ISSN 1009 - 3095 *Journal of Zhejiang University(SCIENCE)* V.1, No.4, P.361 - 369, Oct. - Dec., 2000
http://www.chinainfo.gov.cn/periodical; http://www.zju.edu.cn;
http://lib.zju.edu.cn/English; http://www.zjupress.com

OPERATION BEHAVIORS OF IDEAL INTERNAL THERMALLY COUPLED DISTILLATION COLUMNS*

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Received June.18, 1999; revision accepted Apr.18, 2000

Abstract: A lack of experience in operation is one of the major difficulties associated with the use of advanced energy saving distillation methods. The detailed operational studies of an ideal internal thermally coupled distillation column (ITCDIC) were carried out in this work paved the way for further control and design studies and its practical application.

Key words: distillation, thermal coupling, operational studies
Document code: A **CLC number**: TQ028.8

INTRODUCTION

Distillation consumes a large percentage of the energy used in the chemical process industries. Consequently, there is a significant incentive to improve the energy efficiency of this widely applied separation process. There are various methods using multi-effect columns, side cooler-sideheater, heat pumps and secondary reflux and vaporization (SRV) for reducing external energy inputs by the effective use of heat energy in the distillation system (Umeda, et al., 1979; Linhoff, 1993; Lang, 1996). Energy recovery by heat transfer from the rectifying section to the stripping section is an effective method for energy saving in distillation columns. This method, first proposed by Mah (1977), is called SRV method. Since then, there were extensive studies of SRV (Fitzmorris et al., 1980; Shimizu et al., 1985). ITCDIC is one of the distillation columns where energy savings are realized by the SRV method, which has neither reboiler nor condenser and has large potential for energy reduction (Lueprasitsakul et al., 1990; Lestak et al., 1994; Huang et al., 1997).

However, one of the major difficulties associated with the use of such advanced energy saving columns is lack of experience and intuition in operation (Glinos et al., 1988), e.g., knowledge of the proper number and choice of independent operating variables and policies, the system characteristics and influences of operating variables. This paper deals with the operation of an ideal ITCDIC.

The novel mathematical model and related simulation algorithm of an ideal ITCDIC presented in this paper can be used for further control and design studies, based on the results of which, the system characteristics, such as minimal energy consumption and thermodynamic efficiency, can be achieved directly. The results of our series of detailed operation analyses of the steady and dynamic state, degrees of freedom analysis, steady state and transient behavior analysis, operating line analysis, system characteristic and operation parameter simulation analysis of an ITCDIC can be useful for further ITCDIC study and its practical application. To our knowledge, up to now, nobody has ever set foot in this work, reported here, detailed, thorough

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* Project supported by National Environmental Protection Bureau of China (Huan-Ke-Ke, 1997, No 006)

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and comprehensive analyses of every aspect of an ideal ITCDIC system

MATHEMATICAL MODEL

Schematic diagram

Fig. 1 shows the schematic diagram of the ideal ITCDIC. The rectifying section and the stripping section are separated into two columns. The internal thermal coupling is accomplished through heat exchange between the rectifying and the stripping sections. In order to provide the necessary temperature driving force for moving the heat 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 two sections. Because of the internal thermal coupling, a certain amount of heat is transferred from the rectifying section to the stripping section, which leads to downward reflux flow for the rectifying section and the upward vapor flow for the stripping section. As a result, the condenser and the reboiler are not required and energy savings are realized.

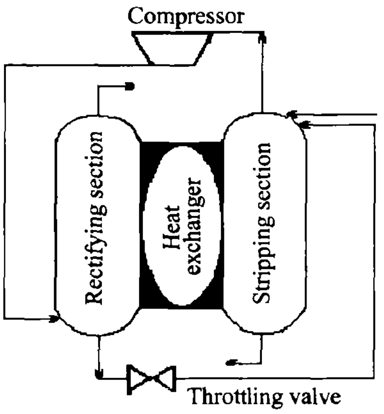

Fig. 1 Schematic diagram of ITCDIC

Modeling

The mathematical model of the ideal ITCDIC is derived by applying energy, composition and overall material balances together with vapor-liquid equilibrium under the following assumptions

(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 being constant;

(11) No vapor and liquid side-stream withdrawal.

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

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

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

$$W_{\min} = F \times RT \times (\sum X_{fi} \ln X_{fi}) \tag{2}$$

where X_{fi} is mole fraction of feed component i. $W_{\min}$ 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 $q = 1$,

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

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

$$E_{\max,\mathrm{con}} = W_{\min} / Q_{\min,\mathrm{con}} = RT \times (\sum X_{fi} \ln X_{fi}) / \{ \Delta H_{b,v} \cdot [1/(\alpha - 1) + Z_f] \} \quad (4)$$

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

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

We choose the compressor work

$$W_{comp} = V_f \times K/(K - 1) \times RT_1((P_2/P_1)^{(K-1)/K} - 1) \quad (6)$$

For gas mixture

$$1/(K - 1) = \sum (Y_i/(K_i - 1)) \quad (7)$$

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

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

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

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

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

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

where D is top distillation product flow rate, $\Delta H_{f,v}$ is vaporizing enthalpy change of feed, $\Delta H_{b,v}$ is vaporizing enthalpy change of column bottom.

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

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

which shows the energy saving's effect directly.

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 presented as follows:

Thermal coupling (Mah et al., 1977; Lestak et al., 1994; Huang et al., 1997)

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

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

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

Mass balances

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

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

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

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

$$V_{j+1} = V_1 + L_j \quad j = 1, \cdots, f - 1 \quad (19)$$

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

Vapor-Liquid equilibrium relationships

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

Component balances

$$H \times \mathrm{d}X_1/\mathrm{d}t = V_2 Y_2 - V_1 Y_1 - L_1 X_1 \quad j = 1 \quad (22)$$

$$H \times \mathrm{d}X_j/\mathrm{d}t = V_{j+1} Y_{j+1} - V_j Y_j + L_{j-1} X_{j-1} - L_j X_j \quad j = 2, \cdots, n - 1 \text{ and } j \neq f \quad (23)$$

$$H \times \mathrm{d}X_f/\mathrm{d}t = V_{f+1} Y_{f+1} - V_f Y_f + L_{f-1} X_{f-1} - L_f X_f + F Z_f \quad j = f \quad (24)$$

$$H \times \mathrm{d}X_n/\mathrm{d}t = - V_n Y_n + L_{n-1} X_{n-1} - L_n X_n \quad j = n \quad (25)$$

Eqs (1) − (25) consist of the dynamic mathematical model of an ideal ITCDIC.

For steady state studies, let

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

the dynamic model becomes steady state model. Where a, b, c are Antoine constants; F is feed rate, kmol/s; H stage holdups, kmol; K is adiabatic index number of gas; L is liquid flow rate, kmol/s; n is number of total stages; P_{vp} is vapor saturation pressure, MPa; P_r is pressure of rectifying section, MPa; P_s is pressure of stripping section, MPa; P represents either P_r or P_s, MPa; q is feed thermal condition; R is general gas constant; t is time, s; T is absolute temperature; UA is heat transfer rate, W/K; V is vapor flow rate, kmol/s; X is mole fraction of liquid; Y is mole fraction of vapor; Z_f is mole fraction of feed; ΔH, ΔS are change in enthalpy and entropy respectively; α is relative volatility; λ is latent heat.

These mathematical models induding the dynamic and the steady state models are efficient for operation studies, and can be used for further control, design and optimization studies.

SIMULATION SYNOPSIS

In the following simulations, a 30-stage ideal ITCDIC is considered as an illustrative example, where a binary mixture of benzene-toluene is separated. Its detailed operation conditions are shown in Table 1.

Table 1 Given operating conditions for simulation

Stage number	30
Feed stage	16
Stage holdups	1.0 kmol
Feed flow rate	100 $\text{kmol}\cdot\text{h}^{-1}$
Feed composition (Benzene)	0.5
(Toluene)	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 $\text{W}\cdot\text{K}^{-1}$
Latent heat of vaporization	30001.1 $\text{kJ}\cdot\text{kmol}^{-1}$
Relative volatility	2.317

Adiabatic index number (K) calculation uses the heat capacity equation of ideal gas. The physical data used in simulation are listed in Table 2.

The simulation programs are programmed using "Matlab Language". The steady state simulation procedure is illustrated as follows

(1) give operation 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 $X_j(k)$.

(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, $X_j(k+1) \rightarrow X_j(k)$, and go to step (4);

(7) calculate $Q_{\text{min,con}}$, Q_{tcd}, X_s from Eqs. (5) - (7), (9) - (11);

(8) calculate $E_{\text{max,con}}$, E_{tcd}, X_e from Eqs. (1) - (4), (8) - (9).

Table 2 Physical data used in simulation

		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	1.133E - 1	1.224E - 1
	C	- 7.206E - 5	- 6.605E - 5
	D	1.703E - 8	1.173E - 8

DEGREES OF FREEDOM ANALYSIS

The degrees of freedom of a processing system are the independent variables that must be specified in order to define the process completely. An analysis of degrees of freedom is very useful for determining the process variables such as manipulated variables and controlled variables.

For a binary mixture system, all the relationships above constitute a system of $6.5n + 10$ equations with $6.5n + 27$ variables. These relations consist of 10 energy calculation relationships, $2.5n$ thermal coupling equations, $2n$ mass balances, n vapor-liquid equilibrium relationships and n component balances. Hence the degrees of freedom (DOF) are

$$\text{No. of DOF} = \text{No. of variables} - \text{No. of relationships}$$

$$= (6.5n + 27) - (6.5n + 10) = 17 \quad (27)$$

These variables can be classified as follows:

Constants (10): $\Delta H_{b,v}$, $\Delta H_{f,v}$, λ, α, $a.b.c$, UA and K_i for $i = 1, 2$;

Externally specified (4): F, Z_f, R_{min} and H;
Unspecified (6. 5n + 13): W_{min}, $Q_{min,con}$, $E_{max,con}$, Q_{tcd}, W_{comp}, K, E_{tcd}, X_e, $Q_{rmin,con}$, X_s, P_r, P_s, q, Q_j for $j = 1,\cdots,f-1$ and X_j, Y_j, V_j, L_j, T_j, $P_{vp,j}$ for $j = 1, 2, \cdots, n$

If given constant variables, the number of degrees of freedom left is 7, which means that only seven variables can be manipulated or specified in order to fully define the ITCDIC system. If the externally specified variables are fixed, the number of degrees of freedom left is 3. For a conventional system such as benzene- toluene system, the stripping pressure, P_s, is 0.1013MPa, hence there are only two manipulated variables such as the rectifying section pressure, P_r, and the feed thermal condition, q, and only two controlled variables also. We can choose the product quality target as the controlled output variable, the top product composition, Y_1, the bottom product composition, X_n, is controlled by the above manipulated variables respectively.

Notice that in practice some constant variables are likely to change along with the operation, such as the transfer rate, UA, will decrease along with the operation. In the following operation analysis, this is taken into account.

SYSTEM CHARACTERISTICS

Fig. 2 shows some system characteristics of the ideal ITCDIC when operation parameters, P_r is 0.2826 MPa and q is 0.5111, other parameters are the same as those in Table 1. For 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 rectifying section and the upward vapor flow for the stripping section. As a result, the flow rates are no longer constant (see Fig. 2b). Fig. 2c shows the thermal coupling condition along with column stages. The difference of temperature distribution along with the column stages (see Fig. 2d) provides the necessary driving force of ITCDIC operation. Compared with the system characteristics of conventional distillation columns, it is obvious that the internal thermal coupling not only causes a change of flow rates but also complicates the heat and mass transfer mechanism in the column.

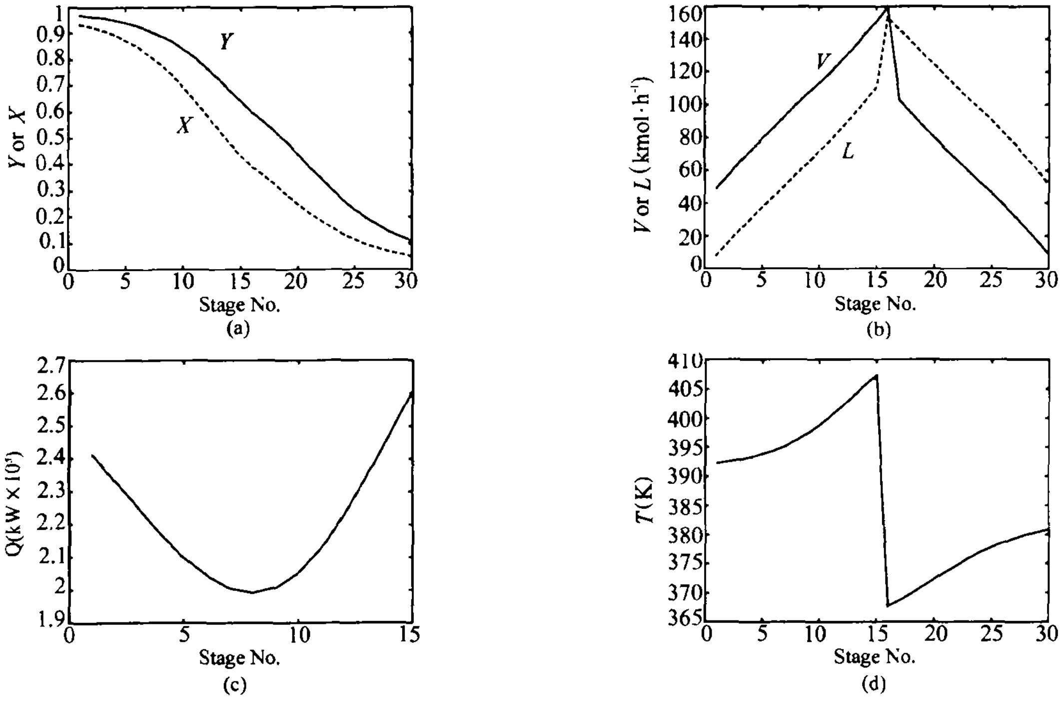

Fig. 2 Some system characteristics figures
(a) composition distribution; (b) flow rate distribtuion; (c) thermal coupling condition; (d) temperature distribtuion

OPERATING LINE

Fig. 3 shows the operation line contrast figure of the ideal ITCDIC, under operating conditions, P_r, of 0.2826MPa and q, of 0.5111. For the conventional distillation column the minimum reflux ratio operation, product quality requirements are the same as those of the ideal ITCDIC. Other parameters are the same as those in Table 1.

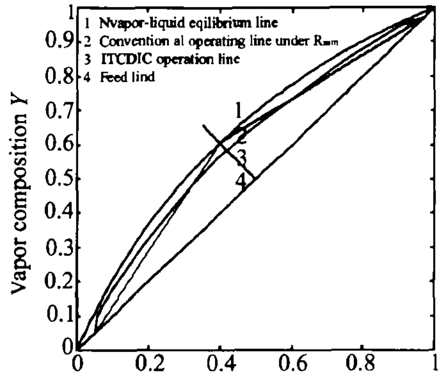

Fig.3 Operating line contrast figure, $P_r = 0.2826, q = 0.5111$

Owing to the internal thermal coupling between rectifying and stripping sections, where the operating line bends away just like the equilibrium line, especially near the top and the bottom stage number, the driving forces of mass and heat transfer of the ITCDIC are significantly reduced compared with the conventional distillation columns (even under minimum reflux operation). Hence the process irreversibility is 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 effect is obtained with the same number of stages at the same energy consumption and energy savings occur in the ideal ITCDIC process.

STEADY STATE BEHAVIOR

The influences of the operating variables on the vapor composition distribution along with the column stages are shown in Fig. 4, where the initial values of the operating conditions are P_r, 0.2826 MPa, P_s, 0.1013 MPa, q, 0.5111, UA, 9803 W/K, F, 100 kmol.h^{-1}, Z_f, 0.5 and the solid lines indicate the above conditions.

Obviously, in all stages, the change direction of the vapor composition is in accord with that of the feed thermal condition and out of accord with that of the feed composition; in the rectifying section, the change direction of the vapor composition is in accord with that of the rectifying section pressure and the heat transfer rate and not in accord with that of the feed flow rate and the stripping section pressure; in the stripping section the change direction of the vapor composition is opposite to that in rectifying section.

Again it shows the feed thermal condition, q, and the feed composition, Z_f, can strongly influence the vapor composition of the ITCDIC; the influences of the pressure of the rectifying section, P_r, and the stripping section, P_s, are inferior; the feed flow rate, F, and the heat transfer rate, UA, have much less influence on the vapor composition. The influence of operating variables on the vapor composition distribution can be expressed by

$$Z_f,\ q \gg P_r,\ P_s > F,\ UA \qquad (28)$$

Furthermore, there are significant differences between the positive and negative responses; which clearly reveals the strongly nonlinear operating behavior in the ideal ITCDIC process. Hence there are very complicated relations and very large influences operation parameters (P_r, q, P_s, UA, F, Z_f) on the composition distributions and the operation behaviors. The feed thermal condition, q and the feed composition, Z_f have dominant roles over the operation. So the former can be regarded as one of the main manipulated variables; the latter, the main outside disturbance; P_r or P_s, another manipulated variable; F, another outside disturbance; UA, the column characteristic variable, which will decrease along with the operating process.

TRANSIENT BEHAVIOR

Fig. 5 shows part of the dynamic behaviors of an ideal ITCDIC. When P_r, P_s, q, UA, F, Z_f change ±20% from P_r, 0.3006 MPa, P_s, 0.1013 MPa, q, 0.5107, UA, 9803 W/K, F, 100 kmol.h^{-1}, Z_f, 0.5 respectively the product qualities (the top vapor composition, Y_1, the bottom liquid composition, X_n) change correspondingly.

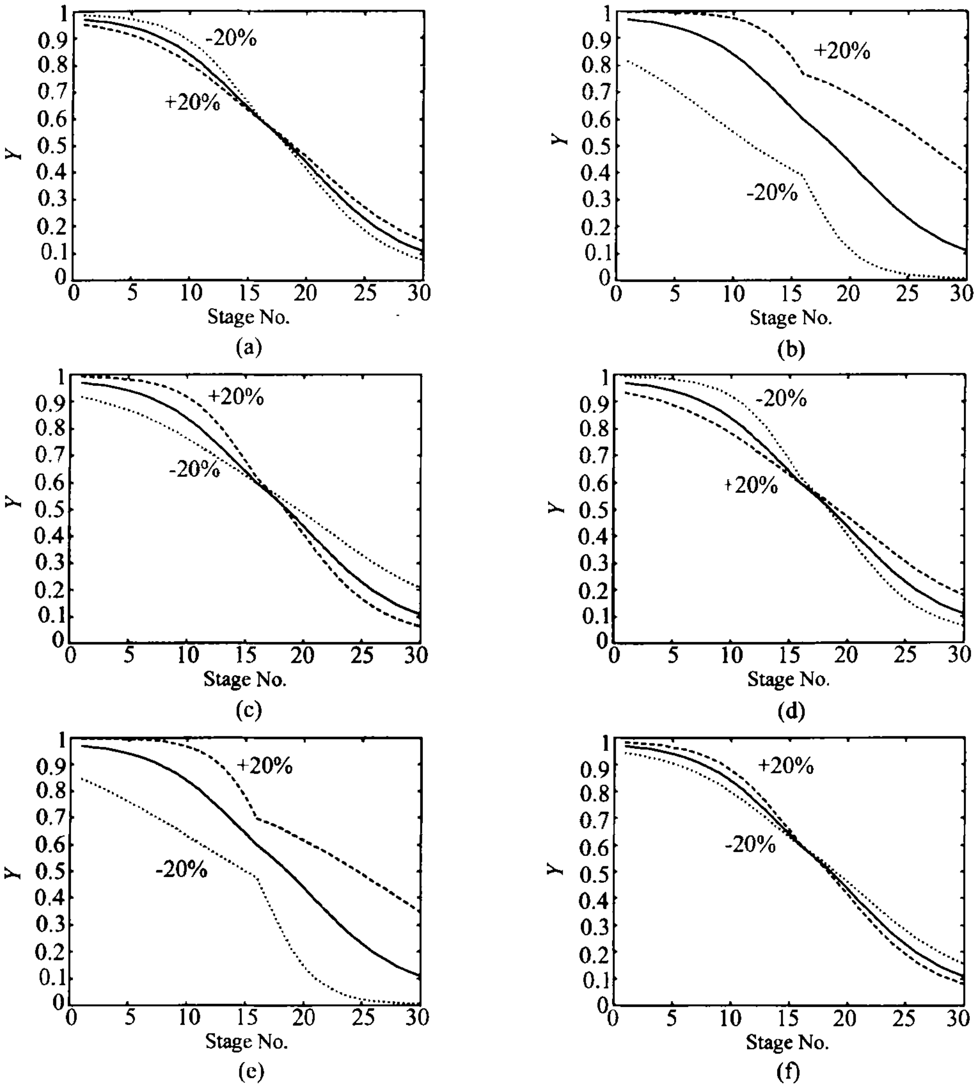

Fig.4 Effects of operating variables a. F; b. Z_f; c. P_r; d. P_s; e. q; f. UA on vapor composition distribution

It shows the feed thermal condition, q, and the feed composition, Z_f, can strongly influence the product quality of the ideal ITCDIC; the influences of the pressure of the rectifying section, P_r, and the stripping section, P_s, are inferior; the feed flow rate, F, and the heat transfer rate, UA, have much less influence on the product qualities. There are significant differences between the positive and negative responses also; it clearly reveals the strongly nonlinear operating behavior in the ideal ITCDIC process.

The above results are in accord with those of steady state, so we can conclude that the ideal ITCDIC process has strongly nonlinear operating behavior and the influence of operating variables on product qualities can be described by Eq. (28). Another notably significant dynamic operating behavior is that the ideal ITCDIC process is self-balancing.

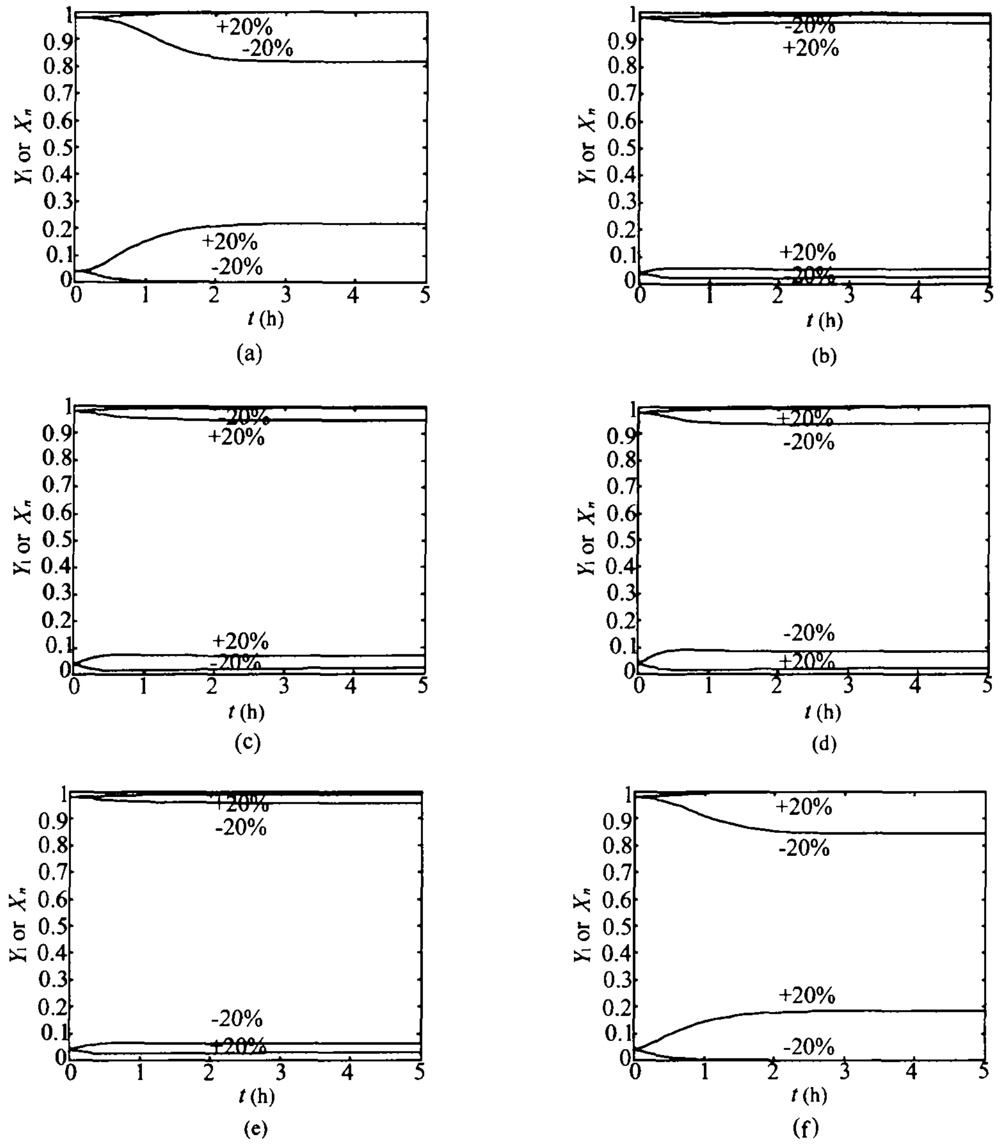

Fig.5 Dynamic responses when a. Z_f; b. F; c. P_s; d. P_r; e. UA; f. q change ±20%, respectively.

SIMULATION RESULTS

Section 6's results show that energy saving can occur in the ideal ITCDIC process, but how much? Based on the result analysis on the degrees of freedom, we chose P_r and q as manipulated variables to appraise the performance of the system and its energy savings. Some simulation results are shown in Table 3. 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 qualities change from 63.73% to 100.00%, for Y_l , from 0.00% to 36.36%, for X_n ; the performance parameter E_{ted} changes from 6. 92% to 21. 03%; X_e changes from 35. 48% to 311.79%; and X_s changes from 37.68% to 75.77%. It shows very complicated relations and very large changes among energy saving, X_s, manipulated variables, P_r, q , and product qualities, X_n, Y_l .

Table 3 Simulation results of Benzene-Toluene system

No.	Manipulated variables		System characteristic						
			Product qualities			Performance parameters			
	q	P_r (MPa)	Y_1/X_n	$E_{max,con}$	E_{tod}	X_e, %	$Q_{min,con}/Q_{tod}$,	10^6 kW	X_s, %
1	0.25	0.1519	0.6373/0.0880	0.0511	0.0813	59.26	4.9122	2.6042	46.99
2	0.25	0.2532	0.6666/0.0003	0.0511	0.0736	44.19	4.9122	2.8764	41.44
3	0.25	0.3545	0.6667/0.0000	0.0511	0.0692	35.48	4.9122	3.0613	37.68
4	0.5	0.1519	0.7708/0.2292	0.0511	0.1173	129.69	4.4928	1.8057	59.81
5	0.5	0.2532	0.9384/0.0616	0.0511	0.1019	99.60	4.4928	2.0779	53.75
6	0.5	0.3545	0.9887/0.0113	0.0511	0.0936	83.29	4.4928	2.2628	49.64
7	0.75	0.1519	0.9091/0.3636	0.0511	0.2103	311.79	4.1562	1.0072	75.77
8	0.75	0.2532	0.9997/0.3334	0.0511	0.1656	224.17	4.1562	1.2794	69.22
9	0.75	0.3545	1.0000/0.3333	0.0511	0.1447	183.23	4.1562	1.4643	64.77

For conventional distillation, the maximum thermodynamic efficiency the Benzene-Toluene system is 5.11%. But for the ideal ITCDIC, in Table 4 the minimum thermodynamic efficiency is 6.92%, enhancing 35.48%, and the related energy saving percentage is 37.68%; the maximum thermodynamic efficiency is 21.03%, enhancing 311.79%, and the related energy saving percentage is 75.77%. Obviously, the ideal ITCDIC can save more energy than conventional distillation.

CONCLUSIONS

From studies of the degrees of freedom, transient and steady state behavior, we can conclude that there are very complicated nonlinear relations and very large influences among operation parameters (P_r, q, P_s, UA, F, Z_f), the product qualities and the operation; again the feed thermal condition, q and the feed composition, Z_f show dominant roles over the operation behaviors and the influences of operation parameters on product qualities can be expressed by Eq. (28); furthermore ITCDIC is a self-balancing process. Studies of the system characteristics, the operating line and simulation results, showed that the internal thermal coupling not only causes changes of flow rates, pressure distributions and temperature distributions but also complicates the heat and mass transfer mechanism in the column. However, its effect of energy savings is marked.

For other systems, such as non-ideal mixture separation, the mathematical model can be applied also, the only thing needed is to change the given conditions, physical data and vapor-liquid equilibrium relationships. We used our study results to develotp related software "ENORM" very useful for further research on ITCDIC. Further investigation is underway to study the control, design and optimization of ITCDIC.

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