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Understanding Temperature Profiles of Distillation Columns

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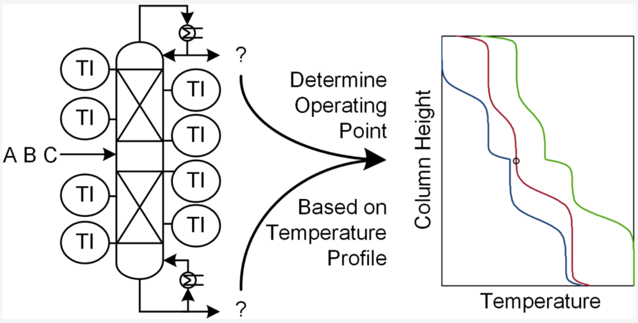
ABSTRACT: Temperature profiles of distillation columns can be measured comparatively easily and can, at the same time, provide detailed information about their operating point. Thus, it is often stated that these profiles are suitable tools to troubleshoot distillation columns. However, the literature also lacks a comprehensive explanation of how temperature profiles should look and what can be read from them. This article systematically investigates temperature profiles of distillation columns with one feed containing two or more components and two product streams. Based on the results, seven simple rules are derived that in the end are used to interpret example profiles in a column with a four-component feed. The rules are found to be suitable tools to understand and interpret temperature profiles properly.



1. INTRODUCTION

The trend toward a more sustainable chemical industry is essential in current times. In this context, a significant lever for improvement can be found in the distillation process, as these are responsible of approximately 3% of the energy consumption in industrially further developed countries.[1,2] Accordingly, it is of great importance to ensure that these columns are operated close to optimal and that not too much energy is used for the separation. A nonoptimal operation of a standard distillation column can in most cases already be observed from its temperature profile over the column height.[3,4] Most columns have temperature sensors at several locations inside the column. For a column without sufficient temperature sensors, a possible solution could be to use the surface temperatures of the column shell as an indication for the internal temperatures.

The expected temperature profile of a binary separation can be easily derived by the now almost 100-year-old graphical approach by McCabe and Thiele,[5] which assumes constant internal flows. The approach can be used to estimate the composition profile from the minimum to an infinite number of stages and also evaluate the impact of nonoptimal feed stages or side rectifiers or condensers.[1,6,7] In combination with the *Txy*-diagram of the mixture, the temperature profile can be derived. The approach of McCabe and Thiele is a standard engineering tool that is probably taught in every chemical engineering course and it helps understanding the general shape of composition and temperature profiles. Nowadays, temperature profiles can also be derived easily in a rigorous manner without assumptions, such as constant molar flows, from flowsheet simulators.

The focus of this paper is the use of temperature profiles to understand and improve the operation. However, without knowledge about how the profiles should look, interpretation is difficult. The authors are not aware of a publication giving an in-depth overview of this topic, even for binary separations. For multicomponent distillation, different statements can be found about the temperature profiles, which at first glance even seem to be contradictory. In summary, the objective of this work is to perform an in-depth analysis of temperature profiles in simple distillation columns for different scenarios and numbers of components in the feed stream in order to enable a deeper understanding of the column operation. For this purpose, the following assumptions are made: The column has no pressure drop, one feed stream, two product streams, and no side streams, the feed is a saturated liquid (liquid fraction $q = 1$), the mixture may consist of two or more components and shows a zeotropic behavior. Based on the results, simple rules are derived that will facilitate the reading of temperature profiles.

The paper is structured as follows. First, the theoretical background is discussed shortly in Section 2, and then a summary of the applied methodology is given in Section 3. Afterward, results are presented in Section 4. The impact of the number of stages on the temperature profiles is evaluated in Subsection 4.1, followed by an in-depth analysis of the occurrence of pinch points at an infinite number of stages in Subsection 4.2, and a study of nonoptimal feed stage locations in

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Subsection 4.3. In each section, simple rules on how to read the profiles are derived, which are then applied to an example case of a quaternary mixture in Subsection 4.4. Section 5 comments on the generalization of the obtained results. Finally, a conclusion is given in Section 6.

2. THEORETICAL BACKGROUND

The temperature profile inside a distillation column (Figure 1) depends both on the feed mixture (composition x_F and flow rate $\dot{F}$), design specifications (total number of stages N and feed stage location N_F), and operational specifications (pressure and one specification for each product stream). During the design phase, all of these degrees of freedom have to be considered, while the design specifications (N and N_F) are fixed during operation, which is the focus of this paper.

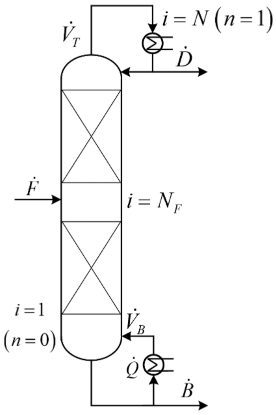


Figure 1. Flowsheet of a distillation column. i denotes the theoretical stage number and n is the relative stage number (eq 2).

When designing a distillation column, two conflicting objectives must be considered, which are the capital costs related to the number of theoretical stages N and the operational costs related to the energy usage (which determines the vapor flow $\dot{V}$).[8] Note that in the following the term "theoretical" is neglected when talking about the number of theoretical stages. There are two extreme design cases: on the one hand the minimum number of stages (N_{min}) with a high (infinite) energy consumption and on the other hand, the minimum energy operation ($\dot{V}_{\text{min}}$) with an infinite number of stages. In the simulations, it is assumed that the energy usage approaches $\dot{V} = \dot{V}_{\text{min}}$ with $N = 4{\cdot}N_{\text{min}}$.[9] The minimum number of stages can be estimated with the Fenske eq 1.[10]

$$N_{\text{min}} = \frac{\ln\left(\frac{(x_{\text{LK}}/x_{\text{HK}})_{\dot{D}}}{(x_{\text{LK}}/x_{\text{HK}})_{\dot{B}}}\right)}{\ln \alpha} \quad (1)$$

Here, x_i is the molar fractions of the components, either the light key or heavy key components (LK and HK, respectively), in the two product streams (see Figure 1), and α is the relative volatility.

In between the extreme cases of N_{min} and $\dot{V}_{\text{min},}$ there are many so-called Pareto-optimal compromise solutions for the design.[6] Even though theoretically all Pareto-optimal designs are "optimal," it is often recommended to operate the column in a region between the two extreme cases where the total costs are minimized,[8] which is usually at around $N/N_{\text{min}} \approx 2$ to 2.5.

In the case of infinite number of stages ($N/N_{\text{min}} \approx 4$ in the simulations), the temperature profiles always have pinch points, which are sometimes also called points of infinitude.[8,11] In these regions, many stages are used to reach infinitesimal small changes in composition. The pinches are visible as zones with an almost constant temperature. Pinch points result from the fact that compositions on neighboring stages are almost the same or, in other words, the operating line almost intersects the equilibrium line so that a high number of stages are needed to achieve minor changes in compositions.

For a given column with a given feed and pressure, only two degrees of freedom (one per product flow) are needed to fully specify the operation and, with this, the product compositions. To visualize all possible separations, a $\dot{V}_{\text{min}}$ diagram[12−14] or alternatively a plot of the reflux ratio versus distillate flow[15] can be used.

The $\dot{V}_{\text{min}}$ diagram (see the "mountain top" borderline in Figure 6 in the result section) shows the minimum vapor ($\dot{V}_{\text{min}}$) demand in the top of the column (i.e., $\dot{V} = \dot{V}_T$) for a sharp product separation (with "pure" products) of a given molar feed flow $\dot{F}$ as a function of the molar distillate flow $\dot{D}$ at infinite number of stages. For the sake of simplicity, the index "T" for the top of the column is sometimes neglected in the following. For a k-component mixture, there are k-1 maxima. Here, all components are present in only one product stream at a time while using the minimum feasible energy input. For ternary (k = 3) or higher mixtures, there are also minima between the maxima. Here, intermediate boiling components are distributed between the product streams. The $\dot{V}_{\text{min}}$ borders separate the feasible operating range into different regions, in which different components are present in the product streams. If a distillation column is operated at a higher energy demand than shown by the $\dot{V}_{\text{min}}$ line, then the products are overpurified (it may seem strange to say "overpurified" since the products are already "pure" but this happens because there are infinite number of stages) and basically energy is wasted. On the other hand, if less energy is used, the separation is no longer sharp and components start to distribute between the product streams. The $\dot{V}_{\text{min}}$ diagram can either be calculated on a short-cut basis, requiring only the relative volatilities or K-values ($K = y/x$) for the components, feed composition, and liquid fraction as input, or it can be obtained rigorously using a flowsheet simulator. For more information about $\dot{V}_{\text{min}}$ diagrams, the reader is referred to literature.[12−14,16]

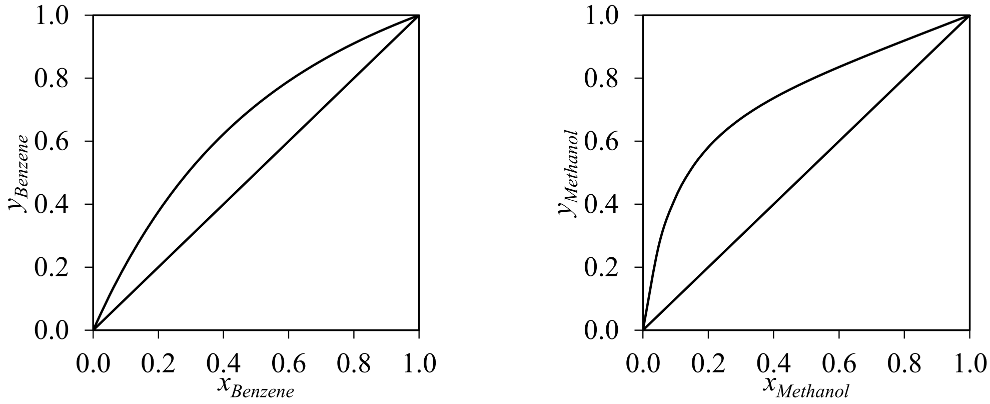
Even though the $\dot{V}_{\text{min}}$ diagram was originally intended for the minimum energy demand case, it was shown that it can also be extended to finite number of stages.[17] The so-called stage-adapted $\dot{V}_{\text{min}}$ diagram helps us understand the actually performed separation task at a given number of stages and energy input.

3. METHODOLOGY

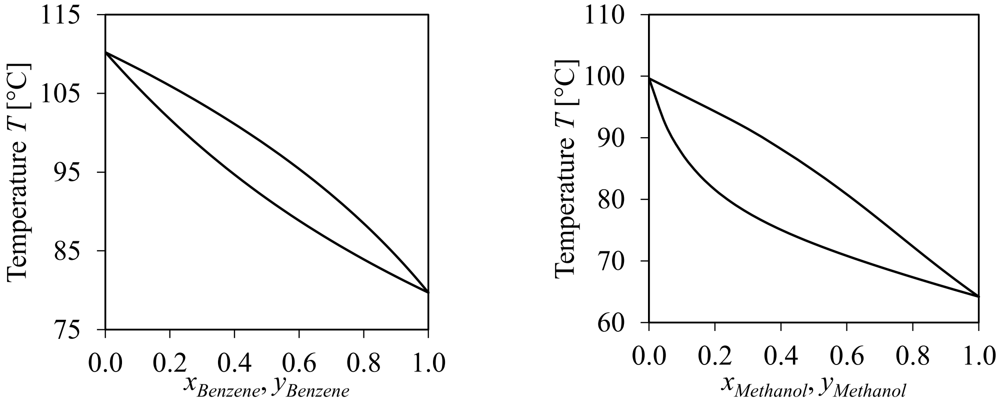
This section briefly summarizes the approach applied in this work. In Section 3.1, the setup of the simulation and optimization is given, followed by the chosen mixtures in Section 3.2.

3.1. Simulation and Optimization.

Simulations of distillation columns are performed in Aspen Plus V11. Pure component properties are from the Aspen Plus internal databank DB-PURE37. As a thermodynamic model, NRTL is used and the interaction parameters are imported from the databank APV110 VLE-IG. The distillation column itself is modeled with the rigorous RadFrac model. For all simulations, the feed stream (see Section 3.2), number of stages, feed stage, vapor rate at the column bottom $\dot{V}_B$ and distillate flow $\dot{D}$ are



(a) *xy*-diagram of benzene/toluene (mixture 1) (b) *xy*-diagram of methanol/water (mixture 2)



(c) *Txy*-diagram of benzene/toluene (mixture 1) (d) *Txy*-diagram of methanol/water (mixture 2)

Figure 2. Phase diagrams of binary mixtures.

specified. The pressure is fixed to 1 bar on all the stages in all cases.

For the evaluation of the simulations, the relative stage number n is sometimes used, see eq 2.

$$n = \frac{i - 1}{N - 1} \tag{2}$$

Similarly, the relative temperature t within the column is calculated with eq 3 based on the actual temperature T and the boiling temperatures (T_b) of the light boiler (LB) and heavy boiler (HB) respectively.

$$t = \frac{T - T_{b,LB}}{T_{b,HB} - T_{b,LB}} \tag{3}$$

For example, a relative temperature of $t = 0$ represents the boiling temperature of the light boiler in the mixture and $t = 1$ is the boiling temperature of the heavy boiler.

In some cases, optimization is performed to determine Pareto-optimal column designs. For this purpose an external multi-objective optimizer is coupled to Aspen Plus. More details regarding the algorithm can be found elsewhere.[18−20] For different numbers of stages, the reboiler duty $\dot{Q}$ is minimized by variation of the feed stage. Product purities are specified to be either above 95 mol % ("non-pure") or 99.8 mol % ("pure"). For separations with distributing components, the recovery of the light key component in the top product and the heavy key component in the bottom product are set instead of the purities. The product flows result based on the mass balance.

3.2. Mixtures.

3.2.1. Mixture 1. The first mixture, which is used for many simulations, is benzene (A) and toluene (B). Here, *p*-xylene (C) and cumene (D) are added, for the ternary and quaternary case, respectively. The boiling points of the pure components at 1 bar are 79.7, 110.2, 137.9, and 151.9 °C respectively. The ternary mixture can be considered as relatively ideal,[21] which can also be observed from the *xy*- and *Txy*-diagrams that are shown in Figure 2a,c. For the simulations, the feed stream is equimolar and saturated liquid (liquid fraction in the feed $q = 1$), with each component having a molar flow of 1 kmol/h.

3.2.2. Mixture 2. As a second mixture methanol (A), water (B) are chosen as they behave less ideal, but they are still zeotropic, as seen in the *xy* and *Txy*-diagrams in Figure 2b,d. The boiling points of the components at 1 bar are 64.2 and 99.6 °C. Again, the feed stream is equimolar, with $q = 1$ and a total flow of 2 kmol/h.

4. RESULTS

In this section, temperature profiles for different scenarios are presented and discussed. Based on the results, simple rules are derived, and new scenarios are chosen and simulated to clarify remaining open questions. The procedure is repeated several times until finally a general understanding is generated. In Section 4.1, the qualitative behavior of temperature profiles as a function of the total number of stages with an optimally located feed is evaluated. With product specification, there is a unique relation between the number of stages and energy demand and also the temperature profile. However, during real column applications, specifications on flows or the feed stage may not be optimally. Section 4.2 thus focuses on pinch zones with a high number of stages but nonoptimal flow specifications. Section 4.3 evaluates the impact of a nonoptimal feed stage at a lower total number of stages. Finally, the derived rules are applied in Section 4.4 to quaternary mixture 1.

4.1. Shape of Temperature Profiles for Optimally Designed and Operated Columns. In this section, temperature profiles of binary mixtures 1 (Section 4.1.1) and 2 (Section 4.1.2) are evaluated for an optimally designed and operated column at infinite and finite number of stages. For a given number of stages, this means that the feed stage is positioned optimally and the product specifications are satisfied. Based on the temperature profiles, a first rule is derived in Section 4.1.3.

4.1.1. Almost Ideal Binary Mixture (Mixture 1). Figure 3 shows the optimal trade-off for the mixture A = benzene and B = toluene for different product purity specifications. In Figure 3 the colored markers correspond to temperature profiles in Figure 4a (99.8 mol % A and B), Figure 4b (99.8 mol % A and 95 mol % B), and Figure 4c (95 mol % A and B).

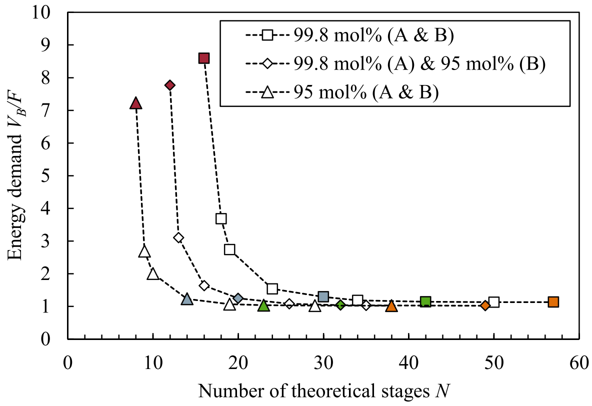


Figure 3. Trade-offs (Pareto-optimal curves) between the number of stages and energy requirement for mixture 1 for three different product specifications. Corresponding temperature profiles are given in Figure 4. The colored points are for $N/N_{\min} \approx 1.1$ (red), $N/N_{\min} \approx 2$ (blue), $N/N_{\min} \approx 3$ (green), and $N/N_{\min} \approx 4$ or more (orange). See also Table 1 for data.

Figure 3 demonstrates the trade-off between energy demand and the number of stages mentioned in Section 2 for three different product specifications (the exact numbers for the colored points can be found in Table 1). The separation can either be obtained with a low energy input and a high number of stages (to the right in Figure 3) or a low column height with a high energy input (to the left in Figure 3) and there are also Pareto-optimal compromises in between. It can be seen that the fronts shift with different product specifications, with the minimum number of stages being a lot more sensitive than the minimum energy demand. In particular, note that the energy demand $(\dot{V}/\dot{F})$ is not reduced much when $N/N_{\min}$ exceeds about 2 (blue points). This agrees with the standard rule of thumb of choosing $N/N_{\min} = 2$ or larger ([10] on page 1125).

Figure 4 visualizes the temperature profiles corresponding to the three product specifications, each shown for four of the colored design points in Figure 3, which correspond roughly to $N/N_{\min}$ of 4 (orange), 3 (green), 2 (blue), and 1.1 (red). Note that a rule of thumb is to choose $N/N_{\min} = 2$ or larger ([10] on page 1125), that is between the blue and green profile. In Figure 4 both axes are normalized 0 to 1. For the normalization of the x-axis (temperature) eq 3 is used and for the y-axis (column height) eq 2.

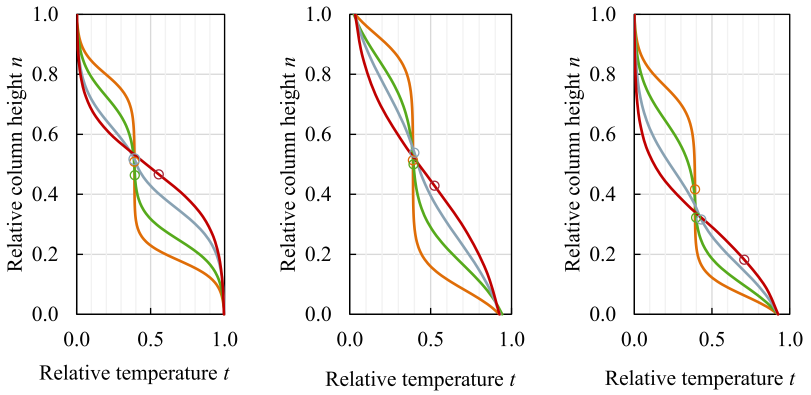
In general, and as expected, the temperature increases from the top to the bottom of the column. The temperature change at the column end gets very small (pinch zone) when the corresponding product has high purity; see Figure 4a, which is because the separation then approaches the corners of the xy-diagram at $x = 0$ and $x = 1$ (Figure 2a). The shape of the temperature profile between the column ends depends on the total number of stages. For a high number of stages (orange, $N/N_{\min} \approx 4$) a pinch zone above and below the feed stage is clearly visible. With fewer stages and more energy required for the same separation task, the pinch zone at the feed stage becomes less pronounced, but it is still visible as a slope change in the temperature profile. This striving of the temperature profile in the direction of the pinch temperature without really ending up in a pinch is in the following denoted as "pinch residue." At a minimum number of stages (red curves), the pinch residue finally disappears. A similar profile is shown by Stichlmair et al.[1] (chapter 4.2 in the book).

Figure 4b shows the temperature profiles with 5 mol % impurities in both products. The shape of the temperature profile around the feed stage is similar to that with higher purities in Figure 4a. However, because of the impure product, there is no constant temperature (pinch) zone at the column ends. With fewer total number of stages, the pinch around the feed again disappears.

Figure 4c shows temperature profiles for one pure product (top, 99.8 mol %) and one impure product (bottom, 95 mol %). In this case, the product flows are adjusted according to the mass balance; thus, the amount of top product, having the higher purity specifications, is reduced and correspondingly the bottom flow is increased. The resulting profiles are as expected nearly a combination of the upper part of Figure 4a and the lower part of Figure 4b. As the profile is now asymmetrical, the optimal feed stage is in the lower part of the column (Table 1). For the opposite case having a nonpure top and a pure bottom product, the profile follows the same pattern and thus is a combination of the upper part of Figure 4b and the lower part of Figure 4a (not shown here).

4.1.2. Nonideal Binary Mixture (Mixture 2). If the mixture is not as ideal as mixture 1, the described patterns may be more difficult to observe. This is illustrated in Figure 5b which shows temperature profiles of mixture 2 (methanol/water) for the case with 99.8 mol % product purities (Figure 5a). In the top part of the column, the range of almost constant temperature is significantly longer than that for the ideal mixture in Figure 4a. This arises from the almost linear slope in the xy-diagram of the mixture at higher x (see Figure 2b). Thus, the operating line is very close to the equilibrium line, resulting in what is called a tangent pinch. Consequently, the temperature in the upper part of the column is almost constant over a large number of stages in all cases.

On the other hand, the pinch zone around the feed location is much less visible. For the ideal mixture (Figure 4) it was found that these feed pinches, in combination with the pinches at the column ends, give a clear indication of how close the column is operated to the minimum energy demand (infinite number of stages). However, in the rather nonideal case in Figure 5b this



(a) 99.8 mol% for both products (colors correspond to the ones of □ in **Figure 3**)

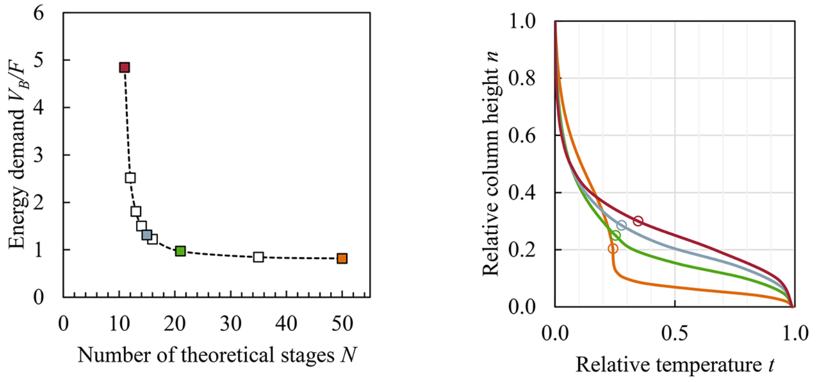
(b) 95 mol% for both products (colors correspond to the ones of △ in **Figure 3**)

(c) 99.8 mol% (top) and 95 mol% (bottom) (colors correspond to the ones of ◇ in **Figure 3**)

Figure 4. Relative temperature profiles for mixture 1 corresponding to points in Figure 3 for $N/N_{\text{min}} \approx 1.1$ (red), $N/N_{\text{min}} \approx 2$ (blue), $N/N_{\text{min}} \approx 3$ (green), and $N/N_{\text{min}} \approx 4$ or more (orange). Circles indicate the optimized feed stage location and the corresponding relative temperature inside the column.

Table 1. Column Specifications Corresponding to Figures 3, 4, and 5. Stages are Counted from Top; The Feed is Optimally Located in Order to Minimize Energy Demand $\dot{V}/\dot{F}$

specifications	color of curve	number of stages N	N/N_{min}	feed stage N_F	relative feed stage n_F	$\dot{D}/\dot{F}$	$\dot{V}/\dot{F}$	$\dot{V}/\dot{V}_{\text{min}}$
mixture 1	orange	60	4.3	30	0.49	1	1.13	1.00
99.8 mol % A	green	42	3.0	23	0.54	1	1.14	1.01
99.8 mol % B (Figure 4a)	blue	30	2.1	15	0.48	1	1.29	1.14
	red	16	1.1	9	0.53	1	8.6	7.61
mixture 1	orange	38	5.4	19	0.49	1	1.02	1.00
95 mol % A	green	23	3.3	12	0.50	1	1.03	1.01
95 mol % B (Figure 4b)	blue	14	2.0	7	0.46	1	1.23	1.21
	red	8	1.1	5	0.57	1	7.23	7.09
mixture 1	orange	49	4.9	29	0.58	0.95	1.02	1.00
99.8 mol % A	green	32	3.2	22	0.68	0.95	1.04	1.02
95 mol % B (Figure 4c)	blue	20	2.0	14	0.68	0.95	1.25	1.23
	red	12	1.2	10	0.82	0.95	7.76	7.61
mixture 2	orange	50	5.0	40	0.80	1	0.82	1.00
99.8 mol % A	green	21	2.1	16	0.75	1	0.97	1.18
99.8 mol % B (Figure 5b)	blue	15	1.5	11	0.71	1	1.31	1.60
	red	11	1.1	8	0.70	1	4.84	5.90



(a) Pareto-optimal column designs

(b) Corresponding temperature profiles

Figure 5. Design trade-off and corresponding temperature profiles for mixture 2 (methanol/water), with both product purities 99.8 mol %. For $N/N_{\text{min}} \approx 1.1$ (red), $N/N_{\text{min}} \approx 2$ (blue), $N/N_{\text{min}} \approx 3$ (green), and $N/N_{\text{min}} \approx 4$ or more (orange). Circles indicate the optimized feed stage location. See also Table 1 for data.

conclusion is more difficult to draw because of the reduced visibility of the pinch caused by the additional tangent pinch.

In the rest of the paper, the focus is on mixtures with more ideal behavior in order to create a basic understanding.

4.1.3. Rule 1 for Temperature Profiles. From the results in this section, a first rule can be derived.

> ***Rule 1. A constant temperature zone (pinch zone) at the column end (top or bottom) indicates an almost pure component in the corresponding product. This pinch zone is observable independently of the number of stages.***

Note that the length of the pinch zone for pure components depends on the vapor−liquid equilibrium (VLE) of the mixture. Consider the equilibrium xy-diagram for mixture 2 in Figure 2b. The y-curve (vapor composition) is well above the diagonal (x = liquid composition) in the heavy end ($x = 0$), thus the pinch at the lower end of Figure 5b is comparably short. If the y-curve is closer to the diagonal around $x = 0$ or $x = 1$, then more stages are needed to reach the corner of the xy-diagram and thus the pinch is longer.

4.2. Pinch Zones at Infinite Number of Stages.

As observed in Section 4.1, pinches might still be visible with a relatively few stages. Thus, understanding their occurrence and location at infinite number of stages may be useful also for practical operation. For this purpose, Subsection 4.2.1 first focuses on a binary mixture followed by a Subsection 4.2.2 evaluation of a ternary mixture.

4.2.1. Binary Mixture. Figure 6 shows feasible binary separations of mixture 1 (A = benzene, B = toluene) in a $\dot{V}_{\min}$ diagram. The black line in the diagram shows the value of $\dot{V}_T/\dot{F}$ needed to achieve sharp separation as a function of $\dot{D}/\dot{F}$.

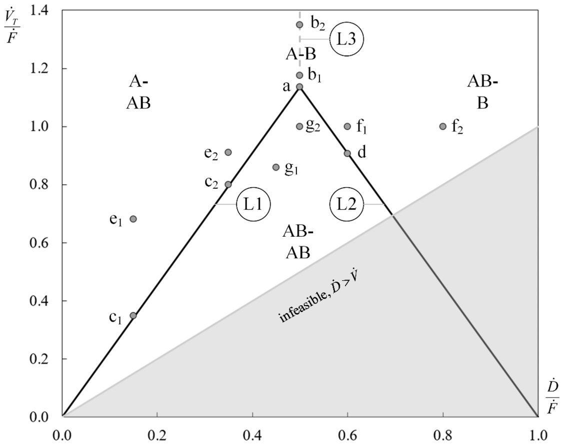


Figure 6. $\dot{V}_{\min}$ diagram for binary mixture 1. The solid lines give the minimum energy ($\dot{V}_{\min}$) required for sharp separation with an infinite number of stages. For the four resulting feasible operating regions, components (A or B) named before the hyphen are obtained in the top product and components named after the hyphen are obtained in the bottom product. Point a: minimum energy separation (at infinite number of stages) obtaining two pure products, along line L3: overpurification of both products. Lines L1 and L2: minimum energy ($\dot{V}_{\min}$) for one pure product. The labeled gray circles indicate operating points to which the corresponding temperature profiles are shown in Figure 7.

As a binary separation is considered, there is one peak in the diagram (point a), representing the minimum energy $\dot{V}_T/\dot{F}$ needed for a sharp separation between the two components with an infinite number of stages. Left below the peak, the line L1 represents the $\dot{V}_{\min}$ operation with pure component A in the top, and where the bottom product contains B with some A. The opposite is the case for line L2, which represents the $\dot{V}_{\min}$ operation when the bottom product is pure B but some B also goes in the top product. Below the "mountain," there are no pure products, as components A and B distribute to both products. Left of the mountain and above line L1, in the region A-AB, one obtains the products as for line L1 but more energy is used than needed. Similar applies for regions AB-B and line L2. Line L2, which separates regions A-AB and AB-B, represents overpurification of both products.

Figure 7 shows temperature profiles corresponding to the gray circles in Figure 6 for the case with $N = 100$ and $N_F = 50$. Figure 7a shows the temperature profile with two pure products at minimum energy operation (point a). As expected based on rule 1, there are pinches at the column top and bottom. Additionally, there are pinches above and below the feed stage (counted as two pinches in the following) with the same temperature as the feed's boiling point (indicated by the circle in Figure 7). Thus, there are four pinches in total, which is also given in the literature as the maximum number of pinches that can be observed at the same time.[22] When using excess energy to reach points b$_1$ and b$_2$ in Figure 6, the pinch zones at the column ends become longer and the pinch zones at the feed stage first become shorter and then disappear; see Figure 7b. Note that the slope change in the temperature profile at the feed stage is not abrupt but is smooth when excess energy is used.

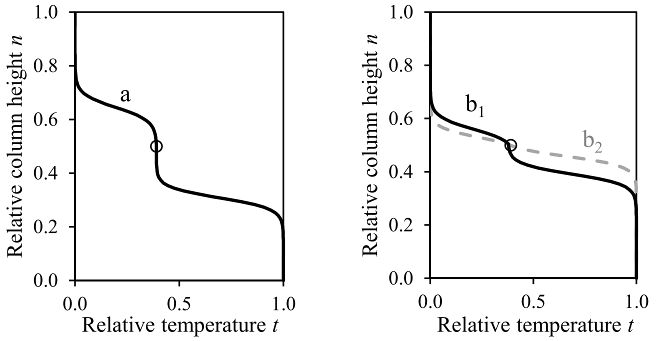
Profiles with one pure and one impure product at minimum energy operation are shown in Figure 7c for points c$_1$ and c$_2$ on line L1, and in Figure 7d for point d on line L2. In both cases, only three pinch zones are observed, as one of the product streams is now impure and overpurified considering the resulting purity. However, there are still pinch zones on both sides of the feed stage (which again is at the feed boiling temperature). Changing the operating point to another location along the same line (compare c$_1$ and c$_2$) does not change the pinch temperatures but only the temperatures at the impure end. As shown in Figure 7e (for points e$_1$ and e$_2$) and Figure 7f (for points f$_1$ and f$_2$), the feed pinch disappears on one side if one of the pure products is overpurified. The feed stage pinch still appears on the other side of the feed stage, but the pinch temperature no longer equals the feed boiling point. With a higher $\dot{D}/\dot{F}$ ratio (points e$_2$ and f$_2$), resulting in more heavy components in the top, all column temperatures increase, including the pinch temperature.

Figure 7g shows the temperature profile when less than the minimum energy is provided; thus, two impure products are obtained (underpurified). There are pinch zones above and below the feed stage, again at its boiling temperature. This pinch temperature does not change when changing the operating point is changed within the area below the $\dot{V}_{\min}$ border (from point g$_1$ to g$_2$). In all areas (not at the borders) where either more or less than the minimum energy ($\dot{V}_{\min}$) is provided (e, f, and g), only one pinch per section is observed.

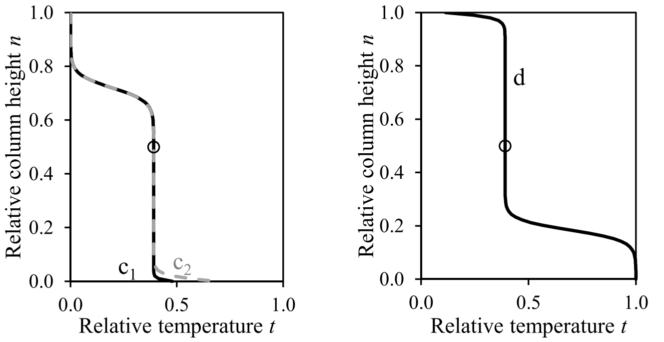
Based on these results, another rule can be derived. Note that a pinch zone that appears both above and below the feed stage is counted as two.

> ***Rule 2. The top and bottom sections can each have a maximum of two pinch zones at the same time. The appearance of two pinches in the same section means that the section is operated at a minimum energy. If only one pinch is visible in a section, the product is either over- or underpurified.***

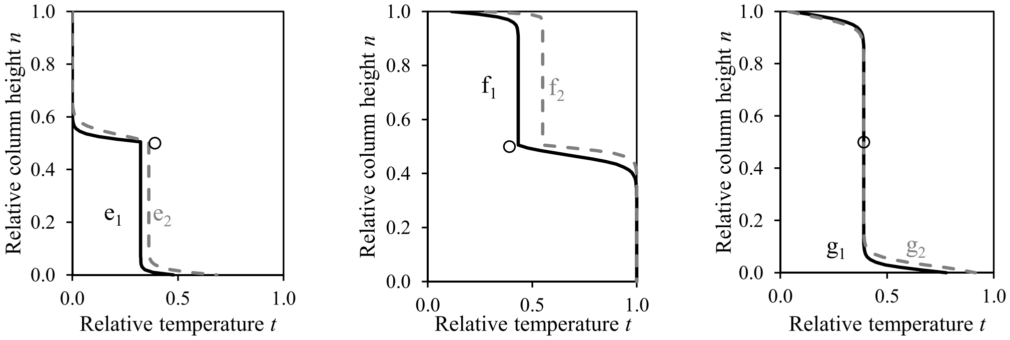
Consequently, for the binary case with minimum energy operation with two pure products (point a), there are two pinches in the top and two in the bottom sections, thus four in total. If only one product is pure (points c and d), then there are three pinches. Over- or underpurification results in only two



(a) A-B, $\dot{V} = \dot{V}_{\min}$ (b) A-B (L3), $\dot{V} > \dot{V}_{\min}$ (top and bottom overpurified)



(c) A-AB (L1), $\dot{V} = \dot{V}_{\min}$ in top, bottom overpurified (d) AB-B (L2), $\dot{V} = \dot{V}_{\min}$ in bottom, top overpurified



(e) A-AB, $\dot{V} > \dot{V}_{\min}$ (top and bottom overpurified) (f) AB-B, $\dot{V} > \dot{V}_{\min}$ (top and bottom overpurified) (g) AB-AB, $\dot{V} < \dot{V}_{\min}$ (top and bottom underpurified)

Figure 7. Temperature profiles at "infinite" number of stages ($N = 100$) for the regions indicated in Figure 6 (binary mixture 1). Circles indicate the feed boiling point and location.

pinches in the whole column (points e, f, g). Note that there may be a transition area where the number of pinches is not entirely clear (b_1).

Another aspect becomes clear when comparing the profiles in Figure 7 in adjacent regions of the $\dot{V}_{\min}$ diagram, thus when transitioning between different product specifications by changing $\dot{V}/\dot{F}$ and $\dot{D}/\dot{F}$. The three pinches at minimum energy operation ($\dot{V} = \dot{V}_{\min}$) for one product (c and d) are at the same location as in the adjacent regions (e/g and f/g). Here, "location" refers to the relative height/position inside the column. For example, region e has pinches at the column top and below the feed stage, region g above and below the feed stage. Profile c, which represents the profile at the border between regions e and g, has pinches at these three locations also, thus at the column top and above and below the feed stage. The same applies for the sharp minimum energy separation A-B (point a). The four pinch locations at column top, bottom and above and below the feed stage are observed in the adjacent regions A-AB (e, top and below feed), AB-B (f, bottom and above feed), AB–AB (g, above and below feed). Based on this, rule 3 is derived.

> ***Rule 3. At the boundaries between neighboring operating regions, i.e. along the minimum energy lines, the location of pinch zones are the same as in the adjacent regions.***

Note that for nonideal mixtures additionally tangent-pinches might appear, as shown in the previous Section 4.1.2.

In order to have a closer look at the temperature and location of the pinches, a ternary mixture is evaluated in the following section.

4.2.2. Ternary Mixture.

The solid lines in Figure 8 show the minimum energy $\dot{V}/\dot{F}$ as a function of $\dot{D}/\dot{F}$ for ternary mixture 1 and the surrounding regions show all resulting feasible product separations. The minimum energy separation for a given

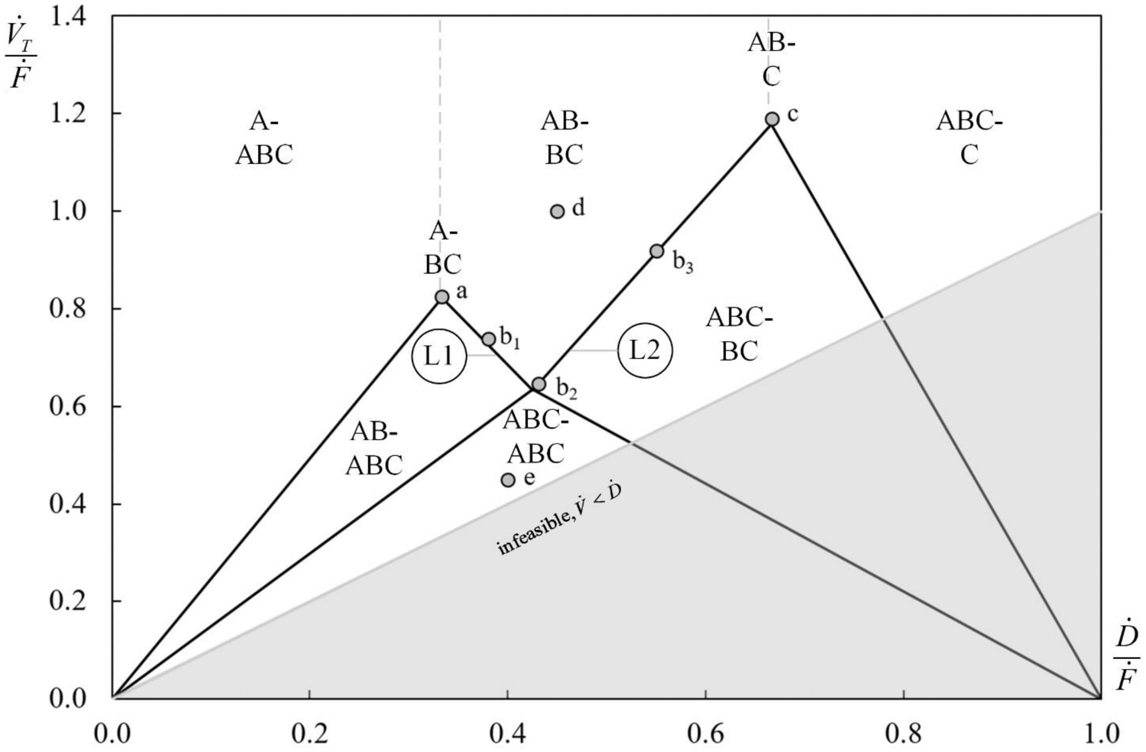


Figure 8. $\dot{V}_{\min}$ diagram for ternary mixture 1. The solid lines give the minimum energy ($\dot{V}_{\min}$) required for sharp separation with an infinite number of stages. For the resulting feasible operating regions, components (A, B, or C) named before the hyphen are obtained in the top product and components named behind the hyphen are obtained in the bottom product. Point a: minimum energy separation obtaining pure A in the top product, point b_2: preferred separation with all A in the top and all C in the bottom while B distributes to both products such that the energy is minimized, point c: minimum energy separation with all C in the bottom. Labeled gray circles indicate operating points with the corresponding temperature profiles in Figure 9.

separation task is along the solid black lines. Note that the $\dot{V}_{\min}$ diagram was calculated only based on feed properties, and the gray circles indicate the actual simulation input resulting in the desired separations. Due to minor nonidealities, these may be located slightly away from the originally predicted values of the $\dot{V}_{\min}$ diagram.

Based on the rules from the previous section, the following is already known about the temperature profiles:

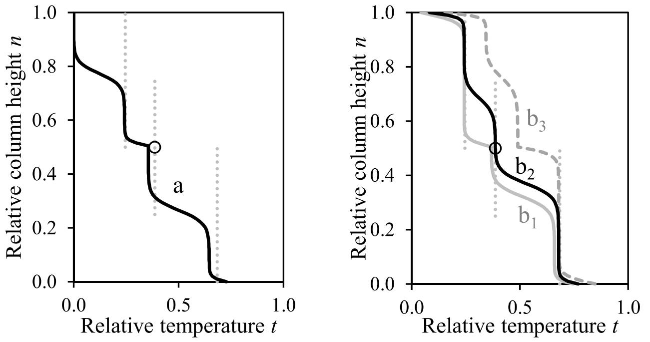
- Rule 1: In region A-ABC there is a pinch at the column top and in region ABC-C at the column bottom.
- Rule 2: At the minimum energy operating points a, b_2, and c there are four pinches.
- Rule 3: a, b_2, and c are adjacent to all feasible regions, so observing the profiles at these points is enough to find all possible pinch locations.

Figure 9a−c show the temperature profiles for the sharp minimum energy separations A-BC, AB-BC, and AB-C (points a, b_2, and c in Figure 8). Additional profiles are shown to assist in making conclusions about the pinch temperatures. Figure 9b shows profiles for the AB-BC separation when either the upper (b_1) or lower column part (b_3) is overpurified (using excess energy for the required separation), while the other section operates at minimum energy. Figure 9d shows the profile when excess energy is used in both column sections for the AB-BC region, and Figure 9e shows the profile in the ABC−ABC region, where too little energy is used and no sharp separation is performed. Composition profiles corresponding to the temperature profiles in Figure 9 can be found in Figure 10.

Profile b_2 in Figure 9b, showing the minimum energy separation AB-BC (b_2), also known as the preferred split, is evaluated first, as it is adjacent to four regions. As expected from Rule 3, temperature profile b_2 has four pinch zones, two are located just above and below the feed stage and have the boiling point of the feed mixture. The two other pinches are not located at the column ends as one may expect from the binary case but are a bit away from the products. This kind of pinch appears if at least one, but not all components except the heavy/light boiler disappear from a product stream,[6] which can be observed from the composition profiles in Figure 10. The temperature change at the column end can be understood a remixing.

Figure 9b also shows temperature profiles when the AB-BC separation is not operated at the minimum but along the lines of L1(b_1) or L2 (b_2). In this case, either the upper or lower column part is overpurified. As expected, based on rule 2, there are then only three pinches observed in the whole column. However, the pinch temperature in the upper column part remains the same along line L1 (compare b_1 to b_2), while the pinch temperature in the lower column part remains the same along line L2 (compare b_2 to b_3). These pinch temperatures are read from the profiles and marked by gray dotted lines in all other diagrams in Figure 9.

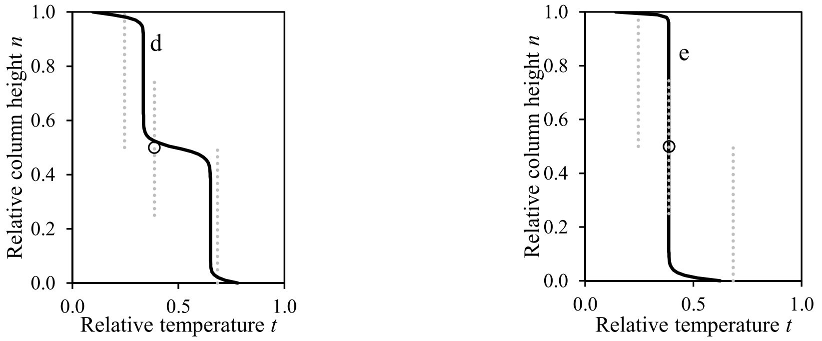
Figure 9a shows the temperature profile for a sharp A-BC split (a) at a minimum energy consumption. As expected, based on rule 2, it has four pinches with one pinch located at the top end of the column (rule 1). There is also a pinch between the column top and feed stage with the same temperature as that of b_1 and b_2. Also, there is a pinch right below the feed stage and finally one in the lower part of the column. Both pinches in the lower column part are different from the ones of b_2 (see the dotted reference



(a) A-BC, $\dot{V} = \dot{V}_{\min}$

(b) AB-BC, $\dot{V} = \dot{V}_{\min}$ in bottom (b_1), top (b_3) and both column parts (b_2)

(c) AB-C, $\dot{V} = \dot{V}_{\min}$



(d) AB-BC, $\dot{V} > \dot{V}_{\min}$ (top and bottom overpurified)

(e) ABC-ABC, $\dot{V} < \dot{V}_{\min}$ (top and bottom underpurified)

Figure 9. Temperature profiles for a large number of stages ($N = 100$) for ternary mixture 1 for the regions indicated in Figure 8. The circle indicates the feed boiling point and its location. The three dotted reference lines are identical in all five subfigures and indicate the invariant pinches (the middle line is the feed temperature). See also composition profiles in Figure 10.

lines). The same only in reverse, can be said for the subfigure c, showing the sharp separation AB-C at minimum energy consumption.

Based on these results, in combination with rule 3, it can be concluded that the constant pinch temperature in the middle of the upper column part of the column is related to the region AB-ABC below the $\dot{V}_{\min}$ borders. Similarly, the constant pinch in the middle of the lower part of the column is related to the region ABC-BC. Interestingly, this pinch temperature does not change when changing the operating point within the region is changed, and this is why it is called "invariant." The invariant pinch of region ABC−ABC, where all components can be found in both product streams, is the feed boiling point as can be observed in Figure 9e. Note that invariant pinches have also be proven theoretically ([23] in Section 3.4.4 and 3.4.5).

When overpurifying the AB-BC separation, the profile in Figure 9d results. There are still two pinches between the column top and bottom, but the pinch temperatures are different from the invariant ones.

Based on the discussion in this Section, rule 4 is derived.

Rule 4. There in an "invariant" pinch temperature when operating at minimum energy or less, which does not change when varying the operating point within the given region of the $\dot{V}_{min}$ diagram. The invariant pinch can be observed in the upper part (e.g., if all components are in the bottom product) or the lower part of the column. If all components are present in both product flows, the invariant pinch is above and below the feed stage and has the feed boiling temperature.

Note that the invariant pinch temperatures depend on the feed composition and condition. Rule 4 is very useful as it can be used to determine whether a column product is overpurified or not. Only if a product is not overpurified can an invariant pinch temperature be observed in the temperature profile.

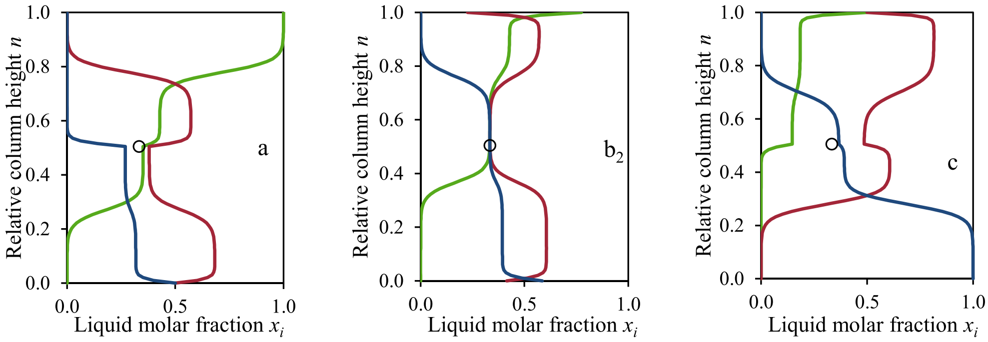
Additionally, for the binary and ternary cases, it was observed that a pinch might be present only on one side of the feed stage with a different temperature than the feed boiling point. Based on Figures 7e, f and 9a, c, d, the reason for this is summarized in rule 5.

Rule 5. A pinch on only one side of the feed stage means that all components are present in the product stream at the corresponding column end. In this case, the pinch temperature does not equal the feed boiling point.

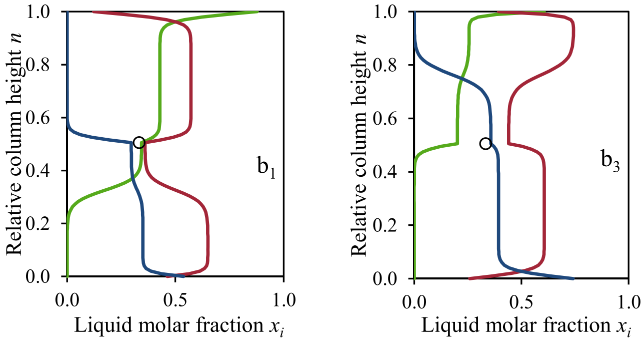
Finally, based on all previously shown profiles and the corresponding composition profiles (Figure 10), rule 6 is derived.

Rule 6. The pinch at the feed stage moves away from the feed and toward the middle or end of the section when one or more components disappear from the corresponding product stream.

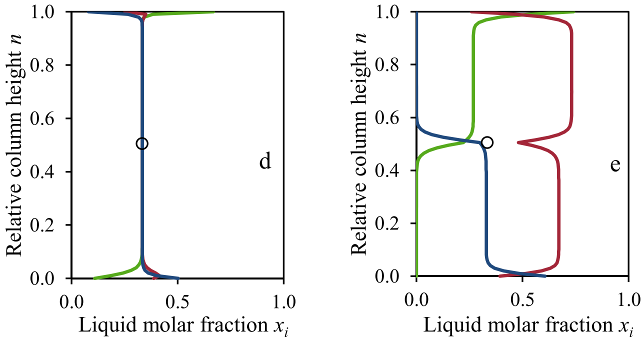
4.3. Impact of Nonoptimal Feed Stage. In Section 4.1, we assumed an optimal feed stage location, and in Section 4.2 the feed stage did not matter because the number of stages was high. Here, we consider the case with a finite number of stages and a possible nonoptimal feed location. This means that in one section, too few stages are provided and in another section too many. The impact of this nonoptimality is shown in Figure 11 for the binary and ternary mixture 1 with $N/N_{\min} = 1.9$. The heat



(a) A-BC, $\dot{V} = \dot{V}_{\min}$ (b) AB-BC, $\dot{V} = \dot{V}_{\min}$ in both column parts (c) AB-C, $\dot{V} = \dot{V}_{\min}$



(d) AB-BC (L1), $\dot{V} = \dot{V}_{\min}$ in bottom, top overpurified (e) AB-BC (L2), $\dot{V} = \dot{V}_{\min}$ in top, bottom overpurified



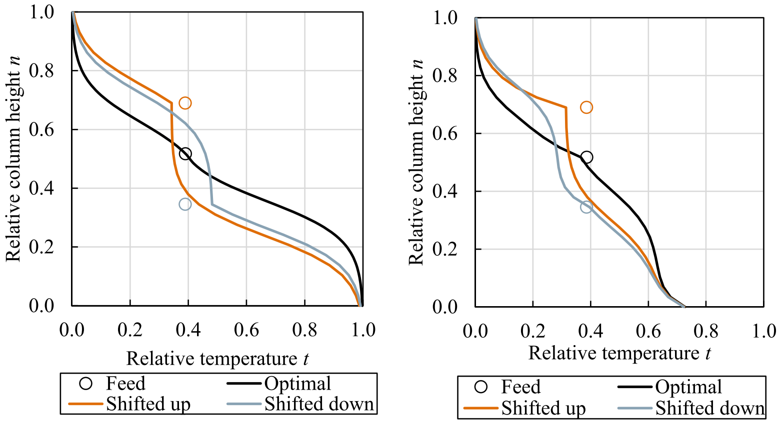
(f) AB-BC, $\dot{V} > \dot{V}_{\min}$ (top and bottom overpurified) (g) ABC-ABC, $\dot{V} < \dot{V}_{\min}$ (top and bottom underpurified)

Figure 10. Molar liquid composition profiles of ternary mixture 1 corresponding to temperature profiles in Figure 9 and operating points indicated in Figure 8. Green: component A, red: component B, and blue: component C.

input at the bottom ($\dot{Q}$) and the product split ($\dot{D}/\dot{F}$) are kept constant at the values of the optimal case. The resulting product purities then decrease.

Figure 11a shows the temperature profiles for binary mixture 1 for three different feed stage locations. In the following, the case when the feed stream is shifted too far up (orange) is described; however, the same conclusions, but reversed, apply when the feed is located too far down (blue). If the feed stage is located too far up, then a pinch appears right below the feed stage. According to rule 5, this indicates that all feed components (A and B in this case) are present in the bottom product. At the same time, the pinches at the column top and bottom end are still visible, although shorter, indicating almost pure products (rule 1). Based on rule 2, the appearance of three pinches means that the column is operated optimally only in one of the two sections. As the lower column part has two pinches, this section is operated close to optimal at minimum energy consumption, whereas the upper column part with fewer stages appears to be not.

Figure 11b shows the impact of a nonoptimal feed stage for the separation A-BC of a ternary mixture. If the feed stage is shifted up (orange), the profile looks similar to the binary A-B case in subfigure a. The only difference is that the second pinch in the lower part is not located at the column bottom but middle. If the feed stage is too far down (blue), then a pinch appears between the feed and top product. Based on rule 6, this means that one or more components disappear from the top product and as this pinch is visible in combination with the one at the column top. Component B is about to appear in the top product, while component C is not present (if C was present, the pinch would be right above the feed stage, rule 5). Again, three pinches



(a) Binary mixture 1, $\dot{V}/\dot{F}=1.29$, $\dot{D}/\dot{F}=0.5$, Optimal: sharp A-B separation,

(b) Ternary mixture 1, $\dot{V}/\dot{F}=0.94$, $\dot{D}/\dot{F}=0.33$, Optimal: sharp A-BC separation

Figure 11. Impact of nonoptimal feed stage location on temperature profiles at $N = 30$. N_F is varied: Optimal $N_F = 15$, shifted up $N_F = 10$, and shifted down $N_F = 20$. In the optimal case, $N/N_{min} = 1.9$ and the top purity is 99.8 mol % A.

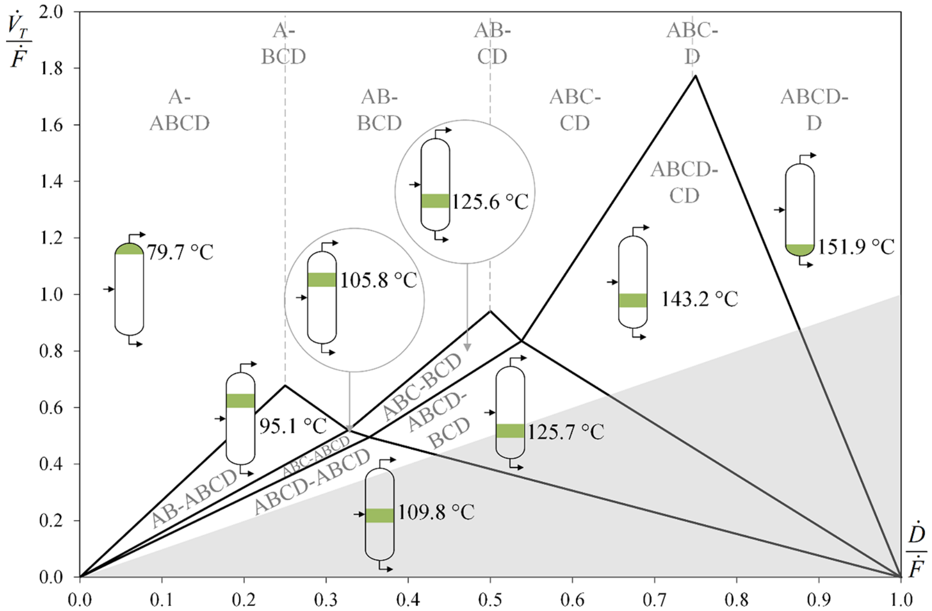


Figure 12. $\dot{V}_{min}$ diagram of the quaternary mixture 1 (benzene, toluene, p-xylene, and cumene) and invariant pinch temperatures determined by simulation. The invariant pinch temperatures and locations (green) are indicated by the small columns in selected regions where they appear.

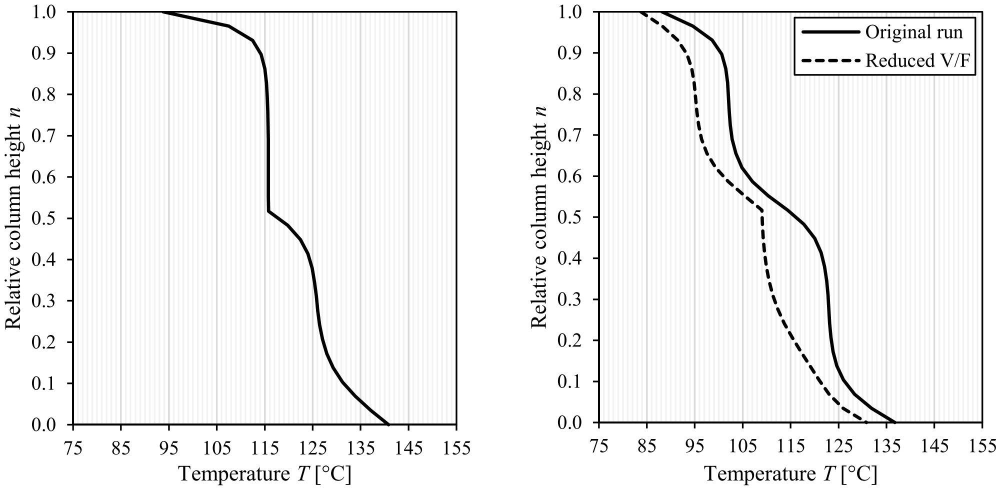
are visible, although those in one column section can be identified much clearer than those in the other one.

In summary, a nonoptimal feed stage means that either the upper or lower section is operated closer to the minimum number of stages, where pinches are less visible, whereas the other section has excess stages, where the pinch is more visible. Based on this, a last rule is derived.

Rule 7. A clearly visible pinch in one section in combination with a poorly visible one in the other section is an indication for a nonoptimal feed stage.

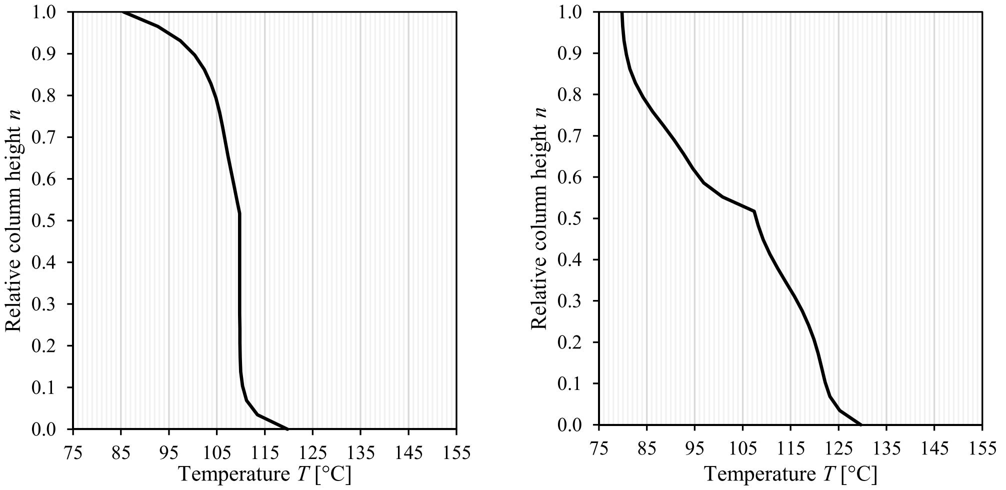
4.4. Examples on How to Determine Operating Point Based on Temperature Profiles. Based on the seven rules derived above, the location of the operating point within the $\dot{V}_{min}$ diagram and thus expected components in the product streams can be derived based on temperature profiles. The only information that is needed in advance are the feed composition, corresponding invariant pinch temperatures and their expected location (upper or lower column part). This information can easily be obtained from a flowsheet simulator by fixing different combinations of $\dot{V}/\dot{F}$ and $\dot{D}/\dot{F}$, and using a column model with many stages (many stages mean that pinches are clearly visible). The choice of combinations can either be random or done in a more sophisticated manner based on the $\dot{V}_{min}$ diagram of the mixture. In the first case, after every simulation, the product compositions have to be checked. Then, in order to guarantee an operation below the $\dot{V}_{min}$ border and not above, $\dot{V}/\dot{F}$ or $\dot{D}/\dot{F}$ have to be changed and it can be observed whether the pinch temperatures change or not. If one pinch does not change, then this is the invariant one for the considered area. With the invariant pinch temperatures and the seven rules, the profiles can be analyzed.

To illustrate the procedure, quaternary mixture 1 (ABCD) is separated in a distillation column with $N = 30$ and $N_F = 15$. The feed stream is equimolar and saturated liquid. First, the $\dot{V}_{min}$ diagram was obtained on a short-cut basis. The K-values of the feed mixture were determined in Aspen Plus to be [2.31, 0.98,



(a) $\dot{D}/\dot{F}=0.52, \dot{V}/\dot{F}=0.72$

(b) $\dot{D}/\dot{F}=0.3$, Original $\dot{V}/\dot{F}=0.8$, Reduced $\dot{V}/\dot{F}=0.55$



(c) $\dot{D}/\dot{F}=0.2, \dot{V}/\dot{F}=0.3$

(d) $\dot{D}/\dot{F}=0.25, \dot{V}/\dot{F}=0.7$

Figure 13. Temperature profiles for the quaternary mixture 1 operated in four different regions. N = 30, N_F = 15.

0.42, 0.29]. Figure 12 shows the resulting $\dot{V}_{\min}$ diagram. Next, for each region in the $\dot{V}_{\min}$ diagram, one operating point is simulated rigorously in Aspen Plus. If the operating point within the region is changed, one pinch temperature stays constant, which is thus the invariant pinch temperature. The resulting invariant pinch temperatures for the example mixture are also given in Figure 12. Additionally, the locations of the pinches is given. It can be observed that the invariant pinches are always located in the upper column part if all of the feed components are obtained in the bottom product. And vice versa, if all feed components are obtained in the top product, then the invariant pinch is located in the lower column part.

Next, to illustrate the use of the rules, temperature profiles for four random combinations of $\dot{V}_B/\dot{F}$ and $\dot{D}/\dot{F}$ with a finite number of stages (N = 30, N_F = 15) were generated, which are shown in Figure 13. Based on the profiles and the rules, in combination with the invariant pinch information from Figure 12, the corresponding operating region and thus the resulting components in the product streams can be identified.

4.4.1. Figure 13a. There is a pinch above the feed stage; thus, according to rule 5, all components are present in the top product. In the lower column part, there is a pinch around 126 °C, which is close to two invariant pinches (rule 4). However, both have components B, C, and D in the bottom stream, and in combination with the known top composition, it is concluded that the operation is located in region ABCD-BCD.

4.4.2. Figure 13b. Consider first the solid line, which is the original profile. There are two pinches in the middle top and bottom part of the column with temperatures 102 and 122 °C. These temperatures are not invariant pinch temperatures, so the column is operated in an overpurification region above the $\dot{V}_{\min}$ borders. However, as both pinches are not located next to the feed stage, one or more components disappear from the top and also from the bottom product (rule 6). In order to determine in which region the column is operated, the energy input $\dot{V}/\dot{F}$ is reduced, as shown by the dashed line. Then, a pinch of around 95 °C appears in the upper column part and one directly below the feed stage. Thus, the new point is in region AB-ABCD and the original case, without a pinch at the column top end, is in region AB-BCD.

4.4.3. Figure 13c. In the lower column part, there is a pinch below the feed stage; thus, all components are present in the bottom product. In the upper column part, the profile is almost linear between relative heights of 0.5 to 0.8. This is an indication that there are two additional pinches affecting the profile. Thus, the column is operated close to a border between two regions (rule 2). Based on rule 3 the approximate temperatures of the pinch residues help in locating the border. The slope increase in temperature around 105 to 109 °C is above the feed stage; thus, the operating point is close to the border between ABC-ABCD and ABCD−ABCD. Additionally, the pinch in the lower column part is significantly longer than the one in the upper column part; thus, according to rule 7, the feed stage is nonoptimal. However, as it does not really make sense to perform such a separation in a real plant, this is not evaluated further here.

4.4.4. Figure 13d. There is a pinch at the column top; thus pure A is expected in the top product (rule 1). Additionally, in the upper and lower parts of the column, there are regions with almost linear decreasing temperatures, which is an indication of two more pinches. Moreover, below the feed stage, a pinch residue is visible. Overall, there are 4 pinches, and thus the separation is a minimum energy operation for the given number of stages. To conclude, as the profile in the upper column part has a distortion in the direction of 95 °C, the profile is located in the A-BCD separation region. Additionally, as the pinch visibility is similar in the upper and lower parts of the column, the feed stage seems to be close to optimal (rule 7).

5. DISCUSSION ON GENERALIZATION OF RESULTS

This article emphasizes the importance of understanding temperature profiles of distillation columns because it can be used to draw conclusions about the column performance and operating point. As the authors are not aware of a similar publication in this context, first, a basic understanding for rather simple standard scenarios had to be generated. For this reason, the results were restricted to a normal distillation column without pressure drop, with one feed stream, two product streams, and without side condenser or reboiler was assumed. The feed mixture was chosen to consist of two or more components, be zeotropic, rather ideal, and saturated liquid. Note that the presented rules were derived based on these assumptions. Although we are certain that the rules can be applied in a broader context, they also need to be validated and extended considering the following aspects:

- The impact of the feed state. Note that this also leads to a change in energy demand of the separation.
- The impact of side condensers and reboilers.
- The impact of additional feed streams.
- Multicomponent mixtures with nonideal but still zeotropic subsystems (e.g., with tangent pinches).
- Azeotropic mixtures. Rule 1, for example, would still be applicable, but the pinch at the column end would then indicate a pure azeotropic mixture instead of a pure component in the product.
- The impact of pressure drop in the column. This affects the boiling temperature of the mixture. It may happen that there is a composition pinch but no more a temperature pinch. Nevertheless, slope changes in the profiles are still observable and pinch zones can still be sensed. One approach may be to make a pressure correction on the temperatures prior to the analysis.
- General rule for location of invariant pinches for mixtures with five or more components.
- The impact of control structure selections.

Evaluating all of these points exceeds the scope of this paper. However, the authors strongly recommend that more research be performed in this area to close this highly relevant gap in distillation theory to enhance the practical applicability further.

6. CONCLUSIONS

Temperature profiles provide important information to interpret the operation of a distillation column. This work gives a comprehensive overview of temperature profiles and how they can be used. The knowledge about pinch points at an infinite number of stages contributes to the understanding of the column profiles also with a finite number of stages, as the temperature profiles still strive in the direction of the pinches. Correspondingly, slope changes in the temperature profile indicate a pinch location without the pinch being fully developed. Seven simple rules are derived to interpret the pinches properly, which are summarized here again:

- Rule 1. A constant temperature zone (pinch zone) at a column end (top or bottom) indicates an almost pure component in the corresponding product. This pinch zone is observable independently of the total number of stages.
- Rule 2. The top and bottom sections can each have a maximum of two pinch zones at the same time. The appearance of two pinches in the same section means that the section is operated at minimum energy. If only one pinch is visible in a section, the product is either over- or underpurified.
- Rule 3. At the boundaries between neighboring operating regions, i.e. along the minimum energy lines, the location of pinch zones are the same as in the adjacent regions.
- Rule 4. There is an "invariant" pinch temperature when operating at minimum energy or less, which does not change when varying the operating point within the given region of the diagram. The invariant pinch can be observed in the upper part (e.g., if all components are in the bottom product) or the lower part of the column. If all components are present in both product flows, the invariant pinch is above and below the feed stage and has the feed boiling temperature.
- Rule 5. A pinch only on one side of the feed stage means, that all components are present in the product stream at the corresponding column end. In this case, the pinch temperature does not equal the feed boiling point.
- Rule 6. The pinch at the feed stage moves away from the feed and toward the middle or end of the section when one or more components disappear from the corresponding product stream.
- Rule 7. A clearly visible pinch in one section in combination with a poorly visible one in the other section is an indication for a nonoptimal feed stage.

The usefulness of the rules was demonstrated for a quaternary separation with a finite number of stages First, the invariant pinch temperatures are determined by simple simulations. Then, in combination with the seven rules, the temperature profiles are analyzed and it can be determined which components are expected in which product stream. This information gives the region location within the $\dot{V}_{\min}$ diagram, and this information can finally be used in order to enhance the column operation, if necessary.

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■ ABBREVIATIONS

Variables

α	Relative volatility
$\dot{B}$	Molar bottom product flow
$\dot{D}$	Molar top product (distillate) flow
$\dot{F}$	Molar feed flow
i	Stage number
k	Number of components in the feed stream
N	Number of theoretical stages
n	Relative column height
q	Liquid fraction of feed
$\dot{Q}$	Reboiler duty
T	Temperature
t	Normalized temperature
$\dot{V}$	Molar vapor flow
x	Molar liquid fraction
y	Molar vapor fraction

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b	Boiling
B	Bottom
F	Feed
LB	Component with lowest boiling point in feed mixture (light boiler)
HB	Component with highest boiling point in feed mixture (high boiler)
LK	Low boiling key component
HK	High boiling key component
min	Minimum
T	Top

■ REFERENCES

(1) Stichlmair, J.; Klein, H.; Rehfeldt, S. *Distillation: Principles and Practice*, 2nd ed.; Wiley-AIChE, 2021.

(2) Fitzmorris, R. E.; Mah, R. S. H. Improving distillation column design using thermodynamic availability analysis. *AIChE J.* **1980**, *26* (2), 265−273.

(3) Górak, A.; Schoenmakers, H. *Distillation: Operation and Applications/edited by Andrzej Gorak, Hartmut Schoenmakers*; Academic Press, 2014.

(4) Rose, L. M. *Distillation Design in Practice; Computer-aided Chemical Engineering*; Elsevier, 1985; Vol. *1*.

(5) Mccabe, W. L.; Thiele, E. W. Graphical Design of Fractionating Columns. *Ind. Eng. Chem.* **1925**, *17* (6), 605−611.

(6) King, C. J. *Separation Processes*, 2nd ed.; *McGraw Hill chemical engineering series, mcc*; McGraw Hill, 1980.

(7) Seader, J. D.; Henley, E. J. *Separation Process Principles*, 2nd ed.; Wiley, 2006.

(8) McCabe, W. L.; Smith, J. C.; Harriott, P. *Unit Operations of Chemical Engineering*, 4th ed.; *McGraw-Hill chemical engineering series*; McGraw-Hill, 1985.

(9) Dejanović, I.; Matijašević, L.; Halvorsen, I. J.; Skogestad, S.; Jansen, H.; Kaibel, B.; Olujić, Ž. Designing four-product dividing wall columns for separation of a multicomponent aromatics mixture. *Chem. Eng. Res. Des.* **2011**, *89* (8), 1155−1167.

(10) Halvorsen, I. J.; Skogestad, S. Distillation Theory. In *Encyclopedia of separation science*; Wilson, I. D., Ed.; Elsevier, 2000; pp 1117−1134.

(11) Shiras, R. N.; Hanson, D. N.; Gibson, C. H. Calculation of Minimum Reflux in Distillation Columns. *Ind. Eng. Chem.* **1950**, *42* (5), 871−876.

(12) Halvorsen, I. J.; Skogestad, S. Minimum Energy Consumption in Multicomponent Distillation. 1. Vmin Diagram for a Two-Product Column. *Ind. Eng. Chem. Res.* **2003**, *42* (3), 596−604.

(13) Halvorsen, I. J.; Skogestad, S. Minimum Energy Consumption in Multicomponent Distillation. 2. Three-Product Petlyuk Arrangements. *Ind. Eng. Chem. Res.* **2003**, *42* (3), 605−615.

(14) Halvorsen, I. J.; Skogestad, S. Minimum Energy Consumption in Multicomponent Distillation. 3. More Than Three Products and Generalized Petlyuk Arrangements. *Ind. Eng. Chem. Res.* **2003**, *42* (3), 616−629.

(15) Górak, A.; Sørensen, E., Eds. *Distillation: Fundamentals and Principles*; Academic Press, 2014.

(16) Ränger, L. M.; Preißinger, U.; Grützner, T. Robust Initialization of Rigorous Process Simulations of Multiple Dividing Wall Columns via V_{min} Diagrams. *ChemEngineering* **2018**, *2* (2), 25.

(17) Ränger, L. M.; Grützner, T. Shortcut Method for Initialization of Dividing-Wall Columns and Estimating Pareto-Optimal NQ -Curves. *Chem. Eng. Technol.* **2021**, *44* (10), 1919−1928.

(18) Bortz, M.; Burger, J.; Asprion, N.; Blagov, S.; Böttcher, R.; Nowak, U.; Scheithauer, A.; Welke, R.; Küfer, K. H.; Hasse, H. Multi-criteria optimization in chemical process design and decision support by navigation on Pareto sets. *Comput. Chem. Eng.* **2014**, *60*, 354−363.

(19) von Kurnatowski, M.; Bortz, M.; Scherrer, A.; Hoffmann, A.; Lorenz, H.-M.; Caraucan, M.; Grützner, T.; Künzle, N.; Küfer, K. Multi-criteria Optimization of an Industrial World-Scale Process. *Chem. Ing. Technol.* **2017**, *89* (11), 1471−1478.

(20) Ränger, L.-M. *Multi-Objective Optimization of Simple and Multiple Dividing Wall Columns and their Operational Flexibility Close to the Optimum*, Universität Ulm, 2021.

(21) Maxwell, J. B. *Data Book on Hydrocarbons:Application to Process Engineering*; Van Nostrand, 1950.

(22) Zhicai, Y.; Di, W.; Zhaoxia, Y.; Ronglan, Z. Evolution of Pinch-Point Zones in Multicomponent Distillation Columns. 1. Rectifying Section. *Ind. Eng. Chem. Res.* **1996**, *35* (8), 2777−2781.

(23) Halvorsen, I. J. Minimum Energy Requirements in Complex Distillation Arrangements. Ph.D. Thesis, Norwegian University of Science and Technology, Trondheim, Norway, 2001.