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SEPARATIONS: MATERIALS, DEVICES AND PROCESSES

Influence of Heat Transfer Across the Wall of Dividing Wall Columns on Energy Demand

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The implementation of a vertical dividing wall (DW) into a distillation column is a well-known concept which can result in considerable energy savings for the separation of multicomponent mixtures. It is commonly known that heat streams across the DW, which are present due to temperature differences between both sides, may either increase or decrease the energy demand for a certain separation task. However, no work has been published so far which explains the maximum influence on energy demand. This article derives the maximum extent to which the minimum energy demand for a given column design can change due to heat transfer across the DW. Additionally, it is illustrated how energy-efficient column operation can be assured even if the total amount of transferred heat is unknown. These results show that the phenomenon of heat transfer across the DW can be handled very well with a suitable control strategy. © 2015 American Institute of Chemical Engineers *AIChE J*, 61: 1648–1662, 2015
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Introduction

Dividing wall columns (DWCs) are a special type of distillation column which contains a vertical partition of the column shell. The presence of such a vertical partition allows to create three or four pure fractions in one distillation column.[1] Without a dividing wall (DW), this task will fail already for a three-component mixture, if only one distillation column is used. In that case, it is not possible to keep the side stream free from both the light and the heavy component with a justifiable energy input. Thus, the DWC can be understood as a combination of at least two conventional distillation columns. For the separation of a three-component mixture, Figure 1 shows a schematic comparison of a DWC and a direct sequence of conventional distillation columns. It is obvious that the DWC case exhibits a reduced number of both column shells and heat exchangers. This, of course, can lead to a considerable reduction of investment costs. In their paper about the industrial application of distillation columns, Kaibel et al.[2] state that DWC technology allows to reduce the investment costs by around 30% in comparison with conventional distillation sequences. Additionally, if designed and operated in a sensible manner, DWCs also have the advantage of consuming less energy than a sequence of conventional distillation columns. Triantafyllou and Smith[3] give an illustrative explanation about the reason for this. If a three-component mixture is separated in a sequence of two conventional distillation columns without side streams, the first column will include a region where the concentration of the middle-boiling component "reaches a peak" before being lowered again toward the end of the column due to remixing effects.[3] In DWCs, these remixing effects can be avoided which is one reason why DWC have the potential to consume less energy for the same separation task.[3] Both the reduction of investment costs as well as the reduction of energy demand make DWCs an interesting alternative to conventional schemes.

The concept of placing a DW as a vertical partition inside of distillation columns has long been known.[4,5] The first patent in this respect was applied for nearly 80 years ago. However, within these early publications, mainly the first advantage of DWC technology is emphasized: the reduction of process equipment in comparison with conventional distillation schemes. One of the first-scientific papers dealing with the second advantage, the reduction of energy demand, was published by Petlyuk et al. in 1965.[6] They use the Underwood equations[7] to calculate the minimum energy demand of DWCs. The authors show that for the separation of a three-component mixture, the minimum energy demand needed by a DWC equals the minimum energy demand needed for the more difficult of the two binary separations.[6] Obviously, this implies a huge potential for energy savings. For high fractions of the middle-boiling component within the feed stream, Petlyuk et al.[6] show that the minimum energy demand for the DWC case might be only 50% of the minimum energy demand needed for a conventional scheme.[6] However, despite these impressive findings, it was not before 1985 that the first-industrial DWC was put in use.[2,8] As then, many different applications of the DWC concept have been reported. Recent publications provide a comprehensive overview about the industrial applications of DWC technology.[8–11] Regarding the high number of industrial applications mentioned there, one is tempted to agree with Kaibel[10] in describing DWCs as having "fully developed to a standard type of distillation column." However, compared with the vast amount of conventional distillation columns, the total number of DWC used in industrial processes is still small.

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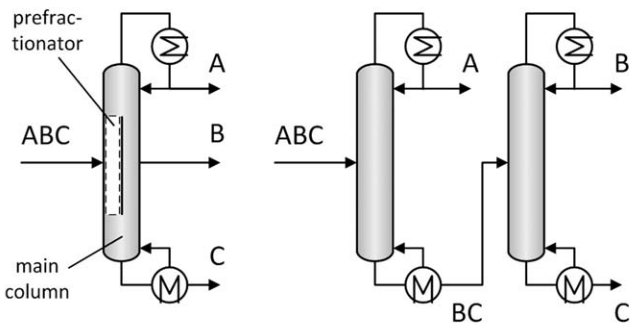


Figure 1. Schematic comparison between DWC (left) and direct distillation sequence (right) for the separation of three components A, B, C.

Why are there still so many industrial processes in which conventional distillation columns are applied but no DWCs? One explanation might be that there are too many restrictions connected with this technology which prevent a more profound use of this concept. In his book about chemical process design, Smith[12] lists common disadvantages of DWC technology which arise as a direct consequence of the process integration step. First, one looses the freedom to choose either different pressures or different materials of construction for each binary separation. Second, one is forced to supply all of the heat at the highest temperature and to reject all of the heat at the lowest temperature present in the system. Third, when designing a DWC, one is forced to choose the column internals on either side of the wall in such a way that the desired vapor split (VS) at the bottom of the DW can be reached.[12] Without doubt, these limitations have to be considered when DWC technology is taken into account as an alternative for conventional distillation schemes. We, however, are convinced that these limitations do not constitute a hurdle which fundamentally prevents a more profound application of the DWC concept in industrial processes than can be seen today. Thirty years after the first-industrial application of a DWC, our experience rather shows that many potential users are still uncertain about whether this column type can really be reliably operated such that considerable energy savings are possible.

How can such an uncertainty be explained? First, one has to point out that for both the design and the precise operation of DWC, more technical knowledge is needed than for the case of conventional distillation columns. Wrong DWC operation (esp. improper choice of the vapor and liquid split (LS) at the DW) causes that the full potential of energy savings cannot be reached. As shown in this article, improper values for the internal split at the DW can even result in an energy demand being twice or three times as big as the energy needed for a sequence of conventional distillation columns. A further reason having the potential to cause uncertainties for potential users of DWC technology is related to the main topic of this article, which is the heat transfer across the DW.

In most of the simulation studies published about DWCs, the heat transfer across the DW was neglected in the past. It is, however, a fact that temperature differences between both sides of the DW will induce heat streams across this wall for basically every DWC. In 1994, Lestak et al.[13] published an article showing simulation results for the separation of a three-component mixture with a DWC. They showed that the energy demand of the column that was needed to reach desired product purities was strongly affected by the heat transfer across the DW. For one case, they observed that the heat duty of the reboiler had to be considerably increased compared to the case without heat transfer. There, the required increase of the reboiler heat duty was more than three times higher than the heat stream that was transferred across the wall. Based on these findings, they concluded that a “small horizontal heat transfer” can induce the need of a “much larger” increase in reboiler heat load in DWCs.[13]

The article of Lestak et al.[13] is still regularly being cited, when it comes to the influence of heat transfer across the wall on the energy demand of DWC.[10,14,15] However, up to now, no additional scientific work has been published that aims to find out why Lestak et al.[13] did observe such a strong effect on energy demand. A scientific publication deriving the maximum influence the heat transfer can have on the energy demand of a DWC is likewise missing. Thus, everyone being interested in DWC technology is faced with an ambivalent situation. A lot of different scientific paper, of which only some are referenced here, have been published that emphasize the ability of DWC to save a considerable amount of energy (typically around 30%) compared with conventional distillation columns.[3,6,16–19] Conversely, Lestak et al.[13] show a 10% rise in energy demand when heat transfer across the wall is considered. Up to now, it has not been cleared whether this is a typical value or if an even higher increase can be expected for certain cases. It is obvious that this ambivalent situation has the potential to create uncertainty when the use of DWCs within industrial processes is considered.

This article, therefore, has two main objectives. First, it is supposed to causally explain the influence of heat transfer across the wall on energy demand of DWC. Based on that, general limits about the influence of this heat transfer on energy demand are to be derived. Second, the article aims to show how energy-efficient operation of DWCs is possible with heat transfer being present between both sides of the wall. By showing that the phenomenon of heat transfer across the DW can be handled very well with a suitable strategy, we want to reduce existing uncertainties and encourage more people of the chemical engineering community to consider the use of DWC within their processes to reduce the energy demand.

To reach these objectives, our article consists of four main parts. First, the strong influence of internal distribution ratios of vapor and liquid streams at the DW on the overall energy demand of DWC is demonstrated for the case without heat transfer across the wall. Next, the reasons for this sensitivity are explained in detail to provide a profound understanding of DWC behavior. After that, a hypothesis is derived on how the overall energy demand of DWCs can be maximally affected by additional heat streams. Remarkably, this hypothesis is derived solely by carrying out a thought experiment. In the third-main chapter, another hypothesis is derived. This one predicts how energy-efficient operation can be assured for DWCs even if the total amount of heat transfer across the wall is unknown. Finally, a simulation study is presented that confirms the validity of both hypotheses derived in the preceding sections.

Understanding the Behavior of DWCs

As mentioned earlier, to determine an energy-efficient point of operation for DWC, more technical knowledge is needed than for the case of conventional distillation columns. When both the column design (i.e., feed location, number of stages, pressure, etc.) and the mass flows of the feed and product streams are given for a conventional column, typical

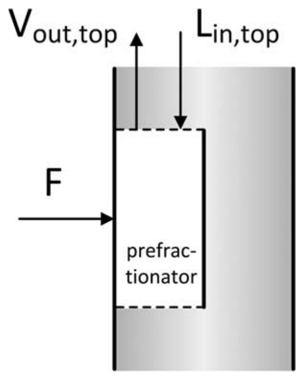


Figure 2. Material streams being used in Eqs. 1 and 2.

simulation models give exactly one reboiler duty that is needed to assure a certain product purity. For DWCs, however, a different picture is obtained. Let us assume that with the use of an equilibrium stage (EQ) model, we have the task to find an energy-efficient operating point for a DWC separating a three-component mixture (A, B, C). Again, both the column design and the molar flows of the feed and product streams are given. Now, in addition to the reboiler heat duty, we have two degrees of freedom: the LS and VS. It was shown that the reboiler duty which is needed to create certain product purities can be strongly dependent on the values which are chosen for LS and VS.[20,21] So, how are the values for VS and LS to be chosen to assure energy-efficient operation?

Importance of internal split at the DW

Halvorsen and Skogestad[21] state that "interesting insights" can be obtained, if one has a look at "how each component moves through the column sections." To do so, they use a variable which was already used by Fidkowski and Krolikowski[20,22] in their articles about the energy demand of DWCs. It is the molar net stream of each component (relative to the amount present in the feed) that leaves the upper part of the prefractionator. This variable is also used in our article. We will, however, focus on the middle-boiling component B. The calculation of this fraction, which is called component split (CS_B) in our work, is shown in Eq. 1. Additionally, Eq. 2 shows the calculation of the molar fraction of the feed stream that leaves the top of the prefractionator. This variable is called feed split (FS). Figure 2 shows the location of the internal streams that are used to calculate both CS_B and FS.

$$\mathrm{CS_B} = \frac{V_{\mathrm{out,top}}\ y_{\mathrm{out,top,B}} - L_{\mathrm{in,top}}\ x_{\mathrm{in,top,B}}}{F_{\mathrm{B}}} \tag{1}$$

$$FS = \frac{V_{\mathrm{out,top}} - L_{\mathrm{in,top}}}{F} \tag{2}$$

Both the component split and the overall FS leaving the bottom of the prefractionator are marked with an asterisk. Following from a basic molar balance around the prefractionator, it becomes clear that both fractions sum up to 1 (cf. Eqs. 3 and 4).

$$\mathrm{CS_B} + \mathrm{CS_B^*} = 1 \tag{3}$$

$$\mathrm{FS} + \mathrm{FS}^* = 1 \tag{4}$$

In general, it can be stated that both the FS as well as the component split are especially affected by the values of LS and VS. For an energy-efficient operation, both the LS and VS should be chosen such that the net flow of the middle-boiling component leaves the prefractionator at both ends of the DW (i.e., $0 < \mathrm{CS_B} < 1$).[21] It is, however, quite interesting that this demand is not met for every combination of LS and VS. Neither the FS nor the component split is limited by values between 0 and 1. Therefore, without having a look at these values, it is easily possible to choose quite unsuitable combinations of VS and LS, where the net flow of middle-boiling component B does not leave both ends of the prefractionator. In such a case, the net flow of B is rather directed to one end of the prefractionator only. This basically means that component B flows in a circle around the DW making the whole idea of this apparatus obsolete. Understandably, if LS and VS are chosen in such a way, the energy demand of the DWC will rise drastically.[21]

In the following sections, by means of simulation studies, it will be illustrated that a proper choice for the component split of middle-boiling component B in the prefractionator is a key parameter having a huge impact on the energy demand of DWC. If one chooses the values for LS and VS in an arbitrary manner without realizing the importance of generating a proper value for the component split, the energy-efficient operation of a DWC is hardly possible.

Column structure and chemical system used for simulation studies

For all simulation results presented in this article, the same hypothetical components A, B, and C are used. The Antoine parameters of these components according to Eq. 5 as well as their boiling temperatures for a pressure of 100 kPa are presented in Table 1. The Antoine parameters are based on a calculation example given in a book by Luyben and Yu.[23] By choosing the same value for C_2 for each of the components, one gets a system with constant relative volatilities, which, in our example, have a value of 1.50 between neighboring components. It is furthermore assumed that the heat of vaporization is constant for all possible compositions, enthalpy changes due to changes in temperature are negligible and the enthalpy of mixture is zero.

$$p_{i,\mathrm{sat}} = \exp\left(C_{1,i} + \frac{C_{2,i}}{T_{\mathrm{abs}}}\right) \tag{5}$$

The DWC which is used in all simulation studies presented in this article contains six segments, each consisting of 50 stages. Additionally, for practical reasons, one stage for the feed stream and another stage for the removal of side product is included. Thus, the column consists of a reboiler, a total condenser, 50 stages above and below the DW, and 101 stages on each side of the vertical partition. Both the column design as well as the required purities for all of the three product streams are shown in Figure 3. An equimolar ternary mixture of A, B, and C is separated into product streams, each with a purity of at least 99.9 mol %. This article gives calculated values for the minimum energy demand that is needed to reach these purities with a given column design. For all of these calculations, a column pressure of 100 kPa is used. The feed stream is always assumed to consist of a boiling liquid phase with a vapor fraction of zero. The same is valid for the three product streams.

Description of simulation model

Within this work, an EQ model based on the well-known MESH equations is used.[24] For the solution of the model equations, the software Aspen Custom Modeler (ACM) by Aspen Technology, is applied. ACM is an equation-oriented simulation tool and is thus especially suited for the

Table 1. Antoine Parameter and Boiling Temperatures for Components A, B, and C

	C_1	C_2 (K)	T_{boil}* (°C)
A	14.810	−3862	105.3
B	14.405	−3862	120.9
C	14.000	−3862	137.9

*For pressure of 100 kPa.

simulation of DWC.[2] Based on the assumptions about the chemical system which are presented in the preceding section, the enthalpy balance of the simulation model simplifies considerably. It can directly be written as a balance of molar vapor streams (Eq. 6).

$$0=\sum_k \left(V_{\text{in},j,k}\right)-\sum_k \left(V_{\text{out},j,k}\right)+\Delta V_j \tag{6}$$

Thus, for the adiabatic case, where none of the stages show heat streams going to the stage or leaving the stage, the molar vapor streams do not change in either of the segments (constant molar overflow). For nonadiabatic cases, a heat stream leaving the stage or being directed to the stage is directly considered as a change in vapor stream (ΔV_j in Eq. 6). The summation symbols in Eq. 6 have to be included for the two stages directly above and below the DW section only. All other stages present in the column only show one vapor inlet and one vapor outlet stream. The final assumption to be mentioned at this point is the general negligence of pressure drop.

Energy demand of DWC without heat transfer across DW

In this section, we show simulation results for the calculation example described above. For the case without heat transfer across the wall, the energy demand is shown as a function of internal split ratios. Additionally, at the end of this section, a control strategy being able to assure energy-efficient column operation is suggested.

To enable a direct comparison with the energy demand needed for a sequence of conventional distillation columns, the energy demand of the DWC is not shown as an absolute value but relative to the minimum amount of energy that is needed for a conventional sequence according to the equations of Underwood[7]. For this, one has to keep in mind that Underwood equations assume an infinite number of stages. Thus, by comparing the Underwood results for a conventional column with those of a DWC with a finite number of stages, one makes sure to present a conservative estimation of possible energy savings with the real savings being even higher.

The definition of this relative demand θ can be seen in Eq. 7. Because of the physical properties of the ideal system looked at in this work (constant heat of vaporization, etc.), the relative energy demand can directly be expressed as a ratio of vapor streams. This means that the terms "relative energy demand" and "relative vapor demand" can both be used for θ in this article. For the calculation example looked at in this work, the minimum vapor demand calculated with Underwood equations[7] for a conventional direct sequence of two distillation columns has a value of 526.8 mol/s.

$$\theta=\frac{V_{\text{reb,DWC}}}{V_{\text{underwood,seq}}} \tag{7}$$

The calculated values of θ for the example summarized in Figure 3 are presented in Figure 4 for the case without heat transfer across the wall. A similar diagram depicting the dependence of energy demand on LS and VS is shown in articles of Halvorsen and Skogestad.[21,25] Figure 4 shows how the energy demand of the DWC is related to VS and CS_B. It is obvious that both the VS as well as the component split of B strongly influence the value of the overall energy demand. If one chooses improper values for these variables, it is possible to create the need for an energy demand which is twice or three times as high as the minimum energy demand for a conventional sequence. This fact has to be kept in mind, when DWCs are planned. If one chooses just an arbitrary combination of VS and LS, one will not get the desired result. As shown in Figure 4, if VS and LS are chosen to have a value of 0.5 each, the resulting CS_B, for example, will be −0.5. Obviously, this totally unreasonable value does not allow for an energy-efficient column operation. This operating point exhibits an energy demand, which is more than 130% higher than for the point with minimum energy consumption ($\theta_{VS=0.5/LS=0.5}=1.46$, $\theta_{\min}=0.62$). With proper values for VS and CS_B, energy-efficient DWC operation is, however, possible. Figure 4 shows a distinct area in which at least 30%

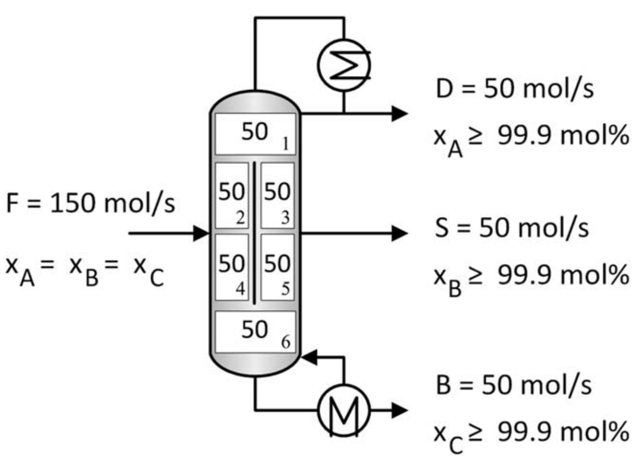


Figure 3. Column setup and separation task used throughout this article.

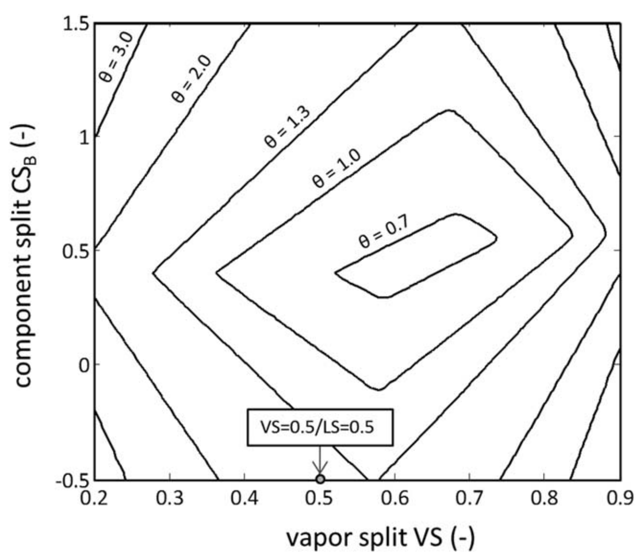


Figure 4. Relative energy demand of DWC as a function of CS_B and VS.

of energy can be saved in comparison to the minimum amount needed for a sequence ($\theta \leq 0.7$).

The fact that energy savings are possible with a DWC in this example is, by the way, not due to special values for the Antoine parameters or due to a certain feed composition. In 1987, Fidkowski and Krolikowski[22] already published a mathematical proof based on the Underwood equations[7] that the minimum energy needed for a DWC to separate a ternary mixture is always less than the minimum energy needed for a sequence. In his PhD thesis, Halvorsen[26] comes to the same conclusion. For an ideal system with constant molar overflow, the author states the adiabatic DWC without heat transfer across the DW to have "the lowest need for vaporization compared to any other adiabatic distillation arrangement for separation of an arbitrary feed mixture into its pure components".[26]

In Figure 4, one can see that it is possible to save at least 30% of energy compared to a conventional distillation sequence for all VS values between 0.52 and 0.73. The interesting thing at this point is that within this region, the optimal values for CS_B are always quite close to 0.5, which means that component B is equally distributed around both ends of the DW. This shows that CS_B is a valuable parameter when it comes to the determination of energy-efficient operating points for DWC. This is because, independent of the particular VS value, the optimal value of CS_B can be estimated quite well in advance. A graphical representation of this fact can also be seen in the upper part of Figure 5. There, the trend shown in Figure 4 is shown for three different VS values. For each of the three VS curves, the optimal value of CS_B is quite close to 0.5. Additionally, the slopes show only moderate values. A change of CS_B by a value of 0.10 will alter the value of relative energy demand by no more than 0.11. Because of that, it is possible to save at least 32% of energy compared to a conventional sequence (i.e., $\theta \leq 0.68$) with a constant CS_B value of 0.5 for all VS values shown in part a of Figure 5.

It is important to realize that, in this context, CS_B can be understood as an alternative for LS. When simulating DWC, one can either choose to specify VS and CS_B. The value of LS will then result from these values. The other possibility is to specify VS and LS. Part b of Figure 5 shows that this choice makes it significantly more difficult to find an operating point with low-energy consumption. First, one can see that the optimal values for LS are by no means constant. They change considerably depending on the value for VS. Second, Figure 5 shows, for example, that in the proximity of the optimal points, the energy demand of the column rises quite drastically, when a LS is chosen which is higher than the optimal value. Because of that, as can be seen in the lower part of Figure 5, the maximum energy savings being possible with a constant LS value are smaller than 5% for the three VS values shown. This can be seen in part b of Figure 5, where the curves for VS $=0.60$ and VS $= 0.70$ intersect at LS $= 0.557$ with an energy demand being higher than 0.95. The most problematic situation, however, arises, when a LS value is chosen which is lower than the optimal one. Then, the desired product purities cannot be reached at all. In total, this shows that for the search of an energy-efficient operating point of DWC, one should rather specify VS and CS_B instead of VS and LS.

This knowledge has a direct impact on the way DWC should be operated in reality. In industrial columns, it is hardly possible to directly adjust the VS value during operation. Usually, this parameter can neither be measured nor set directly. It is rather self-adjusting depending on the flow resistance on both sides of the DW. This means that the value

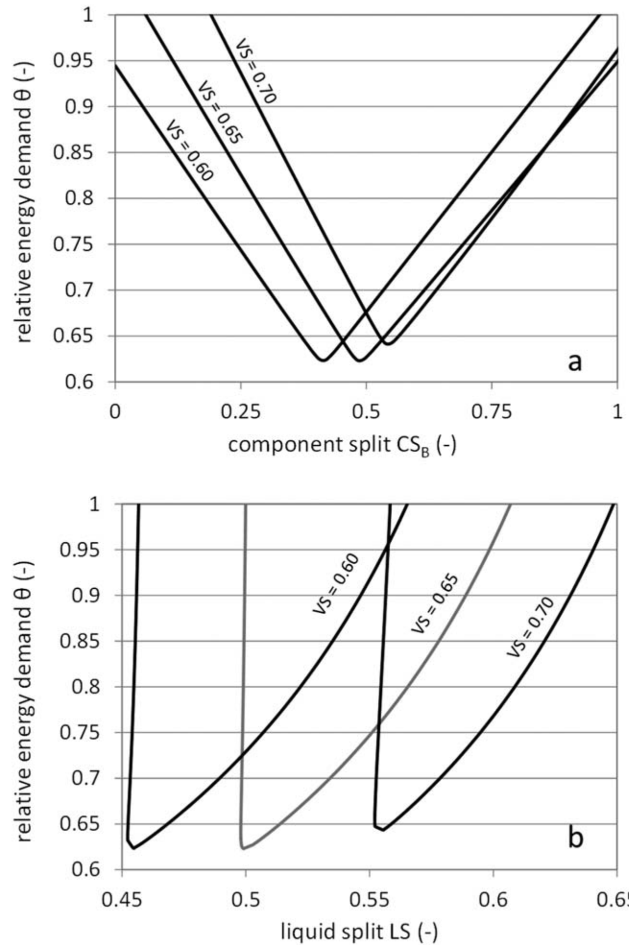


Figure 5. Relative energy demand of DWC as a function of CS_B (a) and LS (b) for different VS values.

of VS can be adjusted roughly by the choice of the column internals on both sides of the wall and the horizontal position of the DW. However, once the column is operated, the exact value of VS is not known precisely. Figure 5 shows that in a situation, where the exact value of VS is not precisely known, it is impossible to guarantee energy-efficient column operation with a constant value for LS. In fact, it is even impossible to guarantee desired product purities being able to be reached at all. For CS_B, however, Figure 5 draws a different picture. Even with a certain degree of uncertainty with respect to VS, a constant CS_B value close to 0.5 will guarantee energy-efficient column operation, for example. The problem, however, is that CS_B, which is a highly valuable parameter for simulation, cannot be measured in real DWC columns either. Luckily, there is a solution to this problem.

The component split has a high impact on energy demand. For CS_B values of 0.4 and 0.6, shown in Figure 6, the energy demand is 10% higher than for the case with $CS_B = 0.5$. It can also be seen, for example, that the temperature within the prefractionator above the feed stage is quite sensitive to changes in CS_B. If the net flow of component B mainly leaves the prefractionator on the upper end ($CS_B = 0.6$), the temperature within this part of the column will rise. Whereas, when B rather leaves the lower end ($CS_B = 0.4$), the temperature will fall. It is, hence, possible to use a temperature sensor in this part of the column for control purposes to keep CS_B at the desired value. The value

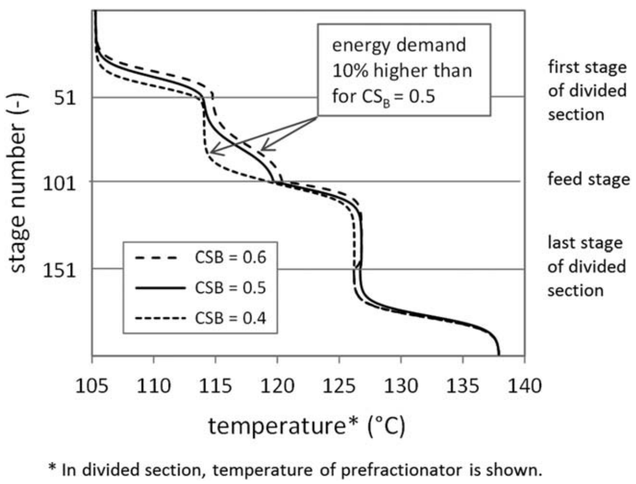


Figure 6. Temperature profiles of DWC with VS = 0.65 for different CS_B values (no heat transfer across DW).

of LS, which can be directly adjusted in real columns, can be used as manipulated variable to keep the temperature in the described section at the right value. This guarantees a suitable value for CS_B and, thus, an energy-efficient operation of the DWC.

Influence of Heat Transfer on Energy Demand

The preceding section of this article gives an overview about how energy-efficient operation can be assured in DWC without heat transfer across the DW. In this chapter, a hypothesis is derived on how this energy demand will be affected, if additional heat streams across the DW are present.

To answer this question, we proceed with a thought experiment. Let us assume a DWC which is operated at the point of minimum energy demand. This means that both the LS and VS are chosen in such a way that the energy demand for the separation task is minimized. For reasons of simplicity, we assume the physical properties of the system in such a way that the assumption of constant molar overflow is applicable. Furthermore, we assume that the number of stages is kept constant for the following considerations as well as the molar feed and product streams. Let us now consider an adiabatic segment of the divided section of the column. In this context, the term "adiabatic" means that no horizontal heat transfer takes place, neither to the surroundings nor between both sides of the DW. For reasons of simplicity, we may assume that the segments on both sides of the wall require the same amount of vapor V. A schematic illustration of such an adiabatic segment of the divided section is shown as "base case" in Figure 7. This figure illustrates the main result of this thought experiment. A detailed explanation of it is given below.

The decisive question, which is to be answered in this section of the article, is the following. Compared to the base case without heat transfer across the wall, how does the minimum overall vapor demand (which is directly proportional to the energy demand) of the DWC change at most due to a heat stream crossing the DW?

To answer this question, one should realize that in this example, from a separation point of view, an increase of vapor streams only has positive effects. We always assume the best possible value for CS_B. Therefore, if a column produces desired product purities with a certain amount of vapor present, an increase of the vapor stream in any of the segments will not deteriorate this situation. It is, however, important to realize that additional heat, and therefore, additional vapor does not have the same effect in every column segment. Depending on the exact location of the segment, the positive influence of additional vapor might be weak or strong. Taking this into account, for our thought experiment, we distinguish between two extreme situations concerning vapor demand in the different segments. Column segments in which the amount of vapor is critical for the overall process are marked gray. It is assumed that the vapor stream which is required in these gray segments has to have a value of at least V to assure desired product purities. Column segments, for which it is assumed that the size of the vapor stream being present inside does not limit the overall process, are marked white for the cases with heat transfer in Figure 7.

For reasons of simplicity, during our thought experiment, we make the assumption that all the heat will cross the DW at one single location. Both the location and the direction of the heat transfer are indicated with black arrows in Figure 7. For the following considerations, it is further assumed that these heat streams always have the same size. Due to the heat stream across the wall, the vapor stream is reduced on one side of the DW and increased on the other side. It is assumed that the heat stream "reaches" the other side without any losses to the surroundings. Therefore, based on the assumption of constant molar overflow, it can be concluded that the vapor stream is increased on one side of the wall by the same value as it is decreased on the other side. For our thought experiment, whose results are depicted in Figure 7, it is assumed that the heat stream across the wall always increases and decreases the vapor stream by a value of X.

We now have a look at the overall vapor demand for all possible combinations concerning the positioning of the limiting (gray) segments. The direction of the heat stream is always assumed from left to right. Because of the symmetry of the problem (vapor demand of V on both sides of the wall for the base case), this can be done without loss of generality. As already mentioned, we are still interested in the operating points with minimum energy demand for a given situation. Therefore, it is obvious that on each side of the DW, at least one gray segment should be present in which the amount of vapor cannot be further reduced. It was explained earlier that in these gray segments, the amount of vapor being

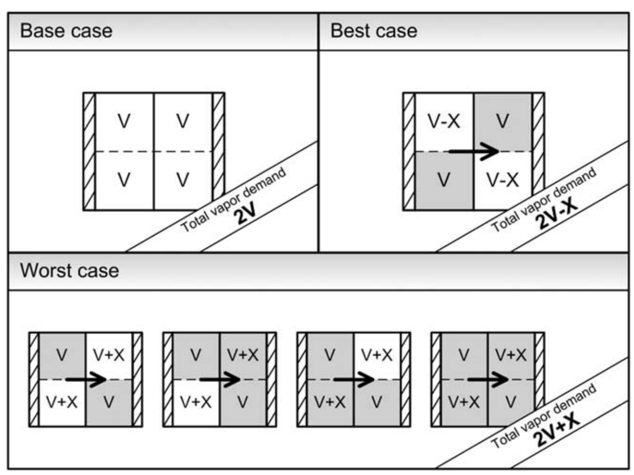


Figure 7. Total vapor demand of DWC for different cases with and without heat transfer across DW (result of thought experiment).

present is critical for the overall process. If we now go through all possible combinations for the positioning of the gray segments with the mentioned constraint that at least one gray segment must be allocated on each side of the DW, we come up with nine different cases. As mentioned earlier, the vapor stream in the limiting gray segments has to have a value of at least V. The amount of vapor being present in the white segments is assumed to be irrelevant. Based on these constraints, the vapor demand for each of the nine different cases can be determined. For one of the nine cases, the vapor demand shows the minimum value of $2V-X$. For four different cases, the maximum value of $2V+X$ can be observed. The remaining four cases show an intermediate vapor demand. As we are interested in the maximum changes of vapor demand due to heat transfer, Figure 7 shows the one case with minimum vapor demand and the four cases with maximum vapor demand and compares these cases with the adiabatic base case, where no heat transfer takes place.

At this point, a short explanation shall be given of how the vapor demand of the different cases in Figure 7 is determined. Let us have a look at the best case. Here, the limiting (gray) segments are located at the lower left and upper right corner. The heat stream is located from left to right. The task was to find the minimum vapor demand for this situation. It was explained earlier that each gray segment in this thought experiment has to have a vapor stream of at least V to meet the desired product purities. At the same time, the vapor streams of the white segments have no limiting effect. We start with a vapor stream V in the lower left corner which is reduced to $V-X$ in the upper left part due to heat transfer across the wall. At the same time, the vapor stream on the right side is increased due to heat transfer at this location. Therefore, in the lower part of the right side, a vapor stream of $V-X$ is sufficient to reach a value of V in the upper part. Thus, the total vapor demand of the best case, which is the sum of the vapor demand for the two lower segments, has a value of $2V-X$.

It should be clear that the best case as well as the worst cases depicted in Figure 7 show ultimate limits of the influence, the heat stream can maximally have on the minimum energy demand of the column. It can, however, be assumed that in reality these ultimate limits are usually not reached. Why is that? For the best case, segments are present that show a vapor stream being smaller than for the base case. To find ultimate limits, we assumed that the reduced vapor stream in these segments will have no negative effect. In reality, however, the vapor stream in the other segments would have to be increased due to this reduced amount. Thus, the actual energy demand will be higher than $2V-X$. For the worst cases, it can be seen that segments are present which show an increased vapor stream compared to the base case. This usually implies that the vapor stream needed in the other parts could be reduced compared to the base case. Thus, the actual energy demand of the worst case will be less than $2V+X$.

The results of this thought experiment can be summarized as follows. It can be seen that the minimum overall vapor demand of the DWC can actually either rise or fall due to heat transfer across the wall. It also becomes clear that the minimum vapor demand for a DWC with heat transfer can never change by more than the size of the vapor stream which is created due to heat transfer across the wall.

During the thought experiment, however, some assumptions were made. First, an idealized chemical system was used, for which the assumption of constant molar overflow was applicable. Second, the heat transfer was assumed to take place at one single location only. Therefore, for real systems and DWCs with heat transfer all along the DW, this result must be expressed differently. As for real systems, the molar heat of vaporization is not always constant, the limits must be expressed in terms of heat streams or energy demand instead of molar vapor streams. So, the hypothesis derived in this chapter is the following.

Compared to the minimum energy demand of the adiabatic base case without heat transfer, the minimum energy demand for the case with heat transfer across the wall will never differ by more than the size of the heat stream which is transferred across the wall.

It is very important to note at this point that the term "minimum energy demand," in this context, is not the minimum demand for an infinite number of stages, but the minimum demand for a given column design (i.e., best operating point in terms of energy consumption). For a mathematical representation of this hypothesis (Eq. 8), the heat stream has to be expressed as the integral of the absolute value for the area specific heat stream across the DW. In Eq. 8, for the base case without heat transfer across the DW, the index "no HT" is used. For the case with heat transfer, the index "with HT" is used.

$$Q^{\mathrm{reb}}_{\mathrm{min,noHT}} - \int_{\mathrm{DW}} |q| \; dA \leq Q^{\mathrm{reb}}_{\mathrm{min,withHT}} \leq Q^{\mathrm{reb}}_{\mathrm{min,noHT}} + \int_{\mathrm{DW}} |q| \; dA \tag{8}$$

If the above considerations are valid, then how can the results of Lestak et al.[13] be explained? Their simulation results, which are carried out with an EQ model, show that starting from an adiabatic base case, an overall transferred heat stream of 1.25 GJ/h results in a required rise in reboiler duty of 4.01 GJ/h. This is a factor of more than 3 and it, thus, seems to contradict our predictions at first sight. A closer look at the results we have shown so far, however, reveals a simple explanation for this. The derived limits on the maximum change of energy demand due to heat transfer in our work (Eq. 8) apply for the operating points with minimum energy consumption both for the adiabatic base case and the case with heat transfer across the wall. While Lestak et al.[13] made sure to create an energy-efficient, adiabatic base case, they did not do so when heat streams across the wall were considered. They decided to keep both VS and LS at the values which were optimized for the base case without heat transfer.[13] This, of course, can result in a drastic rise of energy demand, because the heat transfer across the wall affects the vapor load on both sides of the vertical partition even if the VS at the lower end of the DW is kept constant. This means that the vapor stream leaving the prefractionator is changed and so is the value of the component split for the middle-boiling component (cf. Eq. 1). It is, thus, not surprising that Lestak et al.[13] observe such a strong influence of heat transfer on energy demand. By not adjusting the values for VS and LS accordingly for the case with heat transfer across the wall, the reboiler duty has to be raised unnecessarily high.

Summarizing, one can state that within this section, general limits for the change in energy demand due to heat transfer are derived. The hypothesis (Eq. 8) is formulated that the minimum reboiler duty of a DWC with heat transfer across the wall will differ from the minimum reboiler duty of the adiabatic case by no more than the integral of the absolute values for the heat flux across the wall. In addition to that, the absolute necessity of assuring suitable values for the component split inside the prefractionator is emphasized once more by analyzing the results of Lestak et al.[13]

Energy-Efficient Operation of DWCs

In this part of the article, a hypothesis is derived on how energy-efficient operation is possible for DWCs even if the exact amount of heat being transferred across the DW is unknown. To answer this question, it is first shown how energy-efficient operation can be achieved for the adiabatic case without heat transfer, for our example. Then, in a second step, the actual hypothesis for the case with heat transfer across the DW is derived.

Adiabatic case without heat transfer across DW

As shown in the preceding sections of this article, energy-efficient operation of a DWC does not happen automatically. It is very important to operate the column such that the net flow of the middle-boiling component will leave the prefractionator at both ends of the DW. Otherwise, the energy demand might rise drastically. In practice, however, the value of CS_B can hardly be measured. Therefore, some alternative indication must be used. We already stated that temperature control can be used to guarantee "a suitable value for CS_B and, thus, an energy-efficient operation of the DWC." In the following part, we will confirm this statement with the use of simulation results.

In practice, the LS can be automatically manipulated such that a certain temperature in the divided section is kept constant. By applying such temperature control, the component split of middle-boiling component B can be kept in a sensible range and the column can be operated in an energy-efficient manner. As shown below, for example, the temperature located three stages above the feed stream ($T_{48,2}$ = temperature of stage 48 in segment 2) is a sensible choice for this. At this point, however, the focus is neither on how to determine a suitable location for this temperature nor on the way possible controllers should be tuned. These questions are addressed elsewhere.[27,28]

The suitability of $T_{48,2}$ is shown in Figure 8. It can be seen that for all values of VS shown, this temperature is quite constant for the point of minimum energy consumption. At the same time, if the temperature changes to a higher or lower value, the energy demand of the column rises considerably. This directly corresponds to the behavior shown earlier in Figure 6. Therefore, the temperature on this stage seems to be suitable to be used as an indicator for a sensible component split, and, thus for energy-efficient column operation. In contrast to that, this article already showed that keeping LS at a constant value does not assure energy-efficient column operation.

A summarizing comparison between the two strategies for the case without heat transfer across the wall can be seen in Figure 9. Starting from the base case with VS = 0.65 and minimum energy consumption, it is shown how the required energy demand of the column changes for different values of VS if one either keeps $T_{48,2}$ or LS at their base case values. These base case values are LS = 0.499 and $T_{48,2}$ = 119.4°C. Figure 9 shows that the strategy with temperature control is clearly superior to the other concept. For each individual VS differing from the base case with VS = 0.65, the energy demand for the concept with temperature control is considerably lower than for the case of constant LS. A reason for this can also be seen in Figure 9. For both cases, the CS_B values are shown for a VS value of 0.5. While for the case with temperature control, CS_B shows a reasonable value, the CS_B value for the case with constant LS (−0.48) is far from that. The negative value illustrates that for this situation, the net flow of component B leaving the bottom of the prefractionator is even higher than the amount of B present in the feed. This basically means that component B moves around the DW in a circle, which of course is anything but energy efficient. For some values of VS, it is even impossible to reach the desired product purities with a constant value of 0.499 for LS at all. As can be seen in Figure 9, for VS values higher than 0.65, the infeasible region is directly adjacent to the point with minimum energy consumption. This, of course, is quite problematic. Whereas a VS value of 0.65 results in minimum energy consumption, a VS value of 0.652 already lies in the infeasible region, if LS is kept constant. In this region, the heat duty of the reboiler could be raised to infinity without reaching desired product purities.

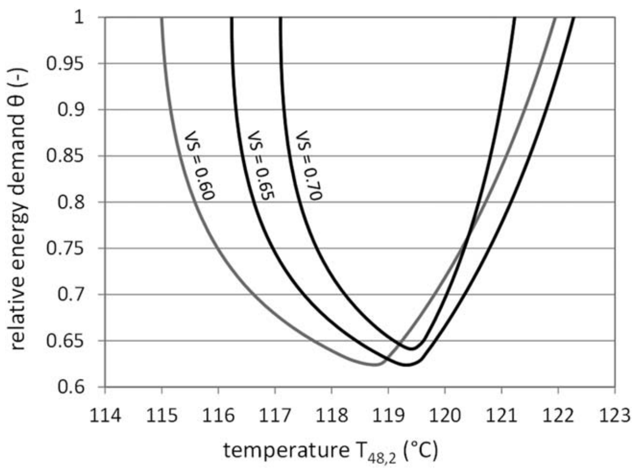


Figure 8. Relative energy demand of DWC as a function of $T_{48,2}$ for different VS values.

How is this possible? To explain this behavior, let us have a look at a certain VS value within the infeasible region shown in Figure 9 (e.g., VS = 0.70). As the desired product purities cannot be reached, one would be tempted to further increase the reboiler heat duty. This, of course, has one positive effect. The vapor streams in each segment of the DWC will increase, which will improve the separation capabilities of the column. At the same time, however, the increasing reboiler heat duty has a negative effect in this situation as well. This negative effect can best be illustrated with Eq. 9, which was derived with a basic molar balance for the case without heat transfer across the wall.

$$\mathrm{FS}=\frac{(\mathrm{VS}-\mathrm{LS})\quad V_{\mathrm{reb,DWC}}+D\cdot \mathrm{LS}}{F} \tag{9}$$

The equation shows that for constant LS and VS values, which are not exactly equal, an increase of the reboiler heat duty automatically changes the value of FS in a linear manner. Thus, in such a situation, if the FS shows a sensible value for a certain starting point, a further increase of the reboiler heat duty will automatically move the FS away from that. Summarizing, one can state that within the infeasible regions shown in Figure 9, the positive effect of a rise in

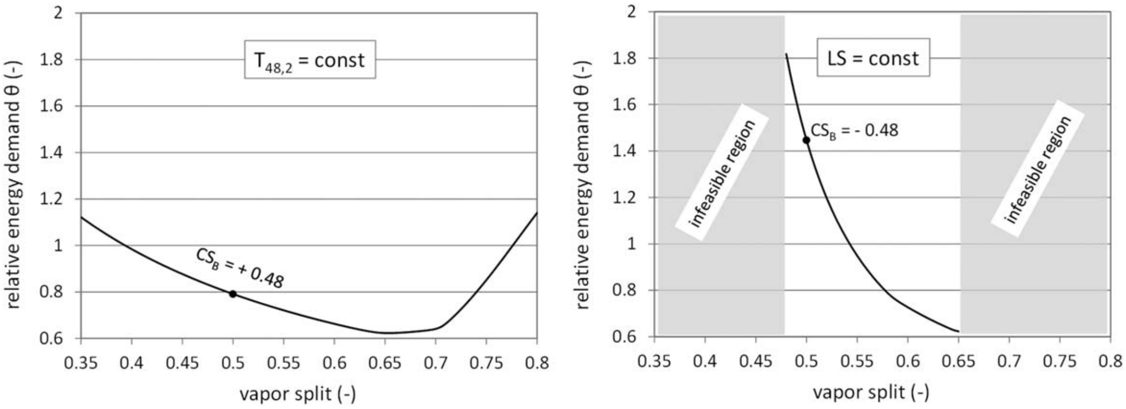


Figure 9. Relative energy demand of DWC as a function of VS for $T_{48,2} = 119.4°C$ (left) and LS = 0.499 (right).

reboiler heat duty simply cannot outpace the mentioned negative effect of creating unreasonable values for the FS.

This section of the article illustrates that controlling a stage temperature with LS to keep the component split in a sensible range is superior to the strategy of constant LS. In our example, it can be seen that the concept with temperature control allows for considerable energy savings for a broad range of VS values (cf. Figure 9). For all VS values between 0.60 and 0.70, the strategy with temperature control assures considerable energy savings of at least 34% compared with a conventional sequence (i.e., $\theta \leq 0.66$). This is very helpful for the practical operation of DWCs because in reality, the VS is usually not known with a high accuracy. Additionally, this section gives an illustrative explanation about the reason, why for constant VS and LS values infeasible regions of operation might occur, in which it is impossible to reach the desired product purities. This finding is also very helpful to develop a comprehensive understanding of the behavior of DWCs.

Case with heat transfer across DW

In the previous part, it was shown how energy-efficient operation of a DWC without heat transfer across the DW can be reached using LS for temperature control. By keeping $T_{48,2}$ at a value of 119.4°C, it is possible to assure energy-efficient column operation for a variety of VS values. If the VS differs from the originally expected value, the LS will be adjusted accordingly to keep $T_{48,2} = 119.4°C$ and thus assure a suitable value for CS_B. If now heat transfer across the wall is present, the only effect this heat transfer has, is to further affect the amount of vapor on either side of the wall. Realizing this, our second hypothesis should be quite obvious.

Control strategies of DWCs that allow for energy-efficient operation for different values of VS also allow for energy-efficient operation when heat transfer across the DW takes place. If, however, a control strategy does not cope well with different VS values, severe problems might arise for different cases of heat transfer across the wall as well.

Confirmation of Heat Transfer-Related Hypotheses

In this section of the article, the validity of the previously formulated hypotheses about the influence of horizontal heat transfer on the energy demand of DWCs is checked with simulation studies for the separation task illustrated in Figure 3. To do so, a first section is presented in which it is shown that the strategy with a constant LS value, which apparently is not suitable to cope well with changes in VS, does not allow for an energy-efficient DWC operation for many cases with heat transfer across the wall either. After that, it is shown that the previously suggested strategy, in which the LS is used for temperature control, copes well with all different situations with heat transfer. Furthermore, it is shown that using this strategy, it is possible to keep the energy demand within the previously predicted limits (Eq. 8) for all analyzed situations.

Constant value for LS

In the previous chapter, it was shown that a constant value for the LS does not allow for an energy-efficient DWC operation if the VS differs from its base case value (cf. Figures 5 and 9). A LS value assuring minimum energy consumption for one specific VS results in high-energy consumption for other values of VS. Therefore, based on the hypothesis derived at the end of the previous chapter, one would expect "severe problems" to arise for certain cases of horizontal heat transfer, if the LS is kept constant. With the use of simulation studies, this is checked and confirmed for the separation task examined in this article.

Description of Simulation Study. The separation example introduced in the beginning of this article is used here again. The physical properties of the hypothetical components as well as information on column design, column pressure, and on feed and product streams can be found there. Starting from the previously described adiabatic base case with minimum energy consumption and a VS of 0.65, four different cases for the direction of heat transfer across the wall are looked at (Figure 10). To provide a complete picture, the influence of heat transfer along these directions is checked regardless of whether they are in agreement with thermal driving forces. Figure 11 shows the temperature profile of the adiabatic base case with minimum energy consumption, which strongly resembles the profile of the optimal operating point shown by Halvorsen and Skogestad.[21,25] It can be seen that heat transfer will basically take place as indicated in Case 3 of Figure 10. By also considering other kinds of heat transfer directions, it is, however, possible to derive a comprehensive picture about the influence which the heat transfer can have on the energy demand of DWC. In addition to the variation of heat transfer directions, the total amount of heat transfer is changed as well. In total, 16 different simulations are carried out to check the influence of heat transfer

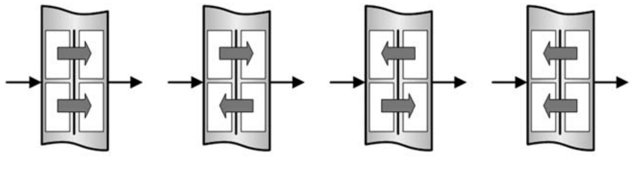


Figure 10. Four different cases for the direction of heat transfer across the DW.

across the DW on the energy demand of the DWC for the case with constant LS.

For our calculations, we assume all stages of segments 2, 3, 4, and 5 (cf. Figure 3) to be equally influenced by this heat transfer. This means that on each side of the DW, 100 stages show a nonzero value for ΔV (Eq. 6). It is assumed that the heat rejected from a stage on one side of the wall is directly supplied to the corresponding stage at the same height on the other side. It is further assumed that regardless of the temperature difference, the total amount of heat transferred between the stages is equal for each stage of these segments.

The following example illustrates how the amount of heat transfer is considered in our calculations. Let us assume the minimum vapor demand of the base case (without heat transfer) to have a value of 100 mol/s and the relative amount of heat transfer to have a value of 5%. This means that 5% of the reboiler heat duty which is needed in the bottom of the column is transferred across the DW. As there are 100 stages "taking part" in heat transfer on either side of the DW, the change in vapor stream on each of the stages has a value of 0.05 mol/s. Depending on the direction of the heat transfer on the particular stage, the vapor stream will either rise or fall by this value from one stage to the next. As in the article of Lestak et al.,[13] however, the VS at the bottom of the DW is kept constant for this simulation study.

Results of Simulation Study. The previously described simulation study is carried out to check whether the heat transfer between both sides of the DW has the expected effects for the case of constant LS. It is expected that the simulation results can be qualitatively predicted with the column behavior, which was observed for varying VS values without heat transfer across the DW.

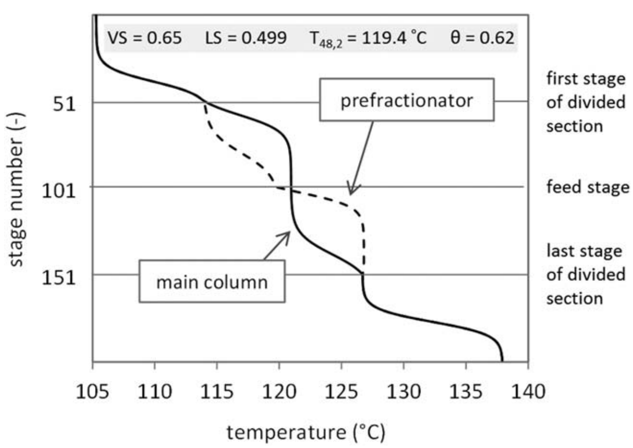


Figure 11. Temperature profile of DWC for operating point with minimum energy consumption (no heat transfer across DW).

What kind of results are to be expected? For the case without heat transfer and with constant LS, Figure 9 shows a strong increase in energy demand, if the vapor load on the feed side is reduced due to a change of VS value compared to the base case. If the vapor load on the feed side is raised, Figure 9 even shows a region directly adjacent to the base case with VS = 0.65, where desired product purities cannot be reached at all. For very small variations of the VS, Figure 9 shows two possible outcomes. The operating point will either show an energy demand close to the base case value or it will be part of the infeasible region. The same results are expected for the four cases with heat transfer across the wall as well. Figure 10 shows that for case 1, the vapor load on the feed side is considerably reduced. Therefore, based on the results seen in Figure 9, a strong increase in energy demand can be expected for this case, if LS and VS are kept at their base case values as done by Lestak et al.[13] For Cases 2 and 3 of Figure 10, it can be seen that the changes of the vapor streams due to heat transfer in the lower part are compensated by the heat transfer with opposite direction in the upper part of the column. Therefore, these cases should produce results, similar to those which can be seen in Figure 9 for very small changes of the VS. The energy demand will either basically stay the same or the production of desired product purities will be impossible. Finally, for Case 4 of Figure 10, it can be expected that due to the increased amount of vapor on the feed side of the DW, the DWC will not be able to produce the desired product purities of 99.9 mol % either.

The results of the simulation study are presented in Table 2. There, one can see that the results which were expected based on the calculation results without heat transfer (cf. right part of Figure 9) are confirmed. As expected, Case 1 shows a strong increase in energy demand which is comparable with the situation shown by Lestak et al.[13] The increase in reboiler heat duty shows a factor of more than 3 compared to the amount of heat that is transferred. Cases 2 and 3 were also predicted quite well. The energy demand will either not change much (Case 2) or the resulting operating point will not allow to produce the desired product purities (Case 3). Finally, for Case 4, the expectations were confirmed as well. For this case, it is impossible to produce desired product purities either. In total, the correct predictions clearly support our hypothesis that strategies showing problems with variations of VS also have problems with certain cases of heat transfer across the wall.

One can see that for most of the cases being looked at, the heat transfer across the wall will have a drastic effect. Only for heat transfer according to Case 2, no big change in energy demand can be seen. Unfortunately, this is not the direction which would be seen in reality for a system like that. As shown in Figure 11, the temperature differences between both sides of the DW will result in heat transfer streams being directed as depicted in Case 3 of Figure 10. For this direction, however, a small relative amount of heat transfer will already prevent the desired product purities from being reached (cf. Table 2), if LS is kept at its base case value. Does this, therefore, imply the need for a perfect insulation of the DW to be able to guarantee energy-efficient column operation?

To answer this question, it is of utmost importance to realize that the heat transfer across the wall is not the primary reason for the drastic effect on energy demand seen in this simulation study. The heat transfer leads to changes in the

Table 2. Change in Energy Demand for Constant LS and VS Depending on Heat Transfer*,†

Relative Amount of Heat Transfer‡ (%)	Direction of Heat Transfer§			
	Case 1 (%)	Case 2 (%)	Case 3	Case 4
1	+3.0	−0.2	inf.	inf.
3	+10.5	−0.3	inf.	inf.
10	+36.9	+0.2	inf.	inf.
30	+112.4	+2.8	inf.	inf.

*VS = 0.65, LS = 0.499.
†Infeasible operating points marked with "inf."
‡Total heat transfer relative to heat duty of adiabatic base case without heat transfer.
§Cases named according to Figure 10.

amount of vapor on both sides of the wall. These changes will, however, only have a drastic effect on energy demand, if a LS value is used that no longer allows to create a sensible component split of middle-boiling component B within the prefractionator. Our simulation results clearly support this conclusion. For Case 2, Table 2 shows a small effect on energy demand. There, the CS_B values are in the range of 0.49–0.52. For Case 1, however, where a huge effect on energy demand can be seen, CS_B values as small as −0.37 are present. It is obvious that a DWC operated in such a way will not be able to allow for energy savings.

If one realizes that the operational problems seen in Table 2 are not primarily due to the presence of heat transfer across the wall, but to unreasonable values of CS_B, the answer to the question posed above is evident. The results shown in Table 2 do not imply the need for a perfect insulation of the DW. The reader is rather advised to care for a control strategy that assures sensible values for the component split. As shown in the next section, a strong increase of the energy demand as well as the occurrence of infeasible regions can thus be prevented.

LS used for temperature control

In the preceding section, a simulation study similar to the one of Lestak et al.[13] is presented. The influence of heat transfer across the wall on the energy demand is analyzed while LS and VS are kept at their base case values. For some cases with heat transfer, considerable problems are shown (cf. Table 2). In this section, it is shown that these problems can be prevented in reality with a suitable control strategy. Additionally, the presented simulation results give further confirmation of the heat transfer-related hypotheses derived earlier in this article.

Description of Simulation Study. The simulation study carried out in this part is run in nearly the same way as the one in the previous chapter. The decisive difference, however, is related to the LS, which is not kept constant here. It is rather used as a manipulated variable assuring $T_{48,2}$ to have a value of 119,4°C. This value was determined and used in a previous section already, where no heat transfer was assumed to take place. Another difference compared to the previous section is related to the VS value. In industrial practice, for a given column design, VS cannot be adjusted directly, but it results from the column internals on both sides creating a certain pressure drop. The VS automatically adjusts such that the pressure drop on both sides of the wall will have the same value. Therefore, as the heat transfer directly affects the vapor streams on both sides of the DW, it also affects the value of VS in real columns. This means that, in practice, the VS value of the adiabatic base case will not equal the VS value of the operating point with heat transfer. Therefore, in this example, VS is not kept at its base case value. In analogy to real column behavior, it is rather determined based on simplified pressure drop correlations. In these, the pressure drop is assumed to be a quadratic function of the molar vapor stream. The equation is set up that a VS value of 0.65 will result for the adiabatic base case (Eq. 10).

$$\left(\frac{1}{65}\right)^2 \sum_{j\in \mathrm{DW_P}} \left(V_{\mathrm{out},j}{}^2\right) = \left(\frac{1}{35}\right)^2 \sum_{j\in \mathrm{DW_M}} \left(V_{\mathrm{out},j}{}^2\right) \tag{10}$$

It must be noted at this point that Eq. 10 is used to calculate realistic values for VS only. At the same time, the assumption still holds that pressure drop on each stage is neglected. This means that for each calculation run presented in this entire article, the pressure on each stage equals the above mentioned column pressure of 100 kPa.

Results of Simulation Study. The results of this simulation study are shown in Table 3. First of all, it can be seen that in contrast to the results for constant LS and VS values (cf. Table 2), this simulation study does not show any infeasible regions. Also, for each of the 16 cases being looked at, the energy demand resulting for the case with temperature control is lower than for the case of constant values for LS and VS. With a look at the CS_B values for both cases, the reason for this becomes clear. As already mentioned, the component split for the feasible operating points shown in Table 2 has values as low as −0.37. For the case with temperature control, the component split shows sensible values in the range from 0.47 to 0.58 without exception for all cases shown in Table 3. We want to emphasize that the suggested control strategy allows to keep the CS_B value in this sensible range even though both the direction and the amount of the heat transfer as well as the VS value change considerably for the different cases analyzed. This confirms the hypothesis that control strategies which allow for energy-efficient DWC operation for different VS values also allow for energy-efficient operation when heat transfer across the DW takes place. At the same time, it can be seen in Table 3 that the energy demand for the temperature control case lies within the limits that were predicted in Eq. 8. For each of the 16 cases in Table 3, the change of energy demand is less than the amount of heat that is transferred.

One, however, has to admit that any kind of regularity regarding the change in energy demand due to heat transfer is hard to identify based on the results of Table 3 alone. Therefore, in addition to these 16 cases, the energy demand resulting from the strategy with temperature control will also be checked for all possible cases of heat transfer in between. The resulting detailed simulation study comprises a total of 960 different cases with heat transfer across the wall.

Description of Detailed Simulation Study. The detailed simulation is run in exactly the same way as the study presented in Table 3. The only differences are that the amount of heat transfer is analyzed with a higher resolution and also different values for the heat transfer are allowed for the upper and the lower part of the column. At the same time, however, the heat stream being transferred inside each segment is equally distributed on all of its stages. For both column parts, a heat stream of up to 15% compared with the total energy demand for the base case is analyzed in 15

Table 3. Change in Energy Demand for Constant $T_{48,2} = 119.4°C$ Depending on Heat Transfer*

Relative Amount of Heat Transfer† (%)	Direction of Heat Transfer‡			
	Case 1 (%)	Case 2 (%)	Case 3 (%)	Case 4 (%)
1	+0.4	−0.2	+0.2	−0.4
3	+1.3	−0.6	+0.7	−1.2
10	+4.5	−1.4	+2.9	−3.5
30	+15.4	−1.8	+10.4	+20.3

*VS calculated with Eq. 10.
†Total heat transfer relative to heat duty of adiabatic base case without heat transfer.
‡Cases named according to Figure 10.

equidistant steps. Again, both directions for this heat transfer are looked at. This assures that all cases shown in Table 3 are part of this study as well.

The following example is intended to explain how the heat transfer is assumed to take place for this simulation study. Let us assume a relative heat transfer of +10% in the upper part of the column and −8% in the lower part. This means that the vapor stream in segment 3 (main side) is raised by a total value of 32.82 mol/s (10% of base case vapor stream), which means that each stage of segment 3 shows an increase of the vapor stream due to heat transfer of 0.6564 mol/s (= 32.82/50). The opposite is true for the stages in segment 2. The negative value for the lower part shows that heat transfer is directed to the prefractionator. Therefore, stages in segment 4 show an increase of vapor stream of 0.5251 mol/s while the vapor stream for all stages in segment 5 is decreased by the same value.

Results of Detailed Simulation Study. Figure 12 gives a graphical illustration about how the energy demand is influenced by heat transfer across the DW. As aforementioned, this detailed simulation study contains all 16 operating points of the simulation study with temperature control, which is shown in Table 3. For a convenient comparison between Table 3 and Figure 12, gray arrows are introduced that indicate the four direction cases used earlier. Within Figure 12, two decisive characteristics can be noted. First, one can see that for small heat streams being transferred, heat transfer directed to the prefractionator is preferable in terms of energy demand. In contrast to this, heat streams being directed to the main column will result in a rise of overall energy demand. According to the results of the thought experiment presented earlier (Figure 7), this behavior can be explained with limiting sections being located in the upper part of the prefractionator and the lower part of the main column's divided section. Second, it can be noticed that heat streams directed to the prefractionator will start to have a negative effect on overall energy demand, when a certain extent is exceeded. Too much heat transfer directed to the prefractionator in either the upper or lower part of the divided section will result in an increase of the overall energy demand. When this happens, the vapor streams in the initially nonlimiting sections become too low.

One should keep in mind that in reality, the heat transfer across the wall will result from temperature differences between both sides. This means that both the amount and the direction of the heat streams cannot directly be influenced during column operation. It was shown earlier in Figure 11 that, for example, the heat streams will cross the DW as indicated in Case 3 of Figure 10. The heat transfer across

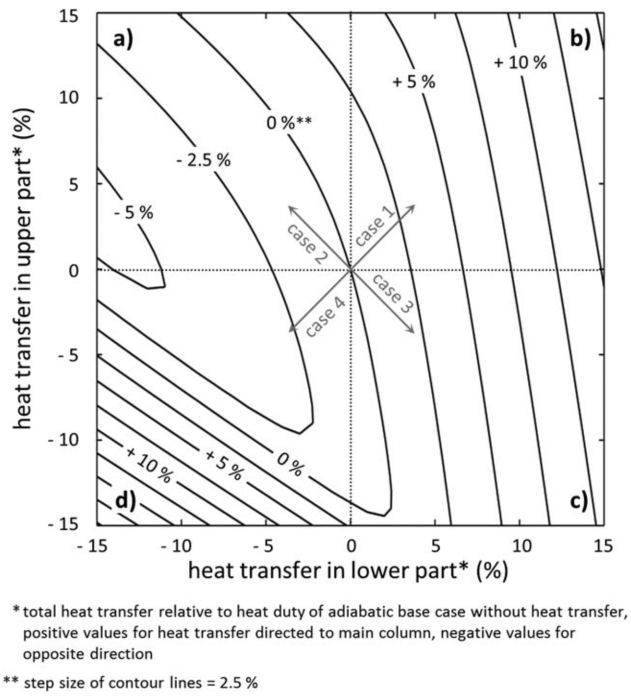
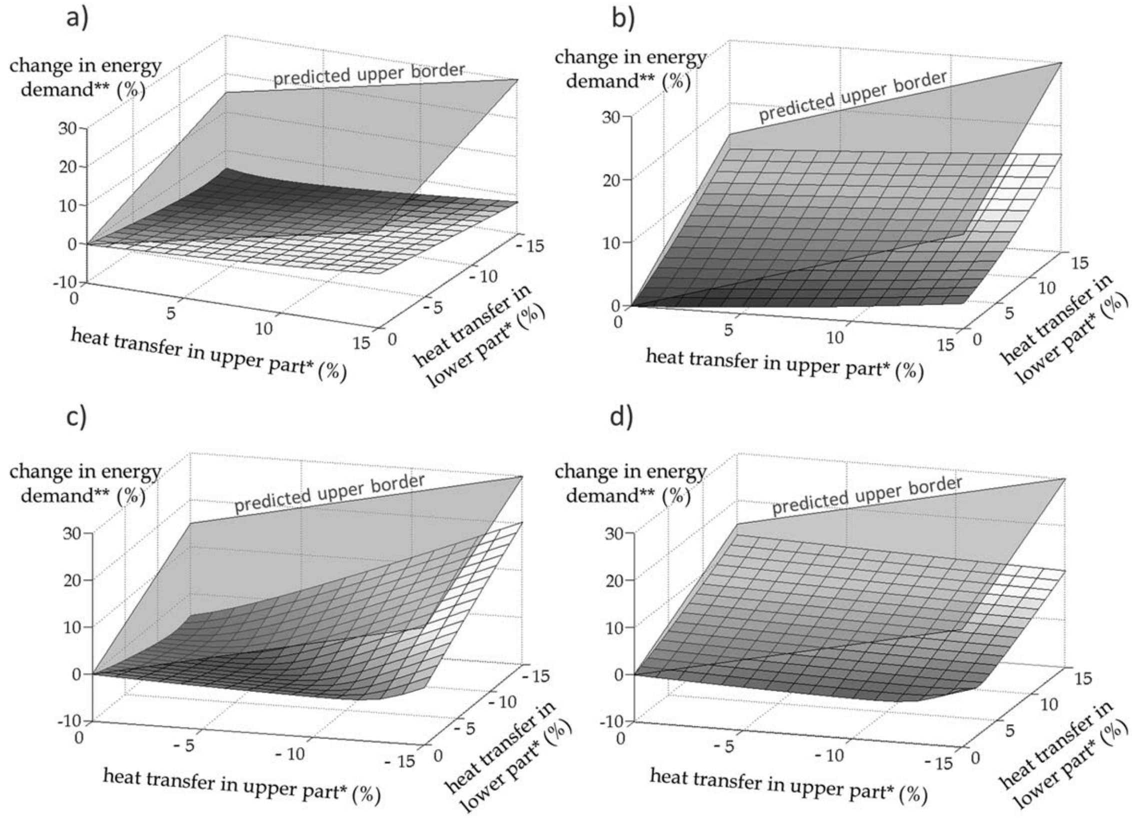


Figure 12. Relative change in energy demand of DWC depending on heat transfer ($T_{48,2} = 119.4°C$, VS according to Eq. 10).

the wall will, therefore, probably lead to an increase of the overall energy demand in this case. The presented strategy with temperature control ($T_{48,2} = 119.4°C$) is, however, able to keep the energy demand within the predicted borders for the minimum energy demand (Eq. 8).

A closer look at the results shown in Figure 12 makes clear that the predicted lower border will not be crossed for any of the operating points. An illustrative example of this fact can be seen for the operating point with minimum energy consumption in Figure 12, which can be found for heat transfer of −15% in the lower part and +3% in the upper part of the divided section. For this point, energy savings of 5.5% compared to the adiabatic base case can be achieved. The total heat transfer across the DW is, however, considerably higher than that (18%). The fact that the predicted upper border will neither be crossed for any of the operating points being part of Figure 12 can be seen in Figure 13. There, a perspective view of the contour plot shown in Figure 12 is given. For all quadrants (a)–(d), the energy demand of the operating points is presented, and it can be seen that none of them shows an energy demand being higher than the predicted upper border, which is shown as a transparent gray layer in Figure 13.

Summarizing, one can state that the energy demand of all operating points being part of Figures 12 and 13 lies within the predicted borders for the minimum energy demand (Eq. 8). The suggested control strategy assures energy-efficient operation of the DWC for all analyzed operating points. Even though heat streams of up to 30% of the total heat duty for the adiabatic case are considered, considerable energy savings compared to a sequence of conventional distillation columns can be achieved for every single operating point. The vapor demand of all operating points being part of Figures 12 and 13 shows values between 310 and 395 mol/s. Thus, relative to the vapor demand of a direct



* total heat transfer relative to heat duty of adiabatic base case without heat transfer
positive values for heat transfer directed to main column, negative values for opposite direction

** change in energy demand relative to heat duty of adiabatic base case without heat transfer

Figure 13. Relative change in energy demand of DWC depending on heat transfer compared with predicted upper border of Eq. 8 ($T_{48,2} = 119.4^{\circ}$C, VS according to Eq. 10).

sequence with an infinite amount of stages (526.8 mol/s), the suggested control strategy assures energy savings of 25–41% for every operating point being analyzed within this study.

Discussion

For the simulation studies shown, we consider an idealized chemical system, we choose a column design with a constant number of stages, and we neglect pressure drop and any kind of maldistribution. Why do we use such a simplified model? One reason to use a very simple model is that by doing so, it becomes very easy for everyone reading this article to check the simulation results and to proceed from there. The main reason, however, is related to one of the main objectives of this article, which is to analyze and understand the fundamental influence of heat transfer across the DW on the energy demand of DWCs. By applying a simple EQ model, we are able to directly focus on the underlying basics of the process which are the material balances and the equilibrium equations. Special fluid dynamic behavior of column internals can be completely excluded from the list of possible causes for any simulation result presented in this work. This decisive feature of EQ models was already emphasized by Taylor.[29] He describes "the essential separation of questions concerning actual equipment design from the material balances and equilibrium equations" as "both the strength and the weakness of the EQ models."[29] Apparently, for the fundamental considerations carried out in this article, this feature is advantageous. Distillation models with a higher level of detail, like the recently presented RNEQ approach,[30] are rather recommended for situations in which the separation efficiency of specific column internals is of interest.

Another question that might arise is if it is necessary to have 50 stages in each of the segments? It is not. Fenske equation gives a minimum number of 34 stages which is needed for a binary separation with $\alpha = 1.5$ and a minimum purity of 99.9 mol %. This article, however, is not dedicated to the question of how many stages should be included in each section in order to find a good compromise between investment costs and energy costs. It is rather dedicated to the question of how DWCs should best be operated to ensure energy savings even in the presence of heat transfer across the wall. To reach this goal, it is totally legitimate to use a column design with more than the minimum amount of stages.

Let us now critically question the difficulty of the calculation example chosen. We show that by using LS for temperature control, it is possible, for our example, to realize considerable energy savings for all different cases of heat transfer being looked at. Compared with the minimum energy demand of conventional distillation columns with an infinite number of stages, energy savings of 25–41% are possible. Is this very good result due to the choice of a calculation example where energy savings can be reached more easily than, for example, shown by Lestak et al.?[13] This is definitely not the case. Our calculation results for constant values of VS and LS show that, for example, it is of crucial importance to assure suitable values for the internal split at the DW. The influence on energy demand, which can be seen for the cases with heat transfer, if LS and VS are kept constant, is even worse than, for example, shown by Lestak et al.[13] For example, a small amount of heat transfer can make it impossible to achieve desired product purities, if LS and VS are kept constant. We show how it is nonetheless possible to assure energy-efficient column operation in practice without knowing the amount of heat that is transferred across the wall. One should, however, be aware that in reality, temperature differences between both sides of the DW can cause certain problems, which can not be predicted with a standard EQ model. One possible problem is given by the fact that mechanical stress might be introduced due to large temperature differences.[2,8,10] A second problem might be caused by undesired wall flow of liquid due to heat transfer across the wall. This is especially important to consider for separation tasks with high-purity demands that are carried out with packings.[2,8]

Conclusions

The energy demand of DWCs shows a strong dependence on the way how liquid and vapor streams are split up at the ends of the DW. To find energy efficient operating points and to develop a control strategy that assures this energy efficiency for all practical situations, the component split of the middle-boiling component within the prefractionator is a highly valuable parameter. Without assuring a suitable value for this parameter, small variations of either the LS or VS can result in a considerable increase of energy demand. It is even possible to create situations in which desired product purities cannot be reached at all. If CS_B is not kept in a sensible range, the same can happen due to small amounts of heat transfer across the DW.

In 1994, Lestak et al.[13] already showed that "a given duty of horizontal heat flow can cause a correspondingly larger increment in the utility consumption." Within this article, it is, however, clarified that such a strong increase can only happen, if the column is not operated at the point of minimum energy consumption. It is confirmed that heat transfer across the DW can actually increase or decrease the minimum energy demand of a DWC. With the use of a simple thought experiment, it is, however, shown for the first time that a heat stream crossing the DW will never change the minimum energy demand of a DWC by more than the amount of heat which is transferred. Knowing this universal limit is important for the design and operation of DWCs, as it reduces the uncertainty about how the energy demand might be affected due to heat transfer across the wall.

The above finding implies that the effect of heat transfer across the wall on the energy demand of a DWC can be kept low, if the column is operated close to the point of minimum energy consumption. This can only be reached with a sensible component split inside the prefractionator. In reality, however, CS_B can hardly be measured. We show how it is nonetheless possible to assure energy-efficient operation of DWCs with heat transfer being present between both sides of the DW. For this purpose, a simple control strategy can be applied that uses the LS as manipulated variable to control a certain temperature which indicates whether CS_B shows a sensible value or not. When developing such a control strategy for a specific separation task, it is typically not even necessary to use a mathematical model that is able to actually consider heat transfer across the DW. One only has to ensure that the selected control strategy is able to assure energy-efficient DWC operation for varying VS values. A proper handling of the case with heat transfer across the DW directly follows from that. For the calculation example shown in this article, it can be seen that the control strategy, which was developed accordingly, allows to generate energy savings of at least 25–41% compared to a conventional sequence for all 960 cases with heat transfer across the wall. We thus showed that the phenomenon of heat transfer across the DW can be handled very well.

This article significantly extents the understanding of how heat transfer across the DW affects the energy demand of DWCs. We hope that the presented findings can help to convince more people from the chemical engineering community of the fact that DWCs are an interesting and promising alternative allowing for considerable energy savings compared to sequences of conventional distillation columns. With a suitable control strategy, DWCs can be operated close to the point of minimum energy consumption even if both the VS value and the amount of heat being transferred across the wall are not exactly known.

Notation

A = area, m^2
B = liquid bottom stream, mol/s
C_1 = first parameter of Antoine equation (Eq. 5)
C_2 = second parameter of Antoine equation (Eq. 5), K
CS_B = molar split of component B in prefractionator (fraction above DW)
CS_B* = molar split of component B in prefractionator (fraction below DW)
D = liquid distillate stream, mol/s
DW_P = set of stage indices j for stages on prefractionator side of DW
DW_M = set of stage indices j for stages on main column side of DW
FS = molar FS (fraction above DW)
FS* = molar FS (fraction below DW)
F = feed stream, mol/s
F_B = flow rate of component B in feed stream, mol/s
L = liquid stream, mol/s
LS = LS at upper end of DW (fraction going to prefractionator)
$p_{i,sat}$ = saturated vapor pressure of component i, kPa
q = heat flux across DW, J/s/m^2
Q^{reb} = heat stream to be supplied in reboiler, J/s
S = liquid side product stream, mol/s
T_{abs} = absolute temperature, K
T_{boil} = boiling temperature of pure component, °C
$T_{j,n}$ = temperature of stage j in segment n, °C
V = vapor stream, mol/s
ΔV = change in vapor stream due to heat transfer, mol/s
$V_{reb,DWC}$ = vapor stream leaving the reboiler of DWC, mol/s
$V_{underwood,seq}$ = minimum vapor demand for conventional distillation sequence calculated with Underwood[7] equations (infinite number of stages), mol/s
VS = VS at lower end of DW (fraction going to prefractionator)
X = change in vapor stream due to heat transfer (for thought experiment), mol/s
x = liquid molar fraction, mol/mol
y = vapor molar fraction, mol/mol

Greek letters

α = relative volatility
θ = energy demand for reboiler relative to minimum demand for direct sequence

Subscripts

B = component B
i = component index
in = inlet
j = stage index (counted from top to bottom)
k = stream index $\in$ [1, 2]
min = minimum energy demand for a given column design
n = segment index $\in$ [1, 2, 3, 4, 5, 6] (cf. Figure 3)
no HT = case without heat transfer across the DW
out = outlet
top = stage index for top stage of prefractionator
with HT = case with heat transfer across the DW

Abbreviations

A, B, C = names of hypothetical components
ACM = Aspen Custom Modeler by Aspen Technology
DW = dividing wall
DWC = dividing wall column(s)
EQ = equilibrium stage
inf. = infeasible
RNEQ = reduced nonequilibrium stage[30]

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