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### The second law optimal state of a diabatic binary tray distillation column

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#### **Abstract**

A new numerical procedure to minimize the entropy production in diabatic tray distillation columns has been developed. The method was based on a least square regression of the entropy production at each tray. A diabatic column is a column with heat exchangers on all trays. The method was demonstrated on a distillation column separating propylene from propane. The entropy production included contributions from the heat transfer in the heat exchangers and the mass and heat transfer between liquid and vapor inside the distillation column. It was minimized for a number of binary tray distillation columns with fixed heat transfer area, number of trays, and feed stream temperature and composition. For the first time, the areas of heat exchange were used as variables in the optimization. An analytical result is that the entropy production due to heat transfer is proportional to the area of each heat exchanger in the optimal state. For many distillation columns, this is equivalent to a constant driving force for heat transfer. The entropy production was reduced with up to 30% in the cases with large heat transfer area and many trays. In large process facilities, this reduction would ideally lead to 1–2 GWh of saved exergy per year. The most important variable in obtaining these reductions is the total heat transfer area. The investigation was done with a perspective to later include the column as a part in an optimization of a larger process. We found that the entropy production of the column behaved almost as a quadratic function when the composition of the feed stream changed. This means that the feed composition is a natural, easy variable for a second law optimization when the distillation column is a part of a process. The entropy production was insensitive to variations in the feed temperature.

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#### 1. Introduction

Distillation is a widely used separation method that requires large inputs of energy (King, 1980). Research is therefore being done to find methods that can replace distillation, e.g. membranes (Baker, 2002). A lot of effort has also been put into the search for improved designs and operation of the conventional distillation columns. One such design is the *heat-integrated distillation column* (HIDIC) (Nakaiwa et al., 2001), while another is the *diabatic* distillation column, where heat is added or withdrawn by heat exchangers on each tray (Rivero, 1993, 2001). We will focus on the efficiency of the latter concept. It has been known for long that

this kind of distillation columns have better second law efficiencies (Fonyo, 1974a,b). Previous work have shown that potentially large savings could be obtained in the use of high quality energy (Sauar et al., 1997; Kauchali et al., 2000; De Koeijer et al., 2004).

The aim of this work is to contribute to a better energy economy of distillation by increasing the energy efficiency. Maximum efficiency is found by minimizing the entropy production in diabatic columns. We continue the work by De Koeijer et al. (2004), who minimized the entropy production in diabatic distillation columns. We shall add to earlier work and show how we can determine, by theory and calculation, the optimal area of heat exchange at each tray. A new numerical solution procedure shall also be reported. We will not yet include aspects related to the practical implementation (like controllability and cost) in this study. The ultimate goal is to include such aspects in the optimization, but there

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are still unanswered questions as of how the operating conditions affect the efficiency: how does the composition and temperature of the feed affect the entropy production of diabatic columns operating at minimum entropy production? What effect does the total heat transfer area and number of trays have? When the kind of optimization we study here, is included in a larger process optimization, the effect of these operating conditions must be known.

More specifically, we shall theoretically study the separation of different mixtures of propane and propene at 15 bar. The mixtures are separated into two product streams with mole fractions of propene equal to 0.95 and 0.05 for the top and bottom stream, respectively. Since the product purities are fixed, the thermodynamical state of the material outputs from the columns are also fixed. For a given separation task, the adiabatic and diabatic column have thus the same net energy requirement. The diabatic column is more efficient in terms of the second law. In the present context second law optimization means to find the amounts of heat transferred locally. Given a certain allowed total heat transfer area, we shall find the distribution of this area, and of the transferred heat, that produces the least entropy. We assume that any kind of cooling or heating medium is available at any temperature. The separation task, number of trays, and total heat transfer area are fixed in the optimization. This problem has not been solved before.

The separation of propene (or propylene) and propane is present in many different chemical plants, especially those producing higher olefins. Olefins are the basic compounds in the making of a large variety of polymers. An additional complication with this separation is that the boiling points are close, which means that the separation must be carried out in columns with many trays and large heat transfer in both the stripping and rectifying sections. Studies so far have mostly been concerned with shorter columns and less heat transfer.

#### 2. Diabatic distillation

We have chosen to study the separation of propylene  $(C_3H_6)$  and propane  $(C_3H_8)$ . This is done in a sieve-plate distillation column (McCabe et al., 1993) with N plates (or trays). A sieve plate is designed to bring a rising stream of vapor into intimate contact with a descending stream of liquid. In lack of rate expressions describing the transfer of heat and mass between vapor and liquid, we assume that the liquid and vapor leaving each tray are in equilibrium (see however Wesselingh, 1997; Kjelstrup and De Koeijer, 2003). We further assume that the sieve-plate column has no pressure drop. The input of new material is done through a feed stream F, entering at a certain tray number  $N_F$ . Distillate D, is removed above the top tray, and bottom flow B, is removed below the bottom tray. Both product streams are liquids at their boiling points. Fig. 1 shows the layout of a distillation column. Traditionally, distillation is done

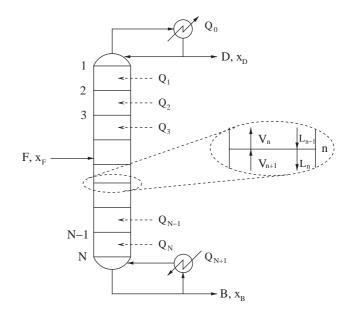


Fig. 1. A diabatic distillation column.

adiabatically, which means that heat is added or withdrawn only in a condenser and a reboiler. No mass transfer is assumed to occur here. In our model, this corresponds to tray number 0 and N+1, respectively. To increase the second law efficiency, heat exchangers may be introduced on each tray in the distillation column, making the column *diabatic*. This allows heat,  $Q_n$ , to be transferred at tray number n. The heat transferred will change the liquid and vapor streams

$$Q_n = V_n h_n^{V} + L_n h_n^{L} - V_{n+1} h_{n+1}^{V} - L_{n-1} h_{n-1}^{L}, \tag{1}$$

where V and L is the vapor and liquid streams, respectively, and h is the enthalpy of the streams. At the feed tray  $(n=N_F)$  and the tray above  $(n=N_F-1)$ , the above equation has an additional term on the right-hand side that includes the heat carried with the vapor and/or liquid part of the feed stream

extra terms = 
$$\begin{cases} -(1-q)Fh_F^{V}, & n = N_F - 1, \\ -qFh_F^{L}, & n = N_F, \end{cases}$$
 (2)

where q is the fraction of liquid in the feed stream. The symbol  $Q_n$  shall for the reminder of this article be referred to as the "duty".

In the modeling of adiabatic distillation columns, the energy balance, Eq. (1), is used with  $Q_n = 0$  for  $n \in [1, N]$ . The material balances, on the other hand, are identical for adiabatic and diabatic columns. Rather than considering *one* tray, these balances are constructed by considering the transport of mass in and out of a control surface covering the top of the column. A total mass balance gives

$$V_{n+1} - L_n = \begin{cases} D, & n \in [0, N_F - 2], \\ D - (1 - q)F, & n = N_F - 1, \\ D - F, & n \in [N_F, N + 1]. \end{cases}$$
 (3)

A similar balance exists for the mass of the light component.

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