Energy saving potential of dividing wall columns identified by $N\dot{Q}$-curves

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Abstract. Dividing wall columns are a promising intensified distillation option for the energy-efficient separation of ternary mixtures. This work aims to quantify their saving potential considering optimal compromises between the total stage number N and energy demand $\dot{Q}$. For this purpose, bi-objective optimizations are performed for different mixtures, purity requirements and feed stream compositions separated in a dividing wall column and compared to results of a conventional direct split sequence. It is found that the resulting Pareto-fronts intersect. This arises from the fact that dividing wall columns require less energy at high stage numbers but the conventional sequences have a lower minimum stage number. In order to quantify this behavior, the dimensionless Decision Number *DN* is introduced and calculated for several cases. The results give a broader insight into the saving potential of dividing wall columns as such an analysis has not been performed systematically yet.

Keywords Distillation, Dividing Wall Column, Optimization, Pareto-optimal, Energy saving

Introduction

Distillation is widely used in chemical industry to separate multi-component mixtures [1]. As it is also energy intensive, it is responsible for a large amount of the global total energy consumption [2]. Thus, more energy efficient distillation processes are highly relevant in order to reduce global warming. One approach to reduce the energy consumption is to use intensified distillation columns called dividing wall columns as shown in Fig. 1b. In the figure the letters A, B and C indicate different components sorted according to their boiling points, where A is the light boiling component. Dividing wall columns are able to separate ternary mixtures into pure products in only one column shell [3]. Usually, ternary mixtures are separated in a sequence of two conventional distillation columns as shown in Fig. 1a. However, in the first column the middle boiling component is remixing with the feed stream resulting in an inefficient separation. In dividing wall columns this remixing is avoided and consequently up to 30 % of energy can be saved [4].

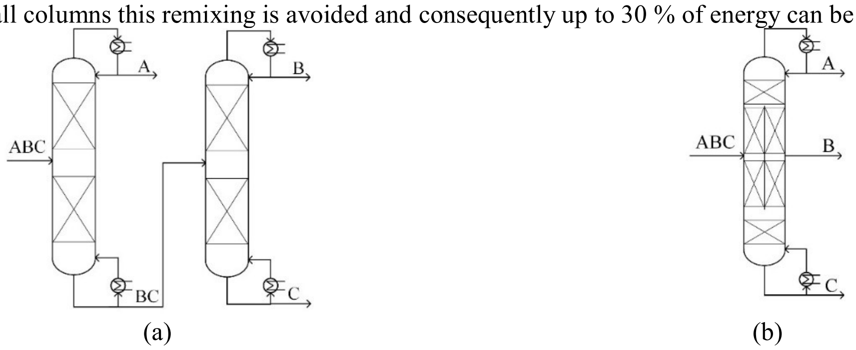


Fig. 1: Two Distillation options for the separation of ternary mixtures. (a) Direct split sequence and (b) dividing wall column.

The optimal design of distillation columns for given product specifications is a bi-objective problem having the reboiler duty/reflux ratio and total stage number as objectives [5]. Correspondingly, there are several Pareto-optimal design options which makes a comparison of different distillation options difficult. In order to anyway quantify the energy saving potential of dividing wall columns often a combined objective function called total annualized costs (*TAC*) is determined and used for comparison with conventional distillation options [6]–[8]. The total annualized costs consider operational and capital costs [9]. The operational costs are mainly affected by the required energy demand, respectively the reboiler duty or reflux ratio, whereas the capital costs are affected by the size of the heat exchangers, the column diameter and height and the internals. The size of the heat exchangers and column diameter are again depending on the required reboiler duty and are thus correlated to the operational costs, correspondingly the only significant

independent capital cost parameter is the height of the column which is given by the required number of theoretical stages. Note that in this contribution the total stage number of dividing wall columns is defined as the sum of stages in all sections, thus for the dividing wall column stages on both sides of the dividing wall are included.
The reformulation of the actually bi-objective problem into a simplified one that expresses the total costs has two main disadvantages. First, different approaches for the calculation of the costs are used in literature and thus the results of different authors are hardly comparable. Second, empirical weightings are combined with the actual objectives prior to the optimization. This simplification is done without knowledge about the effect of the used parameters on the output. Why this could affect the results is explained in the result section of this contribution.
The objective of this contribution is to present a method which quantifies the energy saving potential of dividing wall columns considering $N\dot{Q}$-curves. For this purpose, optimal compromises between the total stage number and the energy demand of distillation columns are evaluated. The procedure is then used to compare the dividing wall column with the conventional direct split sequence.
The following section briefly summarizes the applied methodology and used test mixtures, afterwards results of the performed study are presented.

Methodology

Computational framework

Flowsheet simulations are performed in Aspen Plus V11. For the simulations of column sequences the *RadFrac* model is used, for the dividing wall column the *MultiFrac* model *Petlyuk* is applied. The simulation specifications for the column models are set up and evaluated in Excel, which communicates with Aspen Plus via the ActiveX interface. The optimization problem is also defined in Excel. A bi-objective problem minimizing the energy demand $\dot{Q}$ and total stage number N inside the columns is used in this work. The total stage number is the sum of the stages in each column section, thus for the dividing wall column stages operated in parallel on both sides of the dividing wall are counted separately. As variables the stages in all column sections (thus feed and product stages are included), reboiler duties and the product flows are varied. For the dividing wall column, additionally the liquid and vapor split ratios at the dividing wall are to be considered. Constraints are used on the molar purity of each component in its related product stream.
The multicriteria optimization is performed with an adaptive scalarization scheme provided by the Fraunhofer ITWM [10],[11] using a MISQP solver [12]. Constraints are handled with penalty terms in the objective function. For more details the reader is referred to the literature [10],[11],[13].

Test mixtures

Four ternary mixtures with a feed flow of 3 kmol/h in liquid boiling state are investigated in this study. The mixtures are summarized in Table 1. Additionally, the distribution coefficients K_i of the components in an equimolar mixture are given and the resulting ease of separation index, which is defined according to equation (1) [14].

$$ESI = \frac{K_A \cdot K_C}{K_B^2} \tag{1}$$

Table 1. Ternary mixtures investigated in this work, distribution coefficients are valid for an equimolar feed stream.

Mixture	Component A	Component B	Component C	K_A	K_B	K_C	ESI
M1	Benzene	Toluene	*p*-Xylene	1.91	0.73	0.33	1.08
M2	Hexane	Heptane	Octane	1.79	0.87	0.34	0.82
M3	Methanol	Ethanol	*n*-Butanol	1.79	0.99	0.21	0.39
M4	*n*-Butane	2-Methylbutane	*n*-Pentane	1.84	0.65	0.50	2.15

Results and Discussion

In the following section, first the results of the bi-objective optimization runs are presented. Afterwards, a methodology is introduced to quantify the found behavior which results in the dimensionless Decision Number *DN*. Last, the Decision Number is calculated for the four mixtures, different product purity specifications and feed stream compositions.

Pareto-optima of dividing wall column and direct split sequence

Fig. 2 shows the results of the bi-objective optimizations of the four mixtures in a dividing wall column and direct split sequence, considering at least 95 mol% purity of each product. Details about the calculation can be found elsewhere [13].

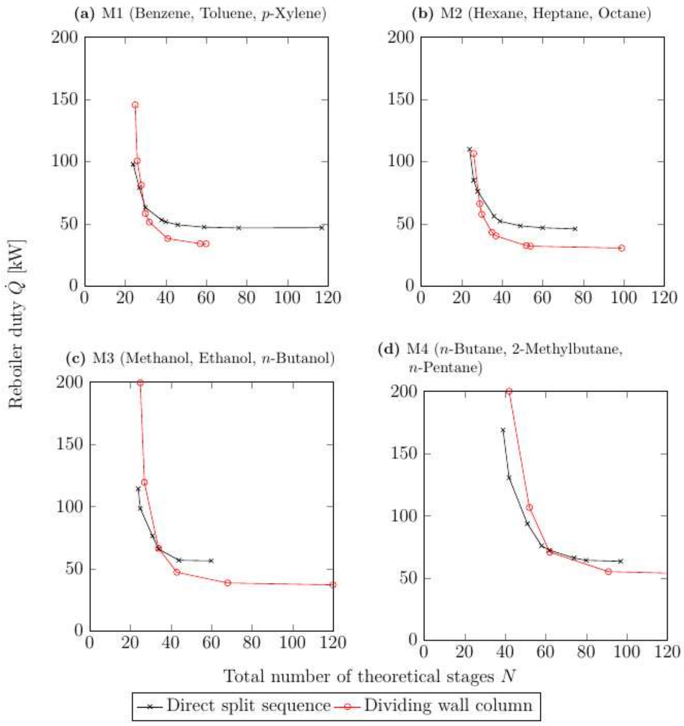


Fig. 2: *NQ*-optima of the four test mixtures in a direct split sequence and dividing wall column.

It can be observed that the Pareto-fronts of dividing wall column and direct split sequence intersect for all four systems. This arises from the fact that the direct split sequence requires a lower minimal stage number while the dividing wall column has a lower minimal energy demand. The location of the intersections seems to depend on the mixture, in Fig. 2b it is close to the minimal stage number and in Fig. 2d close to the minimal energy demand.

At this point it gets clear why the use of different total cost function for comparison of distillation options can be problematic. If the result from a single-objective cost optimization is at a relatively high stage number, the savings of dividing wall columns are in the stated range of 30 %. However, if different weightings are used to determine the cost function and the result is located in the region of the strongest curvature of the Pareto-fronts, the savings of dividing wall columns seem significantly lower, even though exactly the same separation task is evaluated. Therefore, the meaningfulness of such cost optimizations is limited. In order to avoid this problem, the following paragraph aims to quantify the location of the intersection of the Pareto-fronts to enable a more reliable comparison of the saving potential of dividing wall columns.

Quantification of intersection location with Decision Number

Fig. 3 shows a scheme of two intersecting Pareto-fronts of process option *i* and *j*, for the presented example the index *i* relates to the dividing wall column (DWC) and *j* to the direct split sequence (DSS). Additionally, the subscript *is* relates to the intersection location and *min* to the minimal value of one objective. To quantify the location of the Pareto-front intersection, the Decision Number *DN* is introduced, which is defined according to equation (2) [13].

$$DN = \frac{A_2 - A_1}{A_1 + A_2} \tag{2}$$

It relates the areas A_1 and A_2 between the Pareto-fronts on both sides of the intersection to each other. Correspondingly, the *DN* has a value between -1 and 1. At 1 and -1 there is no intersection of the Pareto-fronts, thus at $DN = 1$ option *i*, in this case the dividing wall column, totally dominates option *j*, the direct split sequence, and vice versa at $DN = -1$.

A *DN* which is not equal to 1 or -1 always means that both options (and not just one) have a region where they are more favorable than the other option. For a *DN* close to 1 there is only a small area for which the DSS is beneficial over the DWC. However, for a much larger area the DWC dominates. At $DN = 0$ the areas on both sides of the intersection are similar, thus both options are equally suitable in the bi-objective space. Then, if a column with high stage numbers is to be built, the dividing wall column requires less energy and if a column with low stage numbers should be used the conventional sequence is the better option. Generally, positive *DN*s indicate, that the dividing wall column is more beneficial over the whole feasible range; negative values show that the conventional sequence is preferred overall.

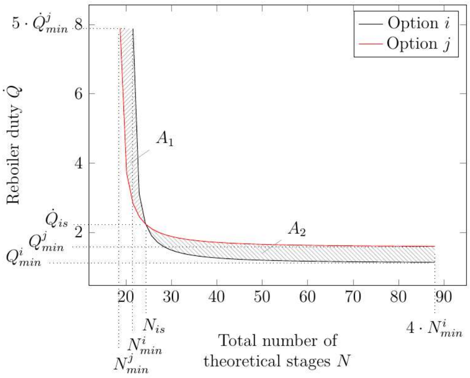


Fig. 3. Nomenclature used for the calculation of the Decision Number *DN*.

To calculate the areas A_1 and A_2, integration boundaries have to be defined. Area A_2 is integrated in *x*-direction between the intersection at N_{is} and $4 \cdot N^i_{\min}$, which approximates an infinite stage number [15]. Area A_1 is integrated in *y*-direction between the intersection at $\dot{Q}_{is}$ and $5 \cdot \dot{Q}^j_{\min}$, which is chosen based on the optimization results [13]. The Decision Number can be calculated by a full integration between the calculated Pareto-fronts, however this is quite time consuming. As a simplification, equation (4) is introduced, which uses the relative location of the intersection according to equation (3). For a detailed derivation of these equations the reader is referred to literature [13].

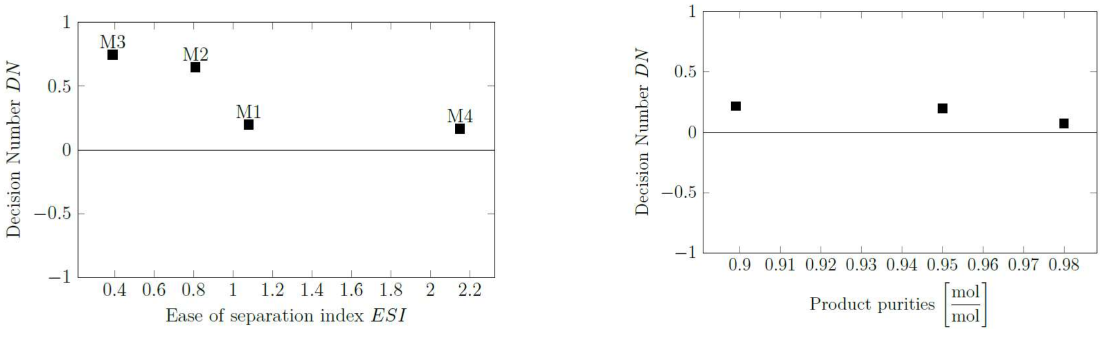
$$\dot{Q}^k_{rel,is} = \frac{\dot{Q}_{is}}{\dot{Q}^k_{\min}} \quad \text{and} \quad N^k_{rel,is} = \frac{N_{is}}{0.97 \cdot N^k_{\min}} \tag{3}$$

$$DN \approx \frac{\ln\left(\left|\frac{\dot{Q}^{DSS}_{rel,is} - \dot{Q}^{DWC}_{rel,is}}{N^{DSS}_{rel,is} - N^{DWC}_{rel,is}}\right|\right) - 0.35}{2.7} \tag{4}$$

Dependence of Decision Number on mixture, product purity and feed composition

In this section equation (4) is applied to determine the Decision Number for different cases. First, Fig. 4a shows the *DN* depending on the *ESI* of the mixtures from Table 1 with an equimolar feed stream and for 95 mol% pure products. These results are based on the Pareto-fronts from Fig. 2. In all cases the *DN* is positive thus overall the dividing wall column is better suited in a large range. The highest saving potential is observed for systems with low *ESI*s, which is valid for mixtures with a more difficult AB than BC separation. Nevertheless, the saving potential decreases with an increasing *ESI*. Correspondingly, for mixtures with high *ESI*s the dividing wall column only has a guaranteed saving potential at high total stage numbers. An opposite trend is found for the dividing wall column in comparison to the indirect split sequence, the corresponding diagram can be found elsewhere [13]. Thus, in comparison to both conventional column sequences, the lowest saving potential of dividing wall columns is observed for mixtures with *ESI*s of 1. With increasing or decreasing *ESI*s the saving potential increases.

Fig. 4b shows the development of the *DN* for an equimolar mixture M1 separated to different product purities, which means that all three components should obtain a certain molar fraction in their corresponding product flow. The *DN* decreases slightly for increasing product purities. However, the effect is rather small.



(a) (b)

Fig. 4. Decision Number comparing direct split sequence and dividing wall column for an equimolar mixture of (a) M1 to M4 at 95 mol% product purities and (b) M1 at different product purities.

Last, Fig. 5 shows the *DN* for mixture M1 reaching 95 mol% pure products assuming different feed stream compositions. Black dots in the diagram indicate the evaluated feed stream compositions. Note that the upper borders of the compositions in these investigations are at 80 mol%, thus the ternary diagram is not filled in the fringe. At 80 mol% of component B the dividing wall column totally dominates the direct split sequence, the other way around can be observed at high fractions of component A. Interestingly, a much less pronounced decrease of the *DN* is observed when the molar fraction of B is decreased while increasing the fraction of component C. In this range the indirect split sequence might be a better option than the direct sequence [16]. Thus, the *DN* comparing dividing wall column and the less suitable direct split sequence does not decrease further if the fraction of component C in the feed stream is increased.

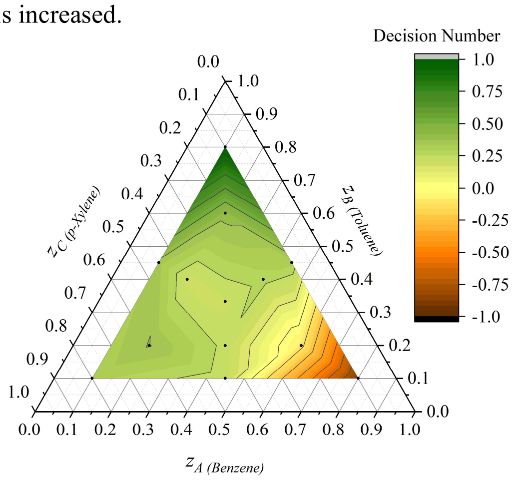


Fig. 5. Decision Number comparing direct split sequence and dividing wall column for mixture M1 in different compositions with 95 mol% product purities.

Summary and Outlook

In this contribution a new approach to evaluate the energy saving potential of dividing wall columns in comparison to conventional distillation options is presented. The approach is tested comparing the dividing wall column with the direct split sequence. For this purpose, first bi-objective optimizations considering the total stage number and the reboiler duty as objectives are performed for the two column versions. It is observed that the Pareto-fronts of the two distillation options intersect, thus none of them totally dominates the other in the bi-objective space. The dimensionless Decision Number *DN*, which can be calculated by a semi-empirical approach, is introduced to quantify this behavior. For the considered test mixtures, it is observed that the *DN* decreases with increasing an Ease of Separation Index *ESI* of the feed stream and increasing product purities. Additionally, it is shown that the *DN* is depending on the feed stream composition. However, the conclusion that increasing fractions of the middle boiling component are always beneficial for dividing wall columns is not totally true. Starting from mixtures with a high amount of the heavy boiling component C, the *DN* increases much weaker if more of the middle boiling component B is added than when starting from a mixture with much of the light boiling component A.

Overall, the *DN* is a simple tool to support the first rough design decision between suitable distillation variants with regard to their energetic suitability. In this work, it was calculated to estimate the savings potential based on results of an optimization. However, it can alternatively be combined with other shortcut approaches that have been published elsewhere [13]. Then, the *DN* can even be calculated only on the basis of feed stream properties and identify the best distillation variant without time-consuming calculations.
In future, first the presented studies should be performed in more detail. The impact of the product purity has to be evaluated further, also a comparison of the dividing wall column with the indirect split sequence and eventually heat integrated distillation options should be performed. Afterwards, the *DN* should be applied to evaluate the saving potential of multiple dividing wall columns that are able to separate quaternary mixtures into pure components [17].

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