

# Energy Efficient Distillation by Optimal Distribution of Heating and Cooling Requirements

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## Abstract

In this paper investigations regarding optimal placement and duty distribution of internal heat exchangers in distillation columns have been carried out based on simulations. In particular the effect of adding 2, 4 and 19 internal heat exchangers to a 19 tray distillation column separating isopropanol and methanol was studied. It is concluded that the minimum entropy production placement of the heat exchangers depends strongly on the degree of separation. The optimum is however rather flat, implying that optimal placement for a nominal operating point performs nearly as well even for significant changes in feed and product compositions. When compared to a conventional column run under the same operating conditions, entropy production for an optimally operating column with four thermally active stages (4TA) is reduced by 25 % as compared to 37 % for a 6TA column and 70% for a column in which all the trays are equipped with heat exchangers.

## Introduction

In spite of its relatively low energy efficiency (typically only a few percent), distillation is still one of the most widely used separation techniques in the chemical industry. This is illustrated by the fact that distillation accounts for more than 3 % of the total energy dissipation in the USA, Mix *et al.* (1978), Humphrey and Siebert, (1992). The energy consumption attributed to distillation has been reported as high as 5-6% within the industrialized countries by Pilavachi (1996).

An immense amount of work has been carried out in the field of heat integration within distillation trains. Most of this work had the purpose of minimizing the use of external utilities in heat exchanger networks (HEN). The major tool for this work has been pinch-analysis which can minimize the external duties when integrating conventional columns, Linnhoff (????).

From a 2<sup>nd</sup> law efficiency point of view, conventional distillation performs very poorly in general. One way of improving this efficiency is to distribute the heat added and removed over the distillation column via heat exchangers. Various methods for optimizing the 2<sup>nd</sup> law

efficiency (minimizing the entropy production, minimizing the exergy loss) for distillation process design have previously been suggested: equipartition of entropy production, Tondeur and Kvaalen (1987); equipartition of forces (EOF), Ratkje *et al.* (1995); equal thermodynamic distance (ETD), Salamon *et al.* (1998).

Assuming a distillation column with  $N$  stages and a heat exchanger on each stage, all methods predict that the entropy production in the column,  $S_{HX}$ , goes to zero as  $N$  goes to infinity (see appendix). In the limit of "large" (but finite)  $N$ , the predictions however diverge. This divergence has been outlined in the coffee cup example of Salamon *et al.* (2000).

From an economical/engineering point of view, an issue that needs to be addressed is how *well* can one do with only a *few* more thermally active stages compared to conventional columns. Optimal tray locations for 4 thermally active stages (condenser + 1 heat exchanger in rectifying section + 1 heat exchanger in stripping section + reboiler = 4 thermally active stages = "4TA") has previously been investigated by Kojier *et al.* (1999), and Siragusa *et al.* (2000).

## Economic vs. Thermodynamic Optimum

The net heat input to a distillation column

$$Q_{net,input} = Q_{added} - Q_{removed} = h_D + h_B - h_F$$

for a specified separation is practically constant. This is true for binary distillation, and applies also to a large extent to multi component distillation with specified product concentrations. The amount of high grade energy added to a distillation column is however not constant, but depends on the sizing and design as well as the operation of the column.

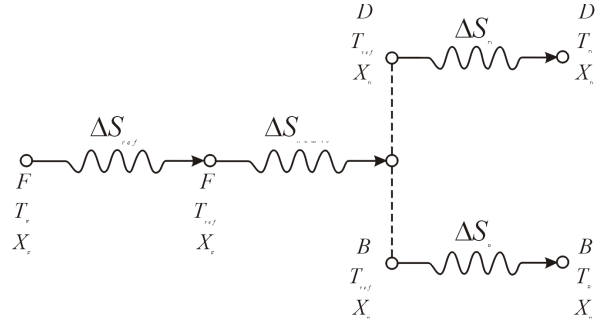
The “true thermodynamic optimum” minimizes the entropy production or, equivalently, the exergy cost. This is carried out by minimizing the quality of the heat input to the column and at the same time maximize the quality of the heat output. This makes it necessary to add heat exchangers on each plate. Possible design procedures for such processes can include the approaches of EOF or ETD.

For industrial applications where the objective is operating at the economical optimum, one can imagine using a “Poor man’s” ETD/EOF distillation column with only a few extra heat exchangers.

In this paper we investigate a “6TA” column, i.e., a column which is equipped with an additional 4 internal heat exchangers. In the following section we describe the model used in the simulations. We compare our results to a conventional column, a 4TA column as well as a column where each plate is equipped with a heat exchanger.

### Entropy Production in Distillation

Figure 1 illustrates the thermodynamic transitions in distillation: 1) a temperature equilibration of the feed from the feed temperature to a reference temperature (e.g. the boiling point of the low boiling component) 2) unmixing of the ideal feed mixture to the two products D and B at the reference temperature and 3) temperature equilibration from the reference temperature to the product temperatures.



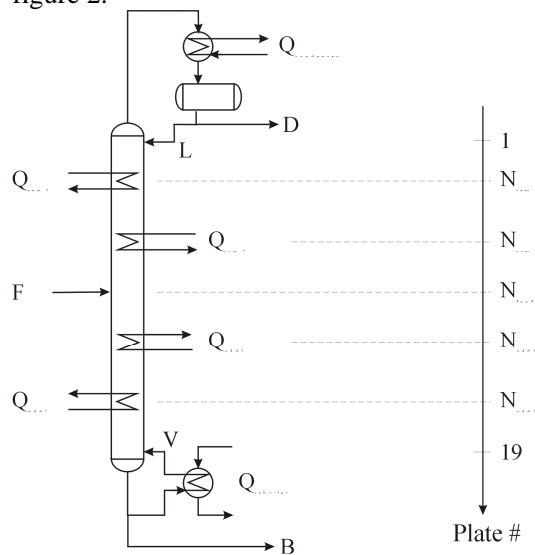
**Figure 1: Thermodynamic transitions in distillation.**

From a thermodynamic efficiency point of view, it is most interesting to look at the entropy change due to irreversibilities – the entropy production. If the subpaths traveled within figure 1 are reversible changes, then the entropy change due to irreversibilities can be formulated as:

$$\begin{aligned} S_{irrev} &= S_{HX} - S_{rev} \\ &= S_{HX} - (S_{ref} + S_{unmix} + S_D + S_B) \end{aligned}$$

### Simulation Model

The simulation model consists of a distillation column with 19 ideal stages, a partial reboiler (1 ideal stage) and a total condenser, separating methanol and 2-propanol. A schematic of the 6TA distillation column model can be seen in figure 2.



**Figure 2: Schematic of a 6TA distillation column model.**

The vapor-liquid equilibrium model used is Soave-Redlich-Kwong. The feed and product specifications are:

Spec.	Value	Unit
$X_F$	50	mole% MeOH
$X_D$	95	mole% MeOH
$X_B$	5	mole% MeOH
$F$	1	mole

The model was implemented in Matlab . The procedure for minimizing the entropy production has been outlined in the appendix together with additional information on the model.

### Results

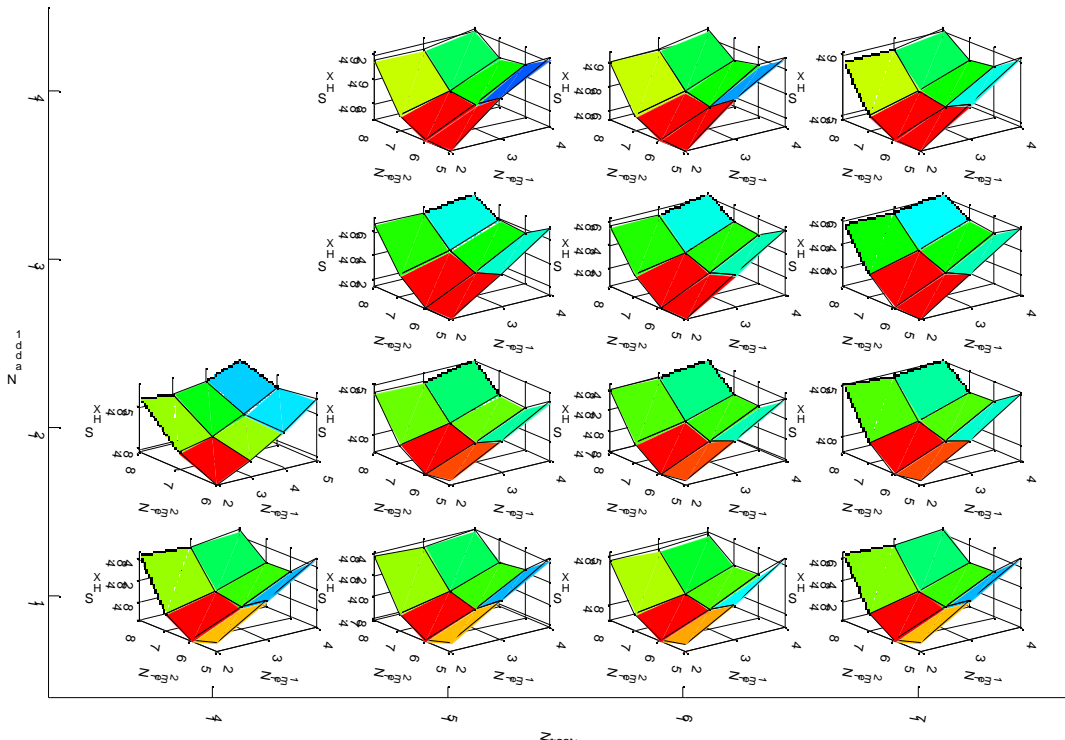
An entropy minimization of the 6TA column was carried out for different TA plate positions. The investigated integer-parameter space was initially:

$$\begin{aligned} N_{rem1} &= 2 : 4 \\ N_{rem2} &= 5 : 8 \\ N_{add1} &= 11 : 14 \\ N_{add2} &= 14 : 17 \end{aligned}$$

In figure 3 a plot has been made over the performed minimization of entropy. The primary x-axis is the TA plate position of the lowest internal heat exchanger  $N_{add2}$ . The primary y-axis is the TA plate position for the upper heat exchanger in the stripping section. For each combination, the entropy change due to heat exchange is plotted as a surface against the heat exchanger combinations in the rectifying section. It is seen that the optimal combination for minimum entropy production within the investigated parameter space is:

$$[N_{rem1}, N_{rem2}, N_{add1}, N_{add2}] = [2 \ 6 \ 12 \ 17]$$

Table 2 shows the heat input of high grade heat, the net heat input (constant), the entropy change due to heat exchange and the entropy production. Table 3 shows the optimal TA plate positions with the corresponding duties as well as the duties for reboiler and the condenser.



**Figure 3:** Minimum entropy production (J/(mol K)) for investigated thermally active tray positions. Main x-axis: lowest positioned heat exchanger ( $N_{add2}$ ). Main y-axis: highest positioned heat exchanger in stripping section ( $N_{add1}$ ). Minor x-axes: highest positioned heat exchanger in rectifying section ( $N_{rem1}$ ). Minor

y-axes: lowest positioned heat exchanger in rectifying section ( $N_{rem2}$ ). Minor z-axes entropy change due to heat exchange.

As can be seen from figure 3, the minimum entropy change does not take place at an interior point but rather it lies on the boundary of the set of allowed parameter values. Thus it was decided to expand the parameter range to also include the tray one position ( $N_{rem1}=1$ ). This was not originally included because it corresponds to a model column which differs significantly from the one shown in figure 1; with  $N_{rem1}=1$ , no reflux is used from the condenser. In figure 4 it is shown that the entropy production is reduced drastically when  $N_{rem1}=1$  is used in combination with the best TA plate choices in the stripping section.

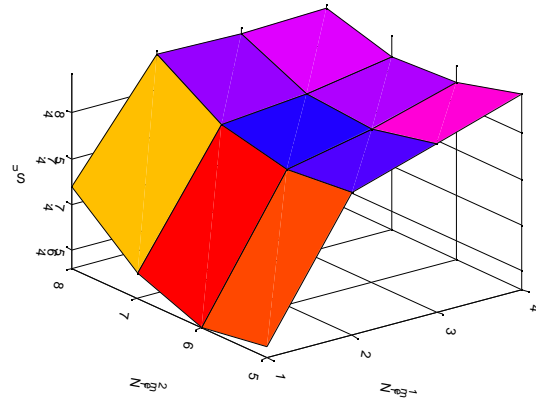


Figure 4: Entropy change (J/(mol K)) due to heat exchange,  $\Delta S_{HX}$ . Where  $N_{rem1}$  is the upper TA plate number in the rectifying section.  $N_{rem2}$  is the lower TA plate in the rectifying section.  $N_{add1}=11$  and  $N_{add2}=15$ .

Column type	Absolute heat input (kJ/mole feed)	Net heat input (J/mole feed)	$S_{HX}$ (J/mole K)	$S_{irrev}$ (J/mole K)
Conventional	50.034	419	5.64	2.71
4TA (optimal)	54.033	419	4.95	2.02
6TA (optimal)	57.074	419	4.63	1.70
ETD (“optimal”)*	???	419	3.76	0.83

Table 2: Comparison of absolute heat input, entropy change due to heat exchange and the entropy change due to irreversibilities for the conventional, 4TA, 6TA and ETD column cases.

\*) The reason why optimal is put in quotes for the case where heat exchangers are put on each tray is that ETD does not predict the true thermodynamic optimum well for small systems, but it does so for larger systems as outlined in Salamon *et al.*

Column type	Rectifying Section			Stripping Section		
	TA plate position(s)	TA plate duty(ies) in (kJ/mol feed)	Condenser duty (kJ/mol feed)	TA plate position(s)	TA plate duty(ies) in (kJ/mol feed)	Reboiler duty (kJ/mol feed)
4TA (optimal)	4	-16.417	-37.197	13	19.016	35.016
6TA (optimal)	1 and 6	-44,564 and -11.759	-	11 and 15	13.924 and 12.566	30.252

Table 3: The optimal positioning and duties for the thermally active plates.

## Discussion and Conclusions

### Simulation model

It would be more reasonable to investigate the true optimum for a “symmetric” column. The column would be more “symmetric” if the

condenser was partial instead of total. As it is in the used simulation model the reboiler constitutes an equilibrium stage - the condenser does not. A better arrangement is to have a deflegmator first (which condenses only what is necessary for reflux) constituting an equilibrium

stage - and then a condenser that takes the heat of condensation out of the distillate product. As the model is now, significant entropy is produced in "pouring" down liquid (reflux) with a lower temperature and different composition to the top tray. It can also be seen from figure 2 that the investigated parameter space for the TA-plates (2:4,5:8,11:14,14:17) should have included the tray 1 position in order to be complete.

#### Operational aspects

One important aspect yet to be analyzed is the operation and control of thermally integrated columns like the 4TA and 6TA.

The overall integration of heat integrated (4TA, 6TA,...) distillation columns will expand the temperature interval of supplied/removed heats and lower the need for external utilities.

Finally it is concluded that in order to perform the separation at the minimum entropy production it is necessary to add 8% and 14% more heat in the stripping section for the 4TA and the 6TA column respectively compared to the conventional case (table 2).

It is also seen that the entropy production can be significantly reduced by adding only 2 extra heat exchangers (4TA), namely 25% compared to conventional distillation. The entropy change due to irreversibilities for the addition of 4 extra heat exchangers (6TA) is 37%.

The optimal tray locations for the thermally active trays are for the 6TA: 1, 6, 11 and 15. In comparison, the 4TA optimal placement of TA plates is 4 and 17.

The optimum is rather flat, implying that optimal placement of TA's for a nominal operating point performs nearly as well in terms of entropy production for even significant changes in feed and product compositions.

### Symbols

Q	-	Heat
D	-	Distillate
B	-	Bottom product
F	-	Feed
x	-	Molar ratio
T	-	Temperature
ref	-	reference state
h	-	enthalpy
S	-	entropy
irrev	-	irreversibility
HX	-	heat exchange
rev	-	reversible
unmix	-	unmixing
N	-	Thermally Active tray location #
addi	-	the i'th addition
remj	-	the j'th removal
	-	change

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## Appendix

### Entropy minimization procedure:

The procedure below was used for minimizing the entropy production for each specified set of TA-plate positions.

- 1) Make an initial guess at the duties of the intermediate TA-plates (using a simplex method),
- 2) Make an initial guess for the condenser duty (using secant method),
- 3) Carry out balancing of column by plate to plate calculation, finding the reboiler duty and optimal feed plate location,
- 4) If balancing is not converging goto (2) otherwise,
- 5) Evaluate entropy production,
- 6) If convergence of entropy production not obtained (minimum entropy production) goto (1), otherwise
- 7) Repeat the procedure for new TA-plate positions.

### Calculation of entropy production:

The change of entropy in the universe for a distillation column can with the given assumptions be formulated as:

$$S_u = S_{HX} + S_{unmix} + S_D + S_B$$

Where  $S_{HX}$  is the entropy change due to heat exchange on the TA-plates, in the reboiler and in the condenser:

$$S_{HX} = \sum_{j=1}^{N_T} \frac{q_j}{T_j} + \frac{q_D}{T_D} + \frac{q_B}{T_B}$$

$S_{unmix}$  is the entropy change of unmixing in the separation.  $S_D$  and  $S_B$  are the entropy changes due to cooling and heating the distillate respectively the bottom product.

The detailed explanations of performing entropy calculations have been outlined in Brown and Siragusa (2000).