MODELING AND OPTIMIZATION ON ENERGY COSTS IN INTERNAL THERMALLY COUPLED DISTILLATION COLUMNS OF NON-IDEAL MIXTURES

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Abstract: Internal Thermally Coupled Distillation Column (ITCDIC) is the frontier of energy saving distillation research. In this paper, an evaluation method on the operating cost and its saving in the ITCDIC processes of non-ideal mixtures is presented. A mathematical model for optimization is first derived. The ethanol-water system is studied as an illustrative example. The optimization results show that the ITCDIC process of non-ideal mixture possesses an enormous potential of operating cost saving. The optimal operation conditions and the maximum percentage of operating cost saving are obtained simultaneously. The process analysis is then carried out and the results show the necessity and importance of optimal design on the rectifying pressure, the feed thermal condition, and the total heat transfer rate. These pave the way for the smooth operation and the further optimal design of ITCDIC processes for non-ideal mixtures.

Keywords: distillation columns, modeling, optimization, process analysis.

1. INTRODUCTION

Distillation remains the most important method used in the chemical industry for the separation of homogeneous mixtures with the amount of energy used in distillation operations being considerable. It takes heat from a heat source at bottom and generally reject most of this heat to a heat sink at the top while performing the task of separation for a conventional distillation column (CDIC), and is thus well known that the CDIC is both energy intensive and inefficient. If the energy removed from the rectifying section could be reused in the stripping section or waste heat was available, energy savings would be achieved in a distillation column.

Energy recovery by heat transfer from the rectifying section to the stripping section is an effective method for energy savings in distillation columns. This method, first proposed by Mah et al. (1977), is called the SRV method. An ITCDIC is constructed in such a manner that the rectifying section and the stripping section are separated into two columns, a compressor and a throttling valve are installed between the two sections and the internal thermal coupling is accomplished through a heat exchanger between them as shown in Fig.1 (Liu, and Qian, 2000), where energy saving is realized by the SRV method, which however has neither a reboiler nor a condenser, can be operated smoothly with two decentralized PID controllers and offers some distinct advantages over CDIC (Liu and Qian, 2000, Huang et al., 1997; Huang et al., 1999).

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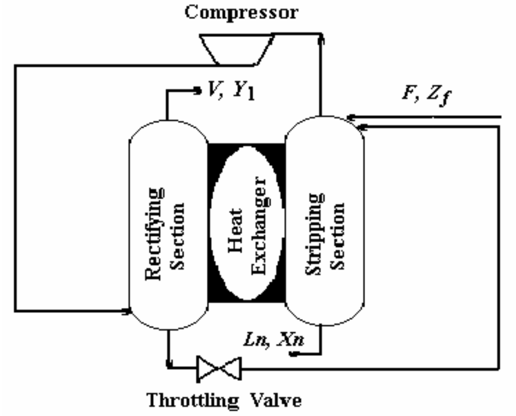

Fig. 1. Schematic diagram of ITCDIC

Because of the internal thermal coupling, a certain amount of heat is transferred from the rectifying section to the stripping section and brings the downward reflux flow for the former and the upward vapor flow for the latter. As a result, the condenser and the reboiler are not required and energy savings are realized. The research of Liu and Qian (2000) has shown that the energy saving could be up to 40-50% compared with CDIC. However, considering the compressor in an ITCDIC uses electric energy, which often takes two or three times more heat energy to generate a unit quantity of work energy and is generally much more expensive than the low-level steam needed by a CDIC, it is very important to explore the operating cost and its saving potential, which is one of the key to decide if the ITCDIC could be widely used. The approach is confirmed by the fact that energy costs usually far exceed the investment costs of a distillation column (Doukas and Luyben, 1978). But how about the operating cost of an ITCDIC, is it economic compared with a CDIC? How much on earth could the operating cost saves? How much is the operating cost saving potential of an ITCDIC process? Little, however, has appeared in the literature on these matters.

The aim of the present work is to explore the operating cost in an ITCDIC of a non-ideal mixture. An evaluating method on energy cost is proposed and a mathematical model for optimization on the energy cost saving potential in an ITCDIC process is then derived. The optimal assessments on the operating cost saving and the related process analysis are carried out, which pave the way for further optimal design of ITCDIC for non-ideal mixtures. From our knowledge, up to now, no one has worked on this matter.

2. EVALUATION OF OPERATING COST

A steady state ITCDIC process of a non-ideal mixture is considered. A CDIC under the minimum reflux ratio operating is chosen as a basis for comparison and assessment of the ITCDIC.

The operating cost of an ITCDIC process includes the cost of electric energy consumed by the compressor, the stream cost to preheat feed and the cooling water cost to cool the vapor distillate. It can be calculated as,

$$C_{ITCDIC} = W_{comp}\, UP_{electric} + Q_{preheat,ITCDIC}\, UP_{steam} + Q_{cool\,,ITCDIC}\, UP_{cool} \quad (1)$$

where W_{comp} is the load of the compressor. The adiabatic compression and the compression efficiency, η, are considered, therefore W_{comp} can be calculated as

$$W_{comp} = V_f\, k\, /\, (k\text{-}1)RT_{\text{in}}((P_{\text{out}}\, /\, P_{\text{in}})^{(k\text{-}1)/k} \text{-}1)/\ \eta \quad (2)$$

The loads of both preheating feed and cooling the vapor distillate are respectively calculated as,

$$Q_{preheat,\ ITCDIC} = F(1\text{-}q)\Delta H_{F,v} \quad (3)$$

$$Q_{cool,ITCDIC} = V_1\ \Delta H_{cool,\ v} \quad (4)$$

The operating cost of a CDIC process operated at the minimum reflux ratio, which is also the minimum operating cost of the CDIC process, is chosen as the comparison basis of the ITCDIC operating. The percent operating cost saving of the ITCDIC process is defined as,

$$X_C = (C_{rmin,CDIC} - C_{ITCDIC})\ /\ C_{rmin,CDIC} \quad (5)$$

where $C_{rmin,CDIC}$ is the operating cost of the CDIC process operated at the minimum reflux ratio, which includes the steam cost for both preheating feed and consumed by the reboiler, and the cooling water cost of the condenser in the CDIC process.

3. A MATHEMATICAL MODEL FOR OPTIMIZATION

The optimization model of the ITCDIC for a non-ideal mixture is derived by applying energy, component and overall material balances, and vapor-liquid equilibrium under the following assumptions:
(1) Perfect liquid and vapor mixing on each tray, the temperature and the composition on each tray being uniform; (2) Vapor-liquid equilibrium for streams leaving each tray; (3) Instantaneous heat transfer from the rectifying section to the stripping section and the transportation of liquid and vapor between trays; (4) Negligible pressure drop and heat loss in each column.

3.1 Objective function

In order to explore the operating cost in the ITCDIC process of a non-ideal mixture, the percent energy cost saving of the ITCDIC, X_C, is chosen as the objective function, which shows the energy cost saving effect directly and could be calculated from Eq. (5) together with Eqs. (1)-(4).

The design parameters including the pressure of the rectifying section, *Pr*, the feed thermal condition, *q*, and the total heat transfer rate, *UA*, are chosen as the optimized parameters. The optimization goal is to find the optimal values of *Pr*, *q*, and, *UA* and obtain the maximums of the operating cost saving of the ITCDIC compared with those of CDIC operated at the minimum reflux ratio, while the product qualities are guaranteed simultaneously.

3.2 Equality constraints

The stages are numbered with the top as Stage 1 and the bottom as Stage n. The amount of thermal coupling in the ITCDIC is then calculated from the following equation (Mah et al., 1977),

$$Q_j = UA(T_j - T_{j+f-1}) \quad j=1,\dots,f-1 \tag{6}$$

The stage temperature can be calculated by Antoine Eq. (7) and the vapor saturation pressure of the *i*th component at the *j*th stage is calculated by Eq. (8)

$$T_j = b/(a - LnP_{vp,ij}) - c \tag{7}$$

$$P_{vp,ij} = P\, Y_{ij} / (\gamma_{ij} X_{ij}) \tag{8}$$

where γ_{ij} is the activity coefficient for the *i*th component at the *j*th stage.

From the component material balance, the following equations are derived,

$$V_2 Y_{i2} - V_1 Y_{i1} - L_1 X_{i1} = 0 \quad j=1 \tag{9}$$

$$V_{j+1} Y_{i,j+1} - V_j Y_{i,j} + L_{j-1} X_{i,j-1} - L_j X_{i,j} = 0 \quad j=2,\dots,n-1 \text{ and } j\neq f \tag{10}$$

$$V_{f+1} Y_{i,f+1} - V_f Y_{i,f} + L_{f-1} X_{i,f-1} - L_f X_{i,f} + FZ_{iF} = 0 \; j=f \tag{11}$$

$$- V_n Y_{i,n} + L_{n-1} X_{i,n-1} - L_n X_{i,n} = 0 \quad j=n \tag{12}$$

According to the total mass balances, the liquid and vapor flow rates are derived as follows

$$L_j = \sum_{k=1}^{j} Q_k / \lambda \qquad j=1,\dots,f-1 \tag{13}$$

$$L_{f+j-1} = L_{f-1} + Fq - \sum_{k=1}^{j} Q_k / \lambda \quad j=1,\dots,f-2 \tag{14}$$

$$Ln = F - V_1 \tag{15}$$

$$V_1 = F(1-q) \tag{16}$$

$$V_{j+1} = V_1 + L_j \quad j=1,\dots,f-1 \tag{17}$$

$$V_{f+j} = V_f - F(1-q) - \sum_{k=1}^{j} Q_k / \lambda \quad j=1,\dots,f-2 \tag{18}$$

From the Vapor-Liquid equilibrium relationships, the vapor composition is obtained as

$$Y_{ij} = K_{ij} X_{ij} \tag{19}$$

where K_{ij} is the equilibrium vaporization ratio and can be calculated from Eq. (20). For a lower pressure system (generally, less than 1.013MPa), it can be simplified as Eq. (20a).

$$K_{ij} = (\gamma_{ij} f^{0}_{ij}) / (\varphi^{V}_{ij} P) \tag{20}$$

$$K_{ij} = \gamma_{ij} P_{vp,ij} / P \tag{20a}$$

where f^{0}_{ij} is the liquid fugacity for the *i*th component at the *j*th stage under a standard state, φ^{V}_{ij} is the gas fugacity coefficient for the *i*th component at the *j*th stage.

Eqs. (6)-(20) constitute the equality constraints of the optimization model of an ITCDIC.

3.3 Inequality constraints

For different product qualities, such as top product composition $Y_1 \geq 80\%$ (mole fraction), bottom product composition $X_n \leq 25\%$ or $Y_1 \geq 75\%$, $Xn \leq 20\%$, they have different optimal values of the design parameters. Constraints should be thereby set on product qualities. For Example, for the controlled compositions

$$Y_{i1} \geq Y_{i,\mathrm{setpoint}},\; X_{in} \leq X_{i,\mathrm{setpoint}} \qquad etc. \tag{21}$$

For the total separation effect, there is

$$FZ_{iF} \geq V_1 Y_{i1} \tag{22}$$

The proper region of the optimized variables must be specified, such as

$$Pr \in [0.1013, 1.013]\ \mathrm{Mpa} \tag{23}$$

$$q \in [0, 1] \tag{24}$$

$$UA \in [7500, 15000]\ \mathrm{W{\cdot}K^{-1}} \tag{25}$$

In order to prove the practicality and feasibility of the composition solution, the following constraints should be set

$$X_{ij} \in [0, 1] \tag{26}$$

$$Y_{ij} \in [0, 1] \tag{27}$$

Eqs. (21)-(27) constitute the inequality constraints of the optimization model of an ITCDIC. Therefore the optimization task can be written as follows

ITCDIC Minimize $f(Pr, q, UA) = -X_c$ (ECSOPT)

Subject to the equality constrains, Eqs. (6-20)

and to the inequality constrains, Eqs. (21-27)

It is a nonlinear programming (NP) constrained optimization problem. A reduced Eq.-oriented Solution Technique1 (Piela et al., 1991), is used to solve process flow-sheet. The Successive Quadratic Programming (SQP) method (Schmid and Biegler, 1994), is used as the optimization algorithm.

4. OPTIMIZATION AND ANALYSIS

In following optimization, a 68-stage ITCDIC is considered as an illustrative example, where a non-ideal mixture of ethanol-water is separated. The maximum of the operating cost saving of the ITCDIC is explored with the maximum of the percent operating cost saving of ITCDIC as the optimal objective function. The energy prices are shown in Table 11 (Ferre et al., 1985). The compressor is assumed to operate with a mechanical efficiency of 80% and be driven by electric motors. The use of a 90% on-stream factor is also assumed. Wilson's method is adopted in the vapor-liquid equilibrium calculation. The operating conditions are listed as follows:

Total number of stages	68
Feed stage	35
Feed flow rate	0.1 kmol·s^{-1}
Feed composition, ethanol/water	0.5/0.5
Top product quality (ethanol)	≥ 80%
Bottom product quality (ethanol)	≤ 25%
Pressure of stripping section	0.1013Mpa

Table 1 Cost of utilities

Utility	Price
Steam	0.0095 \$/kg
Cooling water	0.05 \$/m^3
Electrical energy	0.06 \$/kW·hr

Table 2 lists the optimization results of the ethanol-water system, when top product composition Y_1 ≥80% (mole fraction), bottom product composition, X_n ≤25%. The detailed optimized regions of the optimized variables are given in the table.

The optimization result shows that the maximum of the percent energy cost saving for ethanol-water separation in the ITCDIC process is 38.26% compared with the operating cost of the CDIC operated the minimum reflux ratio, which is absolutely striking and attractive. It reveals that the ITCDIC process of non-ideal mixture possesses a high industrial application value and an enormous economical prospect.

Table 2 The maximum operating cost saving of ITCDIC for the ethanol-water system

		Optimized regions	Optimal results
Quality target	Y_1, %	≥80	80.11
	X_n, %	≤25	25
Optimized variables	Pr, MPa	0.1013~1.013	0.1334
	q	0~1	0.5463
	UA, W.K^{-1}	7500~15000	15000
Goal	Maximum operating cost saving, X_C , %		38.26

Table 3 lists the detailed energy loads and the related operating costs for ethanol-water separation in the ITCDIC process under the optimal operation condition listed in Table 2 and those of the CDIC operated at the minimum reflux ratio. The results show although an infinite number of stages are necessary for the theoretical minimum reflux condition (minimum energy requirement) in a CDIC process, the ITCDIC of a non-ideal mixture can operate with energy cost requirements much more less than that of the minimum value for a CDIC. In the studied case, the operating cost saving for ITCDIC compared with the minimum operating cost of CDIC is 0.214 million dollars annually, which reveals the enormous economical prospect in the ITCDIC process of the non-ideal mixture.

Table 3 Energy loads and operating costs for the ethanol-water system

	CDIC		ITCDIC	
	Load, kW	Cost, K\$/Y	Load, kW	Cost, K\$/Y
Reboiler	1579	217.33	——	——
Preheating feed	1799	247.66	1799	247.66
Cooling	3334	95.40	1778	50.74
Compressor	——	——	84.33	47.57
Total		560.39		345.97

The optimal results in Table 2 and the operating load and cost results in Table 3 reveal that the ITCDIC process for non-ideal mixture can save more energy cost. Based on the optimization program and the optimal results, the following discussion and process analyses are explored and some useful conclusions are obtained as follows:

(1) From the optimal result and the optimal region of the pressure in Table 2, it is seen that the optimal operating pressure of the rectifying section is about 1.5 atmospheric pressures, which is easy to be realized. Fig 2 shows that while the operating pressure of the rectifying section is higher than the optimal operating value, the energy cost saving effect decreases with the operating pressure, which could be explained by the following theoretical analysis. Theoretically, the pressure difference between the rectifying and stripping sections provides the necessary operating driving force for the ITCDIC, with the increasing of the operating pressure of the rectifying section, the operating driving force hereby is increasing, which profit the separation effect. However, the work of the compressor is increasing accordingly and the percent energy cost saving of the ITCDIC is thus then decreasing.

From the curve of Pr- X_c in Fig. 2, it can be seen that the pressure of the rectifying section, *Pr*, has a great effect on the percent operating cost saving in an ITCDIC process and they have a obvious non-linearity. It reveals that optimal design on *Pr* is very important to realize an economical ITCDIC operation of non-ideal mixture.

(2) Table 4 shows the effect of the feed thermal condition, q, on X_c and production quality while the other conditions of the optimal results in Table 2 are kept constant. While q is increasing, Y_1 is increasing, but the bottom composition cannot satisfy the quality constraints; while q is decreasing, X_c is decreasing and the top composition cannot satisfy the quality constraints, but the bottom composition is purer.

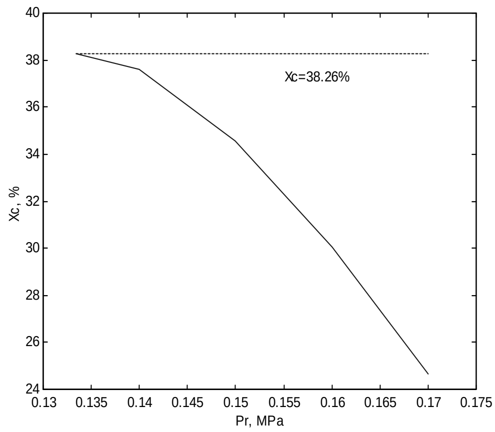

Fig. 2. The changes of the percent energy cost saving of ethanol-water mixture in the ITCDIC process, when P_r changes from 0.1334 to 0.5065 MPa and the other operation conditions of the optimal results in Table 2 are kept constant.

Table 4 Effect of the feed thermal condition on X_c and production quality for the ethanol-water mixture, while the other conditions of the optimal results in Table 2 are kept constant

	Optimal value	When q is changed from the optimal results of Table 2					
	q=0.5463	3%	6%	9%	-3%	-6%	-9%
Y_1, %	80.11	80.45	80.78	81.11	79.74	79.36	78.95
X_n, %	25	26.33	27.62	28.87	23.62	22.19	20.72
X_c, %	38.26	38.63	38.97	39.28	37.87	37.44	36.98

These reveal the complexity among q, X_c and the quality targets, which implies that the optimization procedure on q is necessary to gain the proper optimal design value of q in an ITCDIC process of a non-ideal mixture. From the change scale of Y_1, X_n and X_c in Table 4 while q changes, it shows that the feed thermal condition, q, has a great effect on Y_1, X_n and X_c and the optimal design on the feed thermal condition, q, is very important for the proper ITCDIC operation.

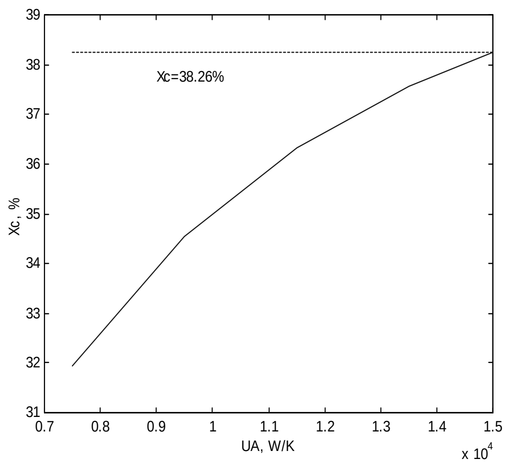

Fig. 3. The changes of percent operating cost saving for ethanol-water system, when *UA* changes from 7500 to 15000 W/K and the other operation conditions of the optimal results in Table 2 are kept constant.

(3) Table 2 shows that the optimal value of the heat transfer rate for the ethanol-water mixture is the upper boundary under the goal of the maximum of the energy cost saving. This implies that for the ethanol-water system, the increase of the heat transfer rate is beneficial for the energy saving of the ITCDIC process as shown in Fig. 3, which shows the influence of *UA* on the percent operating cost saving for the ethanol-water system, while the other conditions of the results in Table 2 are kept constant. In the view of the theory, with the increasing of the heat transfer rate, the amount of the thermal coupling, calculated by equation (6), is increasing, which is profitable to the ITCDIC process and the energy cost is, hereby, reduced under the same finite separation effect.

Fig 3 also reveals that *UA* has a great and complicated effect on X_c. It is thus very important to design an optimal valve of *UA* for a proper ITCDIC operation.

5. CONCLUSIONS

In this work an evaluating procedure of energy cost in the ITCDIC process of a non-ideal mixture is proposed. A mathematical model for optimization on the operating cost saving potential is derived, which include the comparison with the energy consumption and the operating cost of the CDIC operated at the minimum reflux ratio. The optimization and process analysis of ethanol-water system are carried out.

Optimization results show that the ITCDIC of non-ideal mixture possesses a high potential of energy cost saving. Through the optimization of the energy cost saving, it is found that the maximum percent energy cost saving for non-ideal mixtures in the ITCDIC process is close to 40% compared with the operating cost of the CDIC under the minimum reflux ratio operating. It reveals that the ITCDIC process of the non-ideal mixture possesses a high industrial application value and an enormous economical prospect.

Process analysis results show that there exists an optimal design problem for selecting the rectifying pressure, *Pr*, the feed thermal condition, *q*, and the total heat transfer rate, *UA*, in the ITCDIC process of the non-ideal mixture and there are very complicated relations among the energy cost parameters, the product qualities and the optimized variables. It is also found that the optimal operating pressure of the rectifying section is easy to be realized, and while the operating pressure of the rectifying section is higher than the optimal operating value, the energy cost saving effect decreases with the operating pressure. Bearing these in mind is very important for the smooth operation and the optimal design of an ITCDIC process for a non-ideal mixture.

Based on the study of this paper, we have developed a related optimization software 'ECSOPT', which is a convenient tool for quick calculation of the maximum energy cost saving potential and the optimum values of the design variables for the ITCDIC process of non-ideal mixture, and is thereby very useful and significant to further researches on ITCDIC processes of non-ideal mixtures.

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NOMENCLATURES

F	feed rate, kmol·s^{-1}
k	adiabatic index number of gas
K	equilibrium vaporization ratio
L	liquid flow rate, kmol·s^{-1}
P	representation of either Pr or Ps, MPa
Pr	pressure of rectifying section, MPa
Ps	pressure of stripping section, MPa
P_{vp}	vapor saturation pressure, MPa
q	feed thermal condition
Q	energy demand, W
T	absolute temperature, K
UA	heat transfer rate, W·K^{-1}
UP	unit price of loads, \$·W^{-1}
V	vapor flow rate, kmol·s^{-1}
W	thermodynamic work, W
X	mole fraction of liquid
X_c	percent operating cost saving
Y	mole fraction of vapor
Z_F	mole fraction of feed
λ	latent heat of vaporization, kJ·kmol^{-1}
γ	activity coefficient
Subscripts	
comp	compressor
f	feed stage
F	feed
i	component
j	stage number

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