Chinese J. of Chem. Eng., **8** (1) 57—63 (2000)

Thermodynamic Analysis, Simulation and Optimization on Energy Savings of Ideal Internal Thermally Coupled Distillation Columns*

LIU Xingao(刘兴高), MA Longhua(马龙华) and QIAN Jixin(钱积新)**
Institute of Industrial Process Control and National Laboratory of Industrial Control Technology, Zhejiang University, Hangzhou 310027

Abstract Internal thermally coupled distillation columns (ITCDIC) are the frontier of distillation energy saving research. In this paper, a novel energy saving model of ideal ITCDIC and a simulation algorithm are presented, upon which a series of comparative studies on energy savings with conventional distillation columns are carried out. Furthermore, we present an optimization model of ideal ITCDIC, which can be used to achieve the maximum energy saving and find the optimal design parameters directly. The binary system of benzene-toluene is adopted for the illustrative example of simulation and optimization. The results show that the maximum energy saving of ITCDIC is 52.25% (compared with energy consumption of conventional distillation under the minimum reflux ratio operation); the optimal design parameters are obtained, where the rectifying section pressure and the feed thermal condition are $p_r = 0.3006$ MPa and $q = 0.5107$ respectively.
Keywords distillation, thermal coupling, energy savings, simulation, optimization

1 INTRODUCTION

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[1] *et al.*, 1977, is called secondary reflux and vaporization (SRV) method. Since then, there are extensive studies on SRV (Shimizu[2−4], Fitzmorris[5], *etc.*). ITCDIC is one of distillation columns where energy savings are realized by the SRV method, which is the frontier of distillation energy saving research, and has been studied only during the last decade. Takamatsu[6] *et al.*, 1988, first proposed this design idea. During the last decade, some studies have been carried out: Lueprasitsakul[7,8] analyzed the characteristics and the energy efficiency of wetted-wall distillation columns; Huang[9,10] considered control, dynamics and performance evaluation and Matalib[11,12] considered dividing wall distillation columns. The goal of all these studies is energy saving. Therefore, it is very important to study its energy saving directly. However, from our knowledge, there is no minute study on energy savings of ITCDIC up to now. Although there are somewhat related studies, such as: Yang[13,14] studied the operational performance of Petlyuk (a thermally coupled distillation columns of main-tower and second-tower construction) and energy savings of distillation process; Li[15] studied the feasibility of employing Petlyuk distillation tower to save energy.

In this paper, an ideal ITCDIC is considered. An energy-saving model is derived, upon which the system characteristics, such as the energy consumption and the thermodynamic efficiency *etc.*, can be directly achieved. In order to analyze more expediently and more directly, a relevant conventional distillation energy consumption model is given, upon which the percentage of energy savings and thermodynamic efficiency enhancement of ideal ITCDIC can be obtained directly. Then, a simulation algorithm and an optimization model of energy savings are proposed. The optimization of ideal ITCDIC is carried out. For benzene-toluene system, the maximum energy saving and the optimal design parameters of the ideal ITCDIC are achieved.

2 MATHEMATICAL MODEL

2.1 Schematic diagram of the ideal ITCDIC

Fig. 1 shows the schematic diagram of the ideal ITCDIC. The manipulation of internal thermal coupling is accomplished through heat exchanger between the rectifying and the stripping sections. In order to provide the necessary temperature driving force for

Received 1998-08-03, accepted 1999-05-20.
* Supported by the National Environmental Protection Bureau of P. R. China (Huan-Ke-Ke, 1997, No. 006, Project 14), China-Japan cooperative project: "Research on energy savings and alleviating environmental burden in petroleum enterprises" of Institute of Industrial Process Control of Zhejiang University with National Institute of Material and Chemical Research of Japan.
** To whom correspondence should be addressed. E-mail: liuxg@iipc.zju.edu.cn

the heat to be transferred from the rectifying section to the stripping section, the former must be operated at a higher pressure than the latter. For adjusting the pressure, a compressor and a throttling valve are installed between the two sections. Due to 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 rectifying section and the upward vapor flow for the stripping section. As a result, the condenser and reboiler are not required, and energy savings are realized.

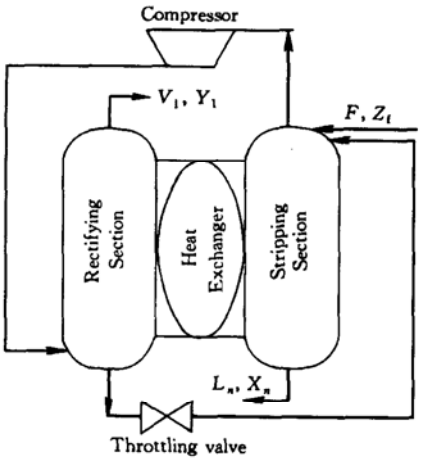

Figure 1 Schematic diagram of an ideal ITCDIC

2.2 Energy calculation model and definitions of the thermodynamic efficiency and the percentage of energy savings of the ideal ITCDIC

Applying energy, component, overall material balances and vapor-liquid equilibrium under following assumptions, the mathematical model of the ideal ITCDIC is derived.

(1) Negligible vapor holdups, liquid molar holdups on each tray being constant;

(2) Perfect liquid and vapor mixing on each tray, the temperature and the composition on each tray being uniform;

(3) Vapor-liquid equilibrium for streams leaving each tray;

(4) Instantaneous heat transfer from the rectifying section to the stripping section and the transportation of liquid and vapor between trays;

(5) Negligible pressure drop in each column;

(6) Negligible hydraulic delay occurring in the liquid flows;

(7) Heat loss and heat capacity change of separation process being negligible;

(8) No time delay in changes of column pressures and feed thermal condition;

(9) Equal and constant latent heat of each composition;

(10) The relative volatility is constant;

(11) No vapor and liquid side-stream withdraw;

(12) The compression efficiencies are 100%.

For a separation process, the minimum amount of thermodynamic energy required to make a complete separation is given by the following equation

$$W_{\min} = F(\Delta H - T\Delta S) \tag{1}$$

For an ideal mixture, Eq. (1) can be expressed as

$$W_{\min} = FRT\sum(X_{fi}\ln X_{fi}) \tag{2}$$

$W_{\min}$ is a thermodynamic term that is independent of any particular process. Actual processes operate with finite driving forces, which are irreversible and consume more energy than the thermodynamic minimum.

For conventional distillation, minimum energy required for separation process ($Q_{\min,con}$) is the minimum reboiler energy requirement. With the use of the McCabe-Thiele diagram, $Q_{\min,con}$ for a binary mixture can be shown to be a function of the heat of vaporization of the bottom product, relative volatility, and feed composition. For complete separation, when feed thermal condition $q = 1$, we have

$$Q_{\min,con} = F\Delta H_{b,v}[1/(\alpha - 1) + Z_f] \tag{3}$$

The maximum thermodynamic efficiency ($E_{\max}$) is defined as the minimum thermodynamic energy ($W_{\min}$) divided by minimum energy required for a separation process ($Q_{\min}$), so for conventional distillation we have

$$\begin{aligned} E_{\max,con} &= W_{\min}/Q_{\min,con} \\ &= RT\sum(X_{fi}\ln X_{fi})/\{\Delta H_{b,v}[1/(\alpha - 1) + Z_f]\} \end{aligned} \tag{4}$$

For ideal ITCDIC, energy required for separation process (Q_{tcd}) is composed with heat of preheating feed and work of compressor (W_{comp}), that is

$$Q_{tcd} = F(1 - q)\Delta H_{f,v} + W_{comp} \tag{5}$$

We choose the compressor work

$$W_{comp} = V_f[K/(K-1)]RT_1((p_2/p_1)^{(K-1)/K} - 1) \tag{6}$$

For gas mixture

$$1/(K - 1) = \sum(Y_i/(K_i - 1)) \tag{7}$$

Then we obtain the thermodynamic efficiency of fully ideal ITCDIC (E_{tcd})

$$E_{\mathrm{tcd}} = W_{\min}/Q_{\mathrm{tcd}} = FRT\sum(X_{\mathrm{fi}}\ln X_{\mathrm{fi}})/[F(1-q)\Delta H_{\mathrm{f,v}} + W_{\mathrm{comp}}] \quad (8)$$

which has profound impact on the overall cost of separation process. Comparing the maximum thermodynamic efficiency of conventional distillation ($E_{\mathrm{max,con}}$) with the thermodynamic efficiency of ideal ITCDIC (E_{tcd}), we can know the energy saving's effect of ideal ITCDIC directly. The percentage of thermodynamic efficiency enhancement of the ideal ITCDIC (X_e) is defined as fellows

$$X_e = (E_{\mathrm{tcd}} - E_{\mathrm{max,con}})/E_{\mathrm{max,con}} \quad (9)$$

For conventional distillation, energy required for separation process under the minimum reflux ratio ($R_{\min}$) operation ($Q_{\mathrm{rmin,con}}$) can be calculated by

$$Q_{\mathrm{rmin,con}} = F(1-q)\Delta H_{\mathrm{f,v}} + [(R_{\min}+1)D - F(1-q)]\Delta H_{\mathrm{b,v}} \quad (10)$$

where D is top distillation product flow rate.

The percentage of energy savings of ideal ITCDIC is defined as follows

$$X_s = (Q_{\mathrm{rmin,con}} - Q_{\mathrm{tcd}})/Q_{\mathrm{rmin,con}} \quad (11)$$

Which shows the energy saving's effect directly.

2.3 Basic equations of the ideal ITCDIC

When the stages are numbered from the top as stage 1 to the bottom as stage n, the basic equations of the ideal ITCDIC are Eqs. (12)—(25)[1,6,9,16].

Eqs. (1)—(25) constitute the dynamic energy saving model of ideal ITCDIC.

Thermal coupling

$$Q_j = UA(T_j - T_{j+f-1}) \quad (12)$$

$$T_j = b/(a - Lnp_{\mathrm{vp},j}) - c \quad (13)$$

$$P_{\mathrm{vp},j} = p/[X_j + (1-X_j)/\alpha] \quad (14)$$

Mass balances

$$L_j = \sum_{k=1}^{j} Q_k/\lambda \qquad j = 1,\cdots,f-1 \quad (15)$$

$$L_{f+j-1} = L_{f-1} + Fq - \sum_{k=1}^{j} Q_k/\lambda \qquad j = 1,\cdots,f-2 \quad (16)$$

$$Ln = F - V_1 \quad (17)$$

$$V_1 = F(1-q) \quad (18)$$

$$V_{j+1} = V_1 + L_j \quad (19)$$

$$V_{f+j} = V_f - F(1-q) - \sum_{k=1}^{j} Q_k/\lambda \qquad j = 1,\cdots,f-2 \quad (20)$$

Vapor-liquid equilibrium relationships

$$Y_j = \alpha X_j/[(\alpha-1)X_j + 1] \quad (21)$$

Component balances

$$H\frac{\mathrm{d}X_1}{\mathrm{d}t} = V_2Y_2 - V_1Y_1 - L_1X_1 \qquad j = 1 \quad (22)$$

$$H\frac{\mathrm{d}X_j}{\mathrm{d}t} = V_{j+1}Y_{j+1} - V_jY_j + L_{j-1}X_{j-1} - L_jX_j \qquad j = 2,\cdots,n-1 \quad \text{and} \quad j \neq f \quad (23)$$

$$H\frac{\mathrm{d}X_f}{\mathrm{d}t} = V_{f+1}Y_{f+1} - V_fY_f + L_{f-1}X_{f-1} - L_fX_f + FZ_f \qquad j = f \quad (24)$$

$$H\frac{\mathrm{d}X_n}{\mathrm{d}t} = -V_nY_n + L_{n-1}X_{n-1} - L_nX_n \qquad j = n \quad (25)$$

3 SIMULATION AND ANALYSIS

For steady state studies, let

$$\frac{\mathrm{d}X_j}{\mathrm{d}t} = 0 \quad (26)$$

The dynamic model becomes steady state model. In the following steady state simulation studies, a 30-stage ideal ITCDIC is considered as an illustrative example, where a binary mixture of benzene and toluene is separated. Its detailed operation conditions are as follows: number of total stages 30; feed stage, 16; feed flow rate, 100 kmol·h^{-1}; feed composition (benzene/toluene), 0.5/0.5; feed thermal condition, 0—1; pressure of rectifying section, 0.1013—1.013 MPa; pressure of stripping section, 0.1013 MPa; heat transfer rate, 9803 W·K^{-1}; latent heat of vaporization, 30001.1 kJ·kmol^{-1}; relative volatility, 2.317.

The simulation studies and the following optimization are carried out using the software 'Matlab'. The simulation procedure is illustrated as follows:

(1) Give operating conditions and physical data: N, f, F, P_r, P_s, Z_f, q, UA; a, b, c; A, B, C, D.

(2) Give termination criteria(ε) that is a measure of the worst case precision required of the independent variables.

(3) Give initial values of $X_j(k)$.

Table 1 Physical data used in simulation and optimization

		Benzene	Toluene
antoine constants	a	15.9008	16.0137
	b	2788.51	3096.52
	c	−52.36	−53.67
ideal gas heat capacity equation parameters			
	A	−8.101	−5.817
	B	1.133×10^{-1}	1.224×10^{-1}
	C	-7.206×10^{-5}	-6.605×10^{-5}
	D	1.703×10^{-8}	1.173×10^{-8}
latent heat of vaporization,kJ·kmol^{-1}		30746	33163

Table 2 Simulation results of Benzene-Toluene system

No.	Manipulating parameters		System characteristic						
			Product quality	Performance parameters					
	q	p_r, MPa	$Y1/X_n$	$E_{max,con}$	E_{tcd}	X_e, %	$Q_{rmin,con} \times 10^6$,kW	$Q_{tcd} \times 10^6$,kW	X_s, %
1	0.25	0.1519	0.6373/0.0880	0.0511	0.0813	0.5926	4.9122	2.6042	0.4699
2	0.25	0.2532	0.6666/0.0003	0.0511	0.0736	0.4419	4.9122	2.8764	0.4144
3	0.25	0.3545	0.6667/0.0000	0.0511	0.0692	0.3548	4.9122	3.0613	0.3768
4	0.5	0.1519	0.7708/0.2292	0.0511	0.1173	1.2969	4.4928	1.8057	0.5981
5	0.5	0.2532	0.9384/0.0616	0.0511	0.1019	0.9960	4.4928	2.0779	0.5375
6	0.5	0.3545	0.9887/0.0113	0.0511	0.0936	0.8329	4.4928	2.2628	0.4964
7	0.75	0.1519	0.9091/0.3636	0.0511	0.2103	3.1179	4.1562	1.0072	0.7577
8	0.75	0.2532	0.9997/0.3334	0.0511	0.1656	2.2417	4.1562	1.2794	0.6922
9	0.75	0.3545	1.0000/0.3333	0.0511	0.1447	1.8323	4.1562	1.4643	0.6477

(4) Calculate $Y_j(k)$, $T_j(k)$, $p_{vp,j}(k)$, $Q_j(k)$, $L_j(k)$, $V_j(k)$ from Eqs. (12)—(21).

(5) Calculate $X_j(k+1)$ from Eqs. (22)—(26).

(6) When $|X_j(k+1) - X_j(k)| < \varepsilon$, go to step (7); if not, $X_j(k+1) \to X_j(k)$, and go to step (4).

(7) Calculate $Q_{rmin,con}$, Q_{tcd}, X_s from Eqs. (5)—(7), (9)—(11), (27).

(8) Calculate $E_{max,con}$, E_{tcd}, X_e from Eqs. (1)—(4), (8),(9).

The initial point can be arbitrarily given to start the simulation and the steady state solution could be reached after a short time of iterations.

Calculation of adiabatic index number (K) uses heat capacity equation of ideal gas

$$c_{p,ideal} = A + BT + CT^2 + DT^3 \qquad (27)$$

The physical data used in simulation are listed in Table 1.

Table 2 shows the simulation results. When feed thermal condition, q, is 0.25, 0.5, 0.75 and pressure of rectifying section, p_r, is 0.1519 MPa, 0.2532 MPa, 0.3545 MPa, the product quality change from 63.73% to 100.00%, for Y_1; from 0.00% to 36.36%, for X_n; the performance parameters E_{tcd} change from 6.92% to 21.03%, X_e change from 35.48% to 311.79%, and X_s change from 37.68% to 75.77%. There are very large changes. So there should be an optimization between manipulating parameters and system characteristic. Obviously, the pressure difference between the rectifying and stripping sections and the feed thermal condition can significantly influence the operation of the ideal ITCDIC. There are very complicated relations among energy saving, X_s, manipulation parameters, p_r, q, and product quality, X_n, Y_1.

For conventional distillation, the maximum of thermodynamic efficiency of benzene-toluene system is 5.11%. But for the ideal ITCDIC, the minimum of thermodynamic efficiency is 6.92%, enhancing 35.48%, and energy saving percentage is 37.68%; the maximum of thermodynamic efficiency is 21.03%, enhancing 311.79%, and energy saving percentage is 75.77%. Obviously, the ideal ITCDIC saves energy more than conventional distillation. The effect of energy savings is marked.

4 OPTIMIZATION AND ANALYSIS

This section provides the optimization problem of ideal ITCDIC energy saving, which is used to find a set of design parameters defined as optimal in some way and may be the minimization or maximization of system characteristics under design parameters.

From the Section 2.2, we know the percentage of

energy savings of ideal ITCDIC, X_s, can show the energy savings more directly. So, we select X_s as the objective function.

For different product quality, such as top product composition $Y_1 \geqslant 96\%$, bottom product composition $X_n \leqslant 5\%$ or $Y_1 \geqslant 98\%$, $X_n \leqslant 4\%$, there should be different optimizing results of energy savings. So a constraint should be set to product quality, such as top product composition $Y_1 \geqslant 96\%$, bottom product composition $X_n \leqslant 5\%$.

For total separation effect, we have

$$FZ_f \geqslant V_1 Y_1 \tag{28}$$

The equality constraints are Eqs. (1)—(26). The optimization attention is to find the optimal design parameters p_r and q, such that the energy saving is maximum and the product quality is guaranteed simultaneously.

The energy saving optimization model of the ideal ITCDIC is presented as follows

ITCDIC min. $f(p_r, q) = -X_s$

s. t. Eqs. (1—26)

Product quality constraints

(such as: $Y_1 \geqslant 98\%$, $X_n \leqslant 4\%$)

$V_1 Y_1 - FZ_f \leqslant 0$

$0.1013\,\text{MPa} \leqslant p_r \leqslant 1.013\,\text{MPa}$,

$0 \leqslant q \leqslant 1$

$0 \leqslant X_j \leqslant 1, 0 \leqslant Y_j \leqslant 1$

It is a nonlinear programming (NP) constrained optimization problem. The optimization algorithm uses the Sequential Quadratic Programming (SQP) method.

A 30-stage ideal ITCDIC is considered as an illustrative example, where a binary mixture of benzene and toluene is separated. Its detailed operation conditions and the physical data used in optimization are the same as those in the simulation.

Table 3 shows the optimization results of energy savings of the ideal ITCDIC. For benzene-toluene system, when $Y_1 \geqslant 98\%$, $X_n \leqslant 4\%$, the optimal percentage of energy savings of the ideal ITCDIC is 52.25%. Table 4 lists other's study results. Comparing the results of Table 4 with those of Table 3, it is obvious that the ideal ITCDIC method saves energy markedly. Energy recovery by heat transfer from the rectifying section to the stripping section is an effective method for energy savings in distillation columns.

Figs. 2, 3, 4, 5 show the system characteristics of the ideal ITCDIC when optimal design parameters p_r is 0.3006 MPa and q is 0.5107. In Fig. 2 the solid line indicates the relation between the liquid composition with stage number, the dotted line, the vapor composition distribution. In Fig. 3 the solid line indicates the relation between the vapor flow rate and stage number, the dotted line, the liquid flow rate distribution. Compared with the system characteristics of conventional distillation columns, it is obvious that the internal thermal coupling not only causes a change of

Table 3 Optimization results of benzene-toluene system

Product quality constrains	Y_1, %	$\geqslant 96$	$\geqslant 98$
	X_n, %	$\leqslant 5$	$\leqslant 4$
Maximum energy savings	X_s, %	52.65	52.25
Achieved optimal design parameters	p_r, MPa	0.2826	0.3006
	q	0.5111	0.5107
System characteristic under optimal design parameters	Y_1	0.9705	0.9800
	X_n	0.0500	0.0400
	$Q_{rmin,con} \times 10^6$, kW	4.3933	4.4768
	$Q_{tcd} \times 10^6$, kW	2.0803	2.1375

Table 4 Other relative study results

Author	Energy savings	Studied system	Column construction	Compared with
Yang[13], 1990	50%	ethyl benzene/ di-methyl benzene	Petlyuk	actual conventional distillation column
Li[15], 1995	33.14%	non-ideal mixture of ethanol/ether *etc.*	Petlyuk	actual conventional distillation column
Mah[1], 1977	54%*	ethylene/ethane *etc.*	SRV.	conventional distillation column
Finn[17], 1993	16%	*i*-butane/ *n*-butane	side rectifier	direct sequence rectifier

*indicate relative steam consumption

flow rates but also complicates the heat and mass transfer mechanism in the column.

Fig. 6 shows the operating contrast figure of the ideal ITCDIC, when operating conditions under the optimal design parameters (p_r, 0.3006 MPa; q, 0.5107). For conventional distillation column, the minimum reflux ratio operating line is under such conditions. Other parameters are the same as those in the optimization.

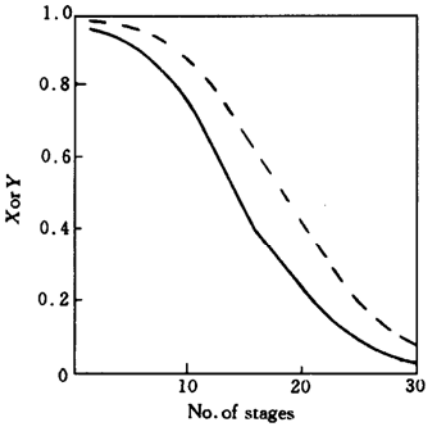

Figure 2 Composition distribution

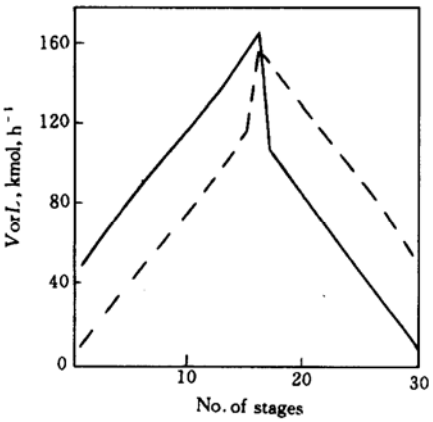

Figure 3 Flow rate distribution

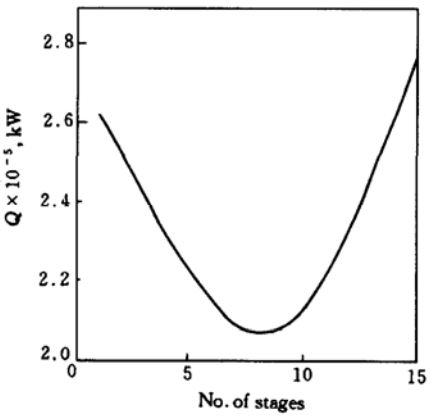

Figure 4 Thermal coupling condition

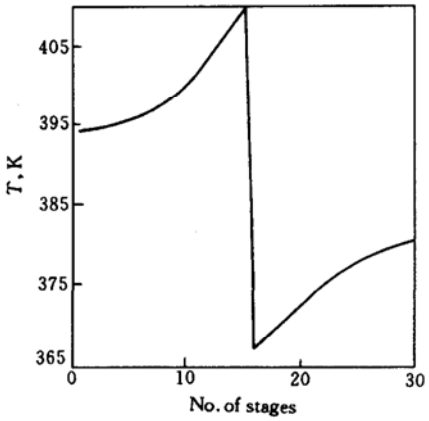

Figure 5 Temperature distribution

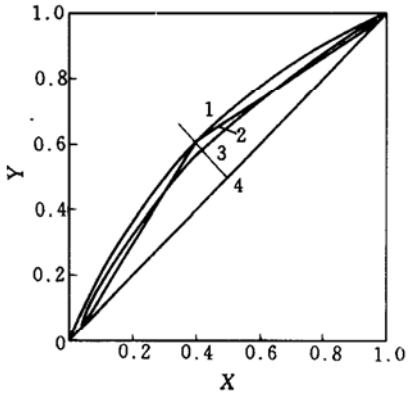

Figure 6 Operating line contrast, $p_r = 0.3006$, $q = 0.5107$

1—vapor-liquid equalibrium line;
2—conventional operating line under R_{min};
3—ITCDIC operation line; 4—feed line

Owing to the internal thermal coupling between rectifying and stripping sections where the operating line bends away quite same as that of equilibrium one, the driving force of mass and heat transfer of ITCDIC has been significantly reduced compared with the conventional distillation columns (even under minimum reflux operation). So the process irreversibility has been significantly reduced. From the viewpoint of thermodynamics, large energy losses for the separation process usually occur due to irreversibility of processes. The result is that either fewer stages are needed to accomplish the same separation or better separation is obtained with the same number of stages at the same energy consumption, and energy savings occur in the ideal ITCDIC process.

5 CONCLUSIONS

On the basis of thermodynamic analysis, simulation and optimization of the ideal ITCDIC, we can conclude that the ideal ITCDIC offers some distinct advantages over the conventional distillation.

For other systems, such as non-ideal mixture separation, the energy saving model can be applied also. The only thing needed is to change the given conditions, physical data and vapor-liquid equilibrium relationships. For different product requirement, we can obtain the different optimal design parameters by the optimization model.

Based on the study of this paper, we have developed a relative software 'ENORM', which is very useful and significant to research further on ITCDIC.

Further investigation is underway to study the dynamic optimization of the ideal ITCDIC that comprises the dynamic control model and series consideration on the system dynamic characteristics and performance of the ideal ITCDIC.

NOMENCLATURE

a, b, c	coefficient of Antoine equation
A, B, C, D	parameters of heat capacity equation of ideal gas
E	thermodynamic efficiency
F	feed rate, kmol·s^{-1}
H	stage holdup, kmol
ΔH, ΔS	change in enthalpy and entropy
K	adiabatic index number of gas
L	liquid flow rate, kmol·s^{-1}
n	number of total stages
p_{vp}	vapor saturated pressure, MPa
p_r	pressure of rectifying section, MPa
p_s	pressure of stripping section, MPa
p	representation of either P_r or P_s, MPa
Q	energy requirement, kW
q	feed thermal condition
R	general gas constant, kJ·kmol^{-1}·K^{-1}
R_{min}	minimum reflux ratio
T	absolute temperature, K
t	time, s
UA	heat transfer rate, W·K^{-1}
V	vapor flow rate, kmol·s^{-1}
W	thermodynamic work, W
X	mole fraction of liquid
X_e	percentage of thermodynamic efficiency enhancement, %
X_s	percentage of energy saving of the ideal ITCDIC, %
Y	mole fraction of vapor
Z_f	mole fraction of feed
α	relative volatility
λ	latent heat

Subscripts

b	bottom
comp	compressor
con	conventional distillation column
f	feed
f	feed stage
i	component
j	stage number
max	maximum amount
min	minimum amount
rmin	minimum reflux ratio
tcd	the ideal ITCDIC
v	vaporization

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