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Entropy Minimization in Design of Extractive Distillation System with Internal Heat Exchangers

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A methodology for entropy production minimization in design of extractive diabatic distillation systems is proposed. The feasibility of the design is obtained by the boundary value method used by Doherty and coworkers, and the optimal design is attained using a genetic algorithm, this strategy allows determine the optimal heat load distribution, and the flows and temperatures for hot and cold utilities. For optimal design of diabatic distillation columns it was employed a multilevel strategy, the first level solves the optimal adiabatic design and the second one determines the optimal heat load distribution in the sequential heat exchangers (SHE), in both levels the feasibility of the designs is forced by a penalty in the objective function, it considers the separation feasibility and the energy balance consistency. The ethanol dehydration by extractive distillation with ethylene glycol is assessed in order to show our optimal design procedure and to compare the diabatic distillation process with the adiabatic one. Results show that this strategy allows to solve the problem, and that with SHE, the entropy production can be reduced expressively: 14% for the recovery solvent column and 16% for the extractive one, compared to the adiabatic columns.

1. Introduction

Traditionally the external heat exchange in distillation columns is done at the top (condenser) and bottom (reboiler) of the column. Nevertheless, a more energy-efficient process can be achieved when the external heat transfer is also allowed in the trays. A better energy usage implies reduction in operational costs and carbon dioxide emissions (Suphanit, 2010).

The maximum second law efficiency in diabatic columns is attained with minimal temperature difference between tray and heat transfer fluid. But that condition can hardly be attained in a real process plant. A way to take advantage of diabatic distillation characteristics is by using sequential heat exchangers in the trays, in this configuration heat transfer utility flows sequentially from one stage to the next; therefore it is only necessary one fluid for heating and one for cooling. Experimental evidence shows a significant improving on the energy efficiency when SHE are used (De Koeijer and Rivero, 2003); the advantages of this configuration can be exploited when a suitable heat load distribution is found.

The aim of this work is to provide a mathematical strategy for optimal design of both single and double feed columns fulfilling the design constraints, such as product composition and recovery of key component. The results may be useful for evaluating, in an early step of design, the advantages of using diabatic or adiabatic distillation.

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2. Mathematical Model

Mathematical model employed in this work is a modification of the boundary value method (Doherty and Malone, 2001), it takes into account the heat transfer in internal stages of the distillation column.
The model comprises mass and energy balances, and the vapor-liquid equilibrium. A feasible design is obtained when the operating profiles from the top and the bottom intersect and the overall energy balance in the column is fulfilled. A detailed derivation of the equations as well as its solving methodology can be found in a previous work (Mendoza and Riascos, 2010).

3. Optimization

3.1 Objective Function

The objective function, *OF*, is formed by two terms (Eq. 1). The first one is the entropy production in the distillation column; the second one is a penalty term which forces the fulfillment of the constraints imposed on the design:

$$OF = \left(\frac{ds_{irr}}{dt}\right)_{DC} + \alpha \sum_{r=1}^{4} \beta_r \tag{1}$$

where α is a weighting factor ($\alpha = 100$), and β_r are binary variables which take the value of zero if the constraint is fulfilled and one if not. The variable β_1 considers the intersection of operation profiles; β_2 the overall energy balance; β_3 and β_4 the minimum temperature approach allowed in condenser and reboiler.
The entropy generated in the column, $(ds_{irr}/dt)_{DC}$ (Mendoza and Riascos, 2010) is:

$$\left(\frac{ds_{irr}}{dt}\right)_{DC} = D\left[s_D - s_F - \frac{\dot{Q}_c}{DT_c}\left(1+\sum_{l=1}^{J}\frac{q_l}{\tau_l}\right)\right] + B\left[s_B - s_F - \frac{\dot{Q}_B}{BT_B}\left(1+\sum_{b=1}^{M}\frac{q_b}{\tau_b}\right)\right] + \left(\frac{ds_{irr}}{dt}\right)_{HEDC} \tag{2}$$

where $\dot{Q}_c$, $\dot{Q}_B$, T_c, T_B are the heat loads (positive when transferred from the heat utility to the stage) and temperatures in the condenser and reboiler respectively. The summation terms represent the heat load in internal stages of the column, $l = 1$ to J are the stages of the rectifying section and the $b = 1$ to M are the stages of the stripping and extractive zones; τ_l and τ_b are stage dimensionless temperatures ($\tau_l = T_l/T_c$, $\tau_b = T_b/T_B$) and q_l, q_b are stage dimensionless heat loads ($q_l = Q_l/Q_c$, $q_b = Q_b/Q_B$); s_D, s_B, s_F are the molar entropies of distillate, bottom product and feed streams. The entropy of the feed is $s_F = (F_r\, s_{Fu} + s_{Fl})/(1+F_r)$ where s_{Fu} and s_{Fl} are molar entropies of the upper and lower feeds and F_r is the feed ratio: $F_r = F_u/F_l$. The last term of the right hand side in Eq. (2) is the entropy production due to heat exchange between utilities and stages, calculated as the product of the heat flow and its thermal force (Kjelstrup et al., 2010).

$$\left(\frac{ds_{irr}}{dt}\right)_{HEDC} = \sum_{l=1}^{J}\dot{Q}_l\left(\frac{1}{T_l} - \frac{1}{T_{f,l}}\right) + \sum_{b=1}^{M}\dot{Q}_b\left(\frac{1}{T_b} - \frac{1}{T_{f,b}}\right) \tag{3}$$

where $T_{f,l}$, $T_{f,b}$ are average temperatures of the cooling and heating utilities in the stage. The sign of the heat load ensures that each term in the Eq. (3) is positive.

3.2 Optimization Strategy

The strategy for optimal design considers two levels: the first level solves the optimal adiabatic design and the second one determines the optimal heat load distribution with sequential heat exchangers (SHE). The stages for the optimal design of adiabatic columns consider:

1. Estimate the minimum reflux ratio of the distillation column, which generates the least entropy production for the separation task in the adiabatic column.
2. Define the operational reflux ratio, which set up the number of stages of the distillation column, the operational reflux is found based on economic criteria.
3. Entropy production of the adiabatic column is calculated after the number of stages and the inlet temperatures of the heat utilities are defined.

The optimal heat load distribution using SHE is achieved allowing heat transfer in the internal stages of the distillation column, and minimizing the entropy production in the column. The maximum heat transfer area is defined knowing the available space given by the column diameter and the tray layout.

4. Case Studies

The methodology was applied on the columns that compose an extractive distillation system for ethanol dehydration with ethylene glycol. The first column is an extractive (double feed) column fed with 0.278 mol s^{-1} of water/ethanol (W/E) mixture, 85% mol E and 15% mol W, it is dehydrated to obtain high-purity ethanol in the distillate (99.8% mol). The upper feed is a water/ethylene glycol (W/EG) mixture, 0.1% mol W and 99.9 % mol EG. Fractional recovery of ethanol in the column is 99.99%. The E/W mixture enters at bubble point whereas the upper feed temperature is 351 K.

The second column (single feed) is fed with the bottom product from the first one, at bubble point, and dehydrates the mixture obtaining EG at 99.9% mol in the bottom stream. Fractional recovery of EG is 99.999%.

Both columns operate at a total pressure of 1 atm, and no pressure drop is assumed; the minima temperature approach in all heat exchangers is 10 K. Reflux ratios of single and double feed adiabatic columns were RR1 = 0.302 and RR2 = 0.65; these values correspond to 1.03 and 1.5 times the minimum reflux of the separation tasks carried out in the single and double feed columns respectively, and they are within the values recommended (Seader and Henley, 1998). The feed ratio in the double feed column was set to Fr = 0.5, based on the economic optimization done by Knight and Doherty (1989).

4.1 Optimization Variables

The optimization variables of diabatic columns were the flows of heating and cooling utilities (m_H and m_C), the reflux and the reboil ratios and the total heat transfer capacity in stages ($0 \leq UA_{stage} \leq 0.2$ kW K^{-1}). The total heat transfer capacity was estimated from experimental data (Kaeser and Pritchard, 2005).

4.2 Thermodynamic Properties and Computational Methods

In liquid phase the activity coefficients as well as the enthalpies and entropies of mixing were calculated using the NRTL model (Seader and Henley, 1998), whereas vapor phases are described by the ideal gas law. Liquid and vapor heat capacities and heats of vaporization were taken from Poling et al. (2008). The heat capacity of heating utility, Dowtherm T™, can be found in the Dow's web page (Dow, 2004). The model was programmed in Matlab™ using a genetic algorithm to optimize the model.

Table 1: Flows and temperatures of heat utilities, and total energy transferred.

		Double feed adiabatic	Double feed SHE	Single feed adiabatic	Single feed SHE
m_c	(mol s^{-1})	4.59	4.34	0.45	0.41
T_C^{in}	(K)	298.1	298.1	298.1	298.1
T_C^{out}	(K)	341.0	343.4	363.0	372.1
m_H	(mol s^{-1})	4.00	0.50	0.29	0.11
T_H^{in}	(K)	432.0	432.0	490.0	490.0
T_H^{out}	(K)	426.5	387.0	475.0	448.8
Q_{added}	(kW)	16.56	16.56	3.52	3.61
$Q_{removed}$	(kW)	-14.80	-14.80	-2.20	-2.29

5. Results and Discussion

The principal results of optimal design for adiabatic and no-adiabatic columns are in Table 1. From energetic efficiency comparison: the entropy generated in the single feed SHE and adiabatic columns were 1.31 and 1.52 W K^{-1} respectively, and the entropy production in the double feed columns were 12.55 W K^{-1} in the adiabatic one and 10.51 W K^{-1} in the SHE one. The reductions achieved in the single and double SHE columns were 13.8% and 16.2% compared with the adiabatic columns.

Entropy production profiles (Figs. 1 and 2) show the reductions are given mainly by the heat load distribution in the stripping zone of the SHE distillation columns.

Vapor and liquid profiles in the stripping zones of the SHE columns differ from the adiabatic ones because in adiabatic ones the external supply of heat is located only in

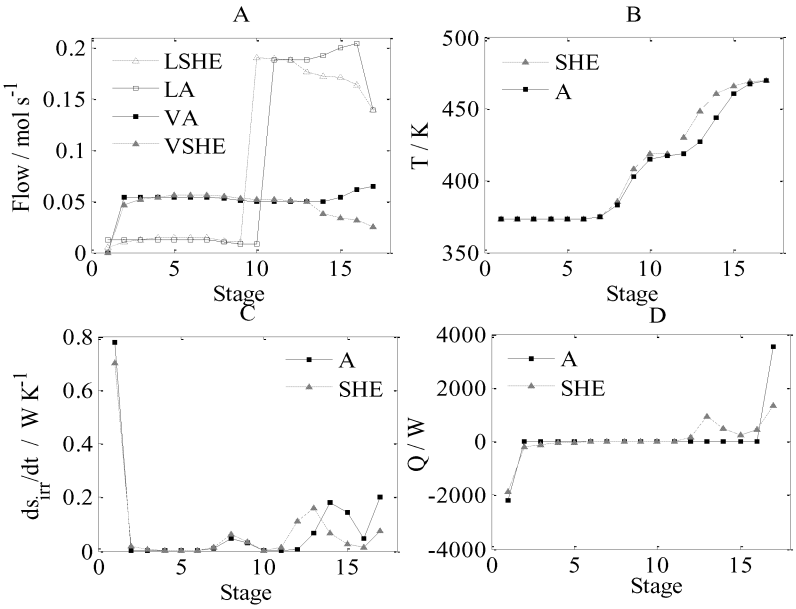

Figure 1: Single feed distillation columns. A. Flows. B. Temperatures. C. Entropy production. D Heat load profiles. LSHE and VSHE are vapor and liquid flows for the diabatic column (SHE); LA and VA are liquid and vapor flows for adiabatic one (A).

the reboiler, whereas in SHE columns, a part of the external heat supply is distributed in internal stages obtaining smoother changes in composition and temperature.
The heat load input is approximately the same in both types of distillation columns, with a maximum difference of 2.6% in the single feed columns (see Table 1). Nevertheless, the SHE columns diminish the energy degradation in the process; this fact is reflected by the reduction of the flows of the heating (62.1% single feed, and 87.5% double feed) and cooling utilities (8.9% single feed, and 5.4% double feed) with respect to the flows required by the adiabatic columns (Table 1), the flow reduction means that the SHE column lessens the demand of high quality energy resources (i.e. the heating flows at the temperatures of 432 K and 490 K).
Another aspect related with entropy production savings in SHE columns is the outlet temperatures of heat transfer utilities: the sequential heat exchangers allow the heat removal, in the rectifying section, at higher temperatures and the heat addition, in the stripping section, at lower temperatures. The gaining in the outlet temperature of the cooling utility in the SHE is relevant if it can be used in a further heat transfer before it comes back to the cooling tower, similarly the lower outlet temperature of the heating utility is advantageous if a part of the heat needed to upgrading its temperature can be obtained from a low temperature heat source.

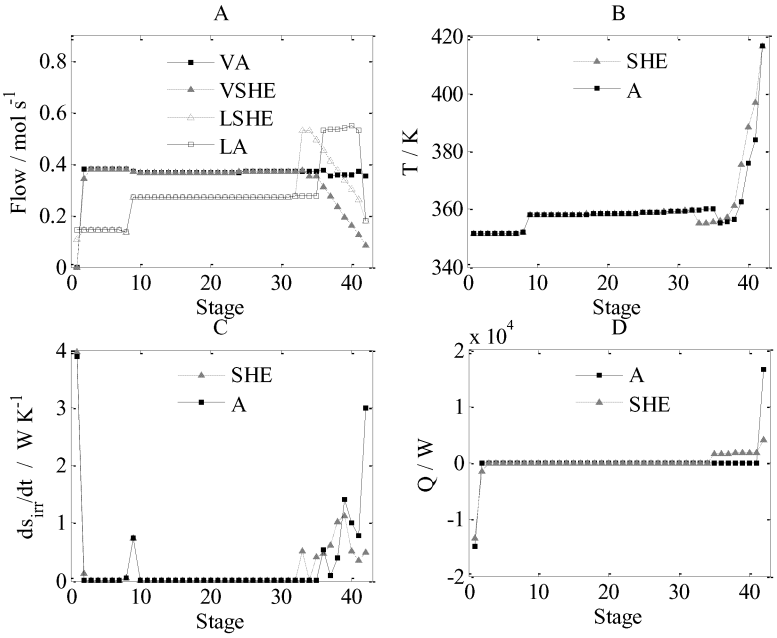

Figure 2: Double feed distillation columns. A. Flows. B. Temperatures. C. Entropy production. D Heat load profiles. LSHE and VSHE are vapor and liquid flows for diabatic (SHE) column; LA and VA are liquid and vapor flows for adiabatic (A) one.

If the inlet temperature of the heating utility would have been an optimization variable the savings in entropy would be reflected in a lower inlet temperature of the heating utility than the required in the adiabatic case (see Kjelstrup et al., 2010). Nonetheless, the lower limit of the heating utility must be greater than the temperature in the reboiler. Using the inlet temperature of the heating utility as an optimization variable depends on the availability of a heat source suitable for upgrading the temperature of the heating

utility; else it is more advisable to use the inlet temperature as optimization variable. In the present work the reduction in the entropy production due to diabatization was lower than the experimental value of 39% reported by De Koeijer and Rivero (2003). They worked with a rectifying column separating water and ethanol, the differences can be explained because of the systems considered and their thermodynamic behavior and the constraints imposed over the distillation columns. In that work, adiabatic and SHE distillation columns with the same number of stages were analyzed, but the separation task carried out by the columns was slightly different, in the present work the entropy production was minimized taking into account columns not only with the same number of stages, but also, with the same separation task; which constraints the optimal design.

6. Conclusions and Outlook

A methodology for optimal design of single and double feed distillation columns with sequential heat exchangers was presented, and it was proven that this kind of columns can be considered as a good alternative to the classical (adiabatic) distillation columns because the entropy production savings obtained by SHE distillation columns lessens the amount of fuel required in the process and the carbon dioxide emissions. The SHE columns can contribute significantly to an energy-efficient chemical industry since distillation is the major separation operation in the chemical industry. There is a need for more experimental information about the heat and mass transfer characteristics of the SHE distillation columns in order to generate more accurate designs.

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