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

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The literature on Dividing Wall Columns (DWCs) has grown extremely rapidly of late, and many researchers have used models for simulating DWCs. With few exceptions, simulations of DWC use interlinked multi-column models based on the equilibrium stage concept. In fact, rate-based (or nonequilibrium) models are more fundamentally sound and more realistic than equilibrium stage models. However, rate-based models are complicated to develop, because more details of the column design, e.g. tray geometry or packing size, and reliable correlations for transport coefficients and pressure drop, are required. This paper describes just such a model, which, via the CAPE-OPEN framework, can be used in any CAPE-OPEN compliant process flowsheet simulation package. We introduce new parallel column model that is rate-based, and equation oriented and can be used to model DWCs of arbitrary configuration. Heat transfer across the dividing wall can be modelled in a straightforward way.
We compare the predictions of the model to experimental data from the University of Texas at Austin. The results of comparisons show good agreement between model predictions and experimental data.

1. Introduction

Dividing wall columns (DWC) have attracted considerable attention in recent years. Our interest is in the modelling of such columns because, up to now, it is often stated, no commercial flowsheet simulation package has yet offered a DWC as a standard module (see, e.g., Dejanović et al., 2010). As a result, nearly all simulations of DWCs – and there are many – employ interlinked multi-column equilibrium stage models in a sequential-modular process simulator. Exceptions include papers by Mueller and Kenig (2007) and Hiller et al. (2010) who modelled DWCs with rate-based models in Aspen Custom Modeler (ACM). (Although models developed in ACM uses equation-based solution techniques, they cannot be generally used to model DWCs with arbitrary configuration without recreating the model if the DWC configuration changes.)
It has long been suggested that equation-based simulators offer some advantages over sequential modular simulators in convergence stability and speed when modelling DWCs (Becker et al., 2001). More recently, Zhou et al. (2018) described an equation-oriented equilibrium-stage parallel column model (PCM) and demonstrated superior convergence when compared to sequential-modular multi-column models when used as a standard module to simulate DWCs with arbitrary configuration. In this paper, our parallel column model framework is extended to use a rate-based stage model. Predictions from the PCM will be compared to data from the University of Texas at Austin (Roach, 2017).

2. Outline of a Parallel Column Model

2.1 Model Description

Rate-based models of counter-current columns have been established now for several decades. A detailed description of a rate-based model can be found in Taylor and Krishna (1993). The building blocks of such a model include:

1. Material balances for each distinct phase
2. Energy balances for each phase
3. Mass and energy transfer rate equations in each phase

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4. Mole fraction summation equations
5. Phase equilibrium equations to model the phase interface(s)
6. Hydraulic equations to account for the pressure drop

We will focus our attention here only on those aspects of the model that differ from a model of a simple column that are required in order to be able to model DWCs. To assist the discussion we show in Figure 1 a schematic diagram of three stages at the top of a dividing wall. Arrows represent material or energy flows, due either to flows from one stage to another, or mass transfer across the two-phase boundaries that are represented by the wavy lines.

It is not possible for the stages of a parallel column model to be numbered so that all material and energy flows are between consecutively numbered stages (see Figure 2 for a demonstration). Thus, the mass and energy balance equations in a PCM must account for flows between stages with any arbitrary number. It is worth noting that for conventional columns there are no streams that connect non-adjacent stages and in divided wall columns there are only a few such inter connecting streams.

Energy transfer across the column shell to the environment and across the dividing wall must be accounted for in the energy balances; we add terms for these energy flows only to the liquid phase balance equation. Modelling of the heat transfer terms is described in detail by Zhou et al. (2018).

The phase equilibrium equations, mole fraction summation equations and mass and energy transfer rate equations in a PCM are functionally identical to those in the standard rate-based model (see Taylor and Krishna, 1993). The only aspect of the rate equations that need concern us is to ensure that the correct column geometry be used in the calculation of the mass transfer coefficients and effective interfacial areas for those stages on either side of a dividing wall.

The hydraulic equations, however, pose a particular challenge since the pressure drop over the wall section(s) must balance. That is, it is the pressure drop that, in practice, determines the fractional flow split to each side of any wall(s). In the application of the model that will be considered below the pressures are estimated from pressure drop models, and vapour split is determined automatically to balance the pressures on two sides. Mass leakage around a non-welded wall is not considered in this work.

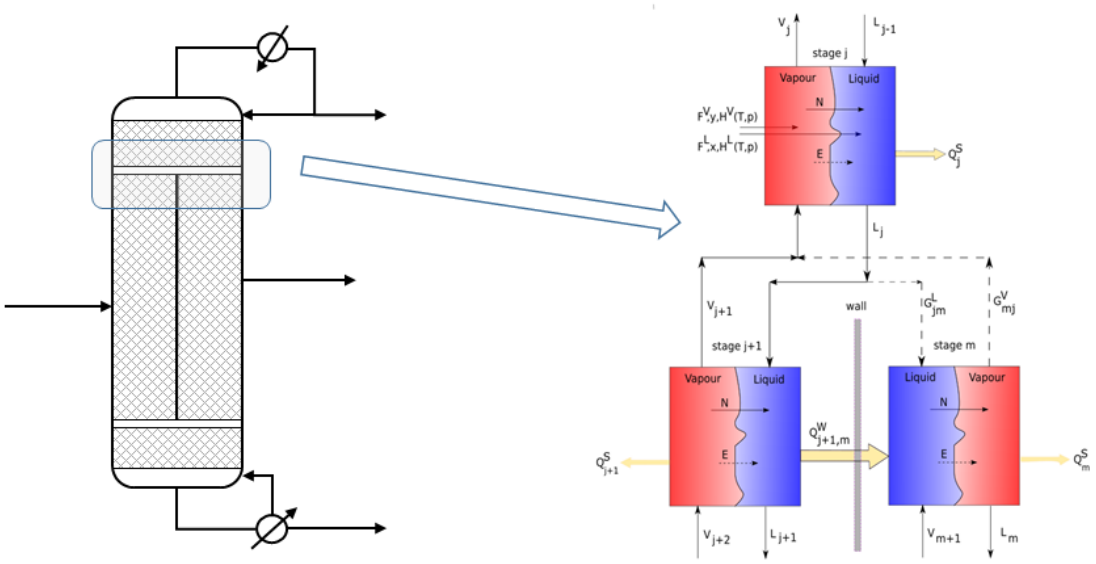

Figure 1: Schematic diagram of sections in dividing wall column and corresponding stage model

2.2 Method of solution

We use Newton's method to solve the equations in a manner similar to the work by Taylor et al. (1994) for conventional columns. An essential and critical aspect of the algorithm is always the generation of initial estimates from which Newton's method will converge. Our rate-based PCM uses the initialization method developed for their equilibrium stage PCM by Zhou et al. (2018). For the simulations described in the next section convergence was attained in most cases in around 10-12 iterations. More iterations sometimes are needed when the wall and shell heat transfer coefficients are "large."

3. Model validation

3.1 Simulation description

A comprehensive experimental study of DWCs has recently been documented in the dissertation of Roach (2017), (see, also, Roach & Eldridge, 2017; Roach et al., 2017). The pilot DWC at the University of Texas, Austin, has 249 inches of Sulzer Mellapak 500Y (estimated from the HETP of 9.5 inches and number of stages provided by Roach) and has an internal diameter of 6.63 inches. There is a welded wall (1/4 inch 304 SS) that divides the cross sectional area more or less exactly in half.
Our model of the Austin DWC has 38 stages in total, with condenser and reboiler included in that number (the same number used by Roach in her equilibrium stage simulations). Figure 2 shows a schematic diagram of the DWC with the stage numbers we used. The feed is to stage 14 and the side product taken from stage 25. Roach describes a large number of experiments carried out with two different chemical mixtures as discussed below. Mass transfer coefficients are estimated from a hybrid model composed of the Rocha et al. (1996) correlation for the gas phase mass transfer coefficient, the Song et al. (2014) correlation for the liquid phase mass transfer coefficient, and the Tsai et al. (2011) correlation for the effective area. The vapour is assumed to be in plug flow, while mixed flow model is used for the liquid phase. (The liquid flow model does not appear to have a significant impact on the results obtained in this study.) The pressure drop is estimated from the model proposed by Kooijman et al. (2002).

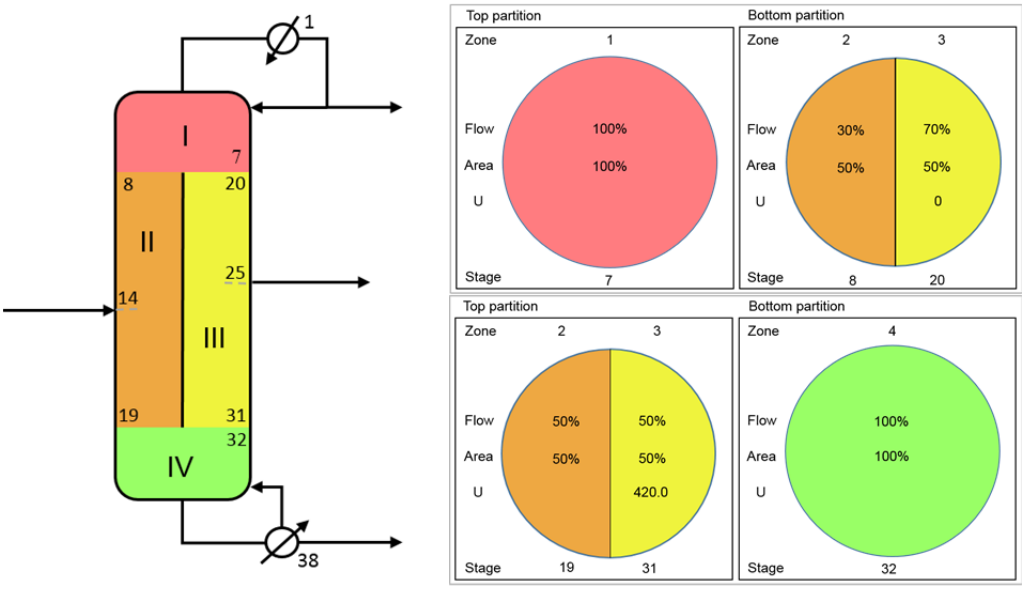

Figure 2: (a) Diagram of the DWC with four packed beds (numbers indicate stages in model); (b) Initial liquid split at the top and vapour split at the bottom of the wall (specified by Roach, 2017).

The hydrocarbon system is composed of n-pentane, cyclohexane and n-heptane. The alcohol system consists of 1-hexanol, 1-octanol and 1-decanol. The NRTL activity model is used to model the phase equilibrium of both mixtures (we used the parameters provided in Appendix D of Roach's dissertation). Vapour pressures were estimated using the correlation in ChemSep (All column simulations were carried out using the parallel column model in ChemSep (www.chemsep.com. For ease of comparison with the original experimental work of Roach (2017) we have used the same units)
We have carried out simulations of all of the experiments described by Roach (2017) using the rate-based PCM described above.

3.2 Simulation results

Three cases are selected for further discussion; specifications for these cases are provided in Table 1 (at the end of this paper). Note that in the simulations of Roach (2017), vapour split ratios are specified to be 50%/50% for all cases, but they are estimated in our simulations. Computed temperature profiles for hydrocarbon case H1 and alcohol case A10ii are shown in Figure 3, together with the corresponding measurements from Roach (2017). The red lines represent the liquid phase temperatures, and green lines show the vapour phase temperatures. Both plots demonstrate good agreement between the predicted values and pilot plant data. The vapour split ratio estimated in case H1 is 50% / 50%, and 46% / 54% in case A10ii.

Table 1: Specifications for Selected Dividing Wall Column Simulations (from Roach, 2017)

Case Number	H1	H12	A10ii
Feed flowrate (lb/h)	101.95	103.48	66.73
Feed temperature (^{o}F)	133.07	139.98	202.39
Feed pressure (psia)	25.00	25.00	1.00
Feed Composition (wt%)			
n-Pentane	26.1	26.7	
Cyclohexane	34.1	33.2	
n-Heptane	39.7	40.1	
1-Hexanol			24.4
1-Octanol			37.1
1-Decanol			38.5
Pressure overhead (psia)	20.00	20.00	0.90
Overall pressure drop (in H_2O)	3.58	3.09	3.29
Wall region pressure drop (in H_2O)	2.11	1.79	1.52
Heat Transfer Coefficients			
Shell (W/m^{2}K)	85.4	85.4	14
Wall (W/m^{2}K)	420	1238	400
Surroundings temperature (^{o}F)	34	65	73.91
Sidedraw rate (lb/h)	35.06	36.23	24.86
Bottoms flow rate (lb/h)	40.45	39.75	25.66
Overhead reflux ratio	2.62	6.62	1.12
Flow split ratios (left % / right %)			
Vapour split specified by Roach	50 / 50	50 / 50	50 / 50
Liquid split specified by Roach (and in this work)	30 / 70	51 / 49	32 / 68
Vapour split estimated in this work	50.1 / 49.9	47.7 / 52.3	46.1 / 53.9
Vapour split estimated when ignoring heat transfer		52.1 / 47.9	

Packing: Sulzer MellaPak 500Y
Specific surface area (m^2/m^3): 507 | Void fraction: 0.975 | Channel flow angle: 45^{o}
Crimp height: 0.0058 m | Channel side: 0.0086 m | Channel base: 0.012 m

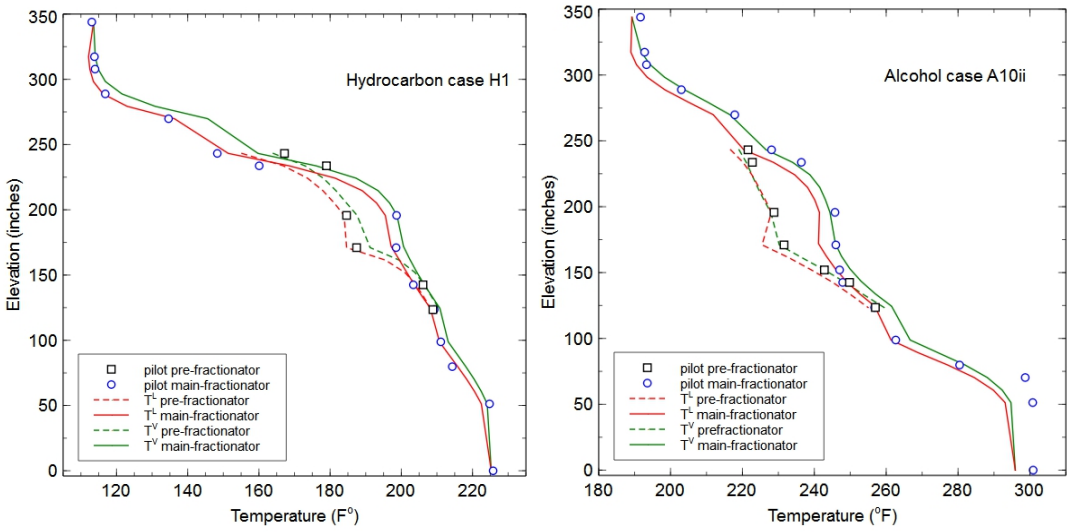

Figure 3: Temperature profiles in the DWC. Data from Roach (2017)

Figure 4a shows the predicted temperature profiles and pilot plant data for case H12. Heat effects (this includes wall heat transfer and heat losses) are not considered in this simulation. However, the predicted temperatures in the pre-fractionator show large deviations from the measured temperatures. Figure 4b shows the improved temperature profiles that result when we include the effects of heat transfer with the heat transfer coefficient for the shell, 85.4 W/m^{2}K, and the wall heat transfer coefficient, 1238 W/m^{2}K, provided by Roach (2017). The vapour split ratios estimated by the model are included in Table 1. We infer that heat transfer effects (both heat transfer across the dividing wall and heat loss) are important in the model of this particular pilot scale dividing-wall column.

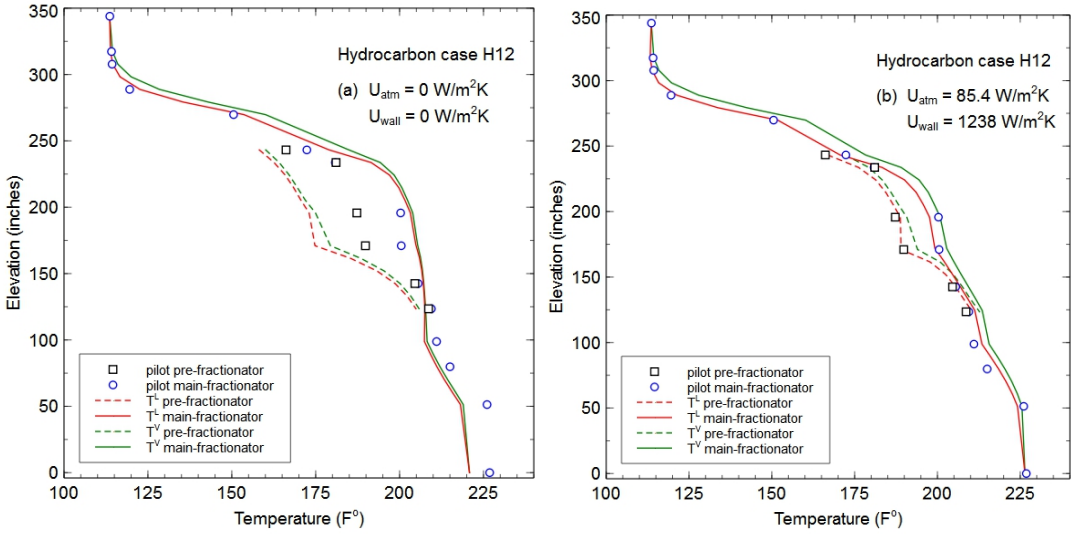

Figure 4: Predicted temperature profiles in hydrocarbon case H12 with (a) no heat transfer, and (b) U_{atm} = 85.4 W/m^{2}K, U_{wall} = 1238 W/m^{2}K. Data from Roach (2017)

All 22 experiments with the hydrocarbon system and all 11 cases involving alcohols have also been modelled using our PCM. Figure 5 shows parity plots of column temperatures in all cases listed in the dissertation, obtained using the rate-based PCM (right) or the equilibrium-stage PCM (left) of Zhou et al. (2018). The statistical data provided in this figure is only for the points in the wall region; the data in the top and bottom sections is not included in these numbers (although points for the top and bottom sections are included in Figure 5). We see that the rate-based PCM gives better predictions for the hydrocarbon cases than does the equilibrium-stage PCM, while both models give comparative predictions to the alcohol cases, with equilibrium-stage PCM performing slightly better.

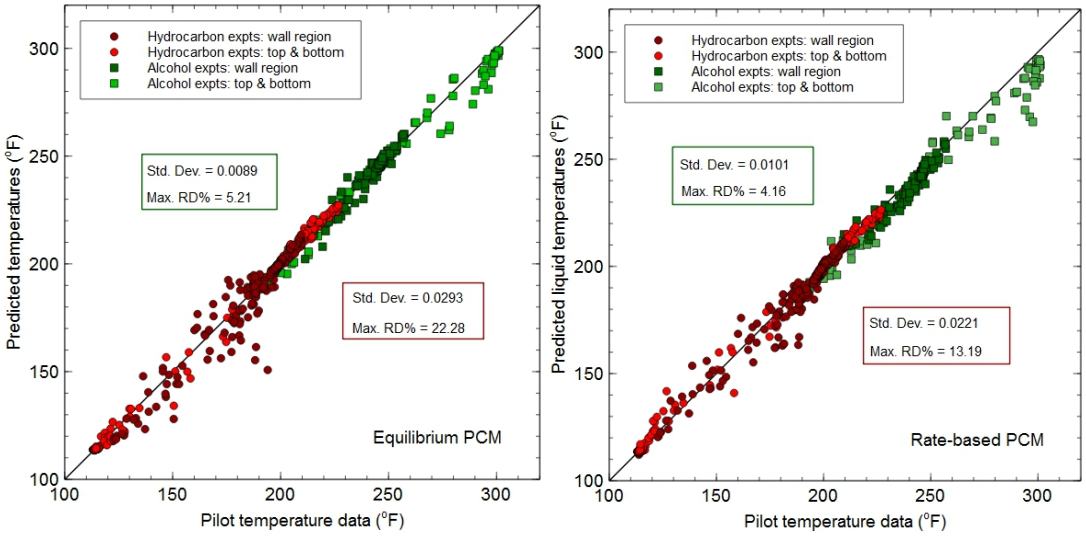

Figure 5: Parity plots of temperatures in dividing wall sections for all case studies in Roach (2017): (a) equilibrium-stage PCM (left) and (b) rate-based PCM

4. Conclusions

In a recent paper, we proposed an equation-oriented equilibrium-stage parallel column model (PCM) that can be used as a standard module to model DWCs of arbitrary configuration. Here, we extend that model to be able to use a rate-based stage model where we take explicitly into account mass and energy transfer. Vapour flow splits are estimated using the pressure balance on both sides of the wall.

The rate-based PCM is validated using an extensive set of experimental data from the recent thesis of Roach (2017). Good agreement between the model predictions and the pilot plant data is found. A comparison of parity plots from the equilibrium PCM and the rate-based PCM show that the rate-based PCM gives better predictions of the experiments with hydrocarbons than does the equilibrium PCM. The hydrocarbon case H12 highlights the importance of heat transfer effects in the DWC simulations.

The proposed rate-based PCM, implemented in ChemSep, can, via the CAPE-OPEN framework, be used in any CAPE-OPEN compliant process flowsheet simulation package as a standard DWC module.

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