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

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Dividing Wall Columns: What Was Said

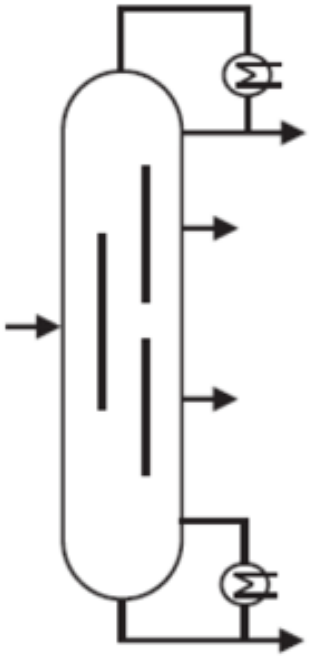
Dejanović et al. (2010) wrote:

*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.*

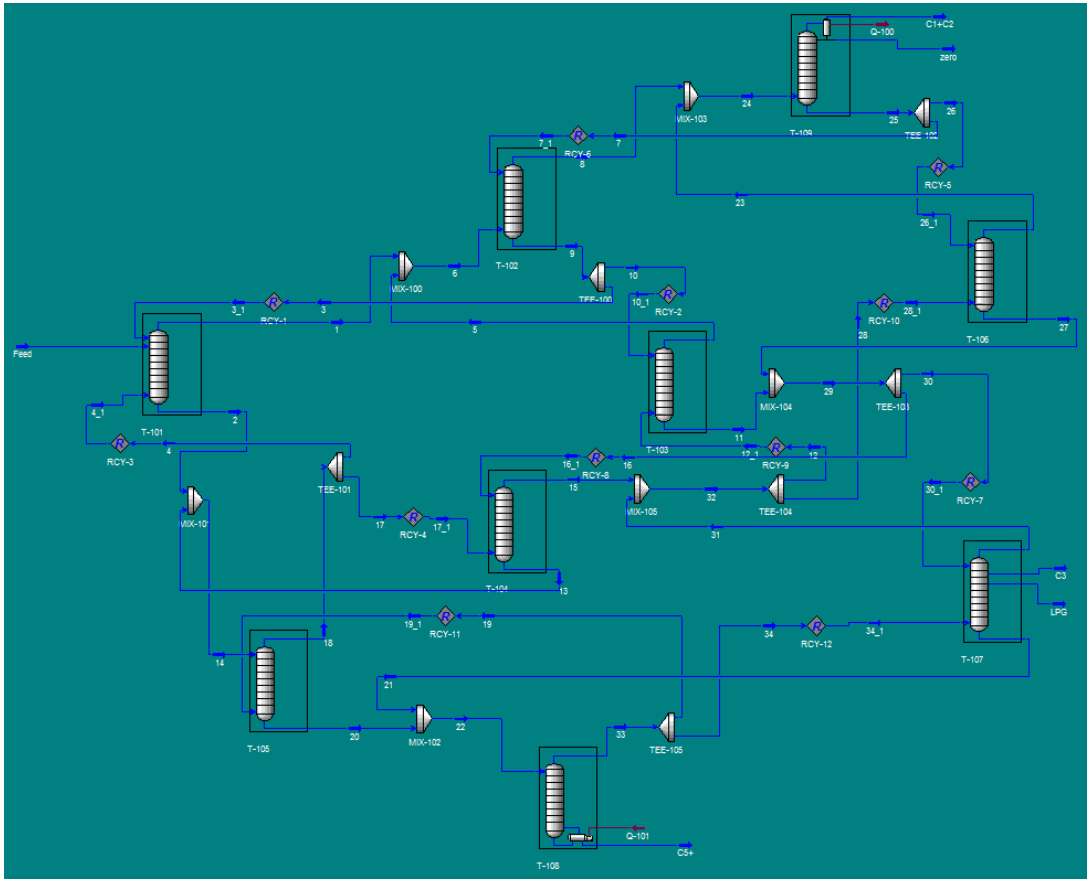
Engineers have, therefore, developed alternative approaches to model DWCs…

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: deviding wall column, double dividing wall column, prefractionator arrangement, Petlyuk column, NGL recovery, distillation* (Master's thesis, Institutt for energi-og prosessteknikk).

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. **This however will occur sooner or later, most probably as a simultaneous, equation based model.***

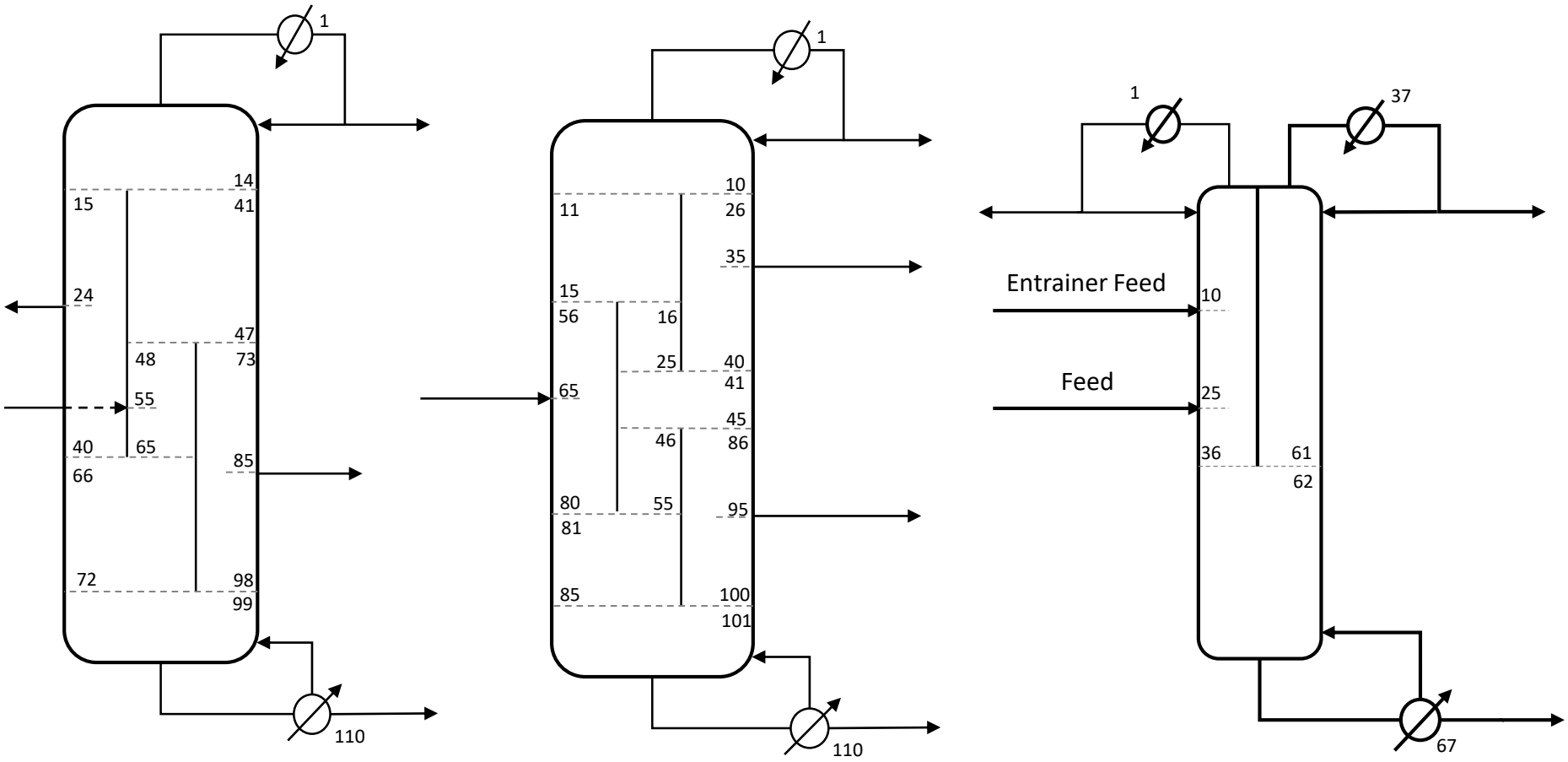
Kaibel (2014) wrote:

*Due to the potential variability of complex internal configurations, there is no dedicated software package for this purpose. … The convergence behavior of programs with sequential operation is **sometimes problematic**. **Equation-based programs normally show better convergence characteristics**.*

But no evidence in support of this assertion had been presented.

Dividing Wall Columns: What We Did

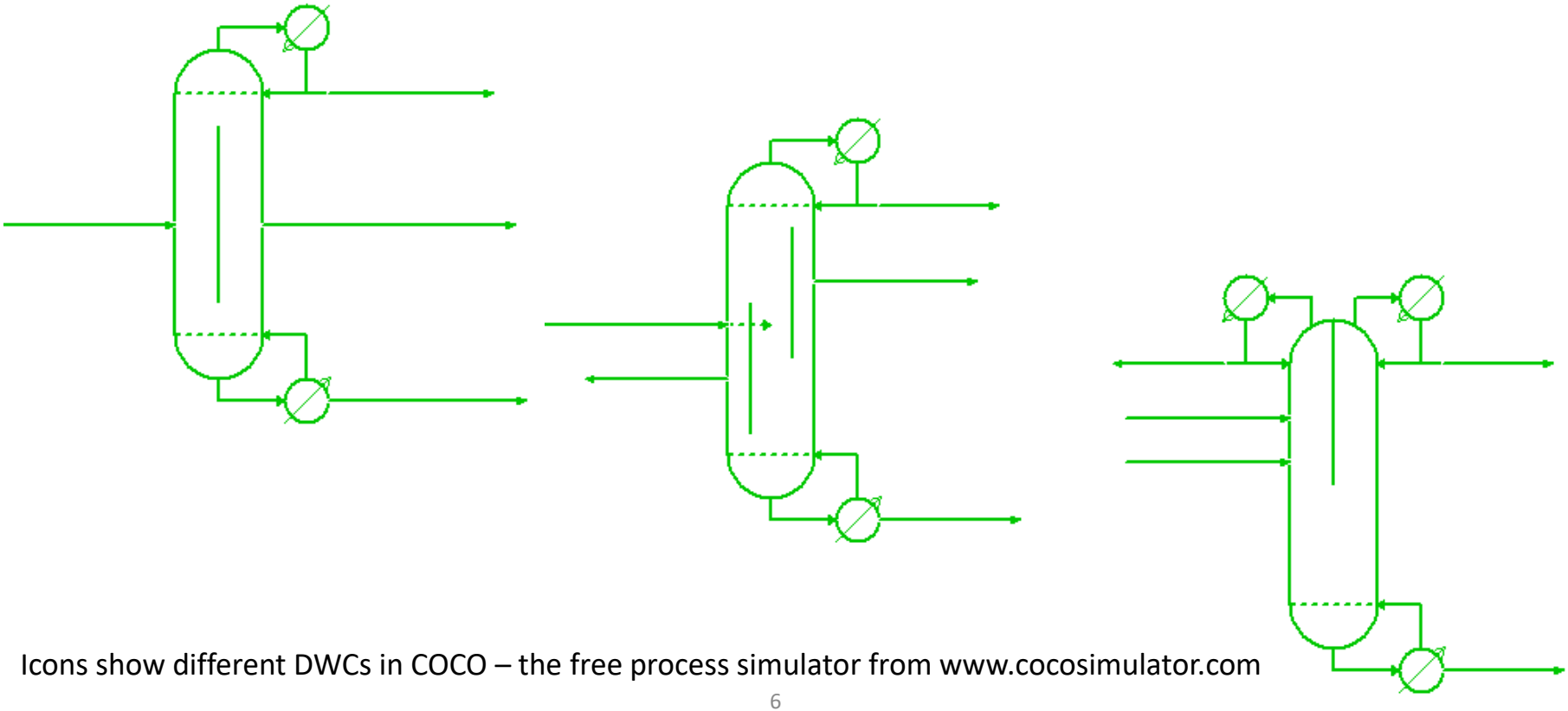
- Equation-oriented parallel column model (PCM)
  - Simulates dividing wall columns (DWCs) of arbitrary configuration



Zhou et al., AIChE Fall National Meeting, Minneapolis, November 2017.

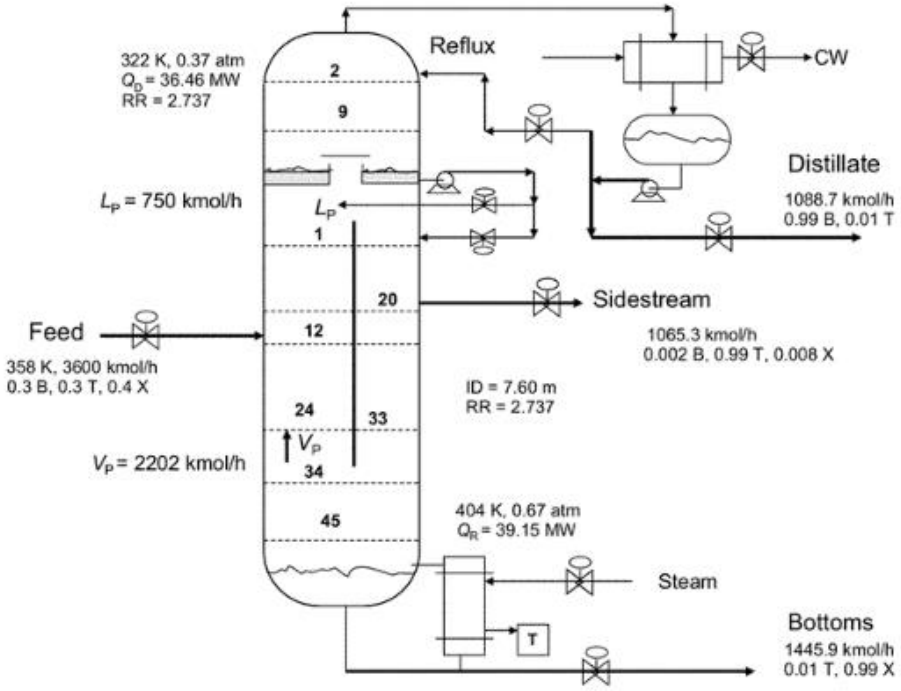
Dividing Wall Columns: What's New

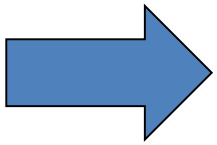
- Integrate Equilibrium Stage PCM in ChemSep
- ChemSep PCM can be used in any CAPE-OPEN compliant process flowsheet simulation package as a standard DWC module
- Rate-based Parallel Column Model

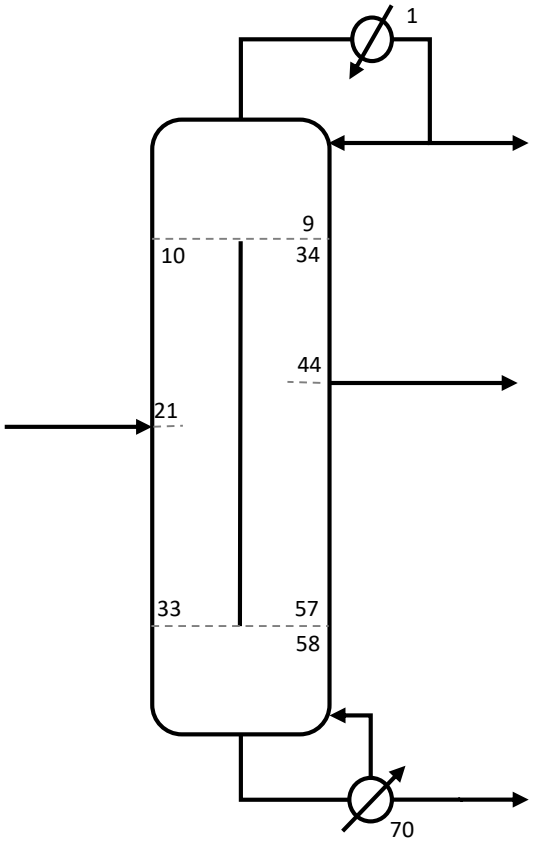


Icons show different DWCs in COCO – the free process simulator from www.cocosimulator.com

DWC Simulation: Luyben BTX Column

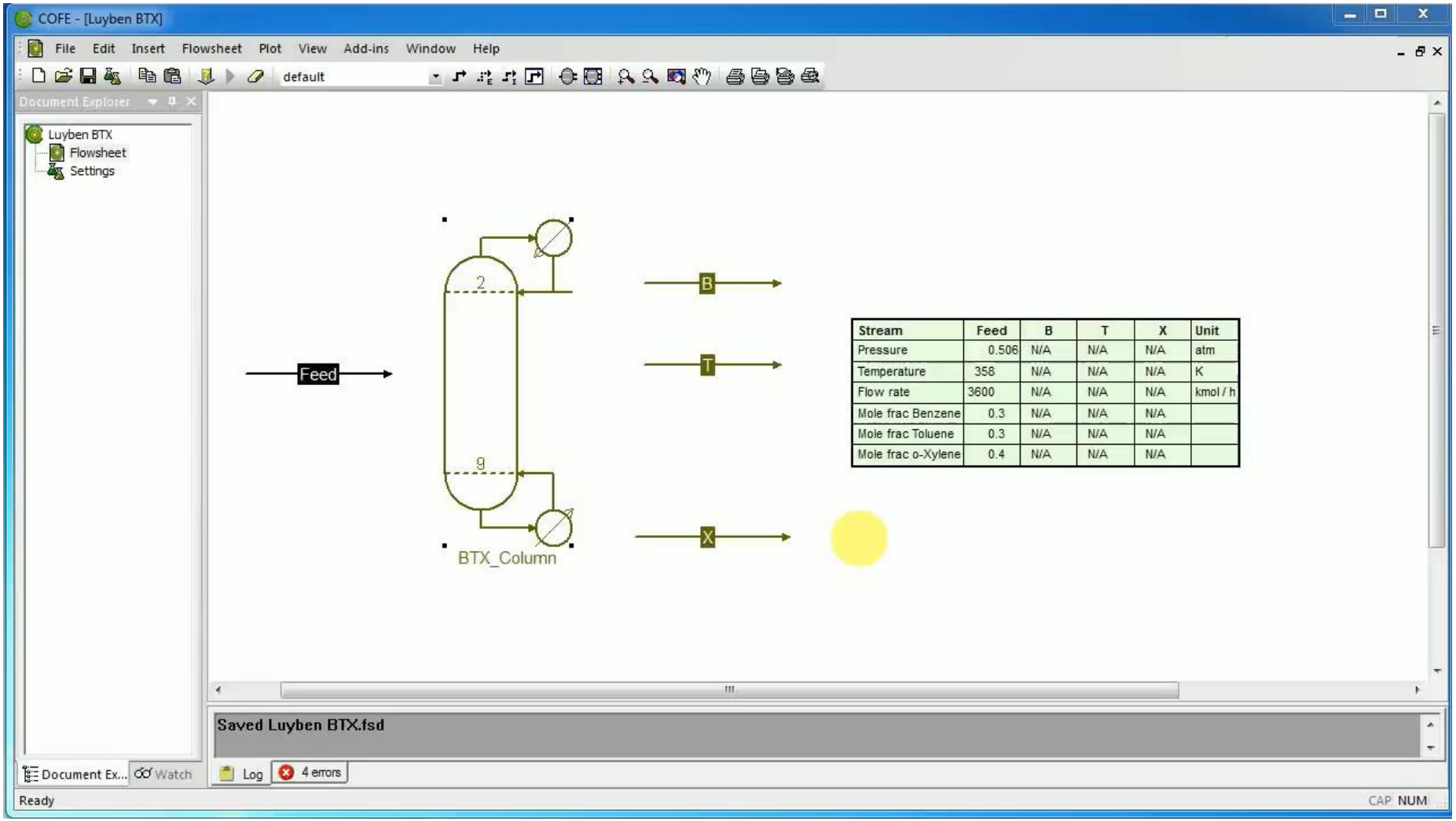




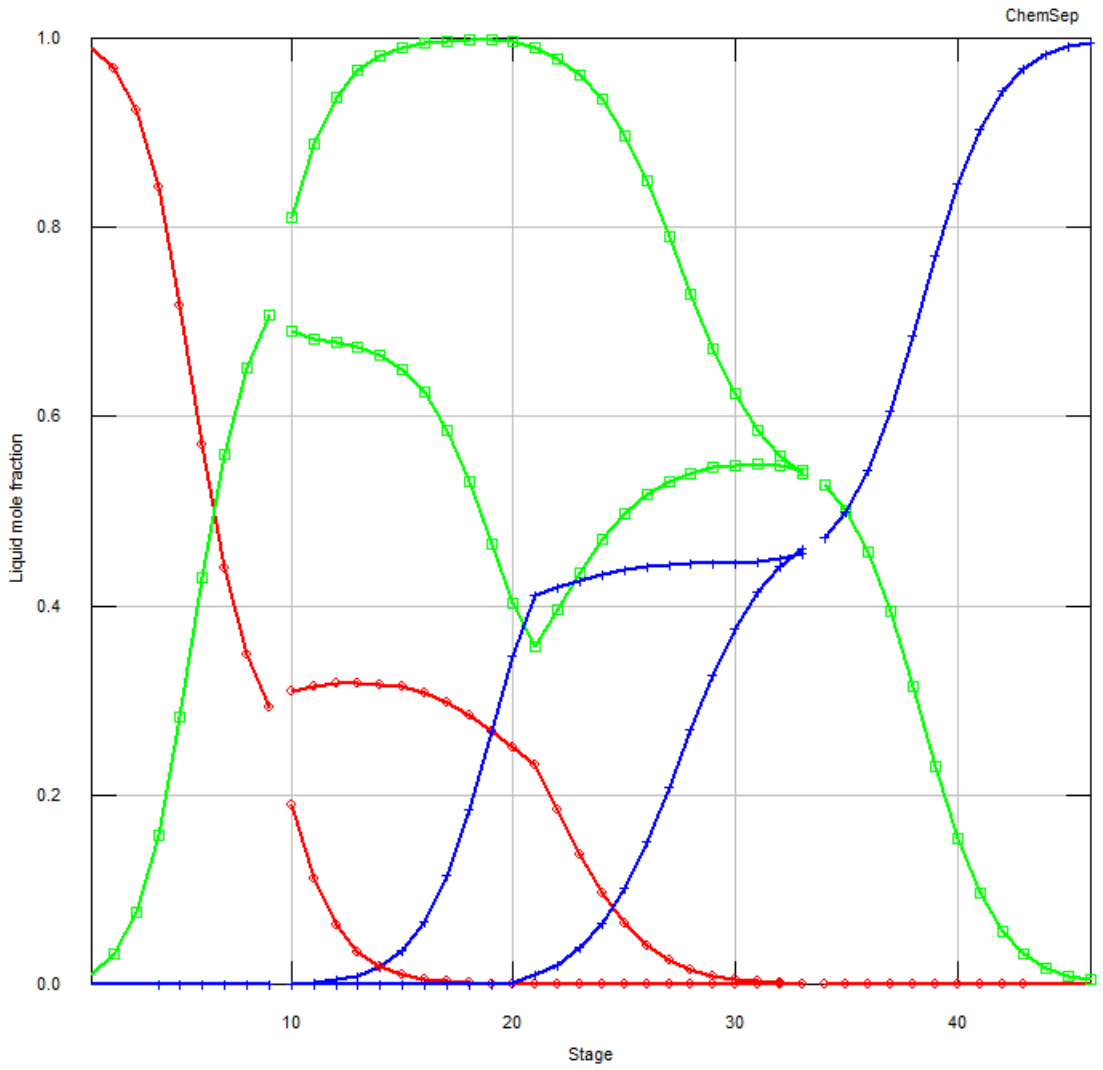


Luyben, W.L. (2013). Divided-wall (Petlyuk) columns, in: Distillation Design and Control Using Aspen Simulation. John Wiley & Sons, pp. 355–384.

DWC Simulation: Luyben BTX Column



DWC Profiles are Intimately Connected



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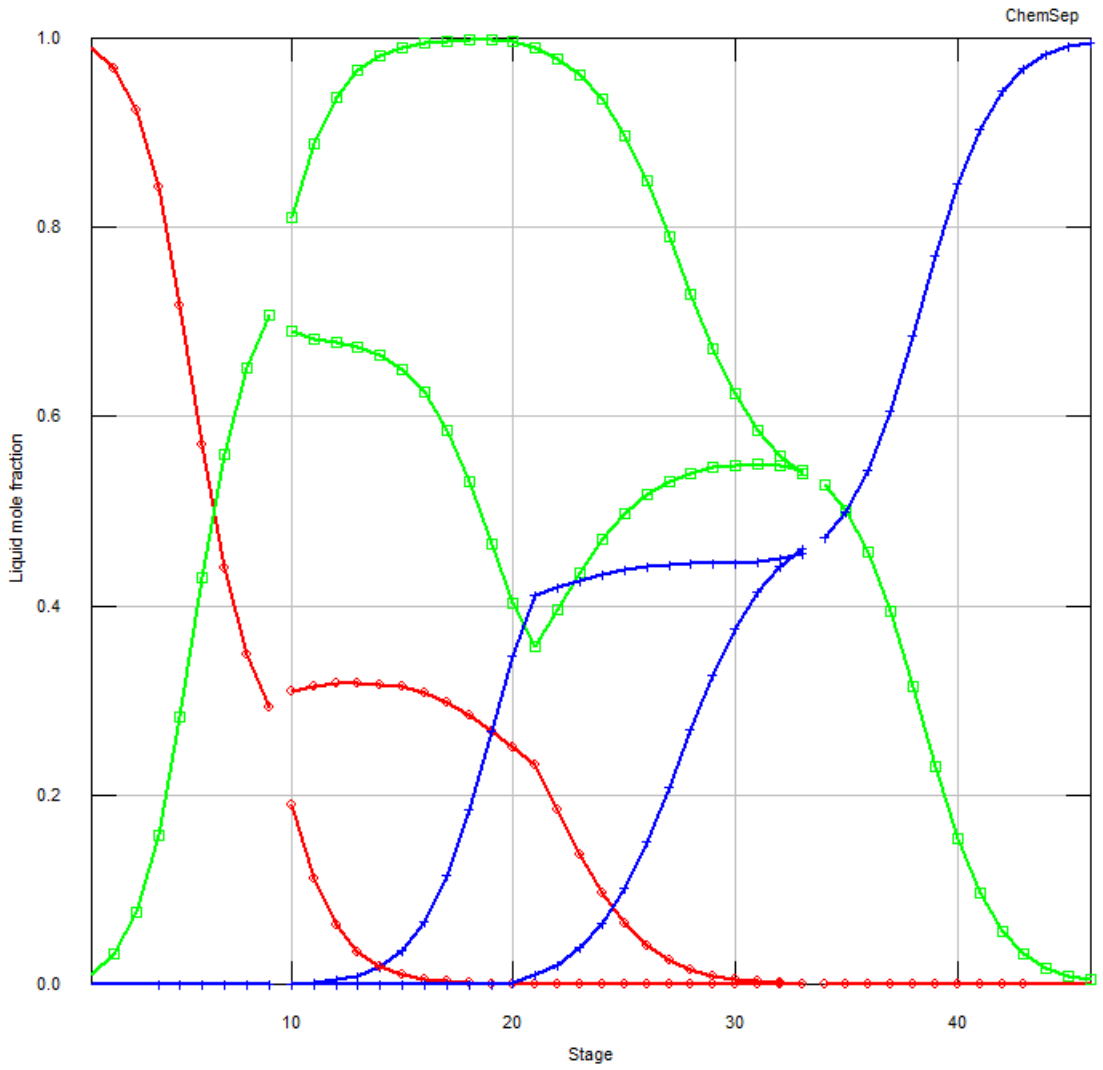


Dividing Wall Columns: What Was Said

Clarkson UNIVERSITY defy convention

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**.*

This, now, has been done.

Kaibel (2014) wrote:

*Due to the potential variability of complex internal configurations, there is no dedicated software package for this purpose. … The convergence behavior of programs with sequential operation is **sometimes problematic**. **Equation-based programs normally show better convergence characteristics**.*

This, also, is true!

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

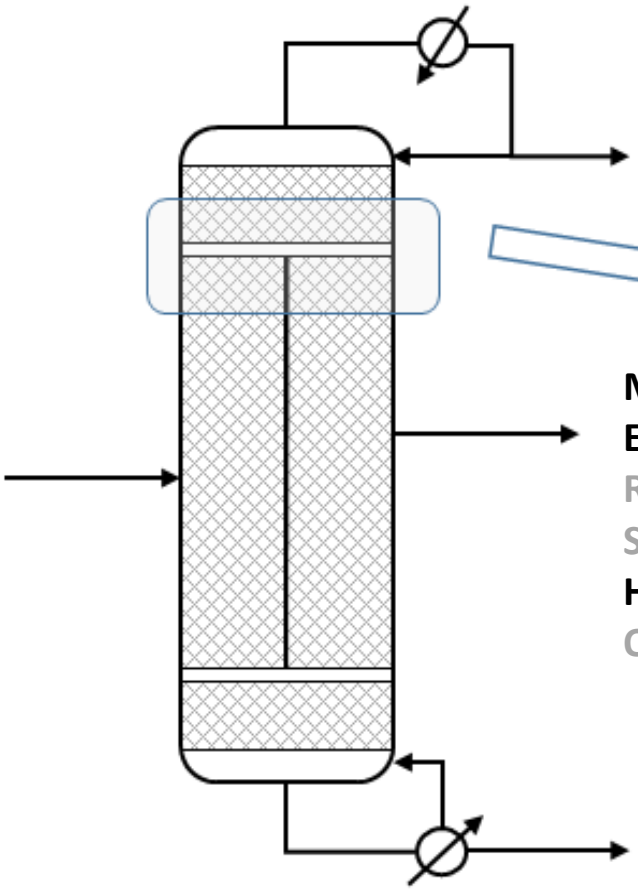
Rate-Based Models

- 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

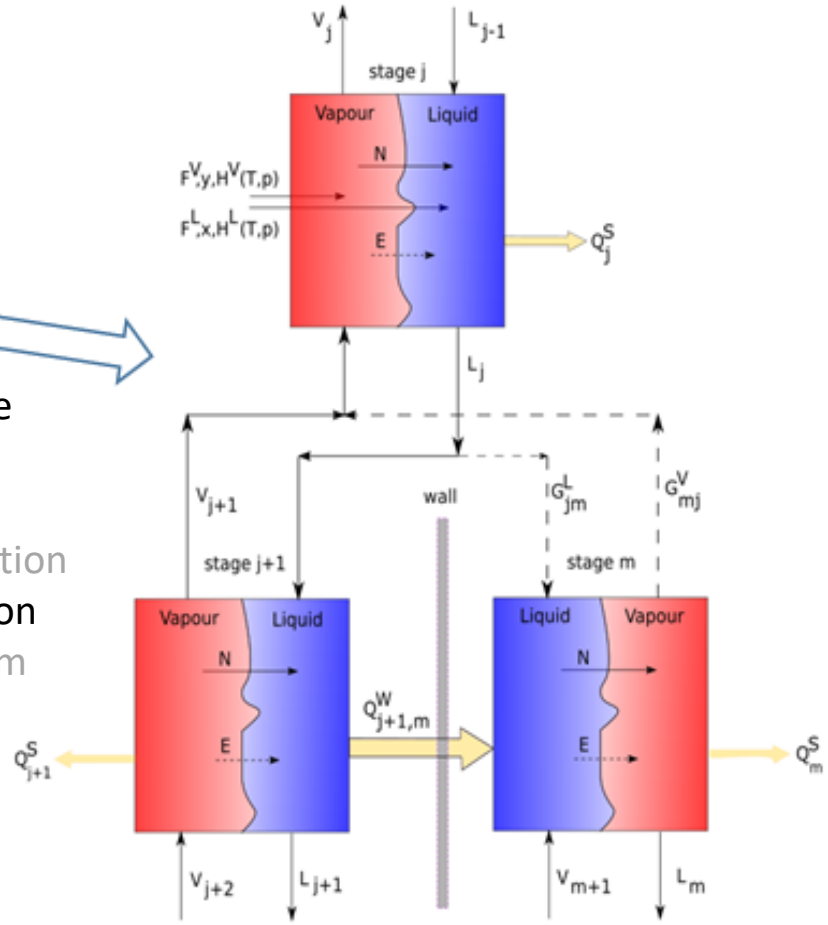
Both used equation-based Aspen Custom Modeler (ACM)

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

Rate-Based Parallel Column Model



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



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

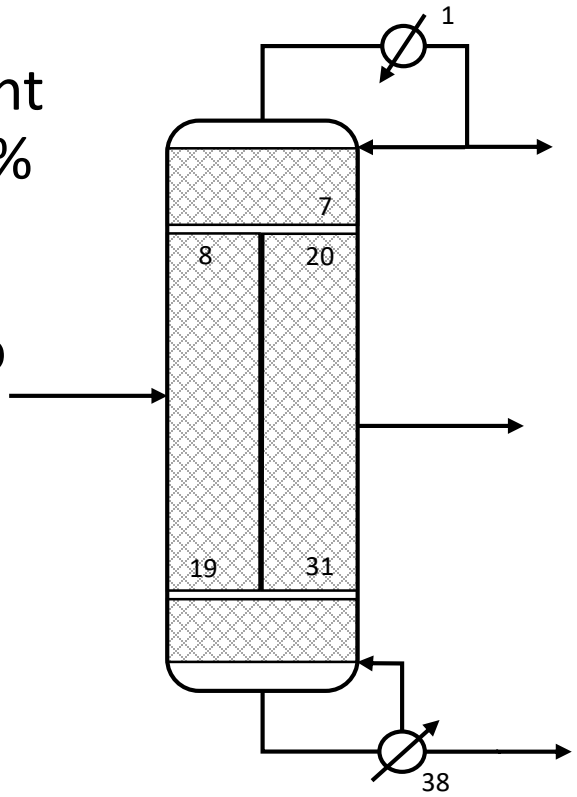
Validation: Experiments of Bailee Roach

- 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).

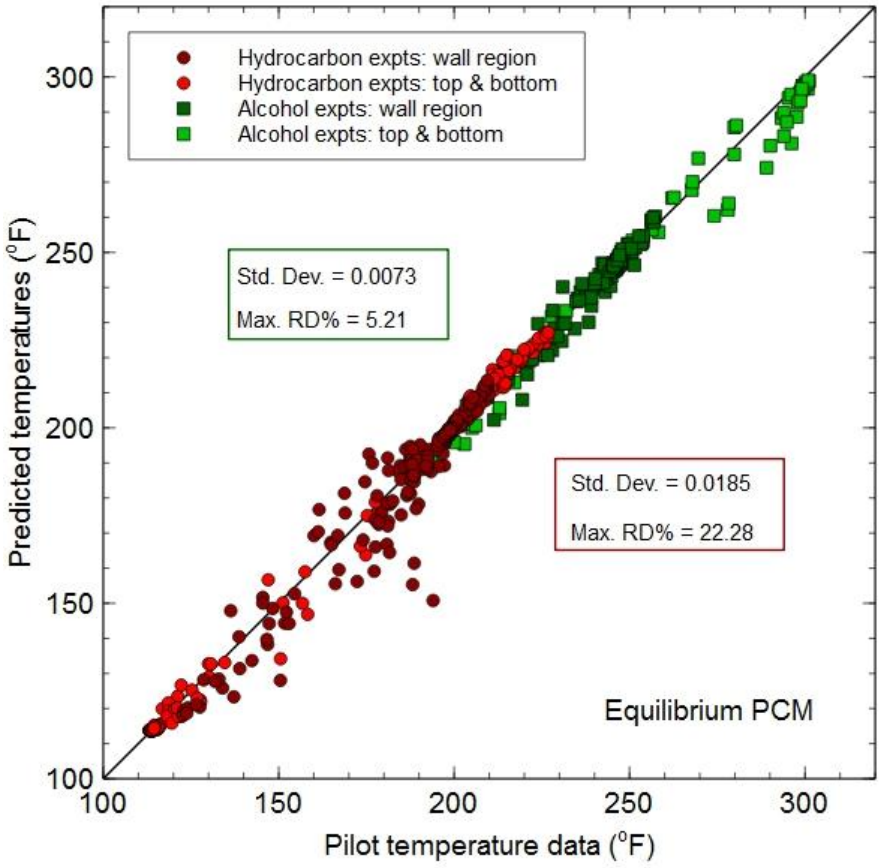
Validation: Experiments of Bailee Roach

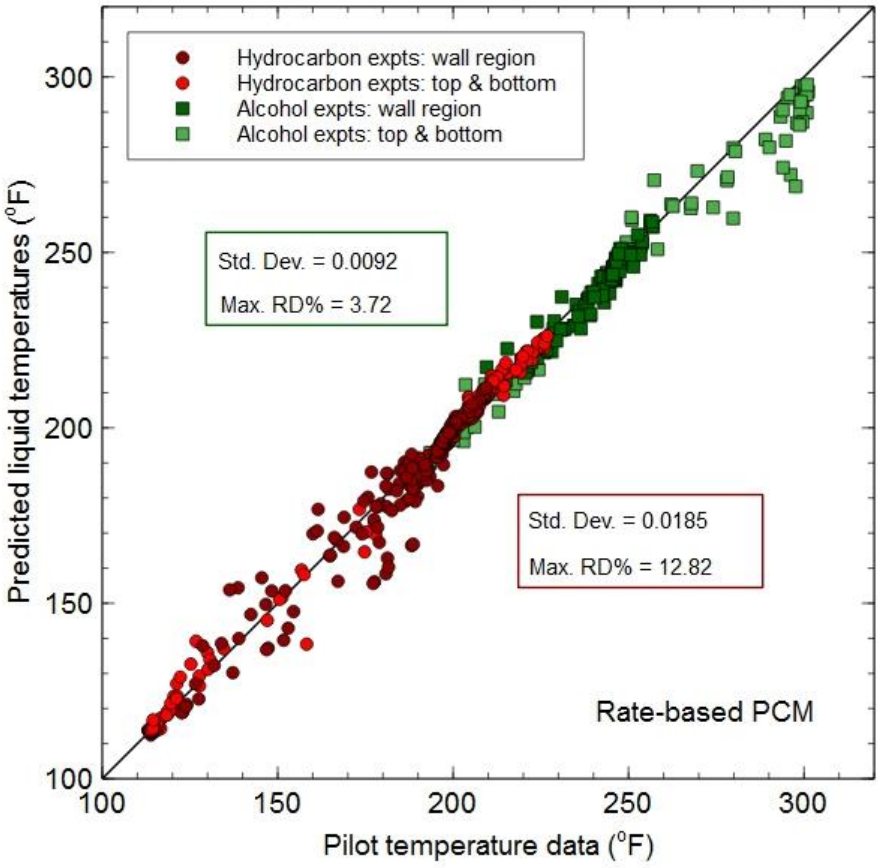
- Column dimensions (from Roach, 2017)
  - Sulzer MellaPak 500Y corrugated metal sheets
  - HETP is given by Sulzer as 9.5 inches/stage
  - Outer column diameter is 6.63 inches
  - Wall is located in the middle of column shell
- Column pressure drop is reported for different bed sections, and vapor split ratio is 50%/50% (from Roach, 2017)
- 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

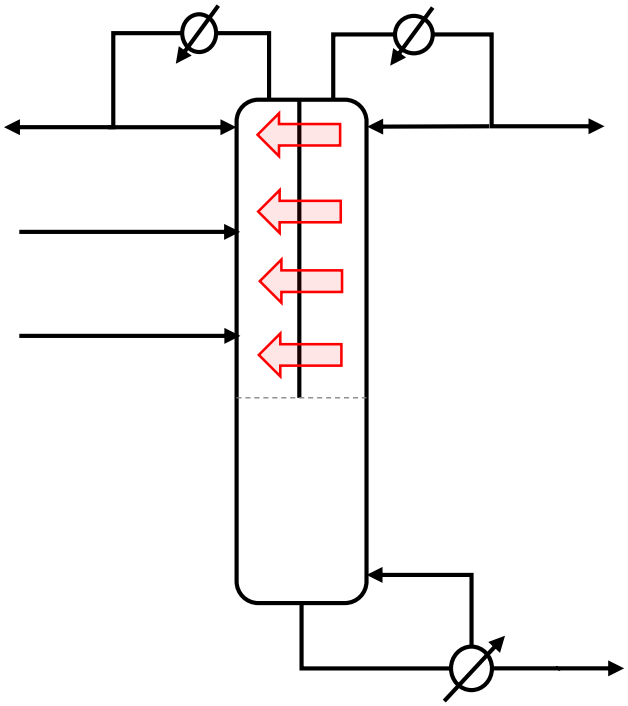
- All experiments from Roach (2017) modeled with PCM

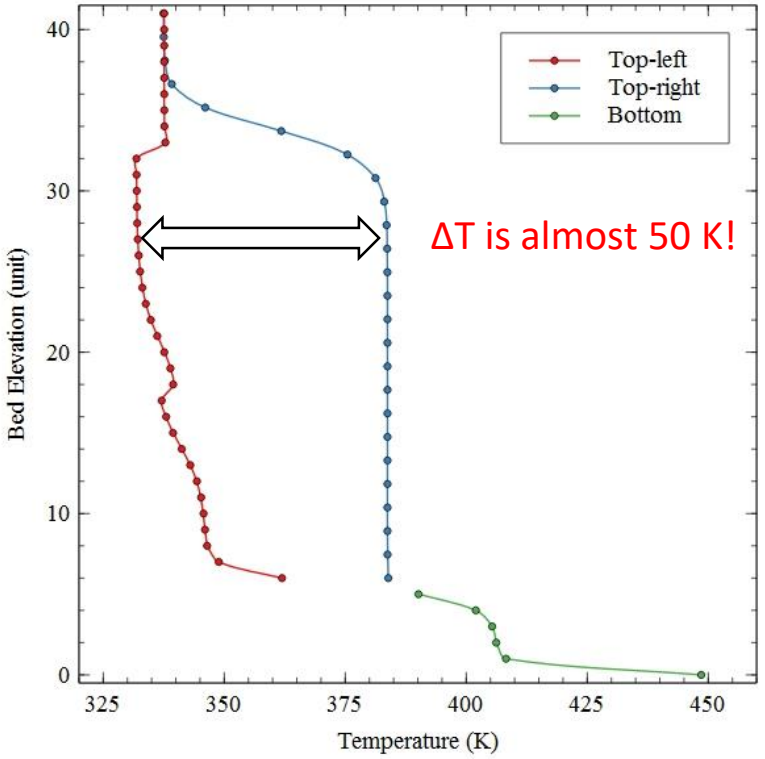




Heat Transfer across Dividing Walls

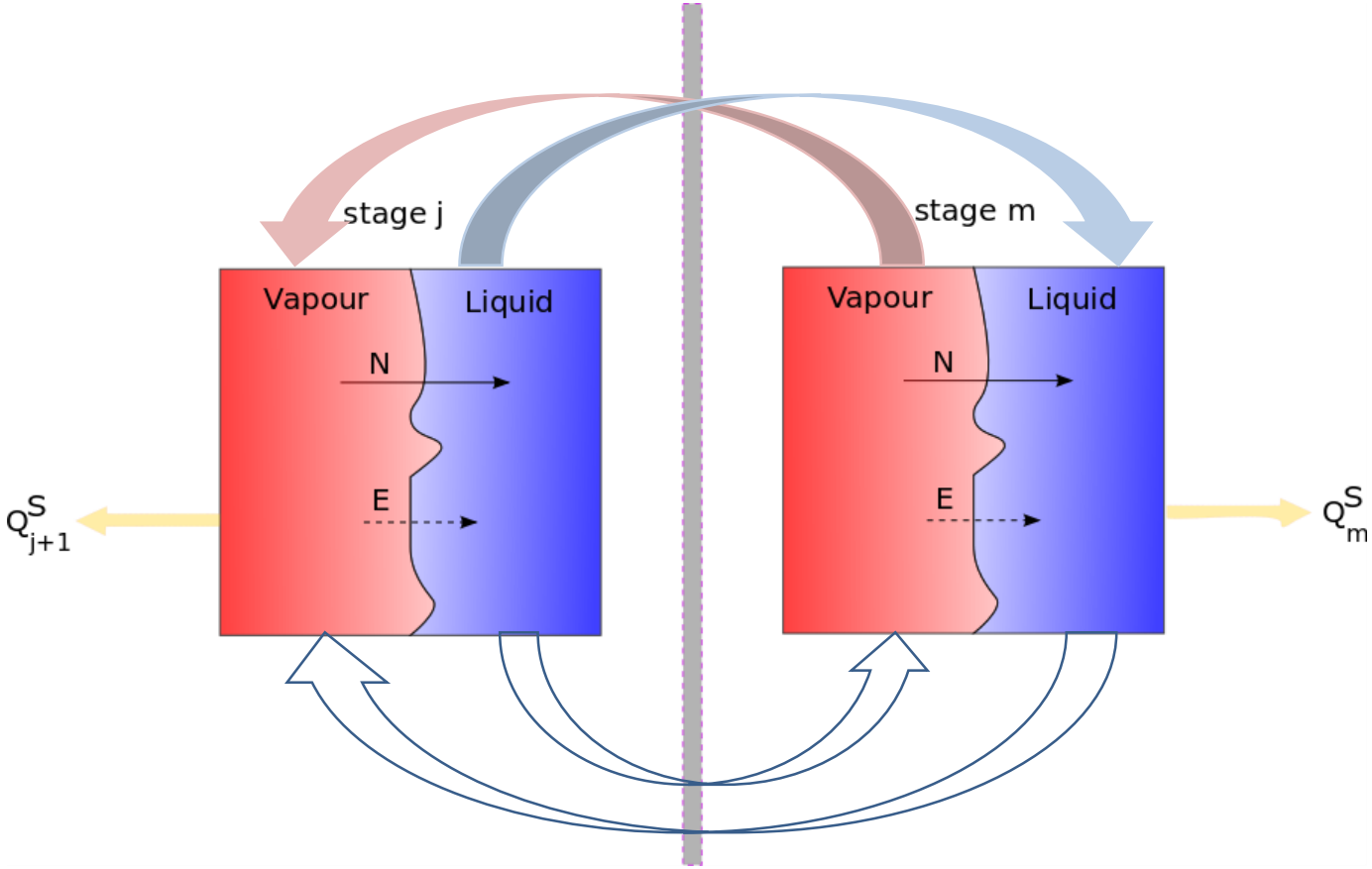
- Dividing walls are not insulators
- Temperature gradients can be significant
- Extremely difficult to include heat transfer in multi-column models
- Very easy to include heat transfer in Parallel Column Model





Heat Transfer across Dividing Walls

- How does heat transfer between distinct phases?



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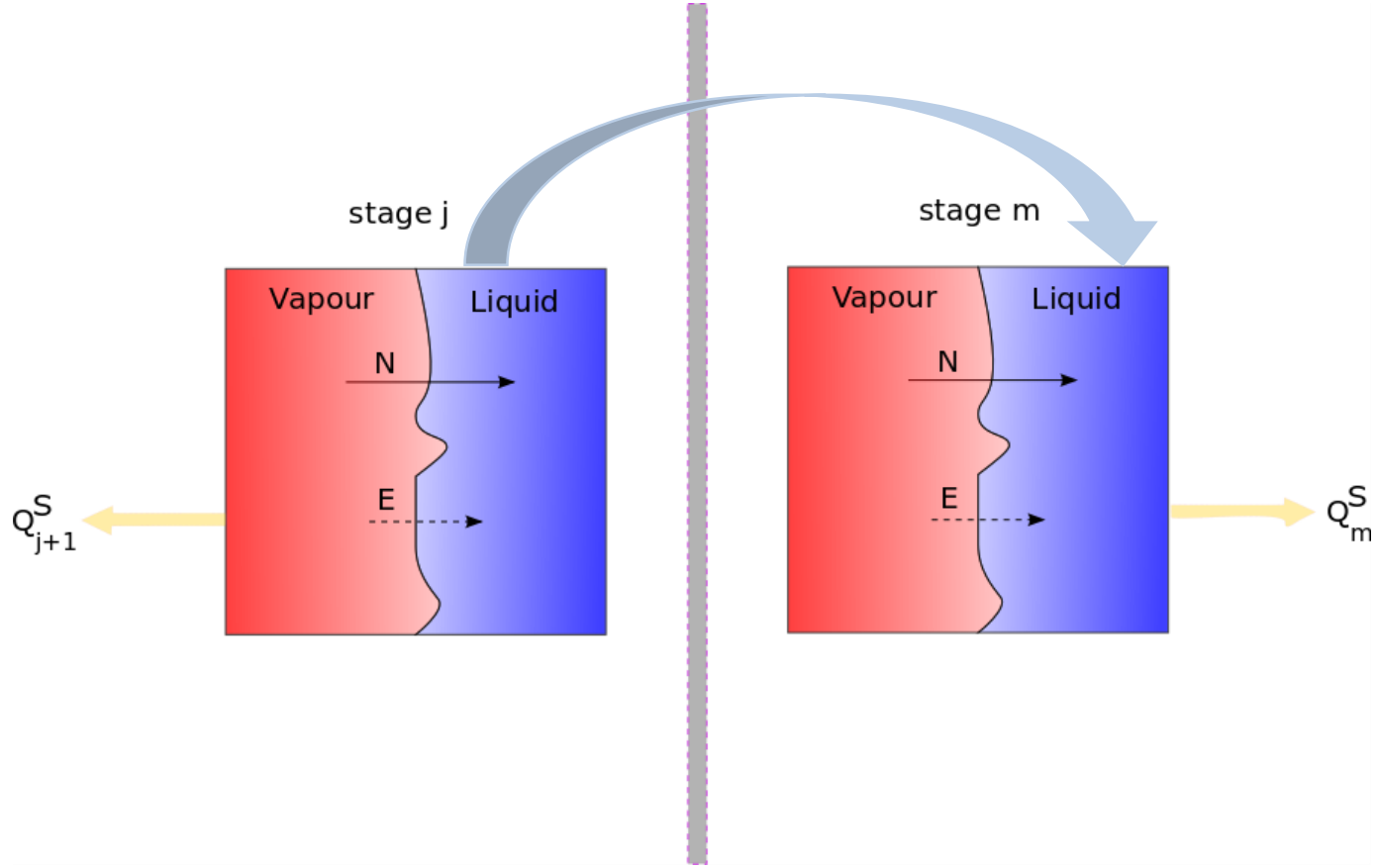
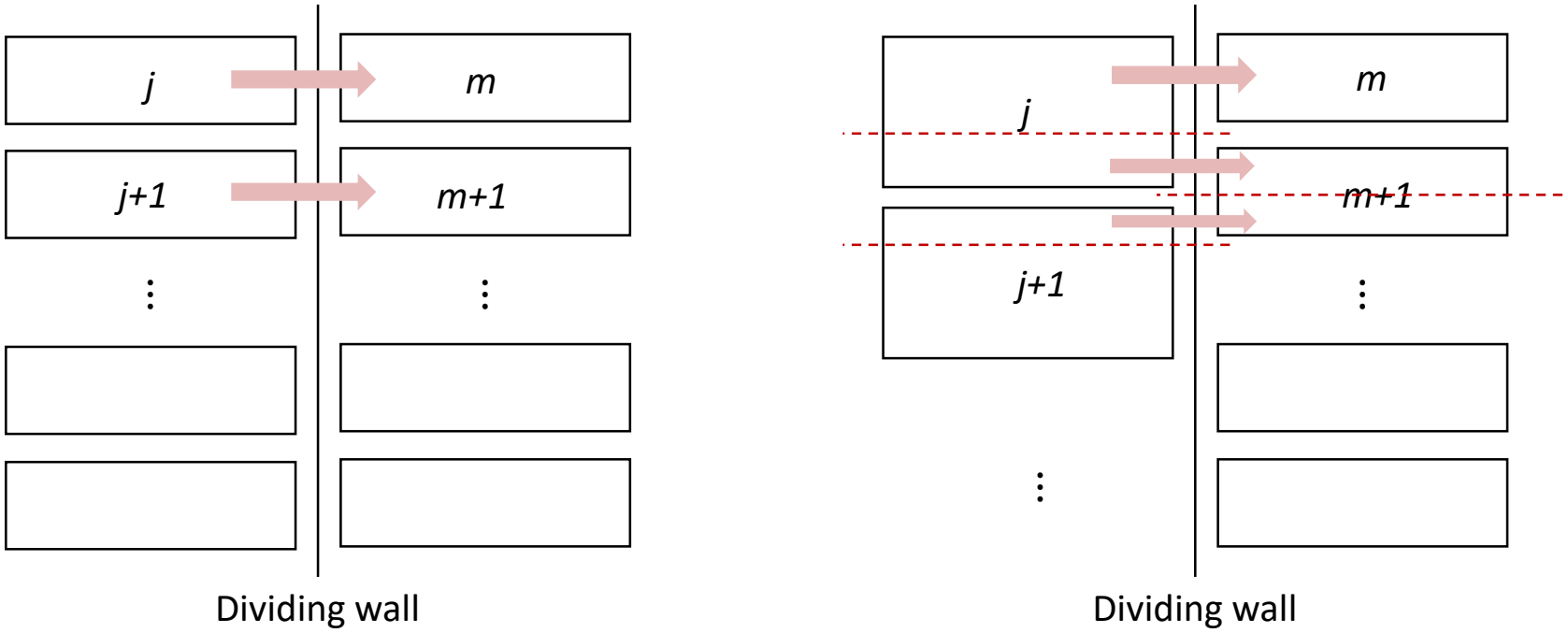


- We assume (for now) that heat transfer occurs between liquid phases

Heat Transfer across Dividing Walls

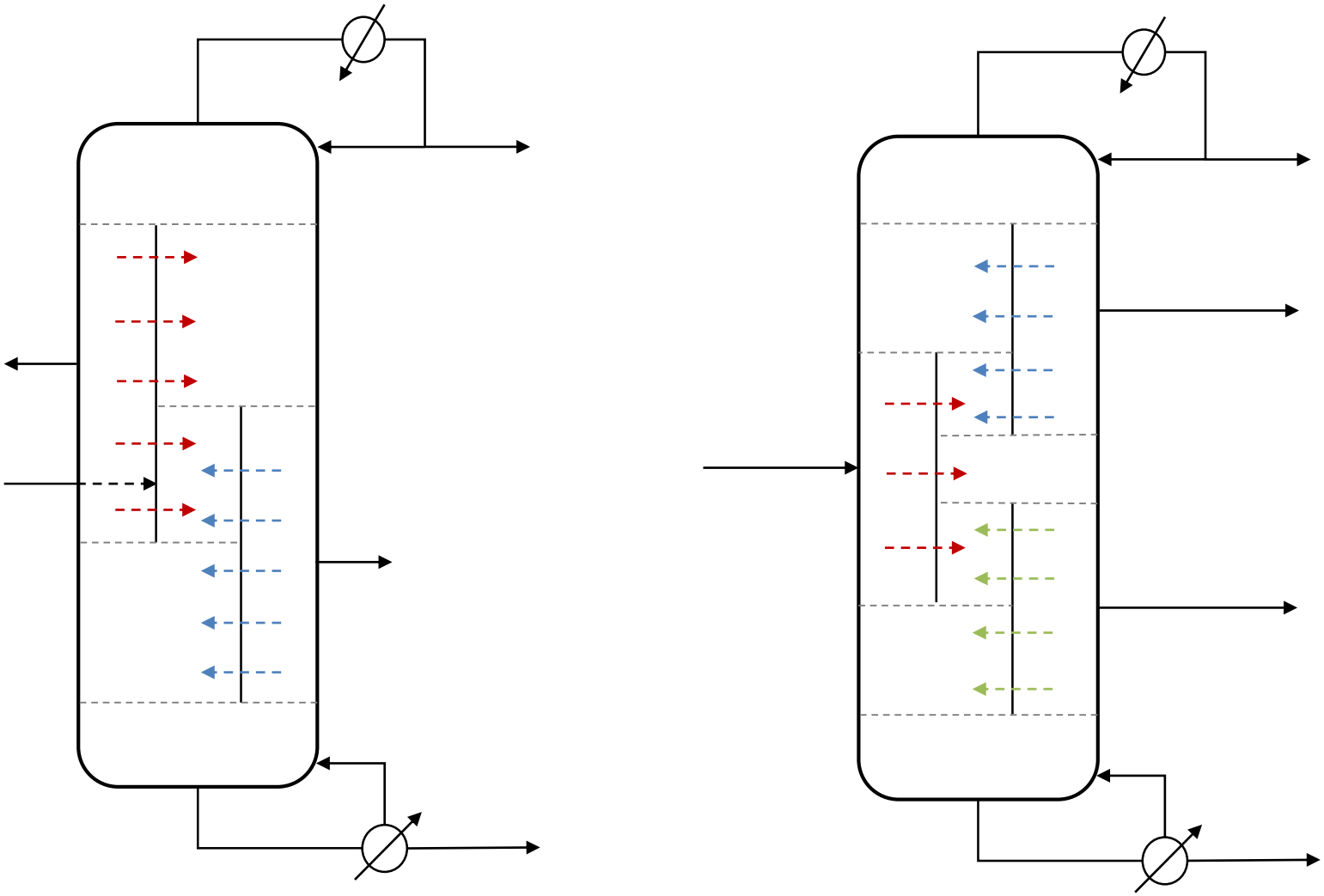
- Number of stages may not align



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

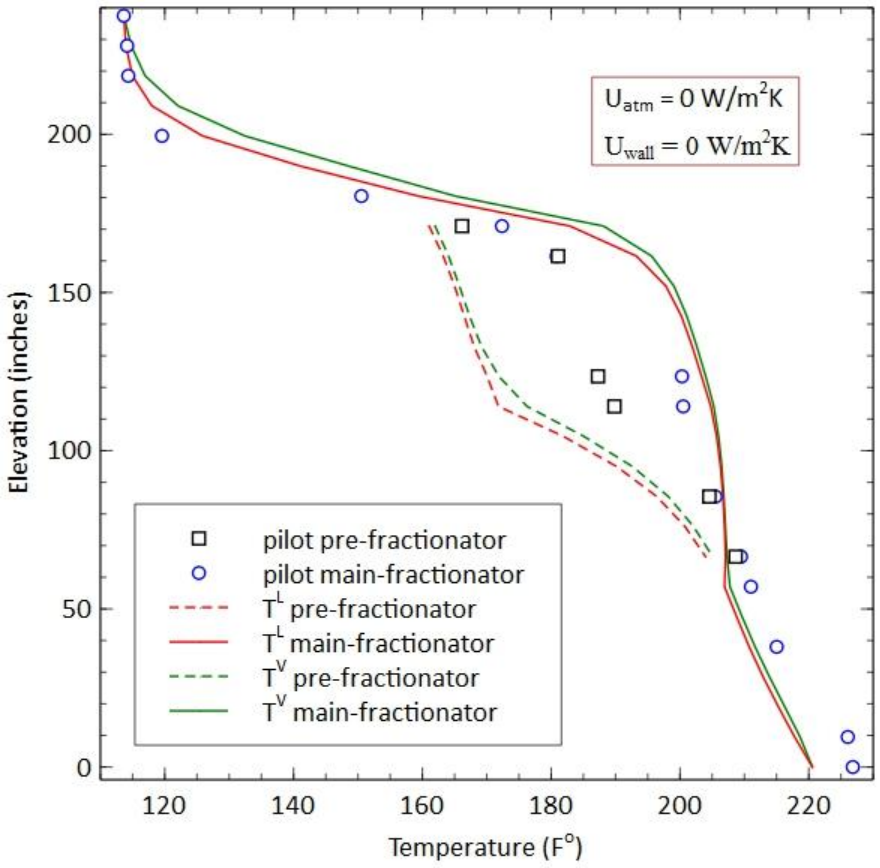
Heat Transfer across Dividing Walls

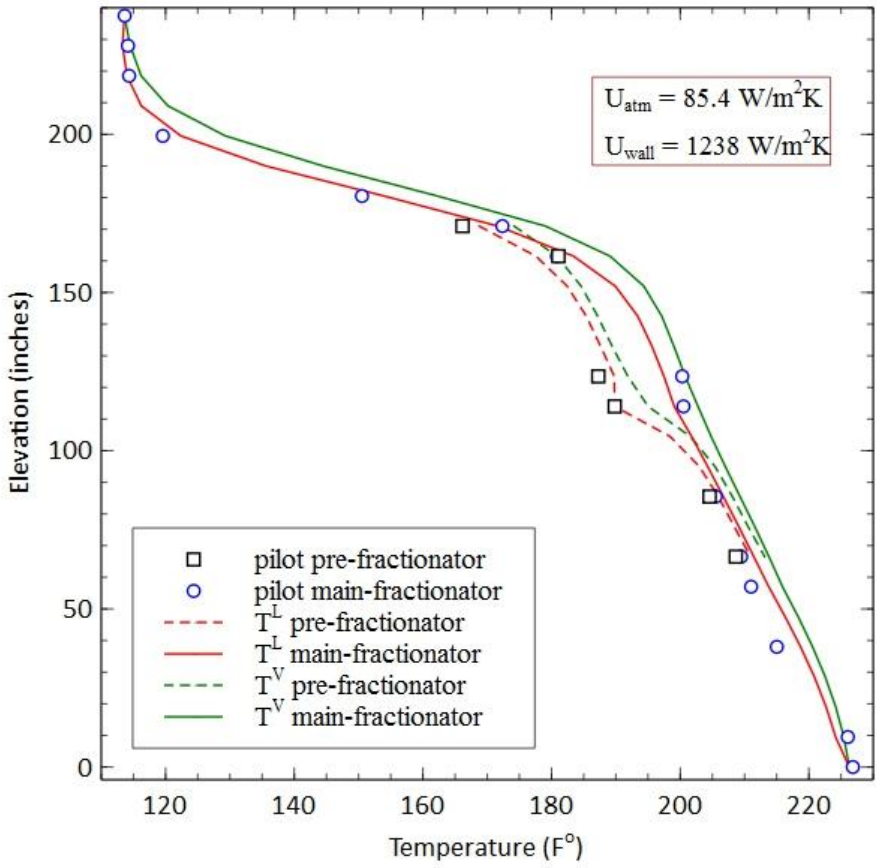
- Multiple walls



Heat Transfer across Dividing Walls

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





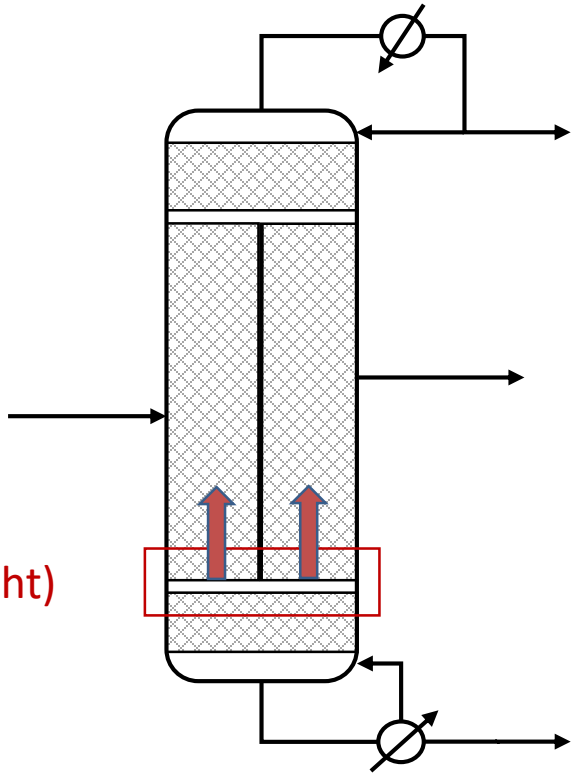
Auto-Adjusted Vapor Split

Pressure balance

$$\Delta p_{left}^{W} = \Delta p_{right}^{W}$$

May need to account for Δp over splitter

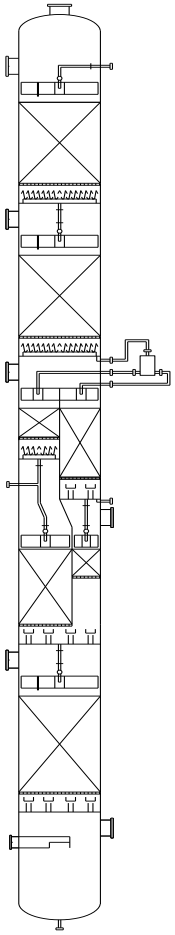
β = Vapor Left / (Vapor Left + Vapor Right)



Pressure equalization is achieved by adjusting β during the simulation

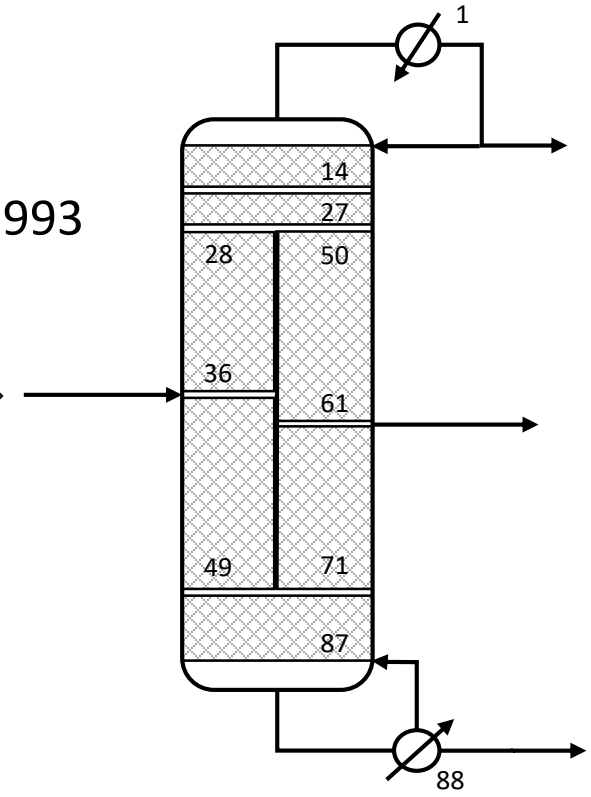
Auto-Adjusted Vapor Split: Dejanović Column

- Aromatics DWC



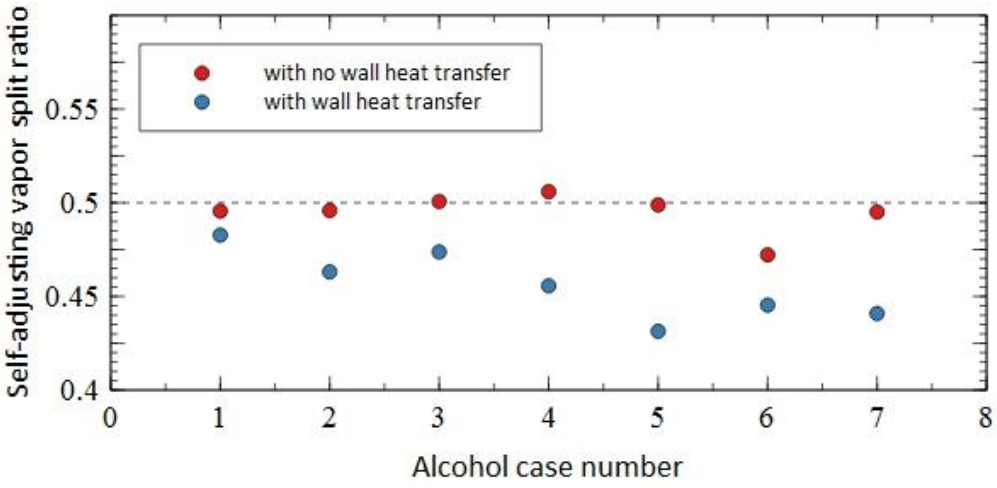
- Pressure drop model: Rocha-Bravo-Fair 1993

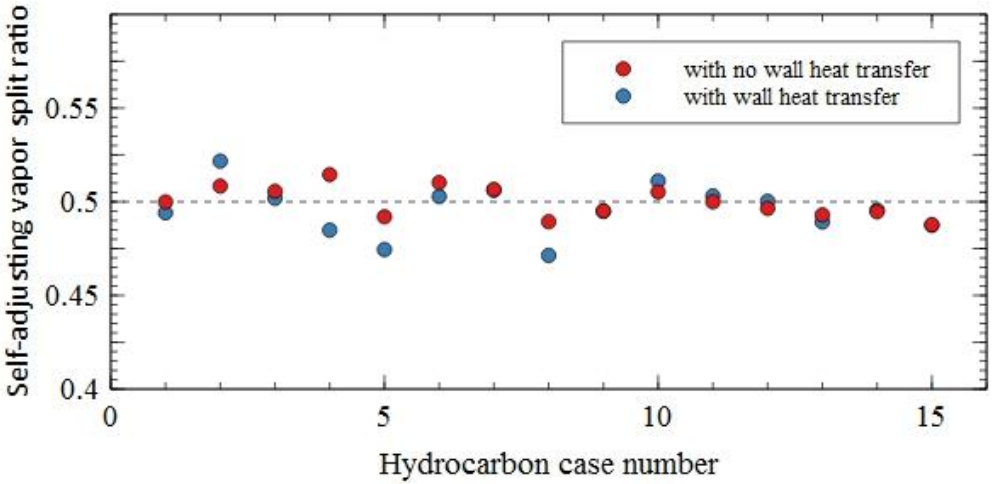
- Vapor Split:
  - Dejanović et al. (2011) 0.6639
  - ChemSep PCM estimate 0.6568



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.

Auto-Adjusted Vapor Split: Experiments of Roach



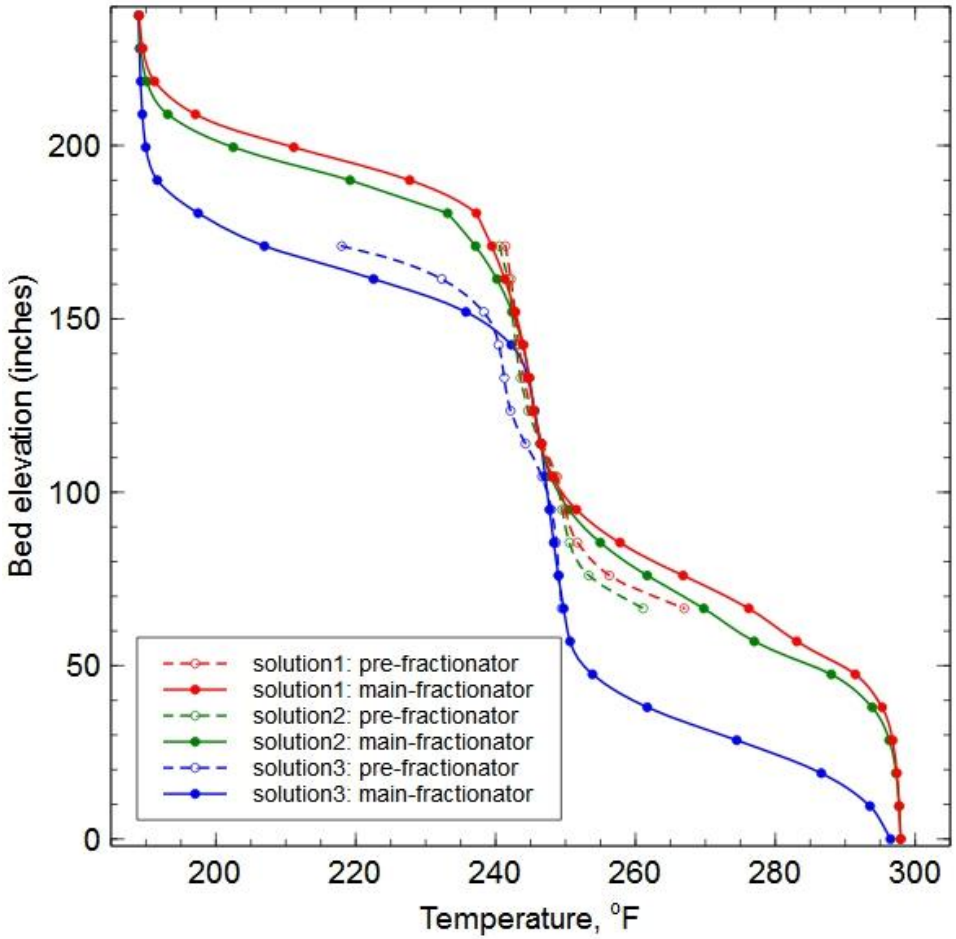


- Wall heat transfer may impact vapor split ratio

Conclusions

- The rate-based PCM
  - Takes very little effort to set up
  - Requires no initial guesses from engineer
  - Converges much quicker than multi-column models
  - Makes it easy to account for heat transfer across walls
  - Vapor split can be calculated (not specified)
- Rate-based PCM in good agreement with pilot plant data
- Vapor split influenced by
  - Pressure drop over walled section
  - Heat transfer across wall
- Mechanistic model for heat transfer between phases is needed
- **Experiments in DWC excellent test of k_L, k_G, and ΔP models**
- And, finally…

DWCs Can Exhibit Multiple Steady States



- Three different steady state profiles for column of fixed configuration and identical specifications
- Example shown left based on experiments of Roach (2017) at University of Texas, Austin
- Almost impossible to find with a multi-column model
- For more on this topic come to ***Distillation and Absorption 2018***, Florence (September 16-19, 2018)