

# Optimization of a Diabatic Distillation Column with Sequential Heat Exchangers

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Diabatic distillation is a separation process in which heat is transferred on the trays inside the column as opposed to classical adiabatic columns where heat is only supplied to the reboiler and extracted from the condenser. Such diabatic columns dramatically reduce the exergy needed to perform the separation. One implementation, particularly suitable for retrofitting applications, uses a single heating fluid circulating in series from one tray to the next below the feed tray and a single cooling fluid circulating in series above the feed tray. The optimal design of these sequential heat exchangers, minimizing the overall rate of entropy production in the separation process, is a difficult optimization problem because traditional algorithms for optimization invariably get stuck. However, an algorithm based on physical intuition for adjusting the temperature profile can find the optimum. The resulting column operation is compared to the optimal operation with independent heat transfer to each tray (the completely controlled diabatic column) and to a conventional adiabatic column. In the former comparison, we find how much exergy is lost by circulating a fluid in series rather than using independently adjustable heat exchanges. In the latter, we find the possible savings available by retrofitting. The comparisons show that most of the potential exergy savings can be captured by diabatization using heat exchangers in series. The potential impact of this technology on the chemical and process industry is enormous because distillation is the single largest energy degrading unit operation worldwide.

## Introduction

An important contribution to exergy savings is through diabatic distillation. Instead of just one heat source (the reboiler) and one heat sink (the condenser), a diabatic column uses a heat exchanger at each tray. Such devices have been investigated<sup>1</sup> as early as 1974 and have recently drawn growing interest.<sup>2–9</sup> Spreading out the heating duties of the reboiler and the cooling duties of the condenser implies potential savings because the reboiler is adding heat at a higher temperature than needed and the condenser is removing heat at a lower temperature than needed (see Figure 1).

Optimal operation of diabatic distillation columns has been calculated before in a number of contexts. The present work goes further in a series of efforts which strive to quantify and minimize the unavoidable irreversibilities associated with different parts of the process. Here, we quantify the amount of irreversibility that is associated with restricting the extra heat supplied to the column to one heat exchange fluid that moves from tray to tray in supplying heat to all of the trays in the stripping section. Similarly, we restrict the

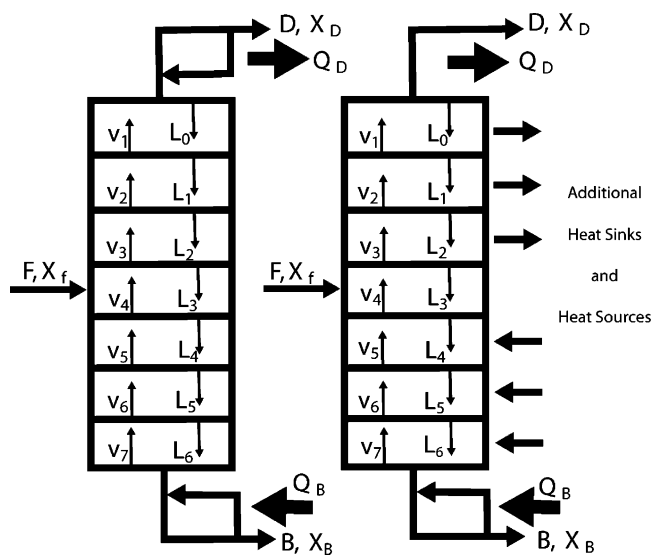
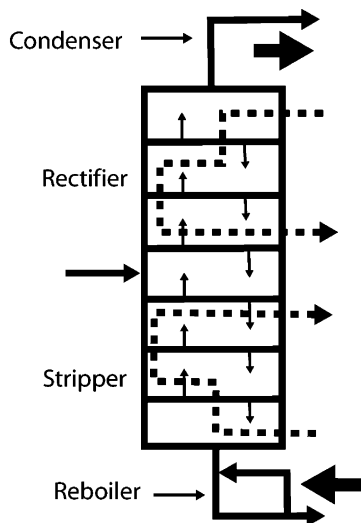


Figure 1. Comparison of an adiabatic column to a general diabatic column.

heat removal to one heat exchange fluid that moves from tray to tray removing heat from the rectification section (see Figure 2). Our previous efforts in this regard found the minimum irreversibility when each tray was

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**Figure 2.** Conventional column retrofitted with serial heat exchangers.

supplied by independently adjustable heat exchangers.<sup>4</sup> Just how much extra irreversibility one has to pay for the loss of independent control of the external temperatures is quantified here for the first time.

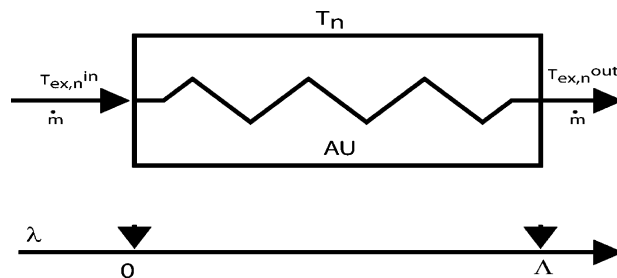
In a steady-state diabatic column, the size of the next temperature step (the temperature difference between the current tray and the next tray) can be adjusted by varying the amount of heat supplied at that tray. An early and general optimization result for columns with equilibrated trays showed that optimal operation, counting only separation losses, in the limit of many trays<sup>2,3</sup> is achieved when these temperature steps are adjusted so the thermodynamic distance between trays is constant.<sup>8</sup>

Recent works have improved on the Equal Thermodynamic Distance Theorem and further support the assertion that diabatic distillation is a way of saving exergy. Two publications<sup>5,9</sup> calculated potential savings without assuming many trays. The agreement between the numerically optimized separation losses and the losses implied by constant thermodynamic length (which provides an asymptotic result for a large number of trays) was found to be excellent down to reasonable length columns.

The next efforts<sup>4</sup> characterized losses due to the inclusion of thermal resistance in the heat exchanger but still allowing the temperature of the heat exchange fluid in contact with each tray to vary freely. The findings were that under optimal operation the heat exchange losses were comparable to the separation losses for reasonable parameter values. Interestingly, the characteristic inverted-U-U shape<sup>7,8</sup> of the optimal heating profile with constant thermodynamic distance was flattened out for short columns and was even further flattened when the effect of thermal resistance was added. This suggested that the serial heat exchanger design considered here could probably be used without a large sacrifice in exergy loss.

## The Problem

**Serial Heat Exchanger Design.** This research concerns the optimal operation of a particular diabatic design with serial heat exchangers.<sup>6</sup> A serial heat exchanger used for cooling is meandered through the



**Figure 3.** Model of heat exchanger on one tray. The parameter  $\lambda$  runs from 0 to  $\Lambda$ .

rectifier, and a separate serial heat exchanger used for heating is meandered through the stripper.

A heat exchange fluid is pumped through the serial heat exchangers to allow heat to be transferred to or from the column. This particular diabatic design will allow a conventional column to be retrofitted with serial heat exchangers with moderate structural changes. Only two piercings of the outer jacket are required for each serial heat exchanger, as shown in Figure 2.

The sample calculations presented here treat the mixture of 50% benzene and 50% toluene, which is separated into the distillate containing 90% benzene and the bottoms containing 90% toluene.

**Variables To Be Optimized.** The serial heat exchanger design has four control variables: (1) the temperature  $T_{ex,1}^{in}$  of the serial heat exchange fluid entering the rectifier; (2) the temperature  $T_{ex,K}^{in}$  of the serial heat exchange fluid entering the stripper; (3) the flow rate  $\dot{m}_r$  of the serial heat exchange fluid in the rectifier; and (4) the flow rate  $\dot{m}_s$  of the serial heat exchange fluid in the stripper. The temperature profile of the distillation column is determined by these four parameters. From these, the total entropy production and thus the exergy losses can be calculated.<sup>9</sup>

**Calculating the Temperature of the Heat Exchange Fluid.** Consider first a model of a serial heat exchanger unit on one tray (see Figure 3). Let  $\dot{m}$  be the flow rate of the heat exchange fluid,  $T_{ex,1}^{in}$  and  $T_{ex,1}^{out}$  be the temperatures of the heat exchange fluid going into and coming out of the tray,  $T_1$  be the temperature of the tray,  $C_p$  be the specific heat capacity of the heat exchange fluid,  $\Lambda$  be the length of the contact area of the serial heat exchanger to the tray,  $\lambda$  be the position along the heat exchanger, and  $UA$  be the product of the heat exchange area  $A$  and the conductivity  $U$  giving the total conductance of the serial heat exchanger unit. The heat flow in a small portion of length  $d\lambda$  is then

$$\dot{m}C_p dT_{ex,1} = \frac{-AU}{\Lambda}(T_{ex,1} - T_1) d\lambda$$

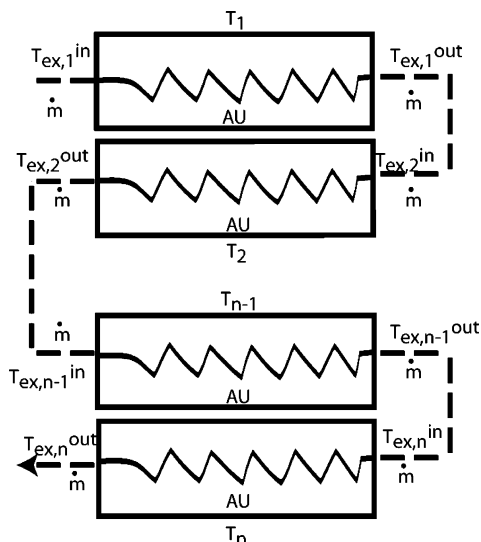
Separating variables and integrating along the length of the heat exchanger gives

$$\int_{T_{ex,1}^{in}}^{T_{ex,1}^{out}} \frac{dT_{ex,1}}{T_{ex,1} - T_1} = \frac{-AU}{\dot{m}C_p\Lambda} \int_0^\Lambda d\lambda$$

Solving the resulting equation for  $T_{ex,1}^{out}$  results in

$$T_{ex,1}^{out} = T_{ex,1}^{in} + (T_1 - T_{ex,1}^{in}) \left[ 1 - \exp\left(\frac{-AU}{\dot{m}C_p}\right) \right]$$

Figure 4 shows a schematic representation of a serial heat exchanger meandering through  $n$  trays of the column. Using the previous equation and knowing the



**Figure 4.** Serial heat exchanger meandering through tray 1 to tray  $n$  of the distillation column.

temperatures of the trays  $T_i$  and the flow rate  $\dot{m}$  of the heat exchange fluid entering the serial heat exchanger, we can calculate the amount of heat transferred at each tray along the heat exchanger.

### The Algorithm

The objective function to be minimized is the total entropy production rate  $\Delta S_u$  of the distillation column from which the corresponding rate of loss of exergy is easily calculated. The four variables to be optimized are the entering temperatures and the mass flow rates of the serial heat exchange fluids. Given a set of values for these variables, the temperature profile inside the column is determined from the nonlinear steady-state conditions. Actually solving for the steady state is a nontrivial task. Because, as mentioned above, all of the operating characteristics of the column are conveniently expressed in terms of its temperature profile, it is natural to start the search for the steady state by guessing a temperature profile, which is then iteratively modified to obtain the steady state. Specifically, for each guessed temperature profile, the excess heats  $Q_{\text{excess}}^n$  on each tray  $n$ ,

$$Q_{\text{excess}}^n = -V_n H_{\text{vap}}(y_n, T_n) - L_n H_{\text{liq}}(x_n, T_n) + V_{n+1} H_{\text{vap}}(y_n, T_n) + L_{n-1} H_{\text{liq}}(x_n, T_n) + Q_{\text{htex}}$$

are determined. Here,  $x_n$  is the mole fraction of light component of the liquid on tray  $n$ ,  $y_n$  is the mole fraction of light component of the vapor above tray  $n$ ,  $V_n$  is the vapor flow leaving tray  $n$ ,  $L_n$  is the liquid flow leaving tray  $n$ ,  $H_{\text{vap}}$  and  $H_{\text{liq}}$  are the molar enthalpies of the vapor and liquid, respectively, and  $Q_{\text{htex}}$  is the heat flow delivered by the heat exchanger to the tray. As these excess heats must equal zero at the steady state, one can use them as penalties in the optimization that are to be minimized at the same time as the minimum of the entropy production is determined. The objective to minimize is then

$$\Delta S_u + M \sum_n (Q_{\text{excess}}^n)^2$$

where  $M$  is a large constant.

Unfortunately, standard optimization methods such as quasi-Newton could not find the optimum. This was due in part to the fact that this is a simulation where only narrow regions of parameter values make physical sense. It was further complicated by numerous local minima and by the high sensitivity of the entropy production on the temperature profile. Therefore, we developed a different approach based on an algorithm using a pseudo dynamics for finding the steady-state temperature profile.

The temperatures of each tray are changed by a small multiple  $\epsilon$  of the excess heat on that tray in each time step; that is, the trays with excess heat are allowed to heat up a little as though this heat were really supplied by the excess heat. The steady state is then found by taking many time steps and changing the temperatures of the trays in each step according to

$$T_n(t+1) = T_n(t) + \epsilon Q_{\text{excess}}^n(t)$$

This algorithm converges to the steady-state temperature profile such that the excess heat at each tray is equal to zero and provides an algorithm to evaluate the entropy production for any value of our controls.

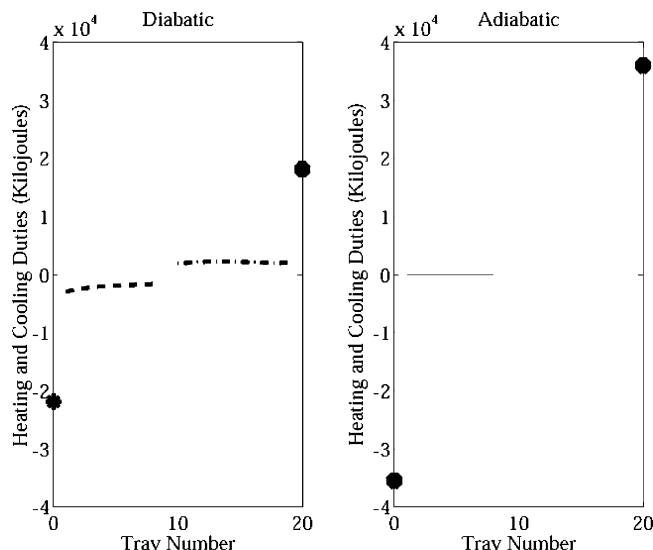
For the minimization of the entropy production, we then employed a standard Nelder-Mead (Simplex) implementation available as `fmins` (MATLAB version 5.x) or `fminsearch` (MATLAB version 6.x) giving robust convergence.

### Results

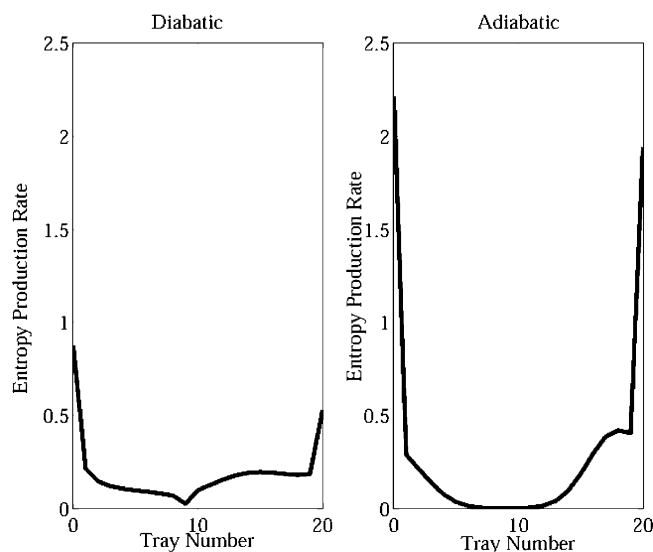
The examples presented here use a conductance  $UA = 500$  W/K on each tray and 10 times this value for the reboiler and the condenser. The feed flow rate is 1 mol/s, and the specific heat capacity of the heat exchange fluid used is taken to be  $C_p = 300$  J/mol·K<sup>-1</sup>. The calculations compare a 20-tray diabatic column and a 20-tray adiabatic column. The results discussed include the heating and cooling duties, the tray-by-tray entropy production, liquid and vapor flow rates, the temperature profiles, the sensitivity of entropy production as the temperature deviates from their optimal values, and the amount of exergy savings as compared to an adiabatic column. It turns out that, because the serial heat exchangers reduce the duty that the reboiler and condenser must perform, a diabatic column with these parameters requires a reboiler that is only half the size of a conventional column and a condenser two-thirds the size of a conventional column.

**Heating and Cooling Duties at Each Tray.** The graphs in Figure 5 show the heating and cooling duties of the condenser (tray 0) and the reboiler (tray 20). The lines on the diabatic column graph are the cooling duties in the rectifier (trays 1–9) and the heating duties in the stripper (trays 10–19).

As mentioned earlier, due to the heating and cooling duties of the serial heat exchangers, the reboiler adds less heat and the condenser removes less heat in a diabatic column, thus resulting in an exergy saving. The reason for the latter is that the temperature drop across which heat from/to the serial heat exchangers is utilized is smaller than the temperature drop from the reboiler to the condenser. The total amount of heat transferred is approximately the same for the two setups. As in the previous studies, it is seen that the optimal heating and cooling loads are essentially constant over the trays.



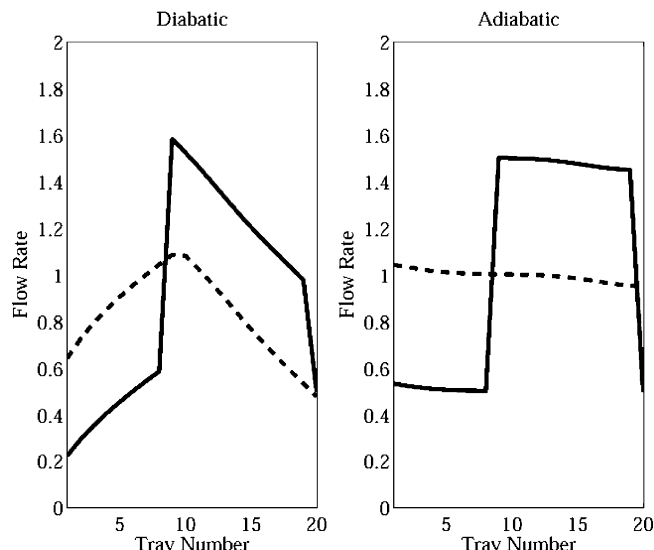
**Figure 5.** Heating and cooling duties of a diabatic column (left) and an adiabatic column (right). The large points represent the reboiler and condenser, while heat exchange on the trays of the column is shown as dotted lines.



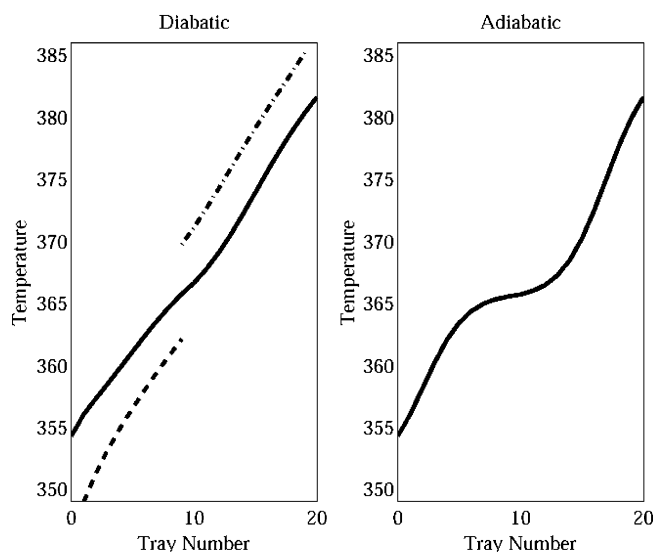
**Figure 6.** Tray-by-tray entropy production rates of the diabatic and adiabatic columns.

**Tray-by-Tray Entropy Production.** As stated earlier, exergy loss is equivalent to entropy production. Note in Figure 6 that the total entropy production rate is significantly lower in the diabatic column and that it is more uniformly distributed; only the feed tray deviates noticeably. This indicates that all of the trays carry more or less the same burden of separation, quite distinct from the performance in the adiabatic column. When comparing the entropy production of the condensers (tray 0), it is observed that the entropy production in the adiabatic column's condenser is approximately twice as large as the corresponding entropy production in the diabatic column. It is also observed that the entropy production in the adiabatic column's reboiler (tray 20) is 10 times larger than the entropy production of the diabatic column's reboiler.

**Liquid and Vapor Flow Rates.** Except for the feed tray, the diabatic column flow rates are noticeably lower than those of the adiabatic column as seen in Figure 7. The significance of lower flow rates is that the column allows cross-sectional area for the serial heat exchangers



**Figure 7.** Liquid (solid line) and vapor (dotted line) flow rates at each tray.

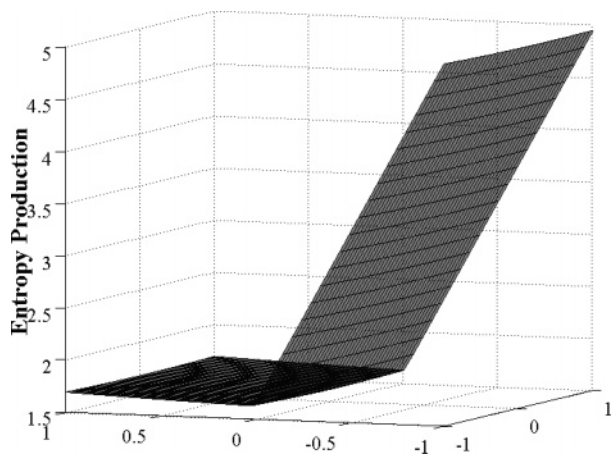


**Figure 8.** Temperature profiles of the diabatic and adiabatic columns. The solid lines are the tray temperatures, and the dotted lines are the temperatures of the heat exchangers.

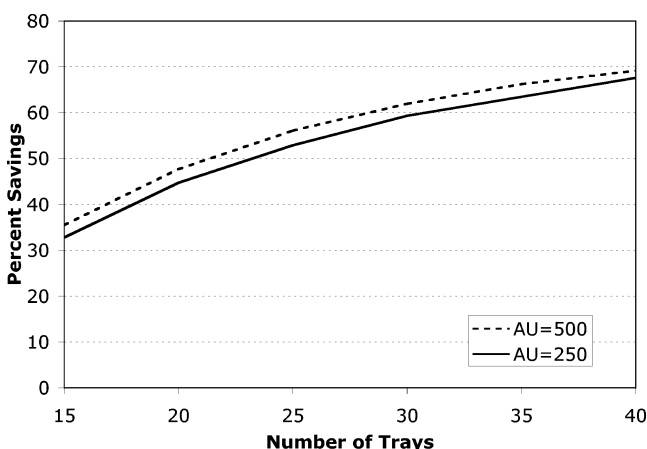
to be installed without interfering with the material flows in the column, implying that a conventional column can be retrofitted with the serial heat exchangers without adverse effects.

**Temperature Profile.** In Figure 8, the middle solid line of the diabatic column chart shows the temperature of each tray in the column; the line below the middle line is the temperature profile for the serial heat exchanger in the rectifier, while the one above is the temperature profile for the serial heat exchanger in the stripper. As for all optimized diabatic columns, the tray temperatures vary almost linearly along the column, indicating that each tray is doing its share of the separation process. The heat exchanger temperatures are mostly a constant difference away, again indicating a uniform dissipation. By contrast, the adiabatic column has very little temperature change across trays 7–12. Thus, the serial heat exchangers help the diabatic column utilize the trays better.

**Sensitivity of Entropy Production.** To investigate the sensitivity of the column performance on the four control parameters (two mass flow rates and two inlet



**Figure 9.** Sensitivity of entropy production rate as a function of deviations from the optimal heat exchange fluid inlet temperatures.

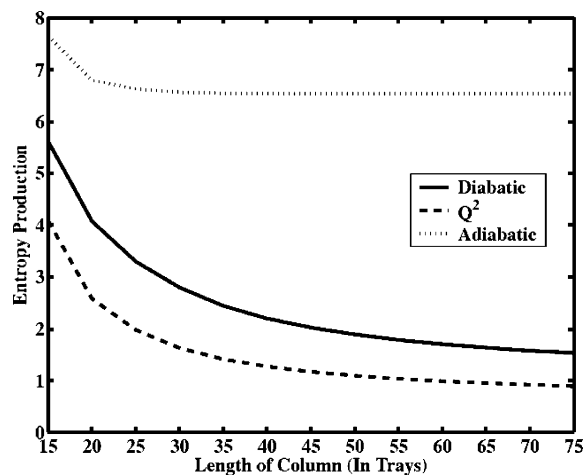


**Figure 10.** Percent savings of entropy production of a diabatic column with serial heat exchange versus an adiabatic column of the same length. A heat exchanger conductance of  $UA = 500$  W/K is drawn in solid line, while  $UA = 250$  W/K is drawn in dotted line.

temperatures) of the serial heat exchangers, the following experiment was conducted. Varying either optimal inlet temperature by 1 K in the direction away from the feedpoint (i.e., slightly larger driving force) will result in an entropy production increase of approximately 15%, while varying either temperature toward the feed point will yield an entropy production increase of 400% (Figure 9). The reason for the latter is a strongly increasing demand on the reboiler and condenser when the serial heat exchangers have a smaller driving force and thus exergetically less efficient operation. This sensitivity is particularly strong for the sequential heat exchange design discussed here because the inlet temperature controls the heat exchange in all subsequent trays.

#### Exergy Savings versus an Adiabatic Column.

Figure 10 shows the potential efficiency improvements by using a diabatic column with serial heat exchange instead of a traditional adiabatic column for the separation process at hand for different length columns. At the short end, a 15-tray column achieves 35% smaller entropy production rate, while at the high end, a 40-tray column can conserve more than two-thirds of the losses, 69%. Generally, the more trays a diabatic column has, the greater the savings, eventually approaching reversible separation for a column of infinite length. Even when the heat exchanger conductance is reduced



**Figure 11.** Entropy production rate comparison between an adiabatic column (dotted), a fully diabatic column (dashed), and a diabatic column with serial heat exchange (solid).

to half, the improvements are still 32% and 67%, respectively.

**Entropy Comparison.** Finally, in Figure 11, we compare the entropy production rates for fully diabatic columns, columns with serial heat exchange, and adiabatic columns over a range of lengths. First, the savings in using a diabatic column are substantial, the more so the longer the column. We also see that there is a price for giving up the total freedom of optimizing the heat exchange on each tray individually and installing serial heat exchangers instead, but it is fairly small, especially for the longer columns. Considering the technical advantages of the serial heat exchange scheme—only four piercings of the column containment rather than two for each tray, and the need for only one heat source and one cold source rather than one for each tray—makes this design most suitable for retrofitting distillation columns.

**Further Studies.** Further studies will be done to find out how entropy can be further minimized using serial type heat exchangers. Studies include adding a fifth parameter that allots the heat exchanger inventory nonuniformly among the trays. Other studies include comparing the present numerical results with a prototype diabatic column under construction in Mexico.

#### Nomenclature

- $V_i$  = vapor rate leaving tray  $i$
- $L_i$  = liquid rate leaving tray  $i$
- $F$  = feed rate
- $x$  = mole fraction of light component
- $x_f = x$  in feed mixture
- $x_D = x$  in distillate
- $x_B = x$  in bottoms
- $Q_D$  = heat removed by the condenser
- $Q_B$  = heat supplied by the reboiler
- $B$  = bottoms production rate
- $D$  = distillate production rate
- $T$  = absolute temperature
- $T_i$  = temperature on tray  $i$
- $K$  = number of trays
- $C_o$  = liquid–vapor coexistence heat capacity
- $\dot{m}$  = mass flow rate of the heat exchange fluid
- $T_{ex,i}^{in}$  = temperature of heat exchange fluid entering tray  $i$
- $T_{ex,i}^{out}$  = temperature of heat exchange fluid leaving tray  $i$
- $U$  = conductivity

$A$  = area  
 $\Lambda$  = length of heat exchanger  
 $\lambda$  = distance along heat exchanger  
 $C_p$  = constant pressure heat capacity  
 $\Delta S_u$  = total entropy production of the process  
 $Q_{\text{excess}}^n$  = unbalanced heat on tray  $n$   
 $M$  = large constant used as a penalty multiplier

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