Distribution of heat exchange in optimum diabatic distillation columns

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Abstract

We improved our model for minimization of entropy production rate in diabatic tray distillation. The entropy production rate had contributions from heat and mass transfer on the trays and from heat exchangers connected to the trays. The area of the heat exchangers were not used as free variables, but calculated from four different area distribution rules. The total heat exchange area and its distribution over the column had a significant effect on the entropy production rate in the system. In the limit of infinitely large forces, the results of an adiabatic column were obtained, as expected. As the forces became smaller, the distribution of the area became more important. The area distribution rule with constant average force in each heat exchanger had the lowest entropy production rate of the rules used. Possible consequences for column design were discussed, and a sketch with the characteristics of an optimum distillation column was presented. Two minimization algorithms were used with similar outcome; the Matlab function fmincon being the fastest.

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1. Introduction

Over the last years, there has been a discussion about minimizing the entropy production rate in diabatic distillation columns [1–6]. A diabatic distillation column has heat exchangers on all trays, and it is known for three decades that this type of distillation produces less entropy, see Fonyo [7,8]. Distillation is a separation method that demands large inputs of energy, and even small improvements can save large amounts of energy. Like this work, nearly all publications are based on simulations. Rivero [6] has given experimental results, however, which confirm that a diabatic column has significantly lower entropy production rate than a conventional adiabatic column (with
The purpose of this research is to provide chemical engineers methods and knowledge about how much energy can be saved in the case of full heat integration. Until now, the focus has been on minimizing the entropy production rate of heat and mass transfer on the trays, i.e. separation. The reason has been to establish the method of mini-
mization [2]. Time has now come to extend the objective function and make the entropy minimization more realistic. Diabatic distillation requires extra heat exchangers, and these produce entropy. The contribution from the heat transfer in the heat exchangers is taken into account in this work. A simultaneous study was presented by Schaller et al. [9]. The minimization was carried out with the temperature at each tray in the column as a variable, while the separation performance and number of trays were constant. Switching to high energy efficiency processes is an important aspect of moving towards sustainable development.

The purpose of this work is to study how the distribution of heat exchange influences the state of minimum entropy production rate in diabatic distillation. We investigate in addition the effect of the size of area used for heat exchange. Four different rules for distributing the heat exchange will be studied. We shall show that the distribution and amount of the heat exchange are important, and will influence the solution for optimal operation. In the optimization, we shall use a Monte Carlo minimization algorithm [2], and an algorithm that uses the function fmincon in Matlab® [10] for confirmation of the results.

2. The system

The system was the same as in de Koeijer et al. [2] but the model was improved (see below). The system consisted of a distillation column with heat exchangers on all trays, see Fig. 1. In this work, only simulations of the system were performed.

Fig. 1. A sketch of the diabatic distillation column.
The column had 20 trays, and split an equimolar benzene/toluene flow (1 mol/s) into a 0.95 benzene mole fraction in the distillate and a 0.05 one in the bottom. The feed and products were liquids at their boiling point. The pressure was constant (10^5 Pa). We assumed equilibrium between the flows leaving each tray. The equilibrium conditions were calculated with the integrated Clausius–Clapeyron equations for a regular solution, with the Margules equation for the activity coefficients. The Margules parameters are $-0.0356$ and $0.0619$ [11]. Temperature dependent heat capacities (see Appendix A) were used for calculating the temperature dependent heat of vaporization.

The system was modelled with a given tray temperature vector ($T_n$), number of trays, in- and output flows, and in- and output concentrations. The equilibrium relations and the mass balances over the trays gave the mole fractions ($x_n$, $y_n$) and the flows ($V_n$, $L_n$). If all flows were positive and all mole fractions between 0 and 1, the duty on each heat exchanger ($Q_n$, $Q_{reb}$ and $Q_{cond}$) followed from the energy balance over each tray. Finally, the entropy production rate was calculated with the objective function described in the next section in Eq. (1).

3. Objective function

The objective function in our second law optimization is the entropy production rate. In the present case, we have:

$$\frac{dS_{irr}}{dt} = BS^B + DS^D - FS^F + \sum_{n=0}^{N} \left(-\frac{Q_n}{T_n}\right) + \sum_{n=0}^{N} (Q_nX_{n}^{HX})$$

(1)

The first four terms on the right-hand side are the entropy production rate due to the heat and mass transfer inside the column. It originates from an entropy balance over the entire column, where the first three terms are the entropy carried with the flow in and out of the column, while the fourth term is the entropy carried with the flow of heat in or out on each tray. The duty, $Q_n$, is the amount of heat transferred per unit of time in one heat exchanger $n$, and varies with the temperature and material flows inside the column. The fifth term $\sum Q_nX_{n}^{HX}$ is the contribution to the entropy production from heat transfer in the heat exchangers [12]. The article by Schaller et al. [9] treats the same objective function. The symbol $X_{n}^{HX}$ denotes the (average) thermal driving force for heat transfer in the heat exchanger. A good approximation $X_{n}^{HX}$ (which was experimentally verified for one column [12]) is:

$$X_{n}^{HX} = \frac{1}{T_n} - \frac{2}{T_n^{\text{in}} + T_n^{\text{out}}}$$

(2)

where $T_n^{\text{in}}$ and $T_n^{\text{out}}$ are the temperatures of the cooling/heating medium flowing in and out of each heat exchanger, respectively. The force is positive when heat is added, and negative when heat is removed from a tray. This makes the contribution of the heat exchangers positive, as it should be. This heat transfer does not couple with the heat and mass transfer between the liquid and vapor phases inside the distillation column. The variables in the minimization are the temperatures $T_n$ in the liquid on the trays.
4. Model for heat exchangers

The heat exchangers are characterized by their area of heat transfer, the flows of the utilities (i.e. heating or cooling medium), the temperatures of the utilities, and the heat transfer resistance. The equations that relate these variables are given in this section. The driving force in the heat exchangers is related to the duty by, see Sauar et al. [13]:

\[ \Delta T_{\text{HX}}^n = R_{\text{HX}}^n Q_n \]  

where \( R_{\text{HX}}^n \) is the average resistance to heat transfer of heat exchanger \( n \). A model for \( R_{\text{HX}}^n \) is required. We apply the film model, and assume that:

- The heat exchanger is a coil, hanging above the sieve, like in Rivero [6].
- The coil on the tray is covered with a liquid film, in which all the resistance to heat transfer is located. There are no dry spots on the coil.
- The film is not affected by the void fraction of vapor on the tray.
- The film is not affected by gas or liquid velocities.
- The conditions in the reboiler and condenser are similar to the ones in the tray heat exchangers. The same resistance model is thus used for the reboiler and condenser.

The simple model for the resistance becomes (see e.g. [14]):

\[ R_{\text{HX}}^n = \frac{\delta}{A_n \lambda_n^L T_n^2} \]  

where \( \delta \) is the constant film thickness, arbitrarily set to \( 10^{-5} \) m, \( \lambda_n^L \) is the thermal conductivity of the liquid on tray \( n \) (see Appendix A), and \( A_n \) is the area of heat exchanger \( n \) (or the area of the film covering the coil). This equation predicts heat transfer resistances from experimental data in Rivero [6] within the same order of magnitude.

It is not necessary to determine the utilities before the minimization. The energy balance over the heat exchangers was used after the minimization was carried out, to design a reasonable heat exchanger network using the area rules below. The energy balance is:

\[ Q_n = \dot{m}_n^{\text{u}} c_p^{\text{u}} (T_n^{\text{u, in}} - T_n^{\text{u, out}}) \]  

5. Area distribution rules

The area of heat exchange, \( A_n \), enters the minimization through Eq. (4) and has not been considered as a variable before. In this work, it was still not introduced as a variable, since this would have increased the calculation times considerably. However, we instead related it to other properties of the column through four different area distribution rules:

1. The, computationally speaking, simplest rule is to take the thermal driving force over the heat exchangers constant. This choice is motivated by earlier findings for minimum entropy production in heat exchangers, see Nummedal and Kjelstrup [4]. Eq. (4) is then not needed in the minimization, but is used afterwards to calculate the area of the heat exchanger on each
tray, $A_n$. Three finite forces were used. A fourth value of the force was set equal to zero to model reversible heat transfer as a limiting case. This rule will be abbreviated as EoF, which stands for equipartition of forces.

2. The heat exchanger area can be taken as a linear function of the vapor flow of the tray. In normal practice [15], the area of a tray varies linearly with the vapor flow. To have approximately the same pressure drop on all trays, we therefore relate the heat exchange area to the vapor flow as follows:

$$A_n = aV_n$$

The value for the proportionality constant varied from 0.1 to 0.9 in the experimental vapor flows and areas of a diabatic column, reported by Rivero [6]. Various values in that range were used in this work. This rule is motivated by an efficient use of space in the column.

3. The area $A_n$ is set equal in all heat exchangers. To use only one type of heat exchanger with the same area, can simplify the column construction.

4. The entropy production rate in each heat exchanger ($Q_n A_{nH}X$) is set constant. Eq. (4) is used to calculate the heat exchange area afterward. This choice is motivated by the proposal of Tondeur and Kvaalen [16] and Johannessen et al. [17]. This rule is abbreviated as EoEP, which stands for equipartition of entropy production.

By application of Eqs. (3) and (4) and one of the rules, we can find the areas of the heat exchangers. The area distribution among the heat exchangers and their effect on the entropy production rate is in focus in this work.

6. Calculations

6.1. The Monte Carlo algorithm

A slightly improved Monte Carlo algorithm, developed by de Koeijer et al. [2,4], was used. The algorithm starts from either a linear temperature profile (i.e. temperature as a function of tray number) or the temperature profile of the adiabatic column. It changes, on a random tray, the temperature with a random step multiplied by a factor $f$. For this changed temperature profile, the vapor and liquid flows, vapor and liquid compositions, heat exchanger duties and entropy production rate were calculated with the heat and mass and entropy balances and equilibrium equations. If the entropy production rate of the new profile is larger, or if the profile is not physically realizable (e.g. a vapor or liquid flow becomes less or equal to zero), the profile is rejected, and a new random step is tried on the previous profile. This check guarantees that the temperature profiles are always realizable. If the entropy production rate is lower, the new profile is accepted. The next step (the improvement over de Koeijer et al. [4]) was to try twice on a tray with an improvement possibility.

The new profile generated in this manner, was used as the next start for a new random step on a random tray. The procedure was then repeated 30 000 times. The factor $f$ was then decreased, and the procedure was repeated. The factor $f$ decreased exponentially in six steps. When the $f$ reached its lowest value, the result was taken as the minimum. In order to test for a
true minimum, the temperature profile was perturbed. The whole procedure was repeated up to 1000 times. If there were no change in the course of a 2–3 h, the procedure was stopped, and a minimum was obtained.

6.2. fmincon in Matlab

Many of the nonlinear programming algorithms today are based upon the solution of the Kuhn–Tucker equations [18]. The Kuhn–Tucker equations are necessary conditions for optimality for a constrained optimization problem. In the function fmincon in Matlab® 6.1 R12.1 [10], the Kuhn–Tucker equations are implemented into a Sequential Quadratic Programming method. Each iteration consists of three main stages:

- Updating the Hessian matrix.
- Solution of a Quadratic Programming problem.
- Line search to find a suitable step.

For more details on Sequential Quadratic Programming, see Gill [19].

It is possible to minimize Eq. (1) using an unconstrained optimization with a given number of trays, in- and outlet concentrations and flows. With a given area distribution rule, the only variables are then the temperatures on the trays. A highly nonlinear optimization problem, like this one, requires, however, that the initial guesses of temperatures are close to the minimum, in order to achieve convergence. While this is tolerable in some cases, a more robust formulation is to introduce the vapor flows as an extra set of variables. In our case, this formulation of the minimization problem proved to be less sensitive to the initial guess of variables. We therefore included the component balances as nonlinear constraints, and used the resulting constrained nonlinear optimization. This approach resembles the one applied to a chemical reactor [20].

6.3. Procedures

A minimization of the objective function in Eq. (1) was first carried out with both algorithms for Rule 1 (EoF) for values of the driving force $\lambda_{\text{HX}}$ 0, 0.00001, 0.0001, and 0.001 1/K. This was done to have a consistency check on the Monte Carlo and fmincon algorithms. The optimum feed tray was found for each force by minimizing the entropy production rate for all possible locations, and selecting the one with least entropy production rate.

The faster algorithm (fmincon in Matlab®) was next used to carry out minimization with Rules 2–4 for values of the driving force $\lambda_{\text{HX}}$ from 0 to 0.001 1/K. The feed tray was fixed on tray number 8 in these calculations. The results were generated using the four rules in the simulation program for the columns, one at a time. For all minimizations, the temperatures, duties, mole fractions, flows, transfer areas, and entropy production rates on all trays were found.

As a reference for the minimization results, the entropy production rate in adiabatic columns were calculated at the same values for the driving force $\lambda_{\text{HX}}$. The duties ($Q_n$) of an adiabatic column are zero by definition, except in the reboiler and condenser. The adiabatic column was modelled with an iterative procedure that altered the reflux ratio until zero duties on the heat exchangers were obtained. The heat transfer area of reboiler and condenser were taken
equal. So, for a given separation, the adiabatic column has a unique temperature profile, reboiler duty, and condenser duty.

Finally, in order to illustrate how the proposed columns can be realized, we calculated the temperatures in and out of the heat exchangers, using data from one optimal column, with water and steam as utility.

7. Results

7.1. Reproducibility by different algorithms

Following the procedures, it was first established for Rule 1 (EoF) that the two algorithms gave the same results for the entropy production rates. Table 1 shows the entropy production rates, total transfer areas and locations of the feed tray for the minimizations with Rule 1. The given transfer areas are the sums of the areas of the intermediate heat exchangers, condenser and reboiler. Agreement within 2% in the entropy production rate was found between the two algorithms for the four thermal driving forces. The same feed tray was also found by both procedures. The results from the Monte Carlo algorithm (see Table 1) were systematically a little higher than the results from Matlab’s \texttt{fmincon}. We assume that this is a consequence of the Monte Carlo algorithm being cut off before convergence. The Monte Carlo algorithm requires large computing time for reaching convergence since it is based on random perturbations. The \texttt{Matlab fmincon} algorithm was also faster by several orders of magnitude, so we proceeded with this.

7.2. Adiabatic column

Table 2 gives the entropy production rates and total transfer areas (including the areas of reboiler and condenser) of the adiabatic columns at the same driving forces and feed tray locations as in Table 1. With increasing driving force, the entropy production rate increased, while the total transfer area decreased. These results are used as a reference for the results of the minimizations.

<table>
<thead>
<tr>
<th>Force (1/K)</th>
<th>$\frac{dS^{\text{irr}}}{dt}$ (W/K)</th>
<th>Area (m$^2$)</th>
<th>Feed tray</th>
</tr>
</thead>
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<tr>
<td></td>
<td>Monte Carlo</td>
<td>$f\text{mincon}$</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>1.7215</td>
<td>1.6889</td>
<td>$\infty$</td>
</tr>
<tr>
<td>0.00001</td>
<td>2.5308</td>
<td>2.4942</td>
<td>4.788</td>
</tr>
<tr>
<td>0.0001</td>
<td>9.3863</td>
<td>9.2726</td>
<td>0.4458</td>
</tr>
<tr>
<td>0.001</td>
<td>74.020</td>
<td>73.949</td>
<td>0.04319</td>
</tr>
</tbody>
</table>
7.3. Rule 1: constant driving force

Beside the agreement between the algorithms, Table 1 shows that the entropy production rate increased with increasing thermal driving force in the heat exchanger. It was smallest for the case of reversible heat exchange ($X_{\text{HX}} = 0$) and largest for the largest driving force ($X_{\text{HX}} = 0.001$).

Fig. 2 goes more in detail and shows the variation in the duty across the column at minimum entropy production rate with the four forces in Table 1. Reversible heat exchange (zero driving force) gave the largest changes in the duty around the feed tray. In contrast, with the largest driving force, the duty was everywhere near zero, except for the last five trays. The duties for the first and last tray were, respectively, $-19.9 \times 10^3$ and $24.8 \times 10^3$ W. Intermediate driving forces gave results between the extreme cases.

7.4. Rules 1–4 compared

Fig. 3 shows the main results of this work: the minimum entropy production rate for Rules 1–4 and the simulations of the adiabatic columns together. It gives the minimum entropy production rate.

![Fig. 2. Duty as function of tray number for simulated columns with minimum $dS_{\text{irr}}/dt$ for Rule 1. The driving force for heat transfer is indicated.](image)
production rate as a function of the total area of transfer for all heat exchangers (including reboiler and condenser) for the area distribution from Rules 1–4, as well as for the adiabatic column, see the Calculations section. The results for the ‘EoF’ line derive from calculations that also give Table 1 and Fig. 2. The results for the ‘adiabatic’ line derive from calculations that also give Table 2. The term ‘linear with vapor flow’ refers to Rule 2, the term ‘constant’ to Rule 3, and the term ‘EoEP’ to Rule 4.

The first rule, EoF, resulted in the lowest entropy production rate for all values of the total area of transfer. Rule 2, that used an area distribution linear with the vapor flow, had always the highest entropy production rate among the diabatic columns. The EoEP rule (Rule 4) gave slightly larger values, and a near parallel curve to the one with constant area (Rule 3). At small transfer areas, Rules 2–4 had a larger entropy production rate than the adiabatic column. When the total area of transfer was large, the four diabatic profiles approached each other, and the entropy production rate was lower than in the adiabatic column. When the total area of transfer became small, the entropy production rates of all five cases approached infinity.

8. Discussion

8.1. The model

The model for the distillation columns is based on several simplifying assumptions. An important one is the assumption of equilibrium between vapor and liquid at the outlet of each tray. Wesselingh [21] argues that this assumption leads to results that have no connection to reality. Our research has the same overall aim as his, to introduce non-equilibrium models for simulations of distillation. This requires more work on the modelling side, however. The
assumption of equilibrium at the outlet on each tray is, in the meantime, an assumption that enables a first calculation of the relative role of the heat exchanger for the minimum in the total entropy production rate. The results must be seen in this perspective.

An alternative to the model for heat transfer resistance in Eq. (4) is to use an empirical correlation with dimensionless Nusselt, Reynolds and Prandtl numbers. No relation could be found in the literature for this specific type of heat exchanger. The model in Eq. (4), that corresponded to the results in Rivero [6], was therefore used. The effect of a pressure drop in heat exchangers and trays was not taken into account here. At large transfer areas, we expect the pressure drop in the heat exchangers to be significant.

Numerical uncertainties in the calculations are within 1–2%. The systematic errors are larger, due to the assumptions mentioned above, the assumption of equilibrium between the flows leaving the tray being the most important. Except for the results given by Rivero [6] there are no experimental results available on diabatic distillation. More experiments are needed for an assessment of the systematic errors.

8.2. Rule 1: constant driving force

We have previously reported that the diabatic column is superior to the adiabatic one, in terms of its second law efficiency [2,4]. This was concluded using a model for heat transfer in the diabatic column that corresponds to the results for zero driving force in Table 1. The results for zero driving force obtained here, are similar to the results reported before [2]. We see now, that the conclusion on the diabatic column holds true, even if the driving force is finite. But the relative gain is smaller, the larger the driving force is, compare Tables 1 and 2. This is understandable, since the total area for heat transfer varies. The larger the driving force, the smaller the area, the larger the entropy production rate, and the smaller is the relative gain. But, the larger the transfer area is, the more expensive the column is.

As the thermal force increases, the addition of heat exchangers has less and less beneficiary effect on the second law efficiency. For thermal driving forces larger than approximately 0.001 1/K (the value used in Table 1), the diabatic column seems to have no justification since the relative saving become smaller than 10%. This is confirmed also by Fig. 2 where Rule 1 with high driving force, approaches the adiabatic column.

By comparing the areas in Tables 1 and 2, we see that the adiabatic column has a smaller transfer area with the same driving force. This is logical because the total amount of transferred heat $\Sigma Q_n$ is smaller in the adiabatic column than in the diabatic column ($\sum Q_n$ is equal for all columns in Tables 1 and 2). Schaller et al. [9] observed duty profiles similar to what we see in Fig. 2.

8.3. Rules 1–4 compared

As was already stated, the area distribution rule with constant driving force (EoF) gave the lowest entropy production rate for all transfer areas, see Fig. 3. This means that the (economic) argument that a diabatic column will always cost more due to unavoidable extra heat transfer area, does not hold in general. However, a diabatic column will always be more complex than an adiabatic column, because the area is distributed over more than two heat exchangers.
The second lowest series of entropy production rates was given by the rule of constant area. So, if it is expensive to build a column with a different heat exchanger on each tray, Rule 3 could be a good alternative. Close to Rule 3 was Rule 4, with EoEP as distribution rule, but the areas derived from using the EoEP rule were, however, not constant over the column. In this work, EoEP performed worse than EoF. Both equipartition theorems originate from a minimization with specific objective function and constraints, which are not fulfilled here. We therefore expect that neither EoF nor EoEP are solutions to the minimization problem. It is interesting however that EoF performs best. The worst performance was from the common design rule of linear vapor flows (Rule 2). So, this rule should not be used.

Fig. 3 also shows that Rules 2–4 had a crossover with the adiabatic column. This means that not all diabatic columns have automatically a lower entropy production rate than the adiabatic column. A diabatic column should not be preferred a priori. Fig. 3 can be used to calculate the relative reduction of entropy production for a certain amount of extra heat transfer area for various rules for area distribution. This relative reduction decreases with decreasing driving forces. So, if extra transfer area is available, it has the highest relative effect in columns with large driving forces. Fig. 2 suggests to add this extra area at the lowest and highest trays for this particular column.

8.4. Optimum column design

A second law optimal (reversible) column was sketched by Fonyo in 1974 [7]. Rivero sketched the diabatic column [6]. With their drawings as a basis, we may now sketch a diabatic distillation column with minimum entropy production rate, see Fig. 4. The sketch is based on the results of this work with reasonable thermal driving forces over the heat exchangers ($10^{-3}–10^{-4}$ 1/K). The column has three special features:

1. The duty profiles in Fig. 2 indicated that heat exchangers are necessary especially for trays near the top and bottom. Therefore, we have only indicated heat exchange at these locations. This is thus the first special feature of the optimal diabatic column.

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![Fig. 4. Sketch of an optimum diabatic distillation column.](image-url)
2. The larger the driving force, the fewer heat exchangers are necessary (but more entropy is produced). The particular optimization must give the number of heat exchangers. The transfer area and duty decrease the further away from reboiler or condenser the heat exchanger is. For this reason, we have illustrated in Fig. 4 that more area is available close to the reboiler and condenser.

3. An outcome of the optimization is that the vapor and liquid flows changes over the trays. In order to maintain the same pressure drop over each tray, and avoid weeping or flooding [15], the diameter of the column should also decrease at the top and bottom trays.

The details of the optimum operation will of course be different from column to column, but the general characteristics should, according to our experience, be captured by the sketch.

8.5. Utility choices

We have up to this point assumed that it is possible to design a heat exchanger network with utilities that can fulfill the energy balance Eq. (5). The entropy production rate was minimized without exact knowledge of the utilities. Given more details on the utilities, the last two terms in the objective function, Eq. (1), can be replaced by \( \sum_0^N \dot{m}_n C_p \ln (T_{n,\text{out}}/T_{n,\text{in}}) \). The problem is now converted into finding a utility that obeys this formula.

In order to illustrate what this means, we calculated with Eqs. (2) and (5), the in- and outlet temperatures of the heat exchangers for a constant driving force of 0.0001 l/K using water (\( C_p = 4180 \text{ J/kg K} \)) and steam (\( C_p = 2000 \text{ J/kg K} \)) as utilities. We chose a constant flow of each utility through the heat exchangers. The values 0.3 kg/s water and 0.4 kg/s steam gave reasonable results, as presented in Fig. 5.

In the rectifying section, the inlet temperature became lower than at the outlet, while both were at least 5–10 K below the temperature on the trays inside the column. The opposite behavior was observed for the stripping section. This ensures that there is feasible heating in the stripping section, and feasible cooling in the rectifying section. The design demands a variety of utilities.
utility temperatures, however. These are probably not available in a plant without a heat exchanger network.

A design where the utilities in each section flow from one heat exchanger to the next, like in Rivero [6], was not possible with the given utilities and results. Unrealistic temperature differences around 1–2 °C between in- an outlet of the utilities were obtained. Furthermore, the temperature differences between outlet and column became negligible, and the flows of utilities were not equal anymore. These results make such a design unrealistic, at least if we use the area distribution following from EoF (constant driving force).

It may be possible, however, to design a diabatic column with equal driving forces over the heat exchangers. Extra equipment and utilities are necessary, however, e.g. valves, pumps, compressors, heat pumps. The design of such columns with realistic heat exchanger networks, is a challenge for future research. In practice, however, economical considerations must also be made, since the second law optimum does not necessarily coincide with the economical optimum.

9. Conclusions

In this work, the effect of the heat exchangers for the minimization of entropy production rate in diabatic columns was reported by means of simulations. Their effect was significant for realistic values of thermal driving forces. For large forces, or small total area, the adiabatic column was not much worse than the diabatic one, however. Out of four different candidate transfer area distributions, the one with equal forces over the heat exchangers had the lowest entropy production, for all total transfer areas investigated. A sketch with the characteristics of an optimum distillation column was presented, and the possible design of accompanying utilities and heat exchanger network was discussed. It remains to be seen whether the conclusions are altered by relaxing assumptions in the model. In the future, a non-equilibrium model should replace our model which assumes equilibrium between liquid and vapor at the outlet of each tray.

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Appendix A.

The heat capacity for liquid and vapor, \( C_p^L \) and \( C_p^V \), relate to the temperature as [22]:

\[
\frac{C_{p,i}}{R} = A_i^{C_p} + B_i^{C_p} T + C_i^{C_p} T^2
\]  

(A.1)

The heat conductivity for the liquid is given by Reid et al. [23]:

\[
\lambda_i = A_i^{\lambda} + B_i^{\lambda} T + C_i^{\lambda} T^2
\]  

(A.2)

For a mixture, the molar average of the two components is taken.
Table 3 gives the physical chemical properties that were used in the simulations.

References


<table>
<thead>
<tr>
<th>Component</th>
<th>Benzene</th>
<th>Toluene</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{boil}$ (K)</td>
<td>353.25$^a$</td>
<td>383.78$^a$</td>
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<tr>
<td>$\Delta_vap H (T_{boil})$ (J/mol)</td>
<td>30 781$^a$</td>
<td>33 201$^a$</td>
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<td>$A^T$ (–)</td>
<td>–0.206$^b$</td>
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<td>$B^C_T$ (1/K)</td>
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<td>$47.052 \times 10^{-3}$$^b$</td>
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<tr>
<td>$B^T$ (W/m K$^2$)</td>
<td>$4.773 \times 10^{-6}$$^c$</td>
<td>$-2.254 \times 10^{-4}$$^c$</td>
</tr>
<tr>
<td>$C^C_T$ (W/m K$^3$)</td>
<td>$-3.78 \times 10^{-7}$$^c$</td>
<td>$-2.47 \times 10^{-8}$$^c$</td>
</tr>
</tbody>
</table>

$^a$ See Ref. [24].
$^b$ See Ref. [22].
$^c$ See Ref. [23].