Simulating Maldistribution in Packed Columns

Hendrik A. Kooijman, Jingsong Zhou, and Ross Taylor
Clarkson University
Potsdam, NY 13699-5705, USA

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1. Introduction

Maldistribution has long be known to be inevitable in packed columns and that it can significantly worsen the separation performance of a packed column. A recent presentation by Spiegel (2018) provides a convenient summary of the research on maldistribution up to relatively recent times.

Parallel column models sometimes are used to investigate the sensitivity of the HETP (the Height of an Equivalent Theoretical Plate) in a packed column due to maldistribution. In such models the vapor and liquid flows are split into two parts, which then enter one of two parallel columns. Billingham and Lockett (2002) proposed a two-column model for investigating maldistribution. Schultes (2000) studied maldistribution by modeling it with three parallel columns in a process simulator, and Stichlmair and Stemmer [3] modeled maldistibution with no less than one hundred parallel columns! Although it is possible to develop a parallel column model using a process simulator, it takes considerable effort to arrange and specify the columns.

Recently, we have described what we call a Parallel Column Model (PCM) (Zhou et al., 2019a,b). While the model was developed with the aim of making it easier to model Dividing Wall Columns (DWCs), we realized that it also is possible to use the ChemSep PCM to model maldistribution in packed columns. Both equilibrium stage and rate-based column models can easily be used within this framework. Our PCM can be used as a tool to study maldistribution inside any CAPE-OPEN compliant process simulation package.

In this paper we review the literature on simulating packed columns with maldistribution. We then show how easily the ChemSep PCM for DWCs may be used to describe maldistribution in packed columns and show how our results match the obtained results of earlier papers. We found a simple bed effectiveness approximation that allows the design of packed beds that are robust for the effects of liquid maldistribution. We illustrate with a practical example involving the design of a commercial scale Argon column (from an air separation plant) with structured packing.

2. Background and Motivation for this Study

The literature on Dividing Wall Columns (DWCs) has grown extremely rapidly of late, and many researchers have used models for simulating DWCs. Zhou et al. (2019a,b) recently described a Parallel Column Model (PCM) for simulating Dividing Wall Columns, Their PCM has been implemented into a column simulation program, *ChemSep*, as a standard unit operation module, that, via the CAPE-OPEN mechanism, can be used within commercial process simulation tools, and thereby ease the task of building DWC models.

In Figure 1 we provide a schematic diagram of three stages at the top of a dividing wall. Arrows represent material or energy flows, due either to physical flows from one stage to another, or to transport across the two-phase boundaries that are represented in the diagram by the wavy lines.

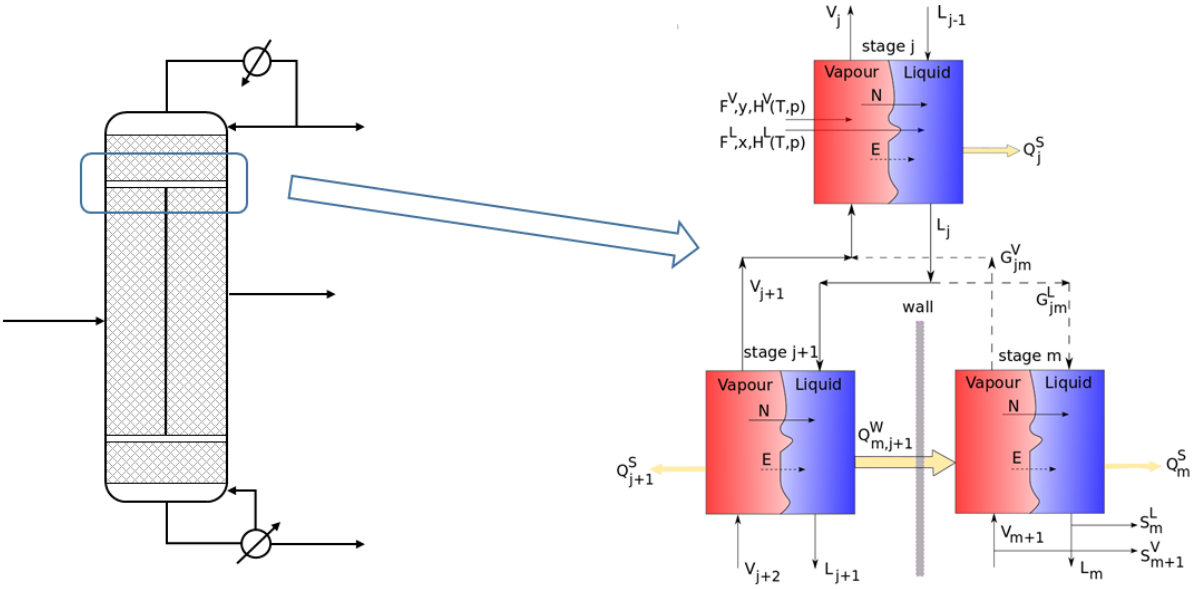

Figure 1: Schematic diagram of sections in dividing wall column and corresponding stage model.
(Source: Zhou et al. 2019b)

Our interest is in the modelling of DWCs came about because, up to now, no commercial flowsheet simulation package has yet offered a DWC as a standard module (see, e.g.,). 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.

Some authors have written in somewhat non-specific terms about their general experience modeling DWCs using a commercial simulator (see, for example,). Kolbe and Wenzel (2004) , for example, had this to say:

Commercial process simulators are not well suited to solving the task of designing a divided-wall column easily, because manual variation of the input is necessary using the commercially available software, which is rather complex and time-consuming.

Using the *ChemSep* PCM can effectively circumvents the tedious procedures of setting up DWCs with multi-column models in a modular process simulator.

Interestingly, parallel column models are not new; engineers have been using parallel column models to describe maldistribution in packed columns for many years. By way of illustration we show in Figure 2 a schematic diagram of a parallel column model used to represent a column used to separate ethylbenzene and styrene. The model was created by D.S. Hubbell for McMullan et al. (1991) who were troubleshooting an ethylbenzene – styrene column that was not performing as expected. The creation of a PCM such as that shown in

Fig. 2 for the purposes of modeling maldistribution is quite time consuming. It is, however, quite easy to create an equivalent ChemSep PCM; a schematic diagram of the ChemSep equivalent is shown in Fig. 3 alongside some results from our simulations of this column.

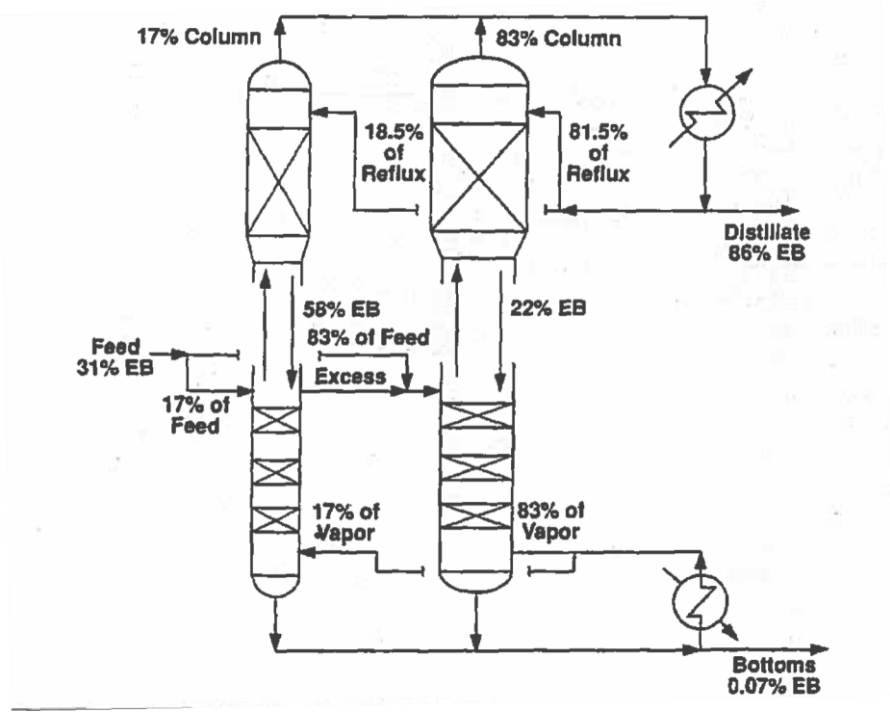

Figure 2: Schematic diagram of parallel column model of ethylbenzene-styrene column. (Source: McMullan et al. 1991)

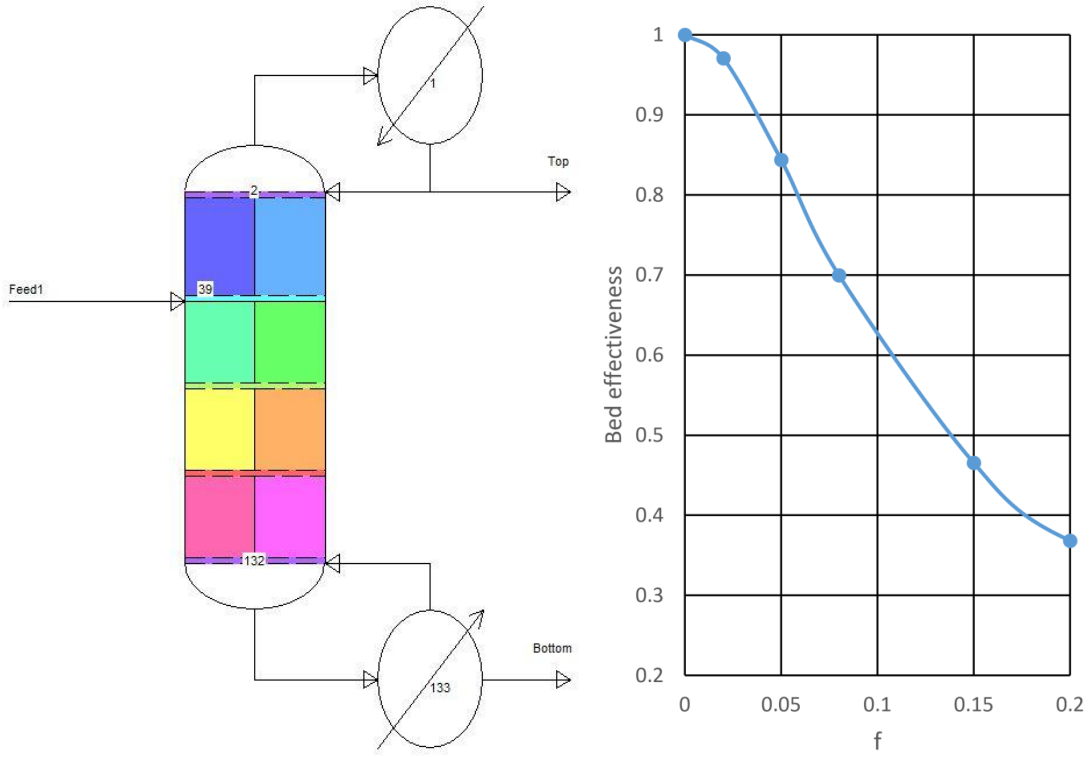

Figure 3: Schematic diagram of equivalent ChemSep parallel column model of ethylbenzene-styrene column. Right hand side shows the effectiveness of the upper bed from simulations.

3. A Trip Back in Time

As hinted at above, parallel column models for studying the effects of maldistribution are not new. In this section we review some of the more important contributions to this field. Note that this is not a comprehensive review of studies on maldistribution, our focus is only on the use of parallel column models for this purpose.

One of the first to employ a PCM was Mullin in 1957. Also in 1957, Manning and Cannon used a bypass model; that is, where a portion of the liquid is diverted to the right hand column, but all of the vapour is directed to the left hand column. They further assume a total condenser at the top and total reboiler at the bottom. Stage-to-stage calculations for a given number of stages and assumed values for the relative volatility and top composition allow calculation of the composition at the bottom of the left column. This stream is mixed with the bypass liquid to provide the composition of the liquid leaving the liquid stream mixer below the beds. That combined stream composition is then used with the assumed overhead composition in the Fenske equation to calculate the number of equilibrium stages that would be needed to achieve that overall separation. If the bypass flow is greater than zero, that number of stages will be less than the number assigned to the left column. The bed effectiveness is then calculated directly from the ratio of the $N_{Fenske}/N_{Specified}$. Figure 4 shows our recreation of Fig. 1 in Manning and Cannon (1957).

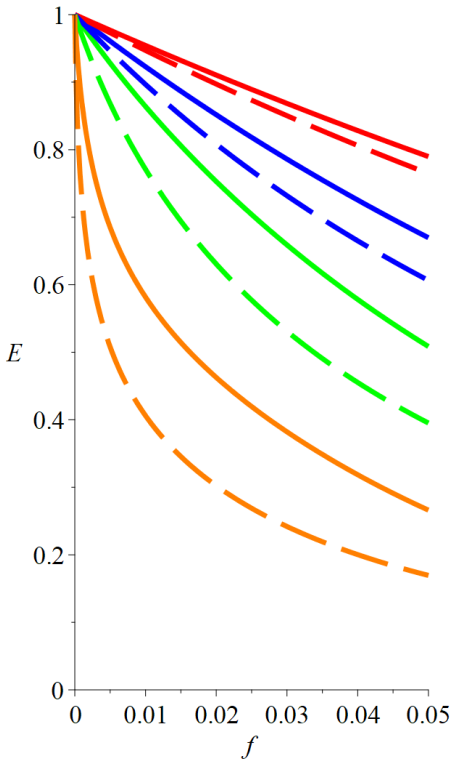

Figure 4: Packed bed effectiveness as a function of liquid phase bypass fraction (f). Recreation of Figure 1 in Manning and Cannon (1957). Solid lines are for $x_{top} = 0.9$. Dashed lines are for $x_{top} = 0.6$. Red = 10 stages, Blue = 20 stages, Green = 40 stages, Dark yellow = 100 stages.

Huber and Hiltbrunner (1966) included in their PCM stages to model radial mixing between parallel column sections. An important result from their paper is that the bed effectiveness (the ratio of the number of stages needed with no maldistribution divided by the number needed to achieve the same separation when subject to maldistribution) is given approximately by

$$E = \frac{1}{1+af^2} \tag{1}$$

where a is a numerical constant and where *f* is the maldistribution fraction.

Yuan and Speigel (1982) studied the effect of maldistribution on the performance of a packed column using a simple parallel column model. As is the case with many (but not all) parallel column models, their model neglects lateral mixing. This leads them to claim that the model is applicable only to large diameter columns. They report that their model shows a significant dependence on the reflux ratio and feed composition. They also report some experimental results that confirm their observations from numerical simulations. In describing their model Yuan and Spiegel wrote:

It is assumed that the column is divided in two partial columns by an imaginary wall, which is impermeable for the vapour and liquid stream.

(It seems to us that a more perfect description of a computer model for a DWC could not be penned.)

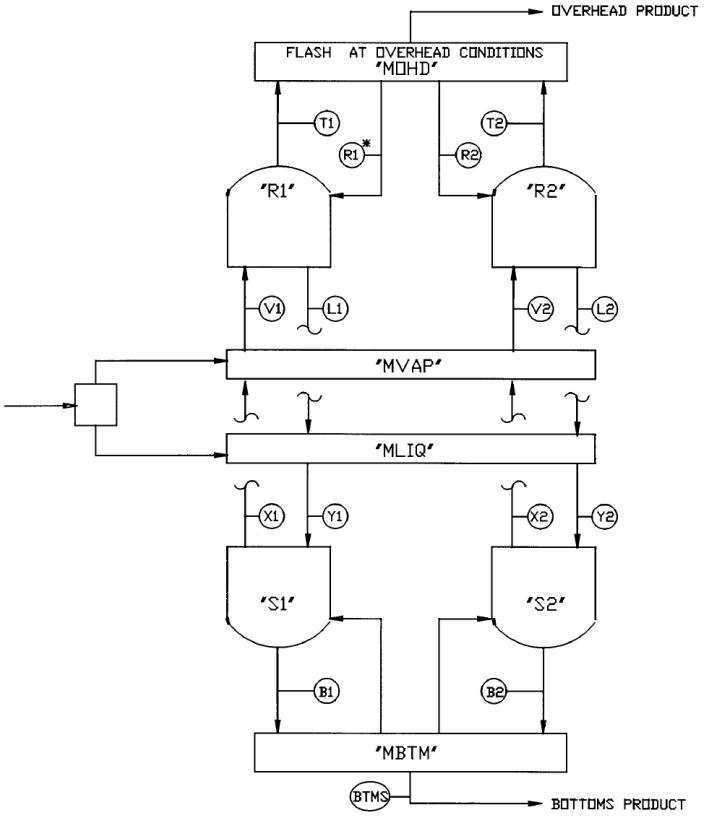

Figure 5: Parallel column model of Martin and Sloley (1995).
(Used with permission of A.W. Sloley.)

Conceptually similar models have been created by Martin and Sloley (1995), Schultes (2000) and Bartlok (2002). A schematic diagram of the PCM of Martin and Sloley – who used Pro/II – is shown in Fig. 5. Martin and Sloley make clear that their approach is not limited to 2 parallel columns. Indeed, they write:

With this model the detail to which maldistribution can be investigated mainly depends upon; the number of unit operations, streams, and recycle loops allowed by the modelling software; the computer time available; and the patience of the engineer. At a limit, every single drip point on a trough distributor could be modeled as a separate tower. On a more practical level, every trough could be analysed as a separate tower.

Schultes (2000) used a PCM to look into the influence of redistribution in packed columns. He used three columns in parallel with redistributors modeled by simple mixers and splitters in an unspecified process simulator. Among other conclusions, Schultes (2000) noted that rectification columns operating close to minimum reflux are particularly sensitive to maldistribution. Figure 7 of his paper, for example, uses 12 column sections (in 3 parallel columns) and 16 mixers and splitters. An equivalent column can be created by the ChemSep PCM as shown in Fig. 6. Redistributors (the stages that span the entire column) are modeled as stages with zero stage efficiency.

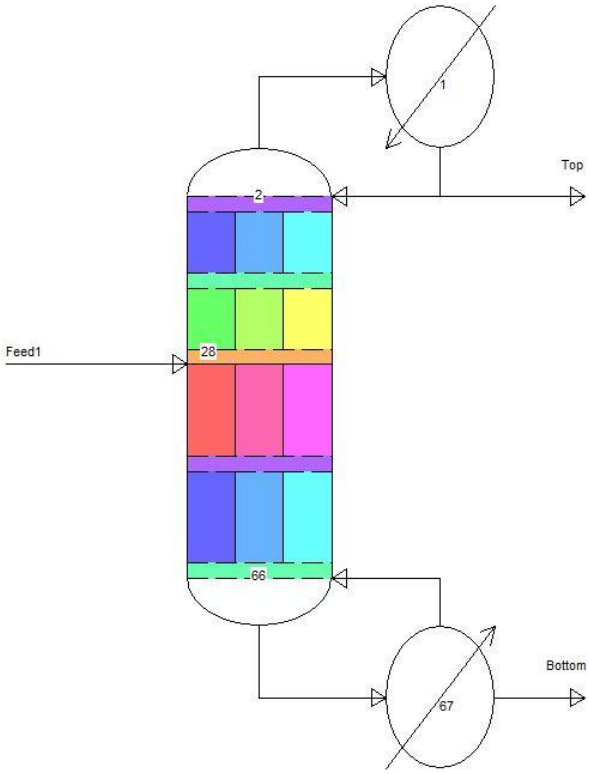

Figure 6: Schematic diagram of ChemSep PCM equivalent to the multi-column model shown in Fig. 7 of Schultes (2000).

One of the most complicated multi-column models for studying maldistribution is that of Bartlok (2002). He created two- and four-column parallel column models in Pro/II. He also allowed for partial vapor and liquid radial mixing by specifying a large number of sidestreams to connect the different column sections. A mixer was use to model a redistributor between the top and bottom beds. His 4-column model is shown in Fig. 7. Bartlok also conducted experimental work and concluded

Man erhält jedoch noch nicht eine vollständige bereinstimmung von Simulation und Messung, ein Verbesserungspotential besteht immer noch.

A translation (courtesy of Google Translate) reads as follows:

However, one does not yet get a complete match of simulation and measurement, there is still room for improvement.

Bartlok's comprehensive study did not result in any journal publications. There was, however, a patent (US 2002/0079597 A1) for a novel distributor design. That patent is assigned to Sulzer Chemtech AG and has been cited in 20 other patents.

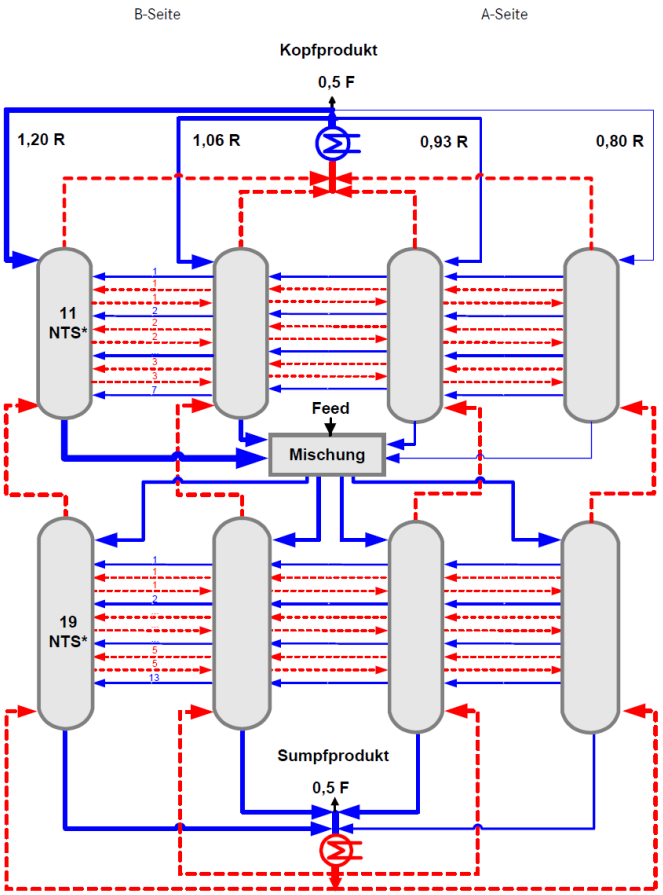

Figure 7: Schematic diagram of multi-column model of Bartlok (2002). (Source, Bartlok, 2002.)

Zuiderweg et al. (1993) developed a “zone/stage” model for estimation of the overall efficiency of a packed column, given a specific initial maldistribution of the liquid phase. The model has two independent calculation steps. The first step calculates the liquid maldistribution on the basis of on a natural flow model as outlined by Stikkelman (1989). In the second step, the influence of this maldistribution on the HETP (height equivalent of a theoretical plate), and thereby on the packing efficiency, is determined.

The effect of the maldistribution on the flow pattern is determined by means of a cell model, whereby it is assumed that a fraction *K* L of the liquid leaving the cell will flow down to the cell below. The remaining fraction of liquid (1 - *K* L) will flow to the adjacent cells below, whereby the flows are split up according to the ratio of the cell surface areas between the cells such as those depicted in Fig. 8. This is referred to as the natural flow model. The underlying idea of the natural flow model is that a liquid flowing down a section of packing will spread according to a diffusional type equation.

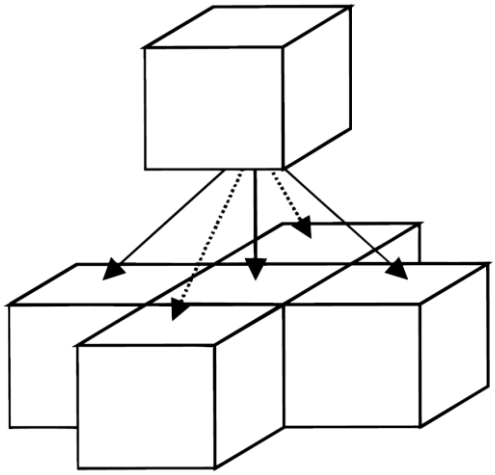

Figure 8: Flow splitting concept of Zuiderweg and coworkers.
(Source of this image: Higler et al. 1999.)

In the classical zone/stage model, as presented by Zuiderweg et al. it was assumed that a stage is split up in a number of annular zones. This model can be used to study maldistribution patterns that are essentially radial. To study arbitrary patterns it is necessary to use a different cell structure; square for example (see Fig. 9).

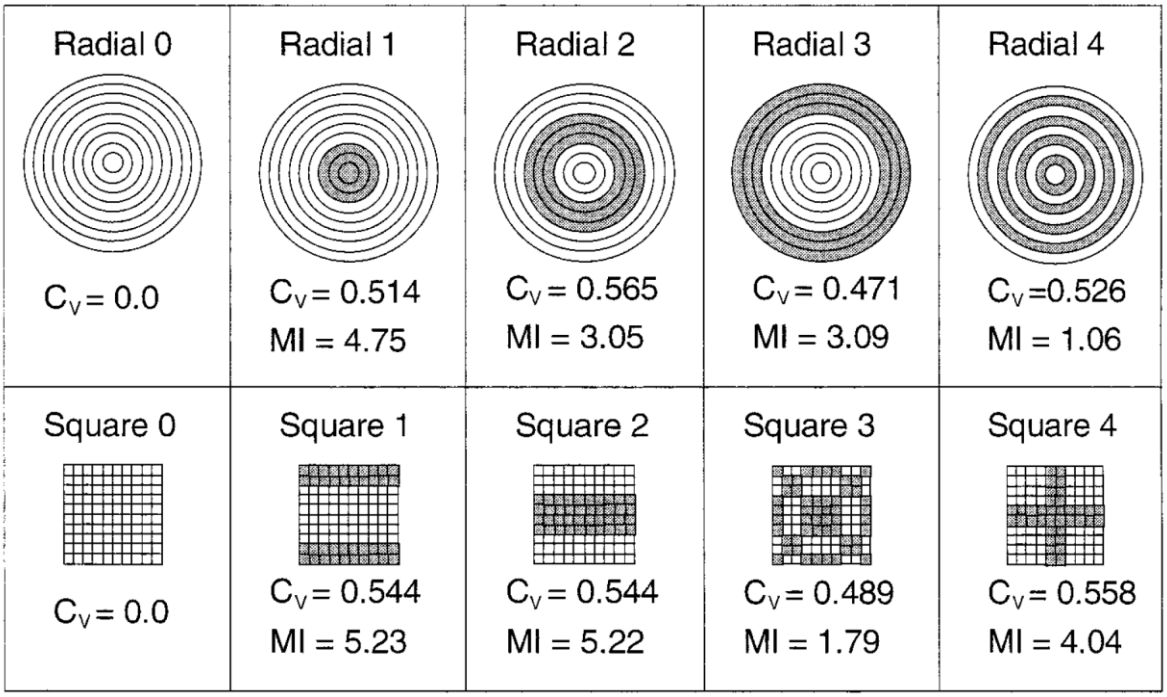

Figure 9: Maldistribution patterns for zone-stage model of of Zuiderweg and coworkers.
(Source of this image: Higler et al. 1999.)

Higler et al. (1999) developed a nonequilibrium version of the zone-stage model for studying the effect of flow maldistribution in structured packings. The model consists of a set of mass and energy balances along with a set of mass- and energy-transfer correlations. Maldistribution is treated by means of a zone/stage approach developed and presented by Zuiderweg et al.

Calculations for some maldistribution cases have indicated that there is some correspondence between the observed deviations of the efficiencies from "ideal" behavior and the currently available methods for reporting maldistribution, the *C*v value and the maldistribution index *MI* (see Fig. 9). It should, however, be noted that, in some cases, these parameters provide inadequate information. It is generally true that maldistribution results in loss of efficiency, but poorer maldistribution does not necessarily lead to poorer efficiency. Simulations show that, even for binary mixtures, packing HETPs can be a function of the height of the packing. Efficiencies and HETPs in multicomponent systems tend to be confusing, and the effect of maldistribution on these parameters is ambiguous. It was shown that, for two ternary systems, that different maldistribution patterns can result in substantial differences in column behavior. In some cases, different maldistribution patterns may lead to completely different products from a column.

Hanusch at el. (2019) have built a very sophisticated model that can be seen to have among its antecedents, the zone-stage model of Zuiderweg that was discussed above but which uses cells in a honeycomb pattern. The flow split-factors are obtained from virtual 3D irrigation experiments. They also created a parallel column model in Aspen Plus.

We have left two important papers for the end of this survey of parallel column models for maldistribution. These are the works of Klemas and Bonilla (1995, 2000) and Billingham and Lockett (2002) (see, also Lockett and Billingham, 2003).

A wide ranging article by Klemas and Bonilla looked at large scale maldistribution, microscale maldistribution, radial spreading, distributor quality, drip point density, levelness, as well as other topics. They modeled maldistribution in binary distillation using a simple PCM based on the Smoker equation.

Figure 10 is our (very good) approximation to a figure in Klemas and Bonilla (2000). It shows the bed effectiveness (or efficiency) as a function of the number of theoretical stages per bed. The lines are color coded by the maldistribution percentage (given the symbol M by Klemas and Bonilla). Thus, the top line for $M = 5$ means that 5% of the liquid flow is diverted to a second parallel section; the bottom line with $M = 30$ means that 30% of the liquid is diverted. This figure shows clearly the now well known result that beds with more stages are significantly more likely to suffer form the negative effects of maldistribution.

Figure 10 was created using the simple equation:

$$E = \frac{1}{1+0.00008(NM)^2} \tag{2}$$

where N is the number of stages in the bed. The approximation is not perfect but it is an acceptable fit to the original figure of Klemas and Bonilla.

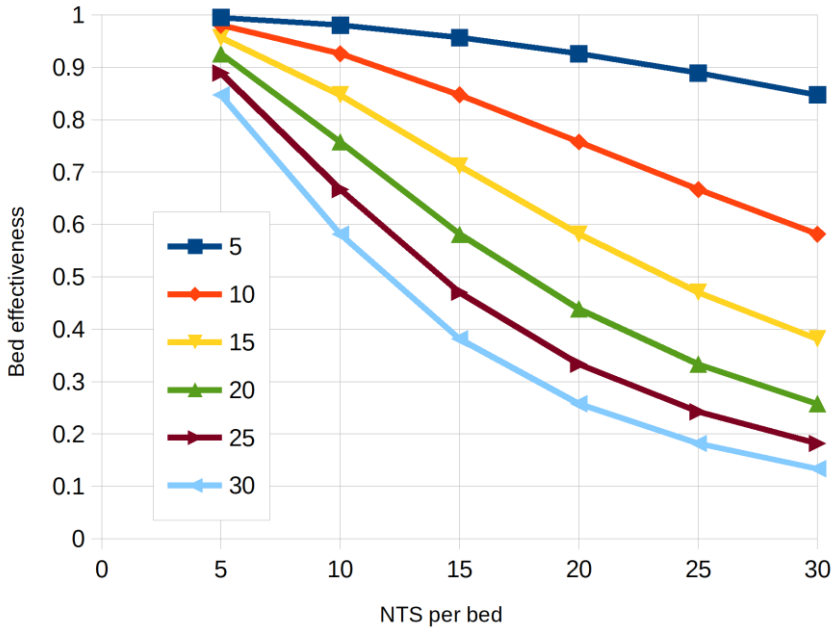

Figure 10: Approximation to bed effectiveness (efficiency) calculation by Klemas and Bonilla (see text for details).

4. Billimgham and Lockett's f_{max}

Billingham and Lockett (2002) wrote:

...it is not obvious to a column designer how to incorporate the output from a conventional column simulation design program into the models.

In other words, how can we extract from the results of a standard simulation of a column (presumably done with a commercial simulator) the extent to which a packed bed is sensitive to maldistribution.

To help address this need Billingham and Lockett used a parallel column model similar to the one shown in Fig. 11. (One small difference is that they did not split the vapor flow as shown in Fig. 11; rather they assumed the gas flow to the base of each column to be the same. We can obtain the same result by specifying a gas flow to the stream splitter that is twice what is needed and a split ratio of 50%.).

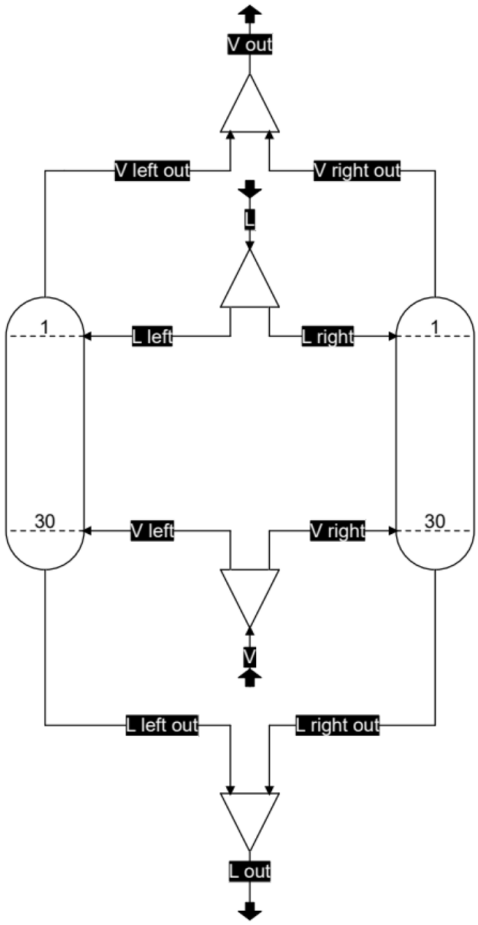

Figure 11: Schematic diagram of parallel column model similar to that employed by Billingham and Lockett (2002).

The equations that model the configuration in Fig. 11 include the mass balances around each splitter and mixer, and the mass balances around each column. In their model f denotes the maldistribution fraction such that:

$$L_{Left} = (1 + f)L \qquad L_{Right} = (1 - f)L \tag{3}$$

(It can be shown that $f \times 100$ used by Billingham and Locket is the same as M used by Klemas and Bonilla.)

Figure 12 is our recreation of Figs. 3-6 in Billinghman and Lockett (2002) who said this:

The calculation procedure involved in the model is relatively straightforward and will not be elaborated here.

Billingham and Lockett used a stage-to-stage calculation to model the column sections and assumed constant relative volatility. However, we wish that they had elaborated more on their calculation procedure since they provide mutually incompatible specifications and it is not always clear which specifications were used in specific figures. For this reason, our Fig. 13 is a close approximation to the figures in Billingham and Lockett but is not an exact match.

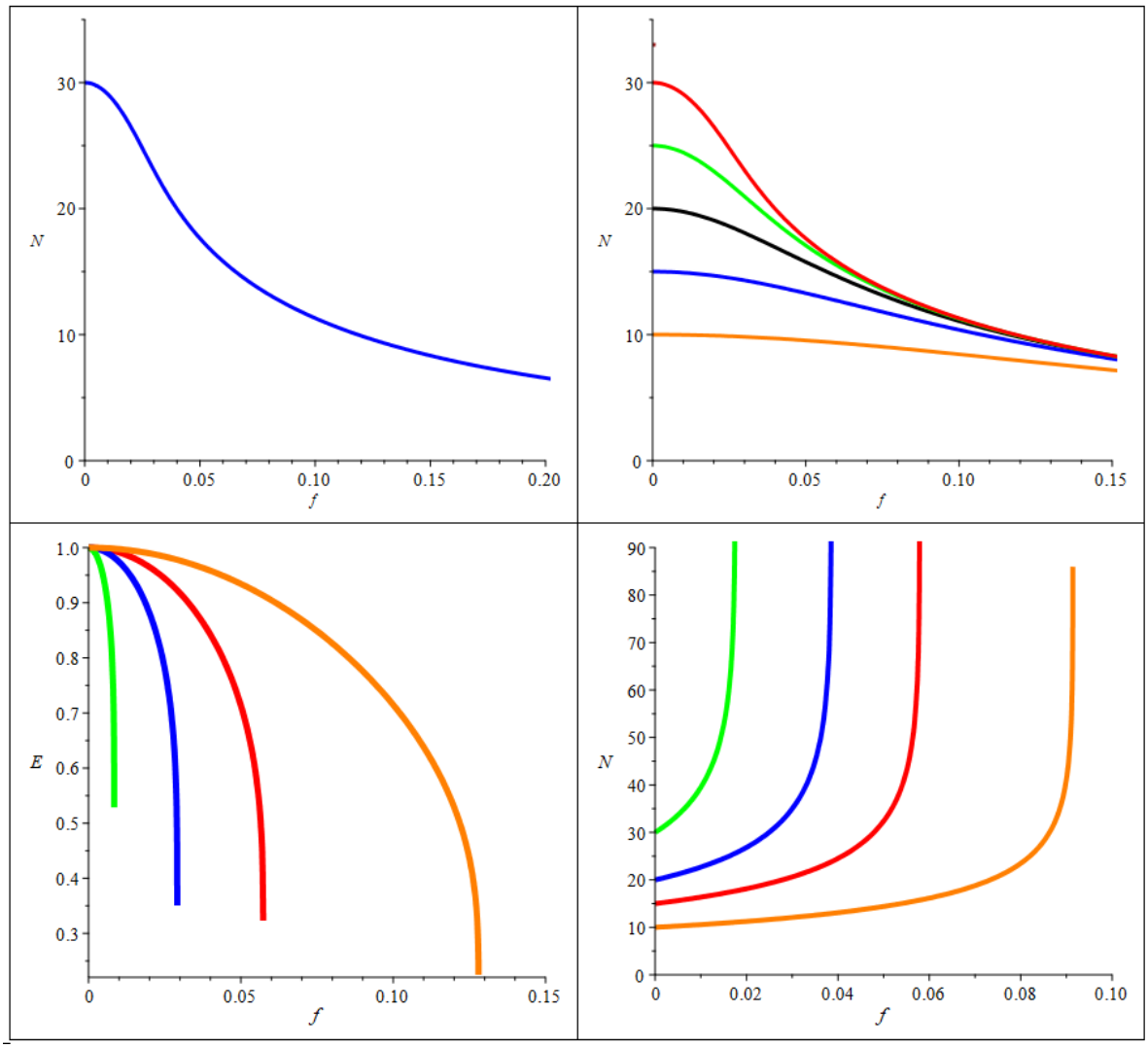

Figure 12: Typical results from the PCM in Fig. 11. These are our recreations of Figs. 3-6 in Billingham and Lockett (2002).

It is important to point out the vertical asymptotes in 2 of these figures. These correspond to the maximum value of f above which no increase in the number of stages can provide the specified separation.

Billingham and Lockett show that f_{max} is given by

$$f_{max} = Y + X - YX \tag{4}$$

where

$$Y = \frac{(y^*_{top} - y_{top})}{(y_{top} - y_{btm})} \qquad X = \frac{(x_{btm} - x^*_{btm})}{(x_{top} - x^*_{btm})} \tag{5}$$

and where the * indicates a mole fraction that is in equilibrium with the other stream at the position indicated by the subscript.

We also used a constant relative volatility model, but we did not use a stage-to-stage calculation when creating Fig. 12. Instead, we used the Martin (1963) equation for these calculations. The Martin equation comes in three forms, one of which is

$$N = \frac{\ln\left(\frac{(y_{top}+A-E_2)(y_{btm}+A-E_1)}{(y_{top}+A-E_1)(y_{btm}+A-E_2)}\right)}{\ln(E_1/E_2)} \qquad \begin{Bmatrix} A \\ E_1 \\ E_2 \end{Bmatrix} \text{depend on} \begin{Bmatrix} \alpha \\ y_{top} \\ y_{btm} \\ x^*_{top} \\ L/V \end{Bmatrix} \tag{6}$$

Equations for the parameters A, E_1, E_2 are given by Martin (1963). The complexity of the Martin model arises from the fact that there are two other equations that might be needed and the choice depends on the values of A, E_1, E_2. Complex root selection is involved in some cases (but that does not mean that the results are complex numbers – again see Martin for details).

The Martin equation is an analytical model in the tradition of the Fenske and Kremser equations, but the Martin equation does not require:

- constant K-values (as are used in the Kremser equation)
- dilute systems (an assumption in the Kremser model)
- constant relative volatility (assumed in the Fenske equation)
- total reflux (the basis for the Fenske equation)
- a condenser and reboiler to be present (part of the Smoker equation derivation)

The model can be applied to systems with curved equilibrium lines and to systems with curved operating lines (Martin shows how). Sadly, Martin's paper has been cited only 20 times and never, as far as we are able to tell, in connection with distillation.

In our calculations the Martin equation is applied to both sides of the parallel column model in Fig. 11. This calculation cannot, in general be made explicit because of the way in which the mole fractions appear in the parameters A, E_1, E_2. To find f_{max} from Martin we search for the vertical asymptotes that can be seen in the two lower plots in Fig. 12. This can be done in a variety of ways one of which involves simply incrementing the value of f. An alternative is to find the tangent (from differentiation of the Martin equation). We used both approaches in this work.

From our calculations with the Martin model as well as with the method of Billigham and Lockett we learn that:

- f_{max} from Martin is an exact match with that from Billingham & Lockett (Fig. 13)
- f_{max} decreases with an increasing number of stages in the bed (Fig. 13 again)
- f_{max} is very sensitive to the choice of thermodynamic model
- f_{max} is very sensitive to the stages selected for calculation using Eqns. (4,5)
- f_{max} can be negative if inappropriate stages are used
- f_{max} depends on what component is used for the calculations in Eqns. (4,5)

- f_{max} value from Billingham and Lockett is always < 1 even when it should be > 1
- f_{max} provides simple way to divide stages over multiple beds
- but no quantitative answer on required extra bed height

Figure 13 shows that the results from the Martin method and that of Billingham and Lockett are the same when using a constant relative volatility model. Differences would be expected if a different model was employed due to the different ways in which the thermodynamics is handled by these two approaches.

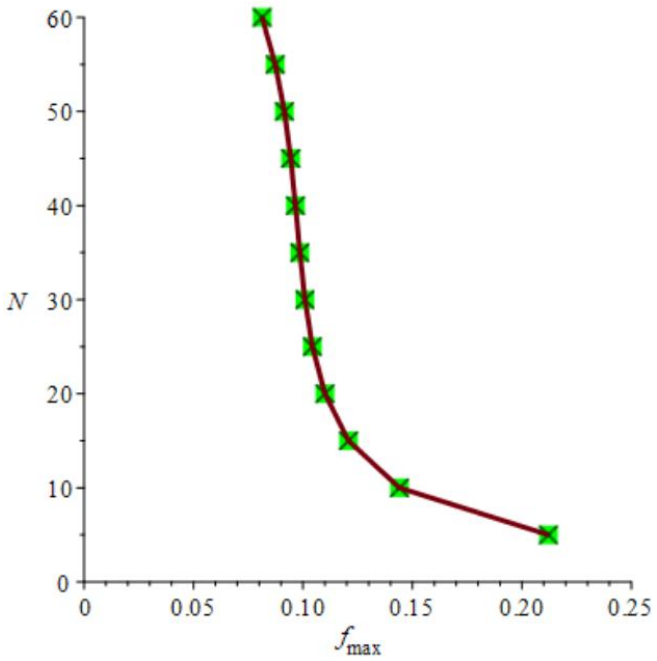

Figure 13: f_{max}:from Billingham and Lockett (2002) method and from the Martin model are in exact agreement.

A final quote from Billingham and Lockett (2002):

Unfortunately, because of the difficulty of predicting the extent of maldistribution, these models can only be used to assess sensitivity to maldistribution rather than as direct design tools.

So the key question can now be posed:

Is there a way to predict the necessary bed height so that the design is insensitive to maldistribution.

The top right quadrant of Figure 12 is the key here. We have developed the approximation given by Eqn. (7) below and shown in Fig. 14.

$$E_{bed} = \frac{1}{1+f^2 N_{bed}/4\, f_{max}} \tag{7}$$

We will illustrate the application of this equation in Section 6 below.

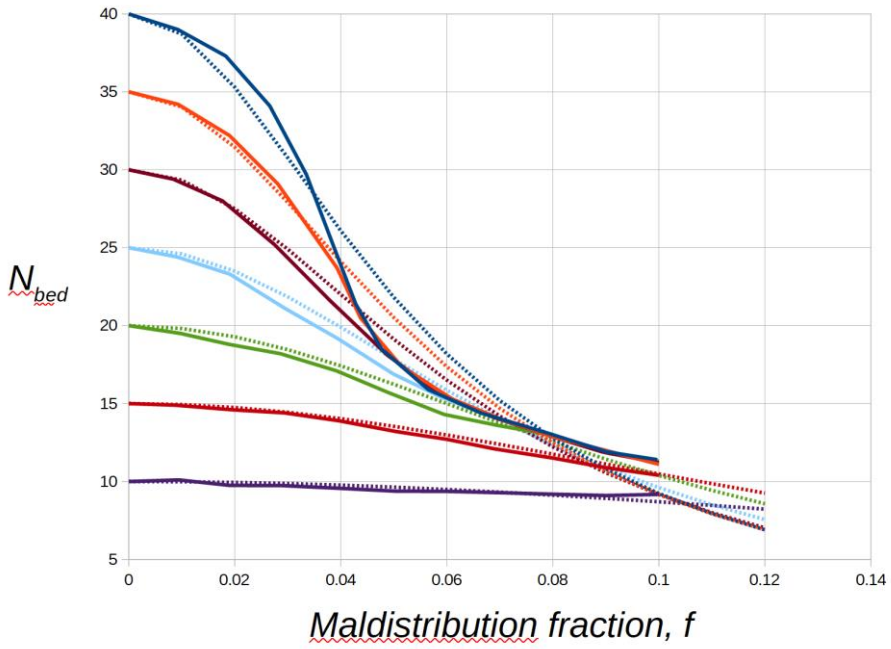

Figure 14: Approximation (dashed lines) to bed effectiveness from Billingham and Lockett (2002).

(We pause here to note that the ChemSep PCM can easily be used to mimic the model of Billingham and Lockett shown in Fig. 11. The model in the figure has a liquid distributor tray above the parallel section and a gas distributor tray below the parallel section. These distributor trays are modeled with a stage efficiency of zero (actually a very small number such as 10^{-6} in order to avoid numerical issues in the simulation). An advantage of using the ChemSep PCM for these calculations is that any thermodynamic model can be used (including a constant relative volatility model as used by Billingham and Lockett). The fraction of liquid sent to the two parallel sections is specified as shown in the figure (at right).)

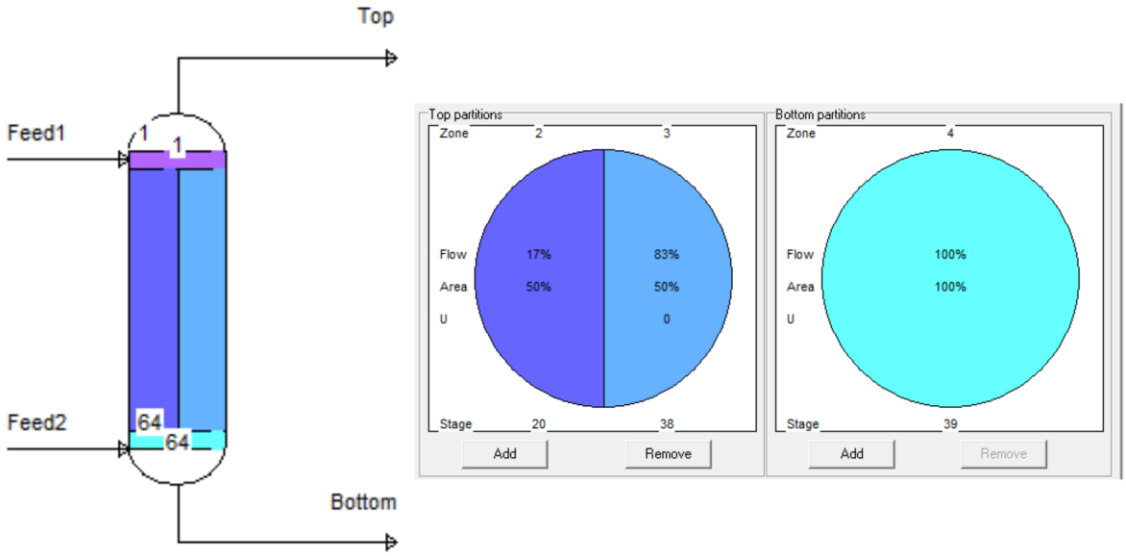

Figure 15: Schematic diagram of ChemSep PCM equivalent to the multi-column model in Fig. 11. Right hand side shows liquid maldistribution specification.

5. Drip Point Density

Liquid maldistribution can be divided into two kinds of maldistribution. The first kind occurs when the initial distribution of liquid is uneven due to unlevel distributors and/or uneven feeding of pre-distributor channels. This could be regarded as a "macro" level type of maldistribution. The second kind is due to (partially) plugged holes in the distributor, imprecisely machined holes, a too low a drip point density (DPD), as well as the maldistribution of liquid due to flow over the packing. The latter is inherent to the packing geometry and materials as well as system properties and occurs throughout the whole bed. These are more "micro" level types of maldistribution. Random packing tends to have much higher inherent maldistribution which frequently shows as increasing wall flow as function of bed height. Structured packing suffers less from wall flow by using wall wipers that direct liquid back into the packing or by extremely tight packing of the metal sheets such that the wall distance becomes similar in size as that of the packing channels. One of the major design factors is the drip point density (DPD) of the liquid distributor. Klemas and Bonilla (1995) addressed the DPD for random packings. More recently, Cai (2018) proposed Eqn. (8) for structured packing:

$$N_{DP} = \frac{1}{\left(16d + \frac{4H}{\tan(a)}\right)h} \tag{8}$$

Our proposal for the drip point density is Eqn. (9) below and follows from an analysis similar to that of Cai in which the liquid from a single drip point contacts N_{wet} sheets but in both directions (Cai's method assumes a single direction).

$$N_{DP} = \frac{P}{A_{wet}} = \frac{1}{2hN_{wet}H\sin(a)} \tag{9}$$

With $N_{wet} = 4$ Eqn. (9) gives:

M250Y: $N_{DP} = 74/m^2$
M250X: $N_{DP} = 104/m^2$
M500Y: $N_{DP} = 151/m^2$
M750Y: $N_{DP} = 225/m^2$

6. Application to Packed Column Design

In this section we show how these pieces can be put together to design a packed column to separate argon and oxygen.

Figure 16 shows a possible flowsheet for air separation. The argon column is highlighted in red. The column is operated at low pressure as shown in the figure.

Of central importance to the successful design of any process is an accurate thermodynamic model. Figure 17 shows the Peng-Robinson equation of state used to model the VLE of the argon – oxygen binary mixture. The left-hand side plot shows the standard PR EOS with a

binary interaction parameter $k_{O2-Ar} = 0.01382$. The right-hand side plot shows the improved model that makes use of the Mathias-Copeman α-function with MC parameter$MC_{1,O2} = 0.32, MC_{1,Ar} = 0.294$. The improvement in the pure component vapor pressures is immediately evident in the right-hand side plot.

Figure 18 shows the oxygen purity as a function of the product to feed ratio in the argon column. The upstream switching of drying beds (to ensure no water freezes in the heat exchangers) cause changes in the feed rates that induce L/V changes in the low pressure argon column. Also, there are different draw rates for waste/pure Nitrogen that depend on how much N2 is produced as a liquefied product. As a result, the Argon concentration in the feed to the argon column can change by 1-2% because the peak of argon shifts up or down the low pressure column. The argon column design needs to be robust to these shifts. Therefore, the steady state simulation may be for a 10% feed (the blue line) but the chosen L/V (or chosen product rate) needs to be set by the 8% Argon feed (i.e. the left hand dashed orange line) and the number of stages is chosen so that the column can handle a 12% Argon feed (i.e. the dotted right hand side orange line). The blue line has too few stages and the green line too many stages. With operation at the L/V at 0.027 the final design point sits above the line of design purity by roughly 13%. That is why this is the line on the side indicates the margin for "Effective Margin Maldistribution" if no extra correction is added onto the HETP. Note that a 9m bed is equivalent to 37 stages including the 13% loss.

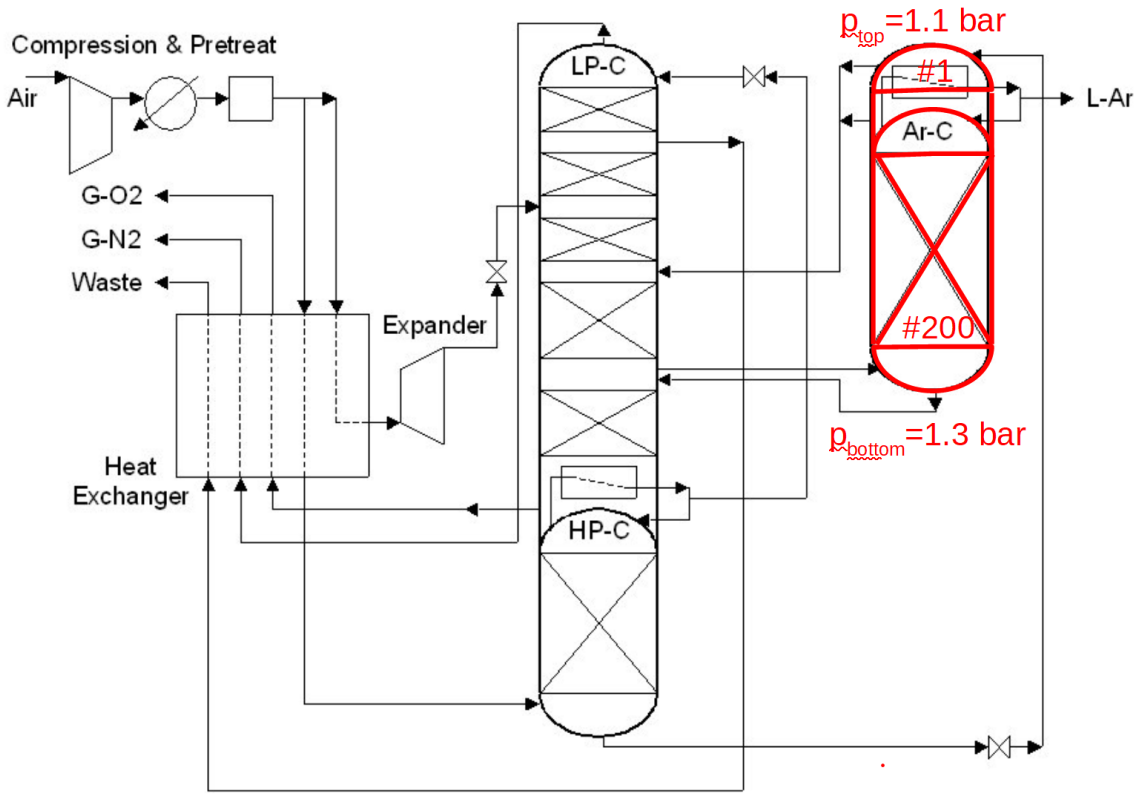

Figure 16: Air separation flowsheet.

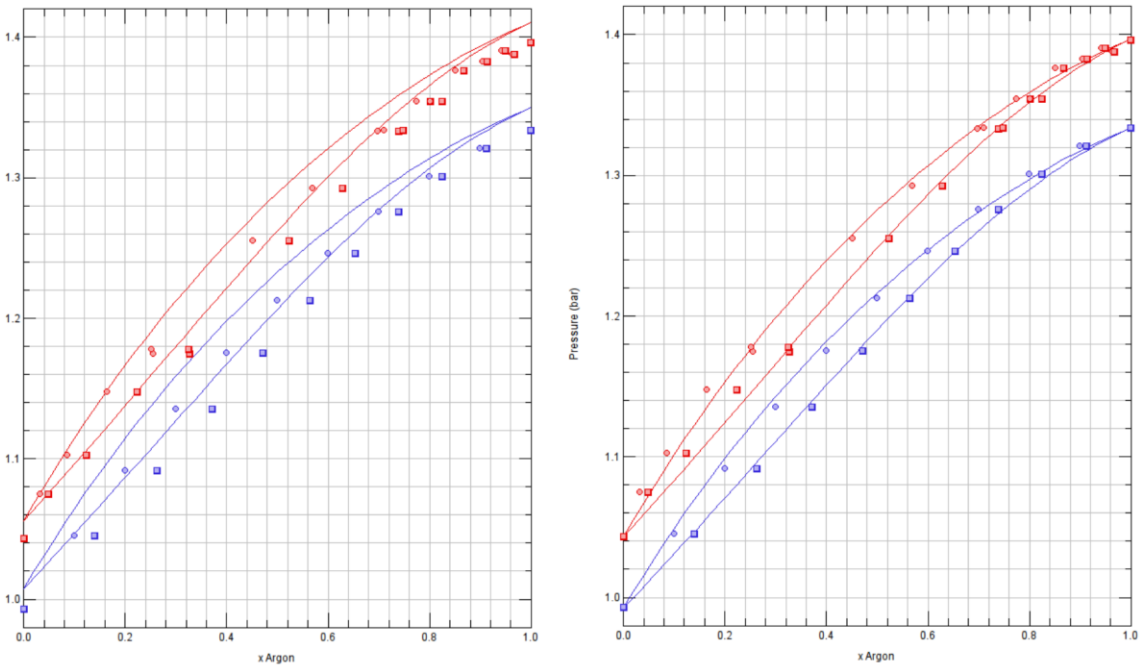

Figure 17: VLE for the argon – oxygen mixture represented by the Peng-Robinson equation of state. See text for elucidation.

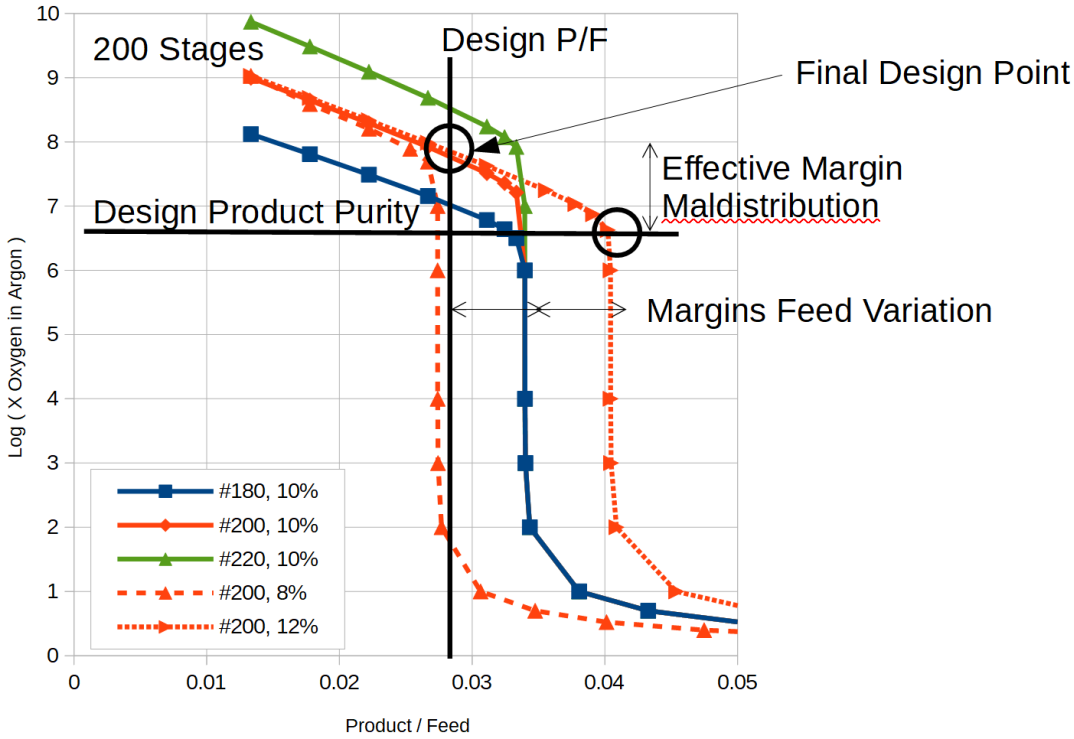

Figure 18: Oxygen purity as a function of the product to feed ratio in the argon column.

Figure 19 illustrates the next step which is to use the ChemSep PCM to assess the significance of maldistribution in this design. For complete understanding we look at maldistribution in beds of differing heights (number of stages) and position in the column. We also vary the maldistribution fraction f as indicated on the right hand part of Fig. 19.

From the ChemSep PCM simulations we created Fig. 20 which shows f_{max} as a function of bed height for the bed at the top of the column (the blue line) and a bed at the bottom of the column (the red-orange line). The results show that the top bed is not especially sensitive to maldistribution, whereas the bottom bed is very sensitive to maldistribution. Figure 21 involves a simple fit to Eqn. (5) of the results of PCM simulations of the argon column.

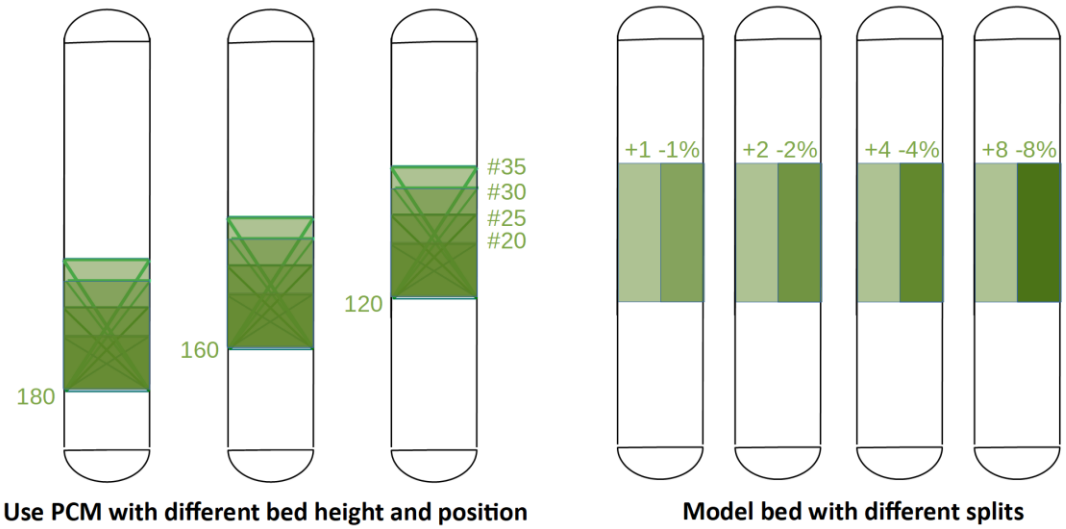

Figure 19: Use the PCM to determine effect of maldistribution.

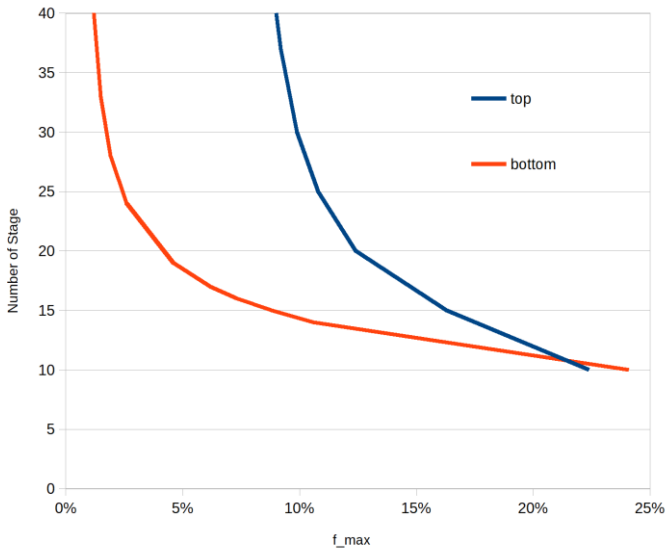

Figure 20: f_{max} as function of the bed depth for beds at the top and bottom of the argon column.

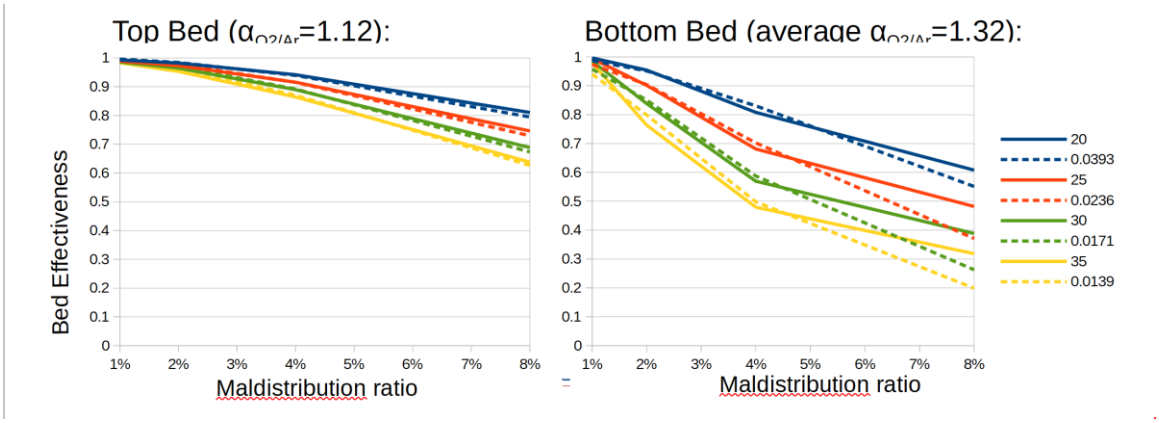

Figure 21: Bed effectiveness for the top and bottom beds in the argon – oxygen column.

Our design method can now optimize the stage distribution over multiple beds.

We start by assuming the maldistribution of the distributor is 1% at turn-down. We then use the Billingham and Lockett method, Eqns. (4,5), to estimate f_{max}. We assume the maximum bed depth is 9m (due to weight restrictions). This is equivalent to 37 stages. The HETP is taken to be 0.215 m and allows for a maximum of 13% loss at turndown.

The automated design calls for 6 beds (5 of 37 stages and 1 of 14) a 50.4% turndown. If we use 35 stages/bed the turndown ratio increases to 54.2% turndown. If we go for 7 beds (5 of 35 stages and 2 of 12) we find only a few extra % at turndown.

A patent by Dean et al. (2000) reaches the same conclusion. There is a feed pinch at the bottom of this parallel column as indicated by the McCabe-Thiele construction in Fig. 22. This makes the bottom of the column sensitive to maldistribution.

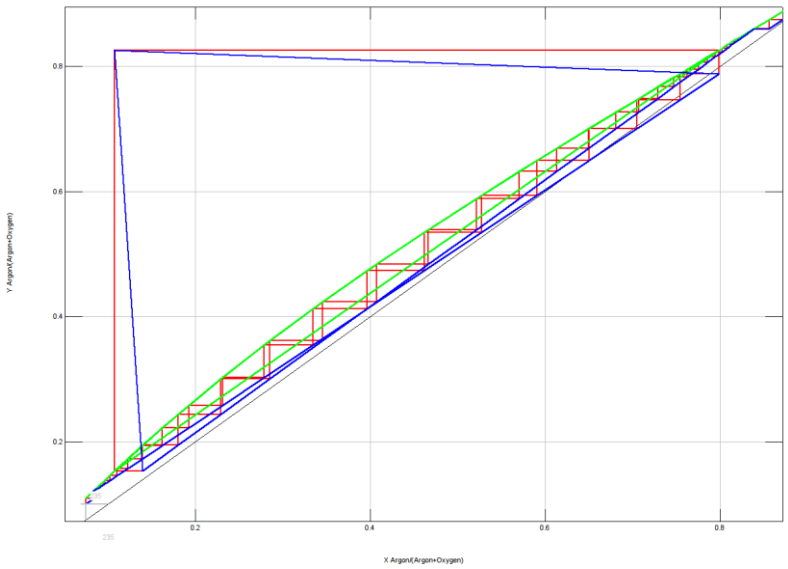

Figure 22: Feed pinch at foot of argon – oxygen column.

7. Conclusions

Any packed bed will suffer from maldistribution and as such, should be designed with sufficient extra height to make it robust for maldistribution. The ChemSep PCM makes it very easy to model maldistribution and come to a robust design that is insensitive to this phenomenon. To ease practical industrial column design, we have proposed a simple approximate formula for a direct calculation of the packed bed effectiveness from a single simulation. This concept can be used to optimize single and multiple packed bed depth(s). The approximation combines the theoretical result of Huber & Hiltbrunner with the concept of a maximum maldistribution fraction as proposed by Billingham & Lockett. It enhances earlier formulations such as that of Klemas and Bonilla by capturing the sensitivity of the bed effectiveness to maldistributiion for feed pinched beds. This was illustrated by the cryogenic separation of Argon in an air separation unit. Further validation of our proposal will focus on the influence of maldistribution in beds with other type of pinches and a numerically more robust alternative for the maximum maldistribution fraction.

Symbols

a	(radians)	Packing angle
A_{wet}	(m^2)	Wetted area of packing
d	(m)	Horizontal distance between ridges
E	(-)	Bed effectiveness (efficiency)
f	(-)	Maldistribution fraction (same as M)
h	(m)	Crimp height
H	(m)	Packing element height
L	(mol/s)	Liquid flowrate
M	(-)	Maldistribution percentage (same as $f \times 100$)
N	(-)	Number of stages
N_{DP}	(/m^2)	Number of drip points
N_{wet}	(/m^2)	Number of sheets wetted by one drip point
P	(m)	Wetted perimeter
α	(-)	Relative volatility
		Function used in EOS models (see discussion around Fig. 16)

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