An Equation-Based Parallel Column Model

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Dividing Wall Columns: Not New Anymore

DWCs with three products

Dividing Wall Columns: Not New Anymore

- DWCs with more than three products

Dividing Wall Columns: Not New Anymore


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

Existing Simulation Strategy

- Dejanović et al. Aromatics DWC

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
Existing Simulation Strategy

- Generally modeled as multi-column systems

Dejanović et al. Aromatics DWC

Four-column model in COCO
Existing Simulation Strategy

- Generally modeled as multi-column systems

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

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
Divided Top Column

Divided Top Column in COCO
(false convergence)

Stage

Flowrate, kmol/h

Liquid
Vapor
Divided Top Column

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

\[ H_j \equiv L_{j-1} H^L_{j-1} + V_{j+1} H^V_{j+1} + F_j H^F_j - (V_j + W_j) H^V_{ij} - (L_j + U_j) H^L_{ij} - Q_j = 0 \]

<table>
<thead>
<tr>
<th>Phase</th>
<th>From Stage</th>
<th>To Stage</th>
<th>Split Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid</td>
<td>27</td>
<td>28</td>
<td>0.5</td>
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<tr>
<td></td>
<td>49</td>
<td>50</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>72</td>
<td>50</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>72</td>
<td>71</td>
<td>1.0</td>
</tr>
<tr>
<td>Vapor</td>
<td>50</td>
<td>49</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>27</td>
<td>49</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>27</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Diagram: [Diagram of column model with stages and flow arrows marked as 28, 27, 50, 49, 72, 71, 87, and 88]
Equation-Based Parallel Column Model

- All equations for all stages solved simultaneously

Dejanović et al. Aromatics DWC

Equation-based ChemSep PCM
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

Temperature, K

Stages

Liquid mole fraction

Benzene
Toluene
m-Xylene
1,3,5-trimethylbenzene

left column
right column
Kaibel Column

Equation-based ChemSep PCM

Kaibel Column

Feed

C2

C3

LPG

C5+

1

2

20

61

21

2

40

72

93

60

100

109

110
Kaibel Column

Stage vs. Temperature (K)

Stage vs. Flows (kmol/h)

Stage vs. Liquid mole fraction

- Ethane
- Propane
- C4
- C5+
Divided Top Column

Divided Top Column

Equation-based ChemSep PCM
Divided Top Column

COCO (false solution)

ChemSep PCM (correct solution)
Divided Top Column

![Graph showing the temperature and mole fraction stages for benzene, cyclohexane, sulfolane, and o-xylene in a divided top column. The graphs display data for top-left and top-right sections of the column.]
Divided Top Column

Temperature gradient across wall can be significant
Dividing walls are not insulators

Heat Transfer
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 \( j \)
- \( \Delta T_j \) – Temperature difference
Heat Transfer

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

\[ R_v = 0.6855 \]

\[ R_L = 0.3641 \]

\[ U_{\text{wall}} = 800 \text{ W/m}^2\text{K} \]
Heat Transfer

(a) Without heat transfer

(b) With heat transfer

U = 800 W/m²K
Heat Transfer

Heat transfer affects product purity

(a) Without heat transfer

(b) With heat transfer
Heat Transfer

What if $U_{\text{wall}}$ goes to infinity...?

![Graph showing temperature vs stage with $U = 600,000,000 \text{ W/m}^2\text{K}$](image)
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
Redistributors modeled as stages with no mass transfer