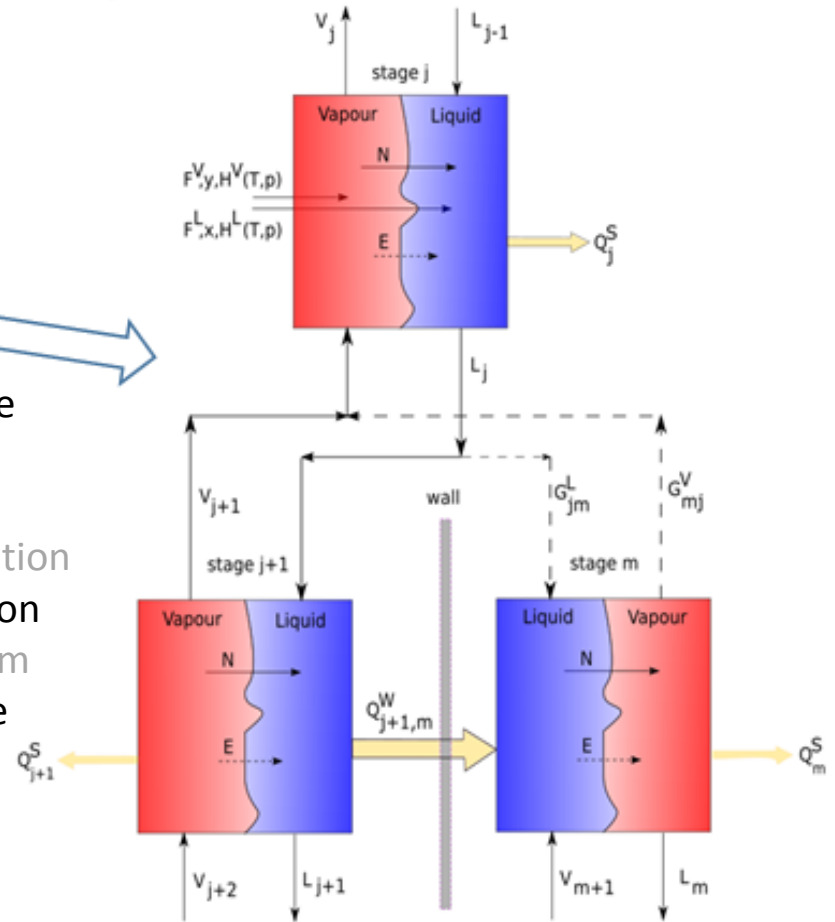
ACM cannot be used to model DWCs with changed configuration without remaking the model

The same applies for other modeling platforms: gPROMS, MOSAIC, ...

Rate-Based Parallel Column Model



- M:** material balance
- E:** energy balance
- R:** rate equation
- S:** summation equation
- H:** hydraulic equation
- Q:** phase equilibrium
- B:** pressure balance



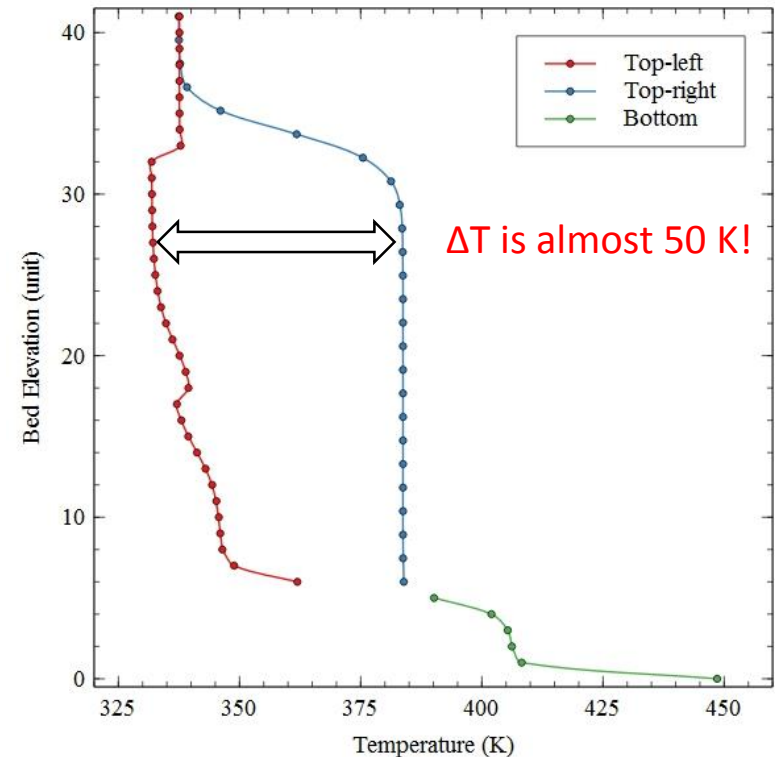
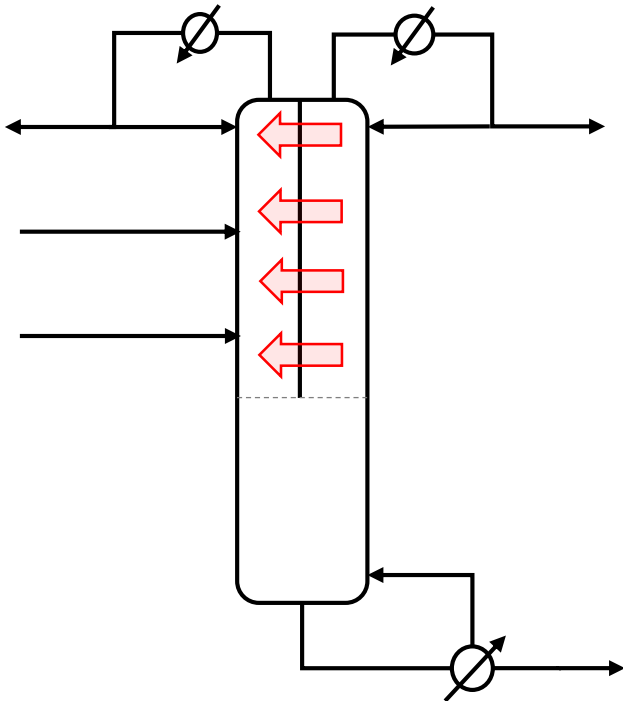
Conventional column: Stages are adjacent AND in sequence

DWCs: Stages are adjacent but all are NOT in sequence

Equations solved simultaneously using Newton's method

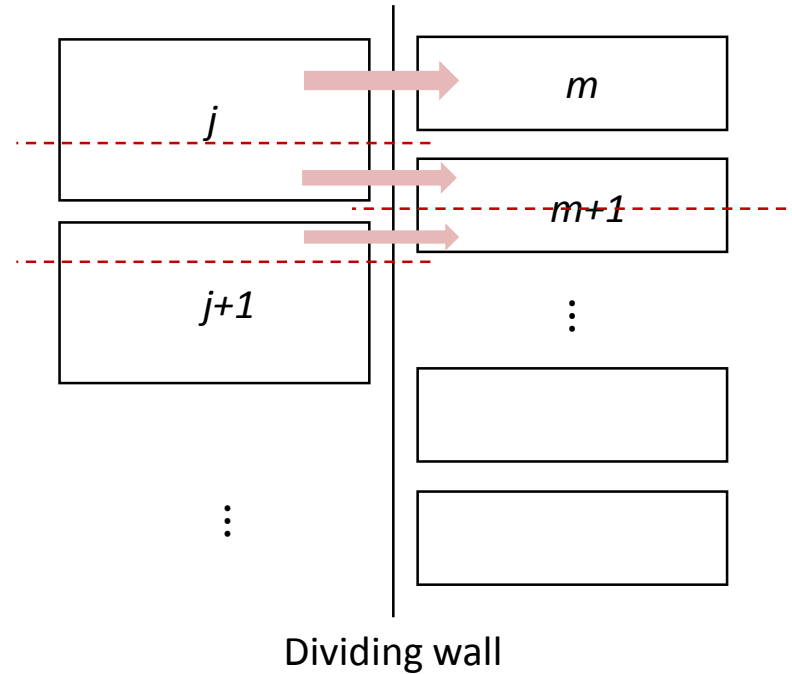
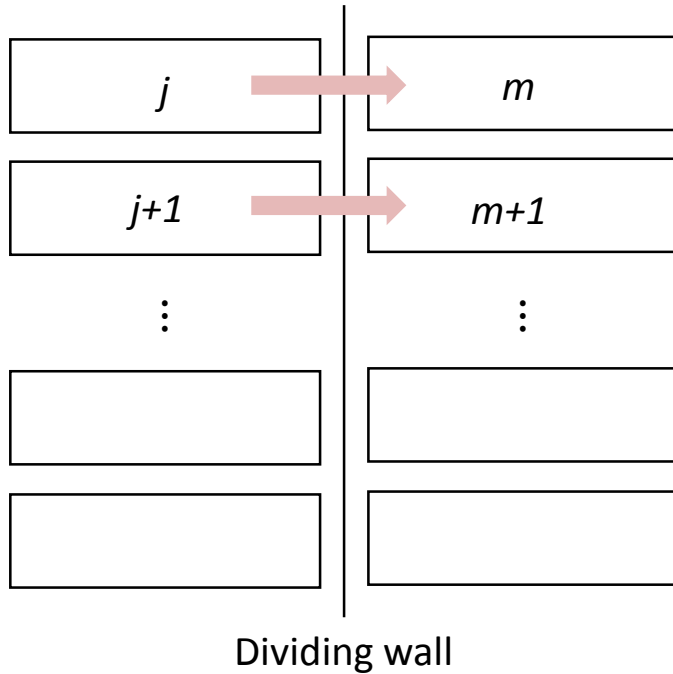
Heat Transfer across Dividing Walls

- Dividing walls are not insulators
- Temperature gradients can be significant
- Can be important for small columns (often used in experimental studies)
- Extremely difficult to include heat transfer in multi-column models
- Very easy to include heat transfer in Parallel Column Model



Heat Transfer across Dividing Walls

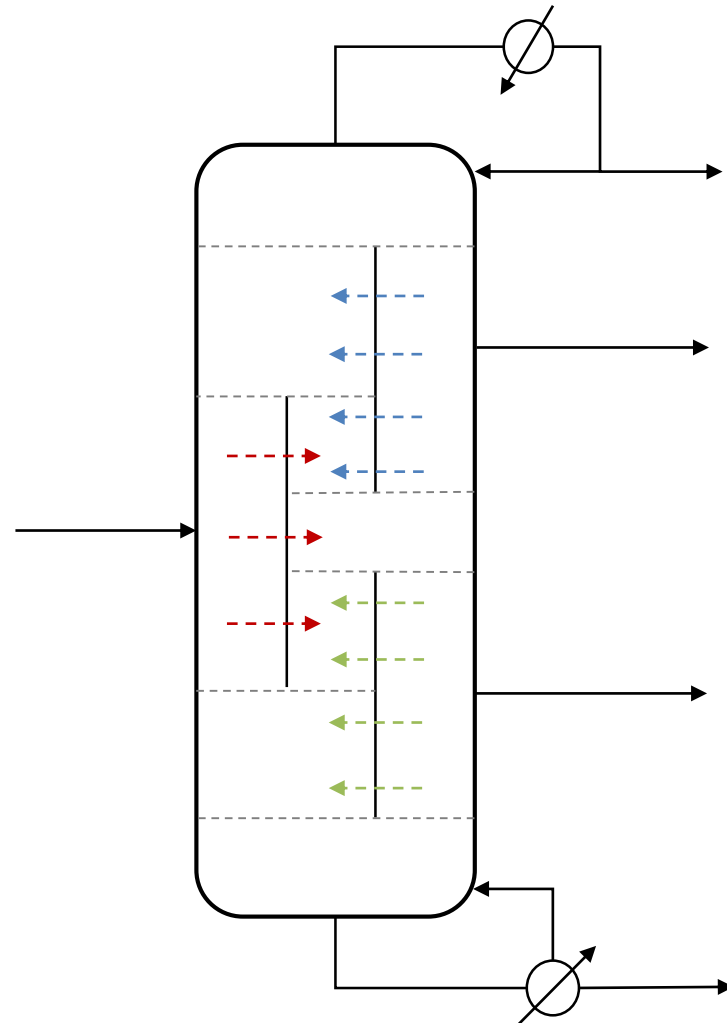
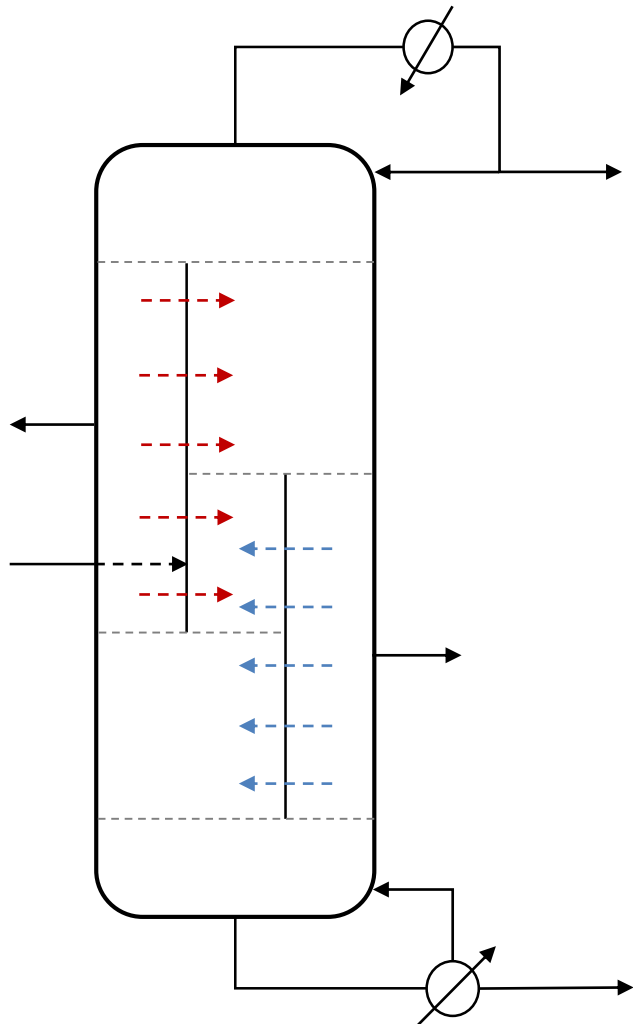
- Number of stages may not align



- Need to account for appropriate heat transfer area for each stage
- Need multiple heat transfer terms for asymmetric walls

Heat Transfer across Dividing Walls

- Multiple walls



Validation: Experiments of Bailee Roach

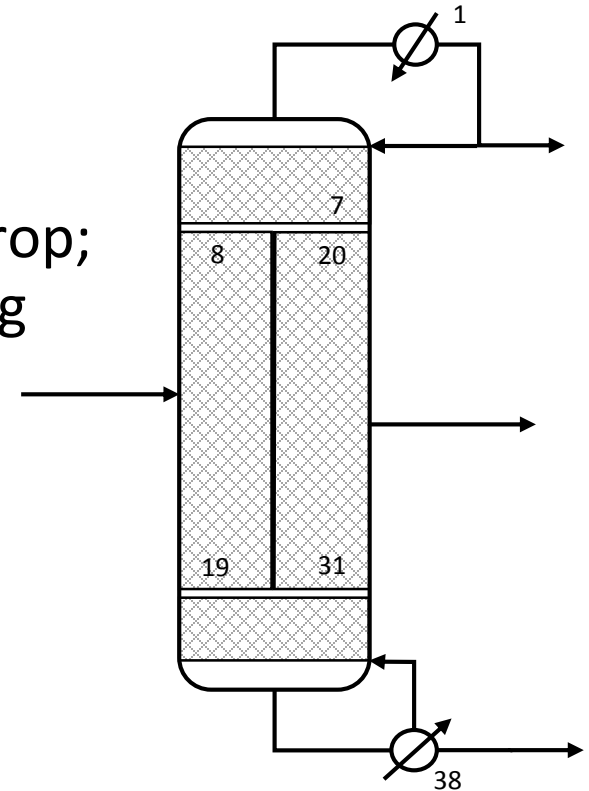
- Data in recent Ph.D. thesis from The University of Texas at Austin
- Two systems investigated:
 - Alcohol System (1-hexanol, 1-octanol, 1-decanol)
 - Hydrocarbon System (1-pentane, cyclohexane, 1-heptane)



Roach, B. J. (2017). *A design model for dividing wall distillation columns* (Doctoral dissertation).

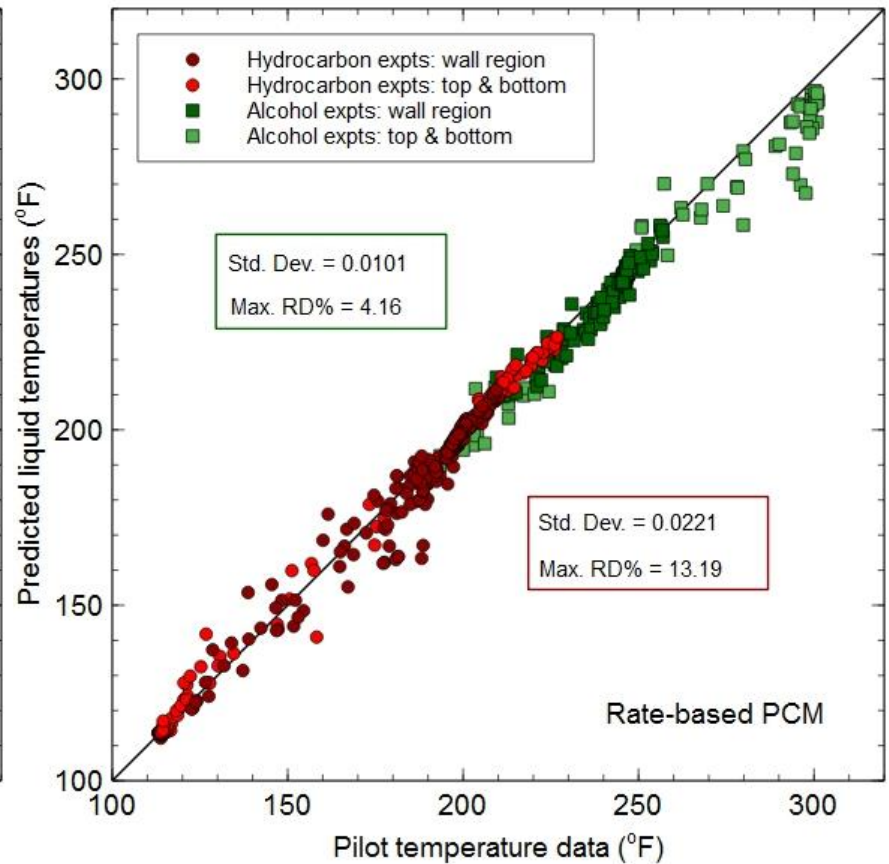
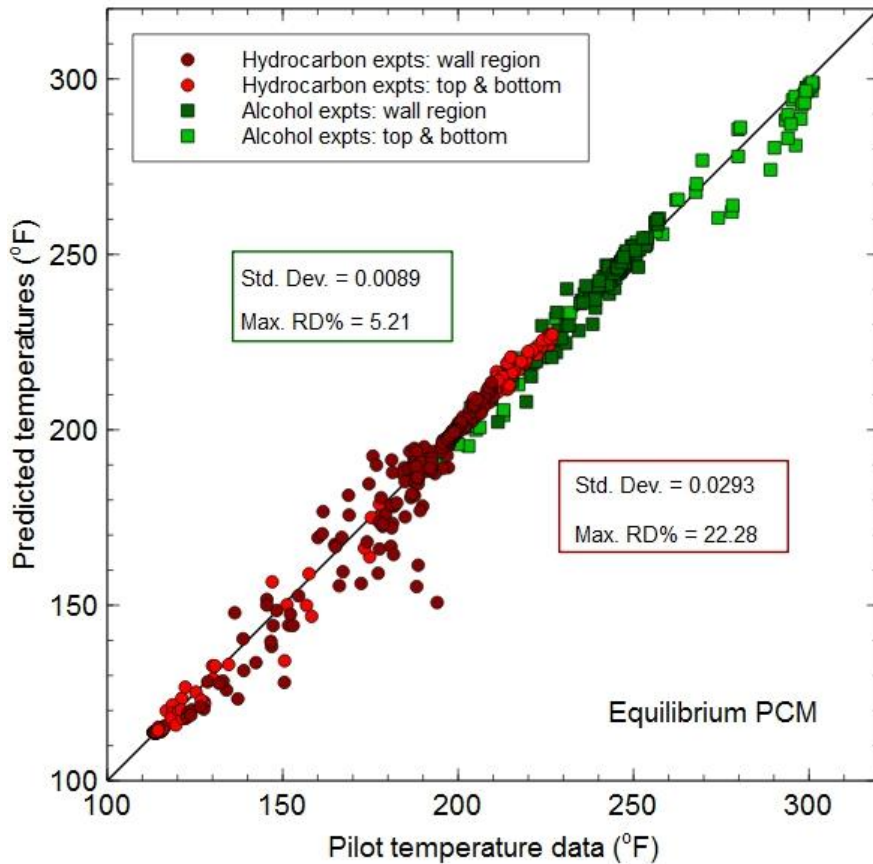
Validation: Experiments of Bailee Roach

- Column dimensions (from Roach, 2017)
 - Sulzer MellaPak 500Y corrugated metal sheets
 - HETP is given by Sulzer as 9.5 inches/stage
 - Outer column diameter is 6.63 inches
 - Wall is located in the middle of column shell
- *Kooijman et al. (2002)* model for pressure drop; Vapor split ratios are estimated by equalizing the pressures on two sides of the wall
- Heat transfer across the wall and heat loss to the surroundings are considered
- Hybrid MTC model
 - k_G : Rocha et al. (1996)
 - k_L : Song correlation
 - a_e : Wang form of Tsai correlation



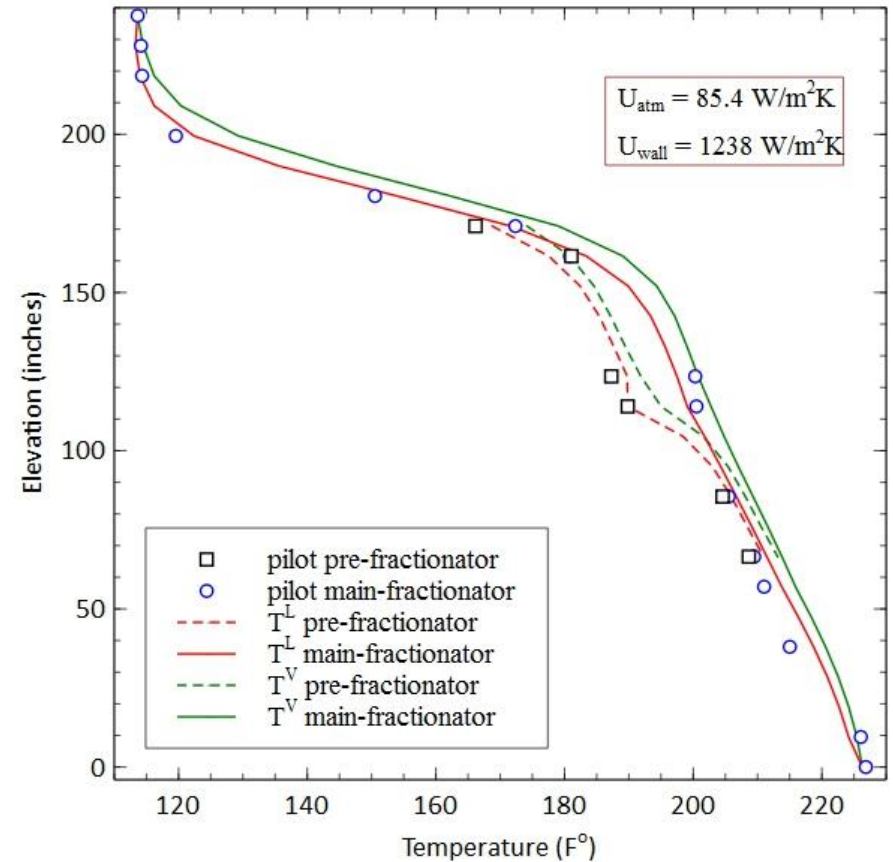
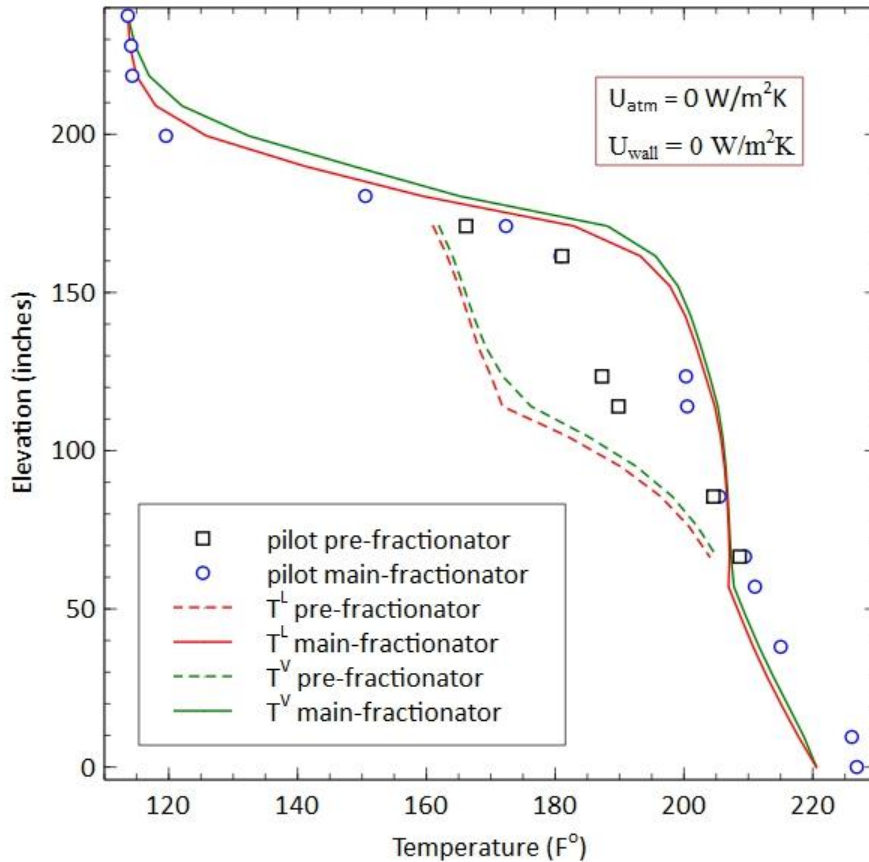
Validation: Experiments of Bailee Roach

- All experiments from Roach (2017) modeled with PCM



Heat Transfer Important in Small Columns

- Case H12: Hydrocarbon Equimolar Feed from Roach (2017)



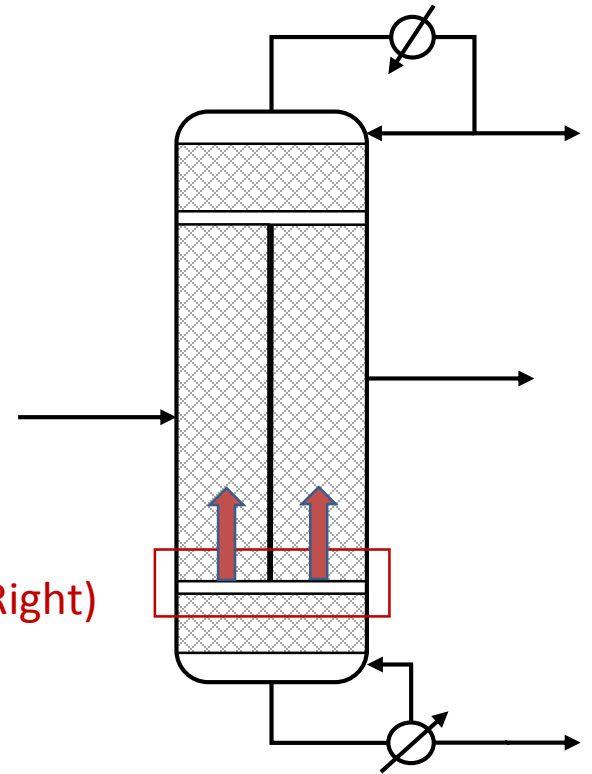
Auto-Adjusted Vapor Split

Pressure **B**alance equation (*B equation*)

$$B \equiv \Delta p_{left}^W - \Delta p_{right}^W = 0$$

Each B equation corresponds to one extra variable, vapor split ratio β

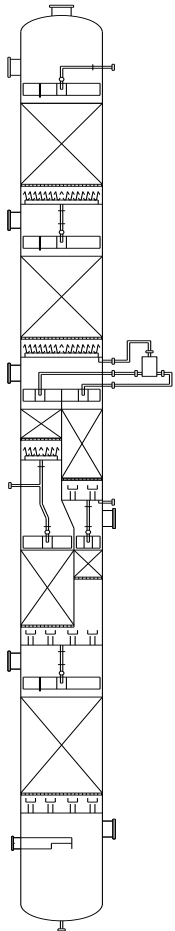
$$\beta = \text{Vapor Left} / (\text{Vapor Left} + \text{Vapor Right})$$



Pressure balance solved simultaneously: β is a result

Auto-Adjusted Vapor Split: Dejanović Column

■ Aromatics DWC

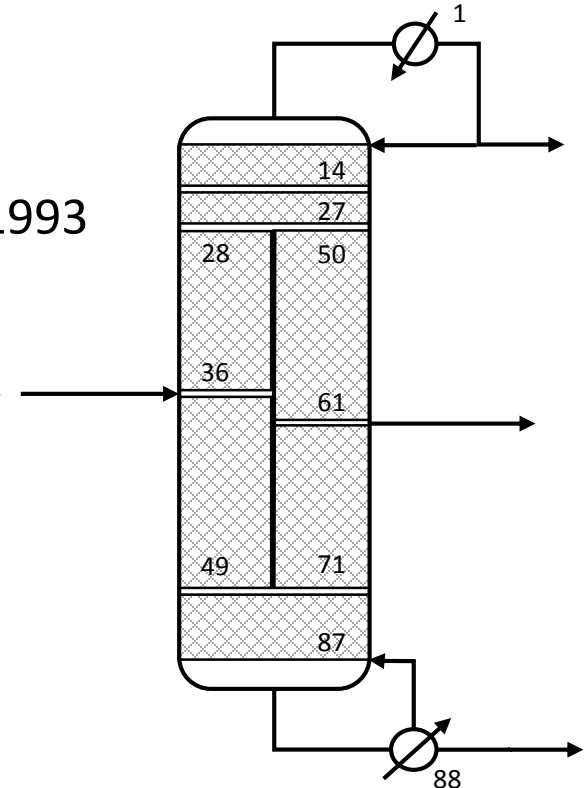


- Pressure drop model: Rocha-Bravo-Fair 1993



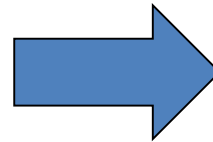
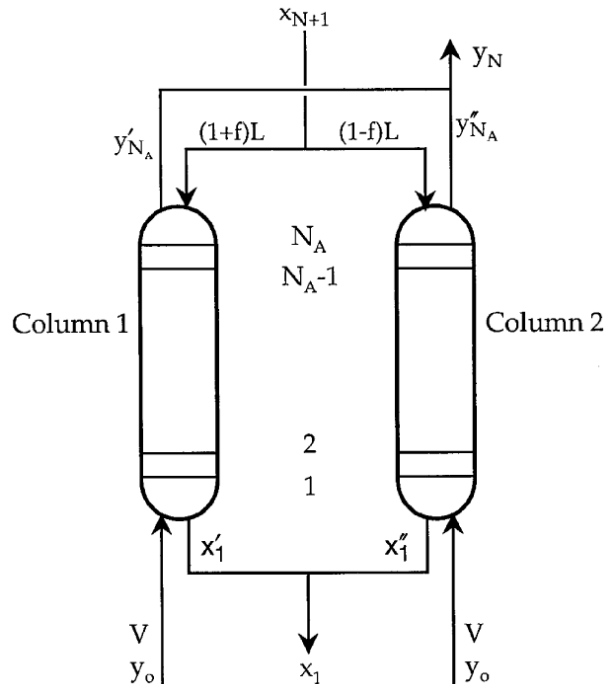
- Vapor Split:

- Dejanović et al. (2011) **0.6639**
- ChemSep PCM estimate **0.6568**

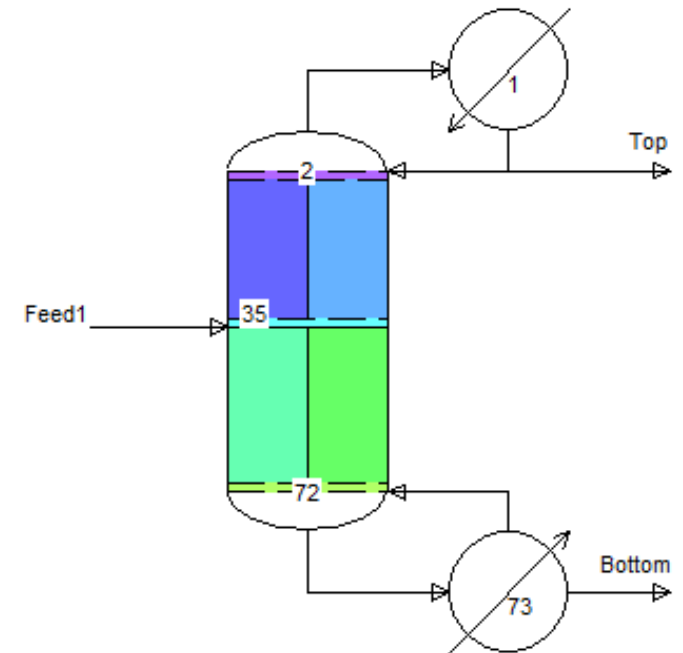


Maldistribution Simulation with PCM

Billingham and Lockett Maldistribution Model



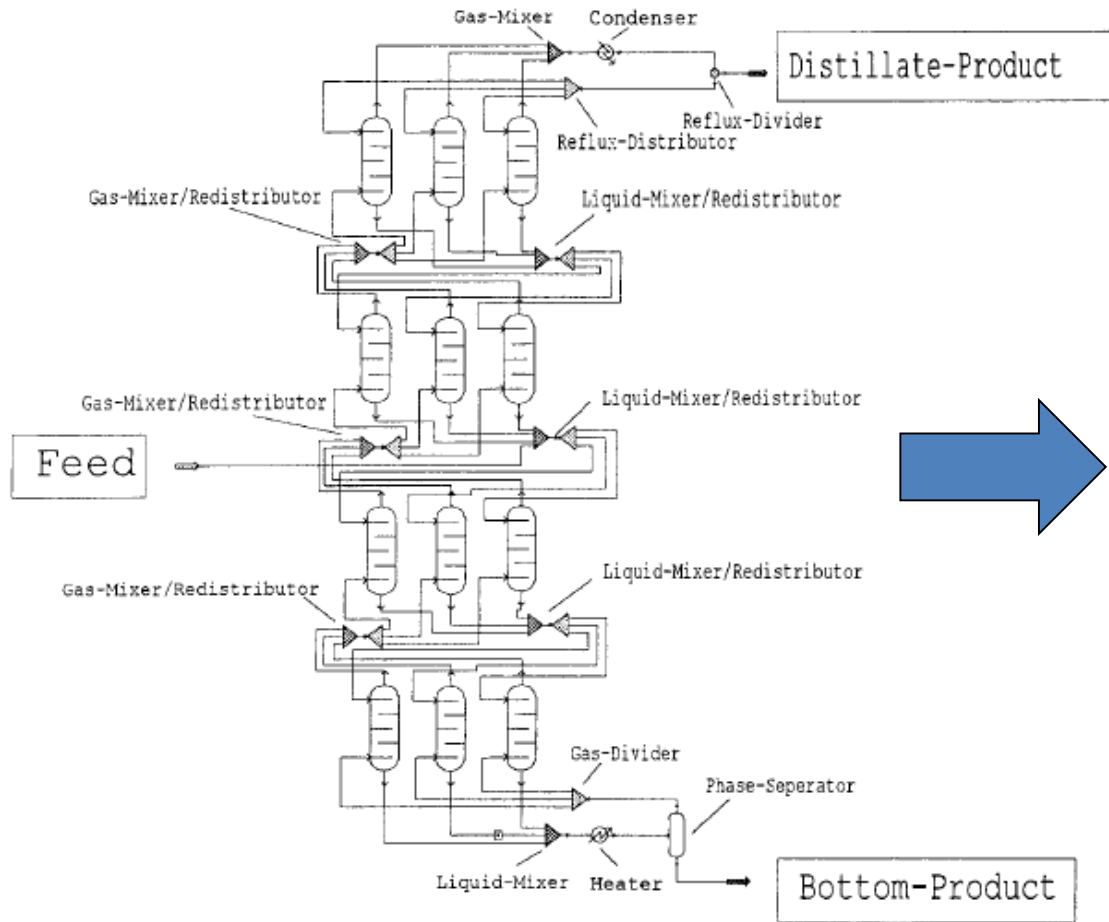
Equivalent PCM Structure



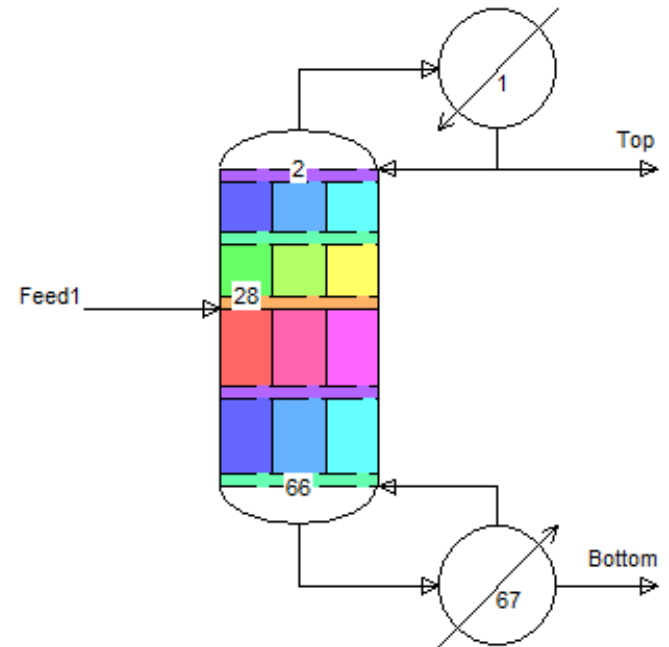
- Redistributors modeled as stages with no mass transfer

Maldistribution Simulation with PCM

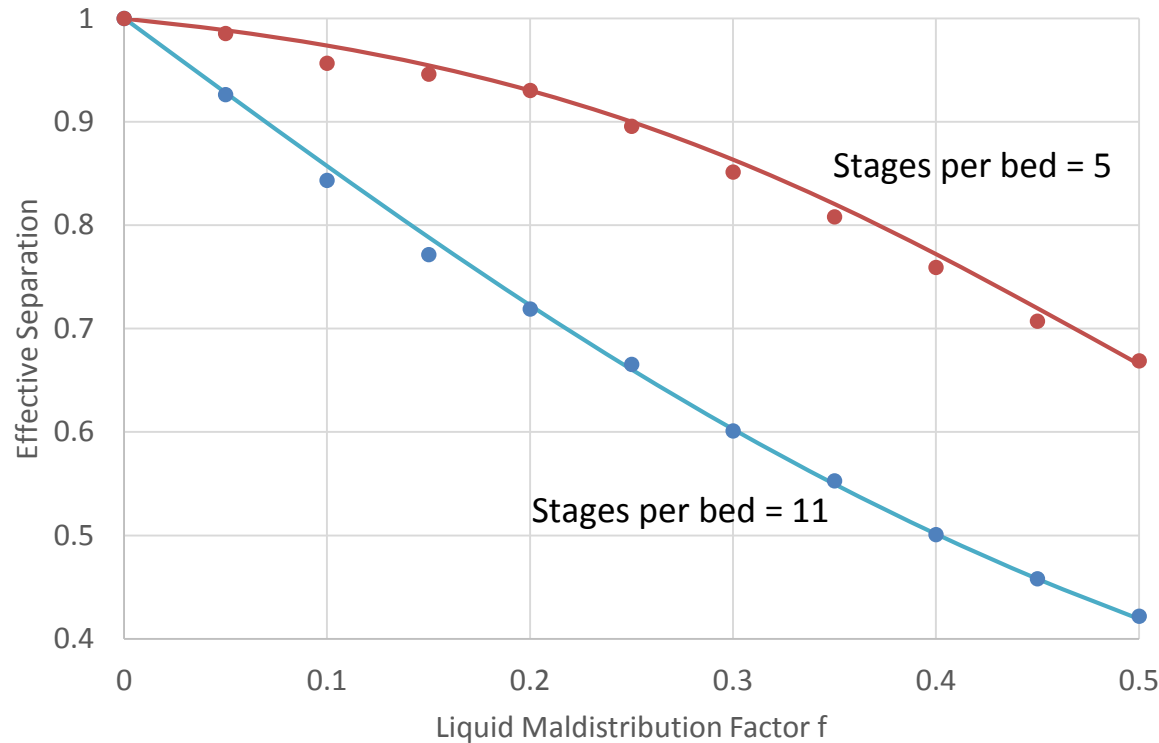
Schultes Maldistribution Model



Equivalent PCM Structure



Maldistribution Simulation with PCM



$$\text{Effective Separation} = \frac{\text{Number of stages without maldistribution}}{\text{Number of stages with maldistribution}}$$

Fractional effective separation as interpolated from the top distillate compositions
Significant influence of the number of redistributors

History of the *free* ChemSep LITE Version

- v5.0 Jan 2005: first CAPE-OPEN compliant version
Maximum 25 compounds, 100 stages
- v6.0 Oct 2006: integration of CAPE-OPEN panel in GUI.
400+ components in pure component data, freely available.
Adaptive icons. Maximum 40 compounds, 300 stages
- v7.0 Jul 2015: ChemSep CAPE-OPEN property packages
- v7.1 Jan 2016: Improved graphics with drag & drop zoom
- v7.2 Oct 2017: Direct export of problems to COCO flowsheets
- v7.3 Feb 2018: Rating panel with connection to vendor tools
- v7.4 May 2018: User defined Group Contribution methods
- **v8.0 Oct 25, 2018: Parallel Column Model for DWCs with one wall, no heat transfer, one condenser, one reboiler**

Conclusions

- The rate-based PCM
 - Takes very little effort to set up a DWC column model
 - Any number of walls
 - Requires no initial guesses from engineer
 - Converges much quicker than multi-column models for DWCs
 - Makes it very easy to account for heat transfer across walls
 - Vapor split can be calculated (not specified)
 - Can be used to model maldistribution in packed columns
- **Rapid design and optimization of DWCs**
- Rate-based PCM in good agreement with pilot plant data
- Experiments in DWC excellent test of k_L , k_G , and ΔP models
- **Simulate simple DWCs using ChemSep LITE**