Energy-Based Targets for Multiple-Feed Distillation Columns

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Invariant rectifying–stripping (IRS) curves are presented for energy analysis of distillation processes. The IRS curves are invariant to the column configuration (that is, feed location and total number of stages) and depend only on the separation problem and the operating pressure of the column. IRS curves are useful to set targets without performing multiple simulation studies. A novel method is proposed to extend the IRS curves, originally developed for simple distillation columns (with single feed and two end products), to complex multiple-feed columns. In the proposed method, a column with n feeds is decomposed into n simple single-feed columns. The IRS curves are generated for these simple columns and the order and location of the feeds are targeted. Then these IRS curves are added in distinct sections demarcated by the feed points to the column to obtain the composite IRS curves for the complex column. Various targets such as minimum energy requirements (that is, minimum condenser and reboiler loads), appropriate feed locations, proper order of feeds, and effect of premixing feeds can be targeted from the composite IRS curves. Thus, the composite IRS curves for complex columns retain all the advantages of the IRS curves established for the case of simple distillation columns. General guidelines are also proposed for appropriate feed preconditioning and side-exchanger duties leading to the design of energy-efficient complex distillation processes.
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Introduction

Complex distillation columns frequently occur in practice. There are thermoeconomic benefits in having feeds entering the column at different locations depending on their flow rates, compositions, and thermal conditions. It has been shown that the minimum reflux—rather than the boiling point, flow rate, composition, or thermal condition—is a better criterion for sequencing feeds in a complex column (Nikolaides and Malone, 1987; Vishwanathan and Grossmann, 1993). However, the energy-saving potential for different column modifications like reflux reduction, feed conditioning, and scope for side reboiler/condenser has not been addressed for complex columns.

Koehler et al. (1995) reviewed the important methods for

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calculating minimum energy requirements for ideal and nonideal distillation, including conventional and complex columns. The methods, which aim to determine the energy requirement for a complex column, belong to three categories: graphical, approximate, and computationally rigorous. Graphical methods extending the McCabe–Thiele diagram for multiple-feed columns have been proposed (Eduljee, 1964; Glanz and Stichlmair, 1997; King, 1980; Kister, 1985a,b). In these graphical methods, the pseudo-binary concept of light and heavy keys was used to analyze multicomponent systems.

Approximate analytical methods extending the Underwood (1948) equation have also been proposed for complex columns (Barnes et al., 1972; Cerda and Westerberg, 1981; Nikolaides and Malone, 1987; Van Winkle, 1967). Analytical equations to approximately calculate the minimum reflux in multiple-feed columns for binary and multicomponent systems (using the pseudo-binary concept) have been proposed by Yaws et al. (1981) and Chou et al. (1986). These methods are useful for preliminary designs and rapid screening of alternatives. However, these approximate methods make simplifying assumptions such as constant molar overflow and constant relative volatility. Most of these methods are based on a trial-and-error approach to determine the minimum reflux for a complex distillation column with predetermined sequence of the feeds.

A mixed-integer nonlinear programming (MINLP) model for determining the optimal location of the feeds and the number of stages for a specified separation in the case of a distillation column with multiple feeds was proposed by Viswanathan and Grossmann (1993). This is a computationally rigorous method that requires no information about the order of feeds. The optimization step automatically determines the order and location of the feeds. However, two major difficulties encountered in the solution of MINLP models are combinatorial explosion and "local optimal" solutions. The former are attributed to the potentially large number of structural alternatives and the latter arise from the nonconvexities in nonlinear process models.

In the conceptual design stage, achievable and reliable targets are set before the detailed design of the flowsheet. The goal of targeting is to quickly reduce the potentially large space of design alternatives to a small set of candidate designs that merit more detailed attention. Different targeting procedures have been developed to analyze heat-exchanger networks to determine the best performance that can be achieved before actual synthesis (Linnhoff, 1993, 1994; Linnhoff et al., 1982; Shenoy, 1995; Shenoy et al., 1998). In conventional design of distillation columns, multiple simulations are required to establish reliable targets for the energy-saving potential for different column modifications like reflux reduction, feed conditioning, and scope for side reboiler/condenser. The temperature–enthalpy (*T–H*) curve, discussed here, for a distillation column provides a useful tool for these purposes.

The *T–H* curve for a binary distillation column at the minimum thermodynamic condition (MTC) can be generated by solving the coupled heat and mass balance equations for the reversible separation scheme (Benedict, 1947; Fitzmorris and Mah, 1980; Fonyó, 1974; Ho and Keller, 1987; King, 1980; Naka et al., 1980). Terranova and Westerberg (1989) extended the approach of Ho and Keller (1987) to multicomponent systems with Underwood's method (1948) for minimum reflux calculation. Carlberg and Westerberg (1989a,b) used the same concept to generate the *T–H* diagram for thermally coupled columns and for simple distillation column sequences. From the converged simulation of a distillation column, Dhole and Linnhoff (1993) described a procedure for generating the *T–H* curve. However, the procedure did not consider the enthalpy balances at the feed stages. A feed stage correction that rigorously considers the mass and enthalpy balances at feed stages was proposed earlier by Bandyopadhyay et al. (1998).

Recently, Bandyopadhyay et al. (1999) proposed invariant rectifying–stripping (IRS) curves (on a *T–H* diagram) that are independent of the feed location, the thermal condition of the feed, and the operating reflux of the column for a given separation problem. The IRS curves are rigorously invariant and provide the absolute minimum utility requirements for binary systems (ideal as well as nonideal); however, they are near-invariant and predict the near-minimum utility requirements for multicomponent systems (where the pseudo-binary concept of a light and a heavy key is used). Procedures have been developed for targeting minimum energy requirement, appropriate feed location, feed preconditioning, and scope for side exchangers for simple distillation columns (Bandyopadhyay, 1999; Bandyopadhyay et al., 1999, 2003). The relation between the IRS curves and the exergy loss in a simple distillation column was recently established by Bandyopadhyay (2002).

In this communication, a decomposition method is presented to extend the IRS approach to complex columns. The composite IRS curves are devised that represent complex columns in the *T–H* space and preserve all the advantages of the original IRS curves approach. Various targets for designing energy-efficient complex distillation processes such as minimum energy requirements, appropriate feed locations, proper sequence of feeds, and effect of premixing feeds can be set directly from composite IRS curves. General guidelines for feed preconditioning and side-exchanger duties are also proposed herein. The composite IRS curves provide a valuable tool for energy analysis of complex columns.

Invariant Rectifying–Stripping (IRS) Curves

Invariant rectifying–stripping (IRS) curves are generated at the minimum thermodynamic condition (MTC), which is defined as a reversible operation for a distillation column with no entropy generation (Bandyopadhyay et al., 1998; King, 1980).

IRS curves

The procedure for the generation of the IRS curves is discussed first. Detailed derivations of the equations that are used in this section are given by Bandyopadhyay et al. (1999). Consider the rectifying section of a column as shown in Figure 1a. Let H_R be the minimum condensing load required to cause separation from x^* to x_D. Then, the overall mass, component, and energy balances for the rectifying section may be combined to obtain the following expression for H_R

$$H_R = D\left[H_V\left(\frac{x_D - x^*}{y^* - x^*}\right) - H_L\left(\frac{x_D - y^*}{y^* - x^*}\right) - H_D\right] = D\left[\left(\frac{H_V - H_L S_R}{1 - S_R}\right) - H_D\right] \quad (1)$$

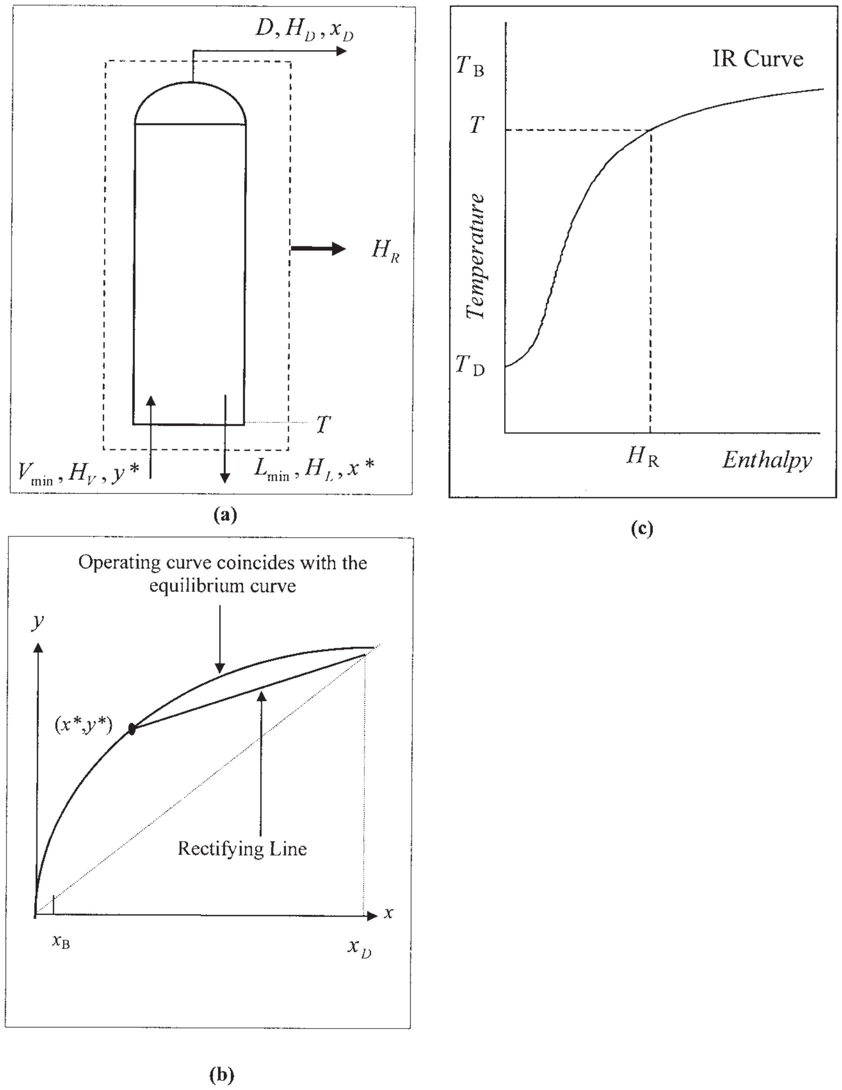


Figure 1. Generation of invariant rectifying (IR) curve.

(a) Rectifying section of a column for determination of enthalpy surplus; (b) rectifying line on *x*–*y* diagram; (c) typical invariant rectifying (IR) curve.

where S_R denotes the slope of the rectifying line (as shown in Figure 1b) and is given by $S_R = (x_D - y^*)/(x_D - x^*) = L_{\min}/V_{\min}$.

The enthalpy surplus in the rectifying section, H_R, may be calculated using Eq. 1 by continuously rotating the rectifying line from $y^* = x_D$ to $x^* = x_B$ along the equilibrium curve with (x_D, x_D) as pivot. This enthalpy surplus is then plotted as a function of the equilibrium temperature to give a T vs. H_R curve, which may be designated the invariant rectifying (IR) curve. A typical IR curve is shown in Figure 1c.

Similarly, consider the stripping section of a distillation column (as shown in Figure 2a) with H_S denoting the minimum reboiling load required to cause separation from x^* to x_B. The overall mass, component, and energy balances for the stripping section may be combined to determine H_S from

$$H_S = B\left[H_V\left(\frac{x^* - x_B}{y^* - x^*}\right) - H_L\left(\frac{y^* - x_B}{y^* - x^*}\right) + H_B\right] = B\left[\left(\frac{H_V - H_L S_S}{S_S - 1}\right) + H_B\right] \quad (2)$$

where S_S denotes the slope of the stripping line (as shown in Figure 2b) and is given by $S_S = (y^* - x_B)/(x^* - x_B) = L_{\min}/V_{\min}$.

The enthalpy deficit in the stripping section (H_S) may be calculated using Eq. 2 by continuously rotating the stripping line from $x^* = x_B$ to $y^* = x_D$ along the equilibrium curve with (x_B, x_B) as pivot. This enthalpy deficit is then plotted as a function of the equilibrium temperature to give a T vs. H_S curve, which may be designated the invariant stripping (IS) curve. A typical IS curve is shown in Figure 2c.

Both these curves may be now plotted on the same tempera-

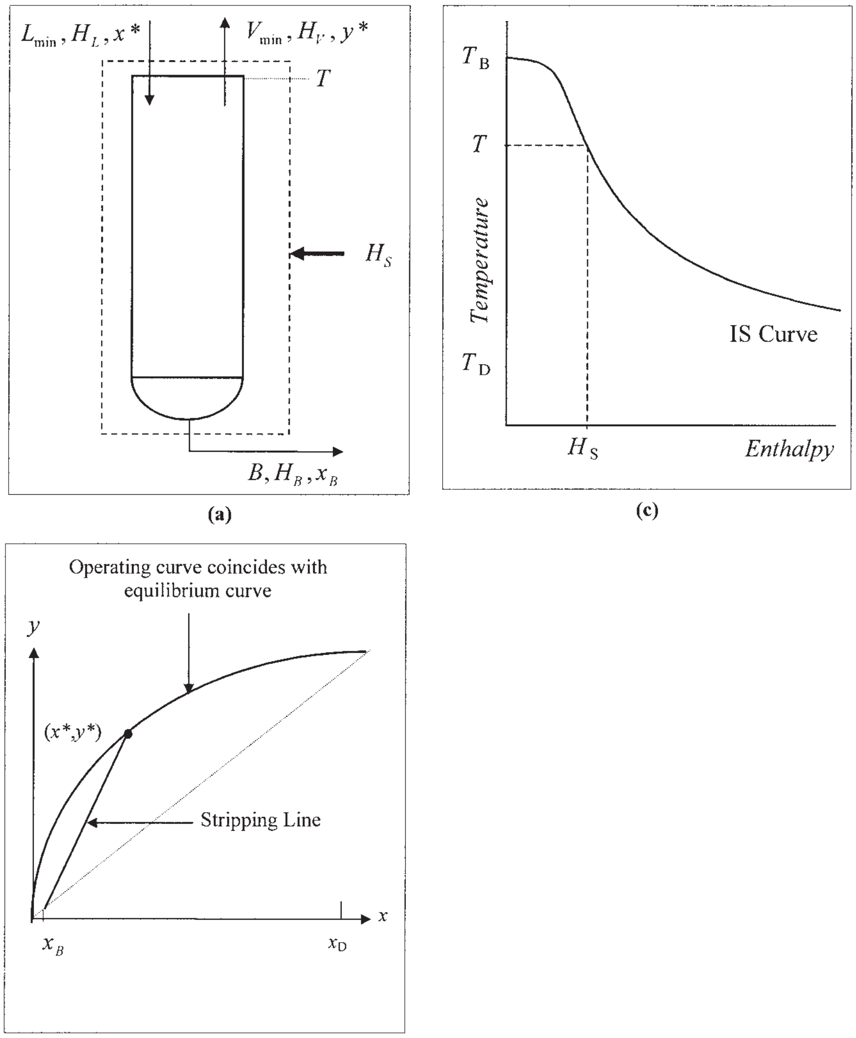


Figure 2. Generation of invariant stripping (IS) curve.

(a) Stripping section of a column for determination of enthalpy deficit; (b) stripping line on *x–y* diagram; (c) typical invariant stripping (IS) curve.

ture–enthalpy (*T–H*) axis to obtain the invariant rectifying–stripping (IRS) curves (see Figure 3). Note that, the enthalpy surplus (H_R) and the enthalpy deficit (H_S) for a distillation problem may be conveniently calculated using Eqs. 1 and 2 for each stage of a distillation column from the output of a converged simulation.

The invariance of the IRS curves for binary systems may be proven from the fact that a binary system has only two degrees of freedom, according to the Gibbs phase rule. Therefore, these curves become deterministic on specifying the operating pressure and separation required. Thus, H_R and H_S are functions of temperature only and are invariant to the total number of stages and the location of the feed in the column. The invariant property of the IRS curves does not hold rigorously for multicomponent systems. However, IRS curves for multicomponent systems show near-invariance to the total number of stages and the feed locations (as demonstrated by Bandyopadhyay et al., 1999).

Feed location and minimum energy targets

The IRS curves may be used to target the feed location and the minimum energy requirement for distillation (Bandyopadhyay et al., 1999). The IR curve and the IS curve are not independent, but are related by the overall component, mass, and energy balances. Combining the mass, component, and energy balances around the feed stage for a column operating at the MTC, the relation between the IR curve and the IS curve can be simplified at the feed stage to give (Bandyopadhyay et al., 1999)

$$H_S = H_R + \Delta \qquad \text{(at the feed stage)} \tag{3}$$

where

$$\Delta \equiv Q_r - Q_c = BH_B + DH_D - FH_F \tag{4}$$

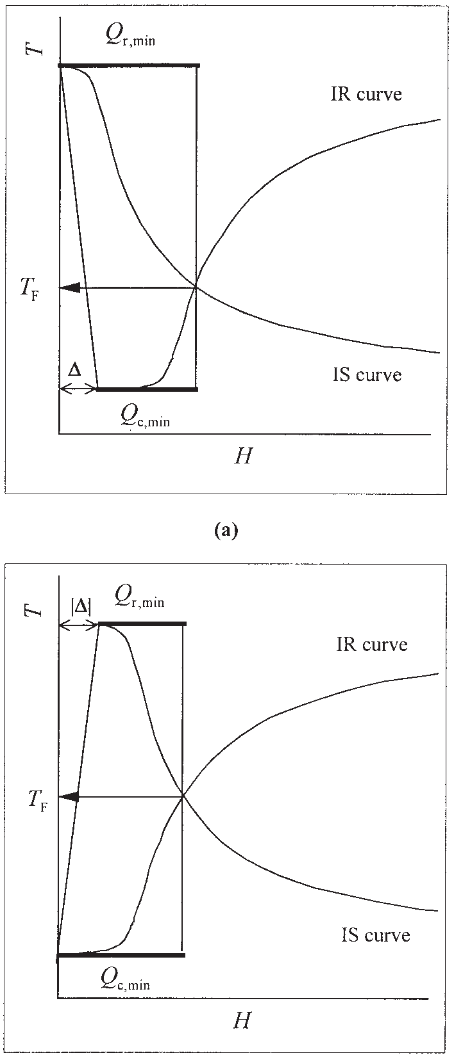


Figure 3. Translated invariant rectifying–stripping (IRS) curves.

(a) $\Delta \geq 0$ ($Q_r \geq Q_c$) and (b) $\Delta < 0$ ($Q_r < Q_c$).

Because Q_r and Q_c are the reboiler and the condenser loads, respectively, Δ corresponds to the constant enthalpy difference for the utility requirements of the column based on the first law of thermodynamics.

Given the fact that enthalpies are relative (that is, the difference in enthalpy is important rather than the absolute enthalpy), the IR curve and/or the IS curve may be translated horizontally. The following convention may be adopted to translate the IRS curves in accordance with Eq. 3. Depending on the sign of Δ (as defined in Eq. 4), the translations may be conveniently classified into two cases: (1) if $\Delta \geq 0$, then only the IR curve is translated to the right by Δ (Figure 3a); and (2) if $\Delta < 0$, then only the IS curve is translated to the right by $|\Delta|$ (Figure 3b). Note that neither the IR curve nor the IS curve is translated for $\Delta = 0$. Mathematically, these translations can be conveniently represented as

$$H_{RT} = H_R + \Delta/2 + |\Delta/2| \tag{5}$$

$$H_{ST} = H_S - \Delta/2 + |\Delta/2| \tag{6}$$

where H_{RT} and H_{ST} are the enthalpy coordinates for the translated IR curve and translated IS curve, respectively. Note that, although the IR and IS curves are independent of feed condition, the translated curves depend on the thermal condition of the feed. Equations 3–6 may be combined to obtain

$$H_{ST} = H_{RT} \qquad \text{(at the feed stage)} \tag{7}$$

Equation 7 defines the criterion for appropriately locating the feed in the column. The appropriate location for the feed may be determined in terms of temperature (T_F) by finding the intersection of the translated IRS curves (Figure 3). A method to convert this target temperature into a stage number for proper feed location was previously suggested by Bandyopadhyay et al. (1999).

After locating the feed from the intersection point of the translated IRS curves in terms of temperature (T_F), the minimum energy requirements may also be determined from the translated IRS curves. The portion of the IR curve below T_F and the portion of the IS curve above T_F may be circumscribed by a right-angled trapezium. Then, the widths of the parallel sides of the trapezium at the top and bottom define the minimum energy targets for the reboiler and condenser, respectively (see Figure 3). Note that a rectangle (rather than a right-angled trapezium) is obtained for $\Delta = 0$. These minimum energy targets are directly related to the minimum reflux target. On the other hand, the operating reflux target (for grassroots cases) and the reflux modification target (for retrofit cases) involve a cost optimization where the trade-off between utility cost (based on the reboiler and condenser loads) and capital cost (based on the column diameter and number of stages) needs to be explored (Bandyopadhyay, 1999).

The pinch on the IRS curves is defined as the point touching the vertical side of the right-angled trapezium. Figure 3 illustrates cases where the intersection point of the translated IRS curves determines the pinch. This is often the case and, mathematically, it requires the IRS curves to be monotonic in nature. However, this may not be the case for nonideal systems (not discussed here for brevity, although the concepts developed are applicable), especially those where a tangent pinch is observed on the *x*– *y* diagram (Bandyopadhyay et al., 1999).

Feed preconditioning targets (including a quantitative method to determine the optimum feed conditioning required to maximize the savings in the reboiler load) as well as targets for the placement of side exchangers have been developed by Bandyopadhyay (1999) and Bandyopadhyay et al. (2003). Thus, the IRS curves allow targets to be established for feed location, minimum energy requirements, thermal condition of the feed, and scope for side exchangers for a simple distillation column (that is, a column with a single feed and two products). In what follows, the generation procedure for the IRS curves is extended to complex columns using a decomposition strategy.

Decomposition of Complex Columns

The proposed method decomposes a complex distillation problem into several separation problems, each consisting of a simple distillation column. Each side product from a complex

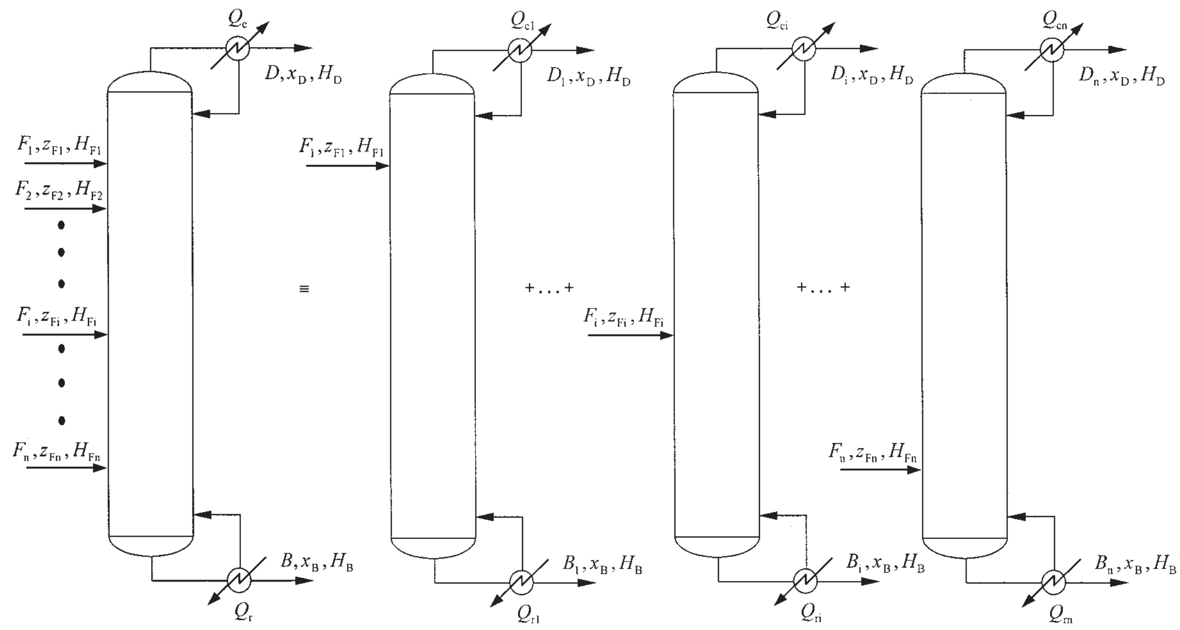


Figure 4. Decomposition of complex distillation column with *n* feeds into *n* single-feed distillation columns.

distillation may be considered as a feed to the column with a negative flow rate (Bandyopadhyay et al., 1998; Kister, 1985a). Therefore, a complex column with multiple feeds and side products is equivalent to a complex column with only multiple feeds where some of the feeds have negative flow rates.

A complex column with *n* feeds is first decomposed into *n* simple columns, as shown in Figure 4. For the *i*th decomposed column, the overall mass, component, and energy balances may be written, respectively, as

$$F_i = D_i + B_i \tag{8}$$

$$F_i z_{Fi} = D_i x_D + B_i x_B \tag{9}$$

$$D_i H_D + B_i H_B - F_i H_{Fi} = Q_{ri} - Q_{ci} \equiv \Delta_i \tag{10}$$

where D_i, B_i, and Δ_i are the distillate flow rate, bottom flow rate, and enthalpy difference (as defined in Eq. 4) of the *i*th decomposed column (Figure 4). It may be noted that for a side product, F_j and the corresponding D_j and B_j are negative. In the decomposition process, the overall mass, component, and enthalpy balances are conserved (given that $D = \Sigma D_i$, $B = \Sigma B_i$, and $\Delta \equiv Q_r - Q_c = DH_D + BH_B - \Sigma F_i H_{Fi} = \Sigma \Delta_i$ where the summation Σ goes from $i = 1$ to $i = n$).

It is important to note that the purity and enthalpy of the end products in the *i*th column are identical to those in the original multiple-feed column. By solving Eqs. 8 and 9, the decomposed distillate and bottom flow rates (D_i and B_i) may be calculated for the *i*th decomposed column with feed F_i (Figure 4) from the following expressions

$$D_i = F_i\left(\frac{z_{Fi} - x_B}{x_D - x_B}\right) \tag{11}$$

$$B_i = F_i\left(\frac{z_{Fi} - x_D}{x_B - x_D}\right) \tag{12}$$

The distillate flow rate (D_i) and the bottom flow rate (B_i) of the *i*th decomposed column may be uniquely determined from Eqs. 11 and 12, which show the contribution of each feed to the end products. On determining D_i and B_i, the values of Δ_i may be simply obtained by substitution in Eq. 10.

The enthalpy surplus (H_{Ri}) and the enthalpy deficit (H_{Si}) of the individual decomposed columns (with product flow rates calculated from Eqs. 11 and 12) may be directly calculated from Eqs. 1 and 2. For this purpose, the enthalpies and compositions on every stage as well as for the feeds and products are required. For binary systems, thermodynamic models for enthalpy and vapor–liquid equilibrium may be readily used. In general, the righthand sides of Eqs. 1 and 2 may be conveniently calculated for each stage of a distillation column from the output of a converged simulation. From Eqs. 1 and 2, it may be noted that (H_{Ri}/D_i) and (H_{Si}/B_i) are constant for every feed. Therefore, it is not necessary to perform *n* simulations for the *n* decomposed columns in Figure 4 to generate the corresponding IRS curves. In fact, from a single converged simulation of the complex column, the translated IRS curves may be obtained through Eqs. 5 and 6 for each of the *n* decomposed columns.

Ordering and locating feeds

The intersection point of these translated IRS curves for the *i*th decomposed column defines the appropriate location of the *i*th feed in terms of temperature (T_{Fi}) in accordance with Eq. 7. This is demonstrated for a two-feed column (discussed in detail as Example 1 later) in Figure 5a.

Physically, Eq. 7 signifies the intersection of the *q*-line for a feed with the equilibrium curve on the *x*–*y* diagram. For a

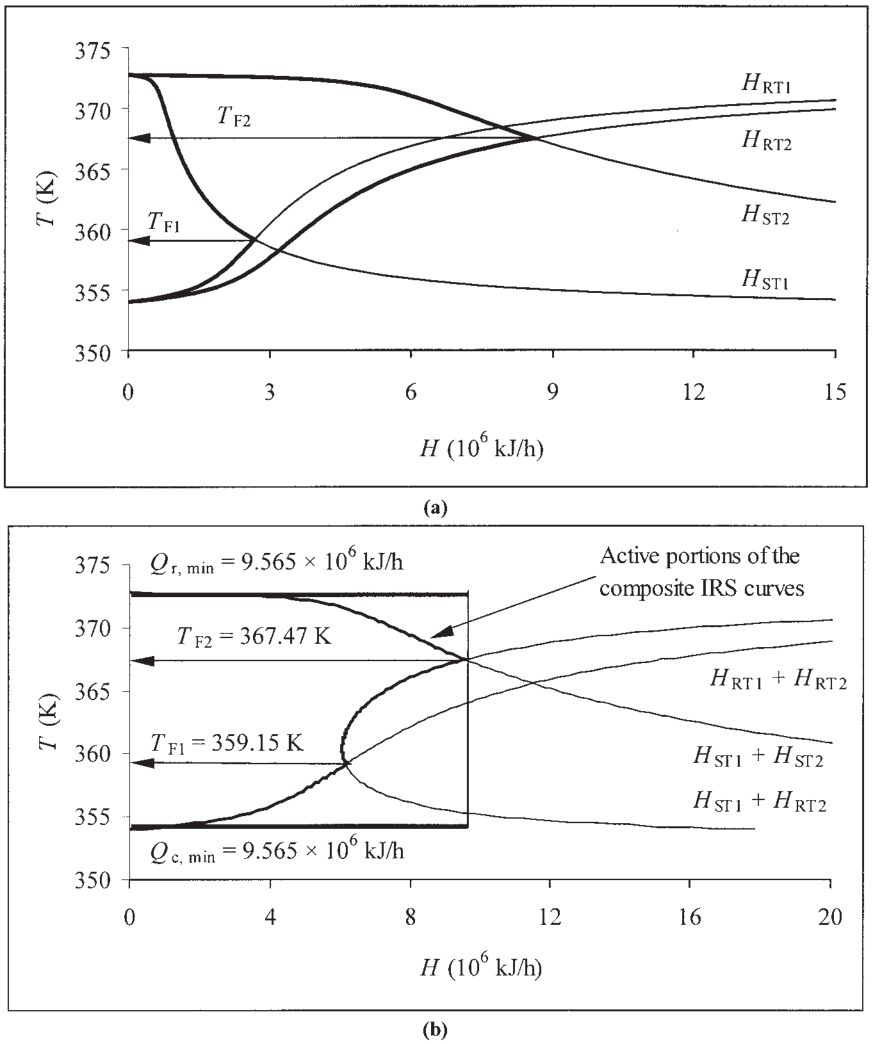


Figure 5. (a) Translated IRS curves for the decomposed columns and (b) the composite IRS curves for the two-feed column.

Example 1 with $F_1 = 50$ kmol/h and $F_2 = 200$ kmol/h.

multiple-feed column, the intersection of the *i*th *q*-line with the equilibrium curve is independent of the intersections for the remaining feeds. Similarly, the intersection of the translated IRS curves for the *i*th decomposed column signifies the appropriate location for the *i*th feed and is independent of the feed location targets for the other feeds. This independence property allows appropriate location of each feed without assuming any predetermined order for the feeds. Rather, the appropriate order for the feeds may be determined by simply arranging the target temperatures (for example, feed F_2 is at a higher temperature than feed F_1 in Figure 5a).

The appropriate location for any feed in a complex column at MTC is independent of the appropriate location of the other feeds. Based on this independence property, the appropriate order of the feeds in a complex column is targeted. Note that the order of the feeds thus targeted is appropriate and accurate for a reversible distillation column or a distillation column at MTC. In general, the order holds for distillation columns operating with reflux more than the minimum reflux required for the specified separation. In some distillation columns operating at higher reflux ratio, the proper order of the feeds may change. This happens only if the *q*-lines of the feeds intersect (on the *x*–*y* diagram). However, in such cases, the energy penalty incurred by not changing the order of the feeds is usually negligible. Note that the order of feeds is not important for initial simulation. Appropriate order of feeds and their appropriate locations can be targeted from the composite IRS curves. These targets can then be validated through a final simulation.

After locating the feeds from the intersection points of the translated IRS curves, the minimum energy requirement for the complex column may be determined by combining the individual translated IRS curves, as described next.

Composite IRS Curves

The portion of the translated IR curve below T_{Fi} and the portion of the translated IS curve above T_{Fi} may be defined as the active portions of the translated IRS curves for the *i*th decomposed column and consequently the *i*th feed. Thus

$$H_{Ai} = \begin{cases} H_{RTi} & \text{for } T \le T_{Fi} \\ H_{STi} & \text{for } T > T_{Fi} \end{cases} \quad (13)$$

For the case of a simple column with a single feed, the active portions of the translated IRS curves are circumscribed by a right-angled trapezium to readily define the minimum energy targets for the column (as in Figure 3). For complex columns, the following procedure is adopted.

Composite IRS curves are generated for the complex column by simply adding the enthalpy coordinates of the translated IRS curves corresponding to all the feeds. The generation of the composite IRS curves is shown in Figure 5b for a typical two-feed column based on the translated IRS curves of the two decomposed columns shown in Figure 5a. The composite IRS curves for the two-feed column are drawn by appropriately adding the IRS curves for the two decomposed columns in three distinct sections demarcated by the feed intersection points. The active portions may be easily identified on the translated IRS curves of the decomposed columns because they are highlighted by heavy lines in Figure 5a. In the section below T_{F1}, the rectifying curves of both the columns contribute to the active portions. In the section above T_{F2}, the stripping curves of both the columns contribute to the active portions. Between the two feeds (above T_{F1} and below T_{F2}) the stripping curve of the first column and the rectifying curve of the second column contribute the active portions. Hence, the composite IRS curves consist of $H_{RT1} + H_{RT2}$, $H_{ST1} + H_{RT2}$, and $H_{ST1} + H_{ST2}$ (Figure 5b). Thus, to produce the composite IRS curves for the two-feed column, only three curves need to be drawn. By induction, for a column with n feeds, $(n+1)$ curves are to be drawn based on the active portions of the translated IRS curves of the n decomposed columns. In Figure 5a, it may be noted that feed F_2 is above feed F_1 as T_{F2} is greater than T_{F1}. Therefore, the section between the feeds F_1 and F_2 constitutes the IS curve for feed F_1 and the IR curve for feed F_2. The section below T_{F1} and above T_{F2} comprises the IR curves for both feeds and the IS curves for both feeds, respectively. Hence, three composite IRS curves are obtained (Figure 5b) by adding the enthalpy coordinates as follows: $H_{RT1} + H_{RT2}$, $H_{ST1} + H_{RT2}$, and $H_{ST1} + H_{ST2}$. The fourth composite IRS curve possible, $H_{RT1} + H_{ST2}$, is unnecessary because the IR curve for feed F_1 and the IS curve for feed F_2 are not active together in any section.

In essence, an n-feed complex column may be decomposed into n single-feed columns for the generation of n sets of IRS curves. Then, their enthalpy coordinates may be added to generate $(n + 1)$ composite IRS curves for the complex column.

Determining minimum energy requirements

In the complex column, the section i between two properly ordered feeds, F_i and F_{i+1} (with $T_{Fi} < T_{Fi+1}$), constitutes the active stripping portions for the feeds below feed F_{i+1} (that is, for all feeds F_j where $j < i + 1$) and the active rectifying portions for the feeds above feed F_i (that is, for all feeds F_j where $j > i$). To obtain the active portions of the composite IRS curves for the complex column, the enthalpy coordinates for the active portions of the translated IRS curves for individual decomposed columns are added together between the intersection points corresponding to the different feeds. Thus, for section i of an n-feed column

$$H_A = \sum_{j=1}^{n} H_{Aj} = \sum_{j=1}^{i} H_{STj} + \sum_{j=i+1}^{n} H_{RTj} \qquad i = 0, 1, \ldots, n \quad (14)$$

Equation 14 ensures that the overall mass, component, and energy balances are satisfied in each of the $(n + 1)$ sections of the n-feed column.

The active portions of the composite IRS curves (H_A) may be circumscribed by a right-angled trapezium, as described earlier for a simple column with a single feed. As before, the widths of the parallel sides of the trapezium at the top and bottom define the minimum energy targets for the reboiler and condenser, respectively (see Figure 5b). Note that in Figure 5b, a rectangle (rather than a right-angled trapezium) is shown as $\Delta = 0$ for this case. Figure 5b illustrates the case where one of the intersection points of the composite IRS curves determines the pinch. This is observed to be the case whenever the IRS curves of the individual decomposed columns are monotonic in nature. Note that the composite IRS curves for the complex column are, however, not monotonic.

Illustrative Examples

For the first three examples, some simplifying assumptions are made that are consistent with the original problem description. The assumptions are no pressure drop losses, ideal vapor phase, and ideal liquid solution. Further, it is assumed that the latent heats of vaporization (λ_i) are equal for both the components and independent of temperature (over the operating temperature range of the distillation column), and the vapor pressure of a component is given by the Clausius–Clapeyron equation. These assumptions imply that the mixture to be separated is an ideal binary mixture of constant relative volatility with constant molar overflow. In the first three examples, $T_A = 353$ K and $T_B = 373$ K, where T_A and T_B are the boiling points of the low-boiling component A and the high-boiling component B, respectively. The latent heat of vaporization λ is calculated using the Clausius–Clapeyron equation from $\lambda = T_A T_B R \ln \alpha/(T_B - T_A)$, knowing the relative volatility α between components A and B. Because $\alpha = 2.05$ for the first three examples, λ is found to be 39.291 kJ/mol. However, it should be noted that the methodology described here is not restricted to cases with these assumptions, as demonstrated in the last two examples. Because the invariance property of the IRS curves is proved based on the Gibbs phase rule, it holds for any binary system, including those with significant heat of mixing effects, irrespective of the number of feeds (or column sections). The problem data for the examples that follow are given in Table 1.

Example 1: two-feed column

This binary distillation problem with two saturated-liquid feeds was originally discussed by Yaws et al. (1981). The data for the flow rates and the feed compositions are given in Table 1.

For this case, the complex distillation column is decomposed into two simple columns. The product flow rates (in kmol/h) may be then obtained by solving Eqs. 11 and 12 as $D_1 = 32.21$,

Table 1. Data for Various Examples

Example		1		2			3			4			5	
System		A and B		A and B			A and B			Acetone–acetic acid			Benzene–toluene–xylene	
Thermodynamic method		$\alpha = 2.05$		$\alpha = 2.05$			$\alpha = 2.05$			Activity coefficient: UNIQUAC fugacities: SRK			SRK	
Operating pressure		—		—			—			101.35 kPa			101.33 kPa	
Feed data	#	F_1	F_2	F_1	F_2	F_3	F_1	F_2	F_3	F_1	F_2	F_3	F_1	F_2
	Flow rate (kmol/h)	50	200	10	40	150	40	160	600	42.18	74.84	50.8	100	100
	Composition (% light component)	60	20	80	52	20	70	55	25	78.5	39.4	27.7	70% benzene 20% toluene	20% benzene 20% toluene
	Thermal condition (q)	1.0	1.0	1.0	1.0	1.0	0.7	0.8	0.9	335.4 K 104.8 kPa	355.4 K 108.9 kPa	366.5 K 117.2 kPa	1.0	1.0
Specifications	Top	98% of A (recovery)		98% of A (recovery)			98% of A			99.06% acetone			99% benzene (recovery)	
	Bottom	97% of B (recovery)		97% of B (recovery)			91.3% of B			99.6% acetic acid			99% toluene (recovery)	

$B_1 = 17.79$, $D_2 = 41.79$, and $B_2 = 158.21$. From the IRS curves for the decomposed columns shown in Figure 5a, the appropriate locations for the feeds may be determined as $T_{F1} = 359.15$ K (corresponds to $x^*_{F1} = 0.60$) and $T_{F2} = 367.47$ K (corresponds to $x^*_{F2} = 0.20$).

Once the composite IRS curves and active portions (Figure 5b) are drawn as discussed in the previous section, the minimum energy targets (in terms of condenser and reboiler loads) are determined from the widths of the circumscribing rectangle ($\Delta = 0$, in this example). The minimum condenser and reboiler duties are equal (9.565×10^6 kJ/h), and correspond to the minimum reflux ratio of 2.29. This value agrees with that reported by Yaws et al. (1981). Note that the second feed defines the pinch and hence the minimum reflux of the column. On the IRS curves, the locations of the feeds are in terms of temperature, which can be converted to feed-stage numbers using the methodology discussed by Bandyopadhyay et al. (1999).

Yaws et al. (1981) studied the effect of feed flows on minimum reflux by changing the flow rates of the feeds (that is, $F_1 = 100$ kmol/h and $F_2 = 50$ kmol/h). On repeating the calculations following the same methodology, it is found that the first feed (rather than the second feed) defines the pinch (Figure 6) and the corresponding minimum reflux equals 1.36 [which is also the value reported by Yaws et al. (1981)].

Example 2: three-feed column

This binary distillation problem with three saturated-liquid feeds (see Table 1 for data) was also discussed by Yaws et al. (1981).

The complex distillation column is decomposed into three simple columns. From Eqs. 11 and 12, the product flow rates (in kmol/h) are obtained as $D_1 = 8.58$, $B_1 = 1.42$, $D_2 = 22.17$, $B_2 = 17.83$, $D_3 = 31.12$, and $B_3 = 118.88$. The IRS curves of the decomposed columns are shown in Figure 7a, and the appropriate locations for the feeds may be targeted as $T_{F1} = 355.87$ K (corresponds to $x^*_{F1} = 0.80$), $T_{F2} = 360.60$ K (corresponds to $x^*_{F2} = 0.52$), and $T_{F3} = 367.47$ K (corresponds to $x^*_{F2} = 0.20$).

The composite IRS curves for the three-feed column are drawn by adding the translated IRS curves of the decomposed columns (Figure 7a) in four distinct sections (that is, $H_{RT1} + H_{RT2} + H_{RT3}$, $H_{ST1} + H_{RT2} + H_{RT3}$, $H_{ST1} + H_{ST2} + H_{RT3}$, and $H_{ST1} + H_{ST2} + H_{ST3}$, as shown in Figure 7b). The composite IRS curve corresponding to $H_{ST1} + H_{ST2} + H_{RT3}$ is C-shaped; however, the composite IRS curve corresponding to $H_{ST1} + H_{RT2} + H_{RT3}$ is not C-shaped because the enthalpy values of the translated IRS curve for H_{ST1} are observed to be relatively low in Figure 7a. When $\Delta = 0$, the minimum energy target determined from the width of the circumscribing rectangle (Figure 7b) is found to be 7.485×10^6 kJ/h. The minimum reflux ratio for the complex column is calculated from the minimum condenser duty to be 2.07, identical to the value reported by Yaws et al. (1981). Note that the third feed defines the pinch and consequently the minimum reflux ratio of the column.

Example 3: three-feed column with two-phase feeds

The data (Chou et al., 1986) for this binary distillation problem with two-phase feeds are given in Table 1. After

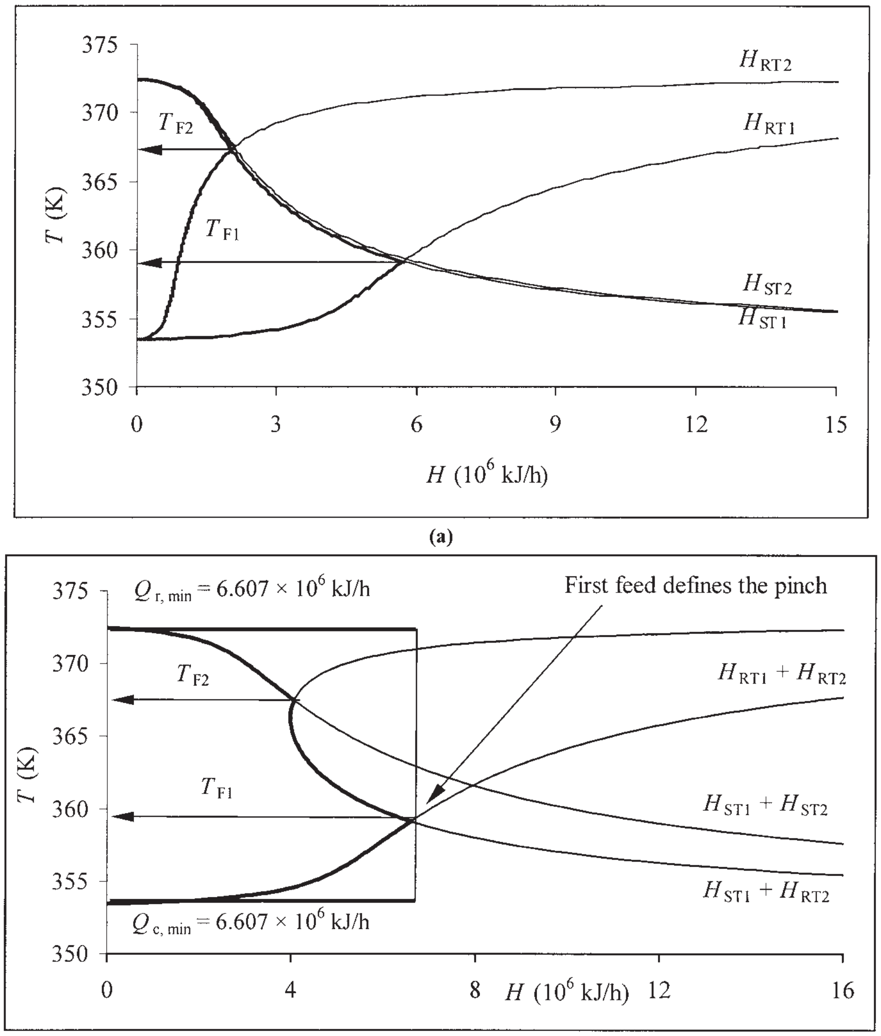


Figure 6. (a) Translated IRS curves for the decomposed columns and (b) the composite IRS curves for the two-feed column.

Example 1 with F_1 = 100 kmol/h and F_2 = 50 kmol/h.

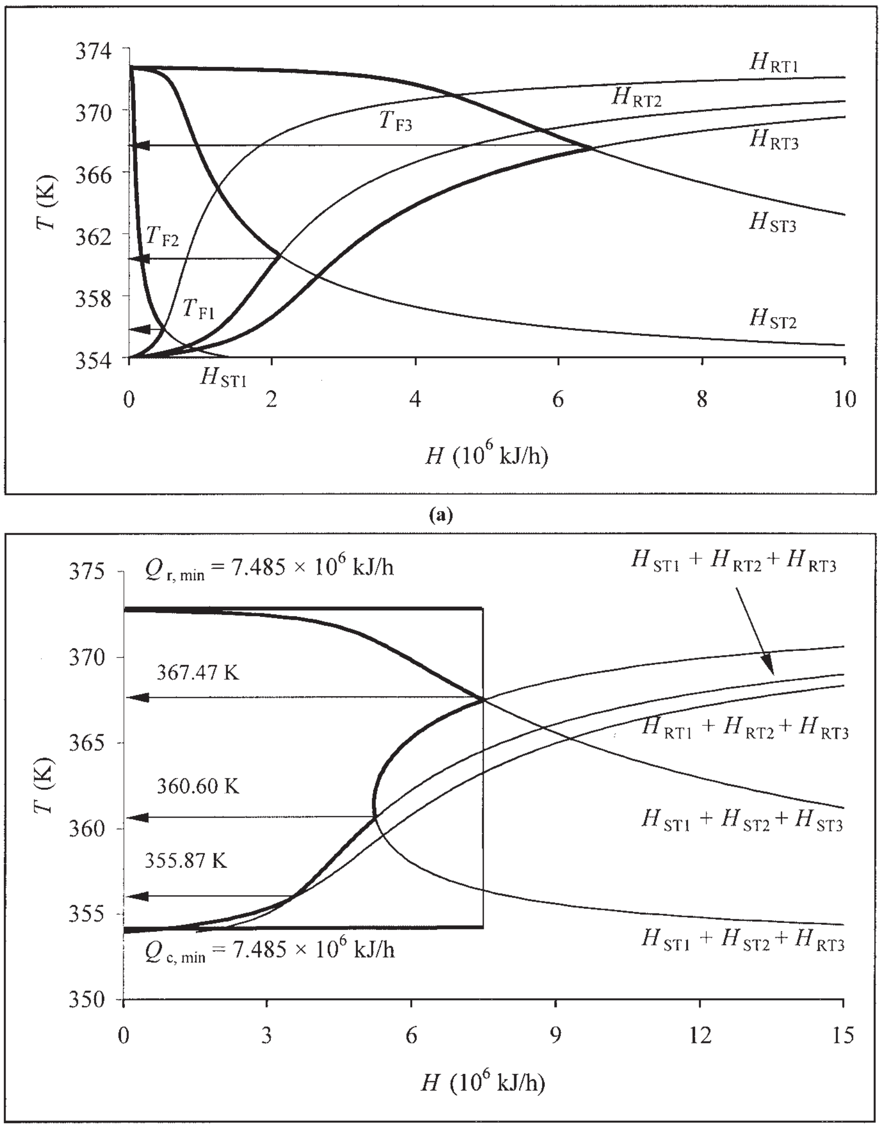
decomposing the three-feed complex column into three simple columns, the product flow rates (in kmol/h) are determined to be $D_1 = 27.46$, $B_1 = 12.54$, $D_2 = 82.97$, $B_2 = 77.03$, $D_3 = 109.58$, and $B_3 = 490.42$. The IRS curves of the decomposed columns are shown in Figure 8a and the appropriate locations for the feeds may be targeted as $T_{F1} = 358.15$ K (corresponds to $x^*_{F1} = 0.658$), $T_{F2} = 360.68$ K (corresponds to $x^*_{F2} = 0.516$), and $T_{F3} = 366.62$ K (corresponds to $x^*_{F2} = 0.235$). It should be noted that the enthalpy differences based on the first law of thermodynamics (that is, Δ_i values) are not zero and are given (in kmol/h) by $\Delta_1/\lambda = -12$, $\Delta_2/\lambda = -32$, and $\Delta_3/\lambda = -60$.

The composite IRS curves consist of $H_{RT1} + H_{RT2} + H_{RT3}$, $H_{ST1} + H_{RT2} + H_{RT3}$, $H_{ST1} + H_{ST2} + H_{RT3}$, and $H_{ST1} + H_{ST2} + H_{ST3}$ (Figure 8b) and are obtained by a procedure similar to that used in Figure 7b. The active portions of the composite IRS curves are then circumscribed by a right-angled trapezium (rather than a rectangle) because Δ is not zero ($\Delta = -4.086 \times 10^6$ kJ/h). The minimum reflux ratio of the complex column calculated from the minimum condenser duty (of 26.364×10^6 kJ/h) is found to be 2.05, identical to that reported by Chou et al. (1986). Note that the pinch is defined by the third feed.

Example 4: three-feed column for acetone–acetic acid separation

In this acetone–acetic acid separation problem with three feeds (Nikolaides and Malone, 1987), the simulations are performed using the PRO/II (1994–1995) software based on the problem data given in Table 1. Stage numbering starts from the top of the column with 1 denoting the condenser. With the feeds at the 4th, 9th, and 16th stages, the simulation for a 22-stage column gives an operating reflux ratio of 0.114 with reboiler and condenser duties of 2.743×10^6 and 2.507×10^6 kJ/h, respectively.

The IRS curves for the three decomposed columns (with $D_1 = 33.39$, $B_1 = 8.79$, $D_2 = 29.58$, $B_2 = 45.26$, $D_3 = 14.05$, and $B_3 = 36.75$ kmol/h) are shown in Figure 9a. The appropriate



(a)

(b)

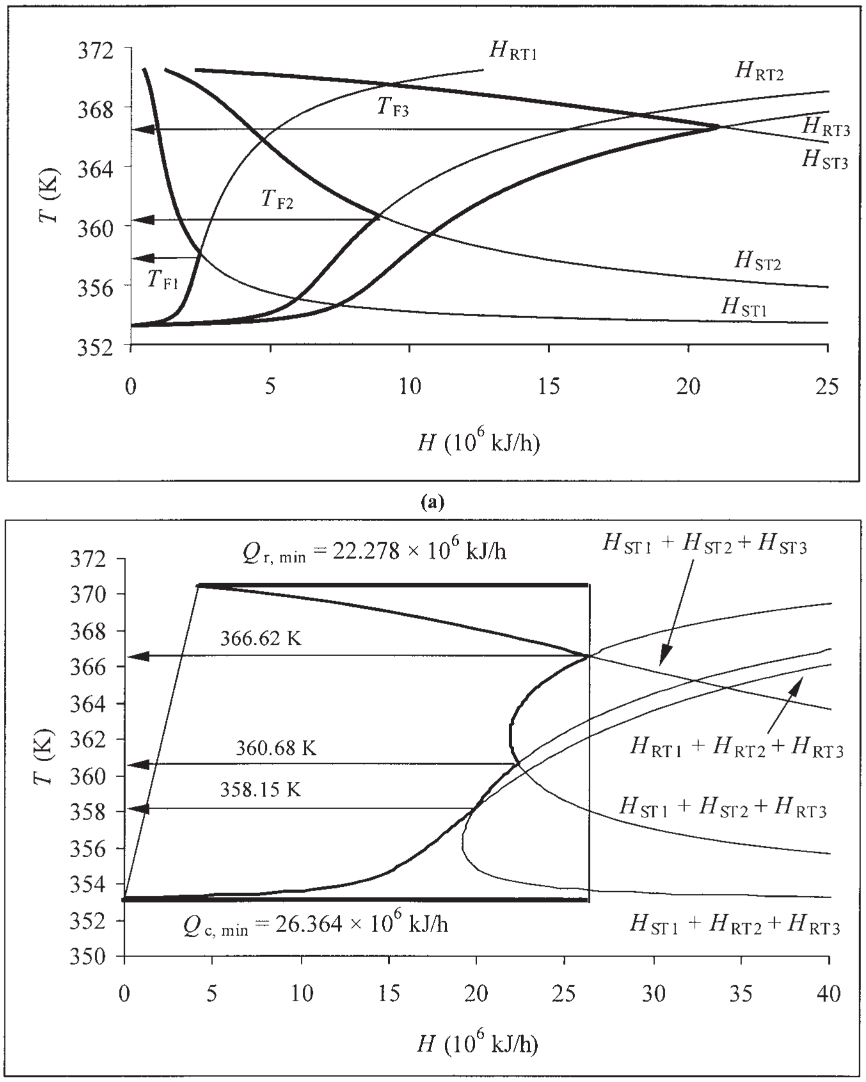
Figure 7. (a) Translated IRS curves for the decomposed columns and (b) the composite IRS curves for the three-feed column.

Example 2.

locations for the feeds may be targeted as $T_{F1} = 336.13$ K, $T_{F2} = 355.93$ K, and $T_{F3} = 364.94$ K.

The composite IRS curves for the three-feed complex column are generated by a procedure similar to that applied in the previous two examples and are shown in Figure 9b. As observed by Nikolaides and Malone (1987), the controlling feed is the first feed, which has the lowest flow rate and the highest composition of acetone. The minimum condenser duty is found to be 2.457×10^6 kJ/h, which corresponds to the minimum reflux ratio of 0.0915. Simulation of a 100-stage column, with the feeds at the 20th, 45th, and 80th stages, yields an operating reflux ratio of 0.0916 with a condenser duty of 2.457×10^6 kJ/h and thereby validates the targets. This target is superior to the minimum reflux ratio based on the Underwood (1948) equation and calculated to be 0.106 by Nikolaides and Malone (1987).

The three feeds may be premixed and fed into the column. Premixing of the feeds causes entropy generation and, consequently, there would be an increase in the energy requirements both in the condenser and the reboiler. In Figure 9b, the distance of the intersection point of the $H_{RT1} + H_{RT2} + H_{RT3}$ and $H_{ST1} + H_{ST2} + H_{ST3}$ curves from the pinch point of the composite IRS curves denotes the increase in energy consumption. The minimum condenser duty for the premixed column is 2.948×10^6 kJ/h, which is 20% higher than the minimum condenser duty for the three-feed column. A similar observation was previously made by Nikolaides and Malone (1987). Note that the increase in the energy requirement for the premixed feeds can be predicted from the composite IRS curves without performing any further simulation.



(a)

(b)

Figure 8. (a) Translated IRS curves for the decomposed columns and (b) the composite IRS curves for the three-feed column with two-phase feeds.

Example 3.

Example 5: two-feed column for benzene–toluene–xylene separation

For reversible multicomponent distillation, the degrees of freedom are still two (Koehler et al., 1991). By arguments analogous to those for the binary case, the system becomes deterministic. The IRS curves are invariant to the feed location and the operating reflux on specifying the operating pressure and the separation. However, the sharpness of separation is generally limited in reversible multicomponent distillation (Fonyó, 1974; Franklin and Wilkinson, 1982), although this limitation can be overcome during the generation of IRS curves using the pseudo-binary concept of a light and heavy key model (Dhole and Linnhoff, 1993; Fonyó, 1974) that defines a practical near-minimum thermodynamic condition (Bandyopadhyay et al., 1999). The invariant property of the IRS curves does not hold rigorously for multicomponent systems because the distribution of the components depends on the operating reflux of the column. Stupin and Lockhart (1968) noted that this distribution bears a nonlinear relationship for any finite operating reflux. However, the temperature vs. composition (*T–x–y*) and the enthalpy vs. composition (*H–x–y*) behaviors of pseudo-binary systems do not change significantly (Campagne, 1993; Johnson and Morgan, 1985) near the minimum reflux for the column. Therefore, the IRS curves for any pseudo-binary system, generated through a simulation with a high number of stages (that is, at a low reflux ratio), show near-invariance to the total number of stages and the feed location (as demonstrated by Bandyopadhyay, (1999) and Bandyopadhyay et al., (1999)).

In binary distillation, one of the components is obviously heavy and the other is light. However, this is not so obvious for reversible multicomponent distillation because the sharpness of separation is generally limited (Fonyó, 1974). As mentioned earlier, the difficulty may be overcome with the pseudo-binary

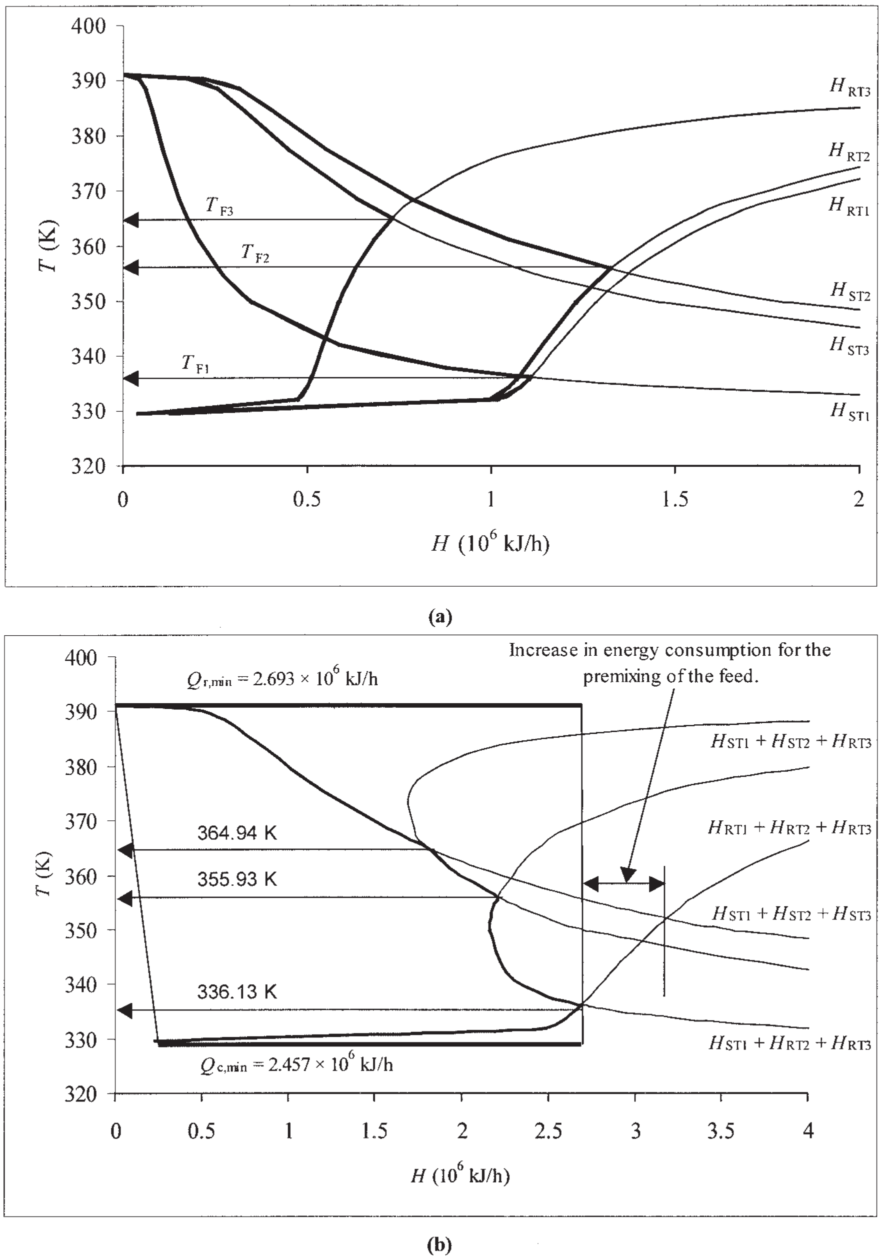


Figure 9. (a) Translated IRS curves for the decomposed columns and (b) the composite IRS curves of the three-feed column for acetone–acetic acid separation.

Example 4.

concept of a light and heavy key model (Fonyó, 1974) that defines a practical near-minimum thermodynamic condition (Bandyopadhyay et al., 1999). The key components are usually specified by the designer. Light non-key components are clubbed with the light key, and heavy non-key components with the heavy key. Distributed components can be clubbed with the light or heavy key depending on their *K*-values. In the case of crude distillation, the key definition varies from stage to stage and keys can be defined according to the *K*-values of the pseudo-components or by comparing stage compositions (Dhole and Buckingham, 1994). It must be noted that the shape of the IRS curves and the reflux modification targets depend on the key definition. Except for strongly nonideal mixtures, the minimum reflux separation of multicomponent mixtures exhibits a pinch point in each half of the column. When the column products do not contain one or more of the components present in the feed, the pinch point is closer to the product outlet for that half of the column and does not coincide with the feed stage (Koehler et al., 1995). In general, the pinch point determining the minimum reflux is not known a priori. However, only the pinch point controlling the minimum reflux is detected by pseudo-binarization, and hence the minimum energy consumption predicted is close to that calculated through a rigorous calculation (Bandyopadhyay et al., 1999).

The simulations for this benzene–toluene–xylene separation problem with two feeds are performed using the Design-II

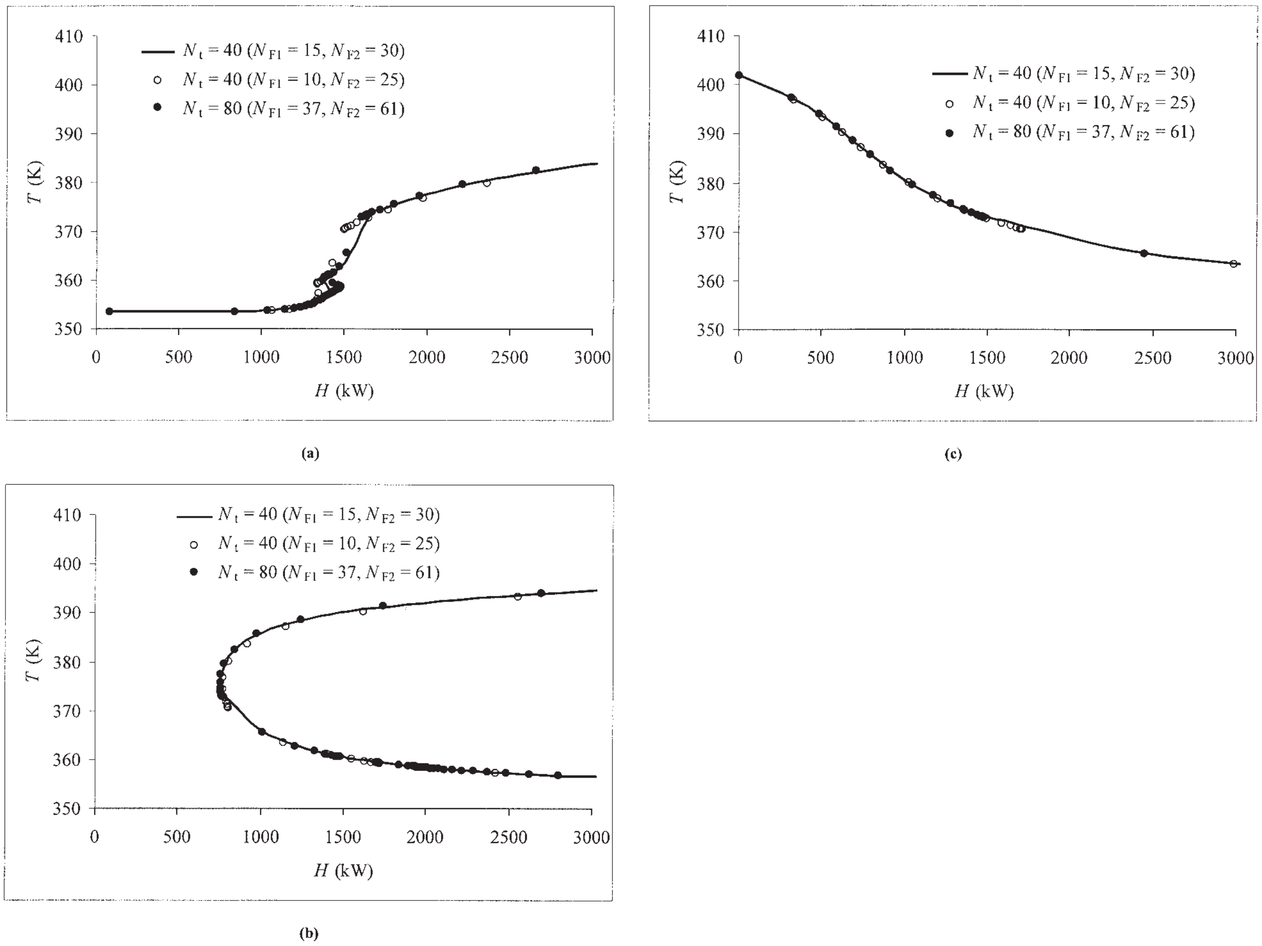


Figure 10. Near-invariant property of composite IRS curves for multicomponent system on varying feed locations and total number of stages.

(a) $H_{RT1} + H_{RT2}$, (b) $H_{ST1} + H_{RT2}$, and (c) $H_{ST1} + H_{ST2}$.

(1999) software based on the problem data given in Table 1. For this multicomponent separation of the two-feed column, Figure 10 shows data for composite IRS curves generated from three different simulations on varying the feed stages (N_{F1} and N_{F2}) and the total number of stages (N_t). The three data sets define practically unique composite IRS curves for $H_{ST1} + H_{RT2}$ and $H_{ST1} + H_{ST2}$; however, the data points for $H_{RT1} + H_{RT2}$ show a certain degree of scatter (within 2%). It may be concluded that the composite IRS curves are only near-invariant for multicomponent systems, and the practical targets provided by them need to be finally verified through rigorous column simulation.

In Figure 10a, the scatter is attributed to the fact that the controlling pinch in the rectifying section is well developed only for values close to the minimum reflux (that is, high N_t). It is therefore meaningful to generate the IRS curves from a converged simulation with a high number of stages. The simulation of the 80-stage column (with feeds at the 37th and 61st stages) gives reboiler and condenser duties of 1.481 and 1.407 MW, respectively, with an operating reflux ratio of 0.856.

For the purpose of generating the IRS curves, benzene is considered as the light key and toluene and xylene are grouped as the heavy key. The IRS curves for the two decomposed columns (for $D_1 = 70.07$, $B_1 = 29.93$, $D_2 = 19.43$, and $B_2 = 80.57$ kmol/h) and the composite IRS curves for the two-feed complex column are shown in Figure 11. The appropriate locations for the feeds may be targeted as $T_{F1} = 361.1$ K and $T_{F2} = 383.3$ K. It should be noted that the decomposed IRS curves (for H_{RT1} and H_{RT2}) and the composite IRS curve ($H_{RT1} + H_{RT2}$) are nonmonotonic in nature. This is generally the case for the sharp separation of multicomponent systems. The pinch is defined by the $H_{RT1} + H_{RT2}$ curve and not by any particular feed intersection point (Figure 11b). The minimum condenser duty turns out to be 1.403 MW, which corresponds to the minimum reflux ratio of 0.852. Simulation of a 122-stage column, with the feeds at the 61st and 86th stage, yields an operating reflux ratio of 0.854 with a condenser duty of 1.406 MW and thereby validates the minimum reflux and energy targets.

Discussion and Conclusion

A simple methodology has been proposed to extend the IRS curves from simple single-feed columns to complex multiple-feed columns. In this methodology, a complex n-feed column is decomposed into n single-feed columns by calculating the

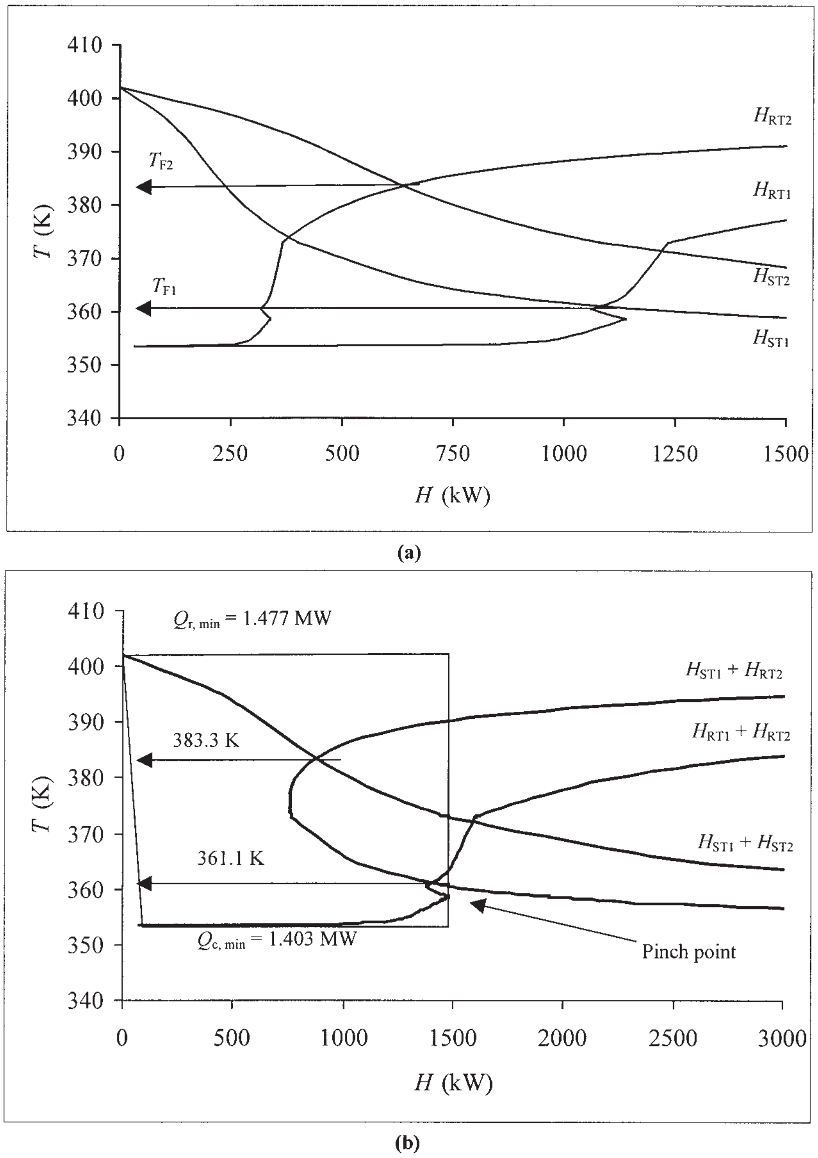


Figure 11. (a) Translated IRS curves for the decomposed columns and (b) the composite IRS curves of the two-feed column for benzene–toluene–xylene separation.

Example 5.

contribution of each feed to the end products. Side products may be considered as feeds with negative flow rates in this decomposition procedure. The IRS curves are generated for each of these *n* decomposed columns and their enthalpy coordinates are then appropriately added in distinct sections demarcated by the feed intersection points to obtain ($n + 1$) composite IRS curves for the complex column. The methodology is rigorously valid in the case of binary systems because here the H_{ST} and H_{RT} terms are directly proportional to the bottoms and distillate flow rates. So, addition of the enthalpy coordinates of the translated IRS curves of the decomposed columns will give the composite IRS curves for the actual complex column. In the case of multicomponent systems, the decomposition may not be rigorously valid. However, as demonstrated through an example, the decomposition holds practically good for targeting purposes of multicomponent complex columns arising from the near-invariant nature of the IRS curves.

Although the focus herein has been on minimum energy and feed location targets, the composite IRS curves have the potential to provide targets for feed preconditioning and side exchangers. The effect of the feed preheating (or cooling), in terms of the decrease (or increase) in the reboiler duty and increase (or decrease) in the condenser duties, can also be determined from the IRS curves, as demonstrated by Bandyopadhyay et al. (2003). From the study of different complex columns, a general principle can be devised for better energy efficiency of distillation processes: feeds below the pinch should be cooled and feeds above it should be preheated. Furthermore, the significance of the pinch, in the context of side exchangers for distillation, may be stated as follows: no (side-)reboiling below the pinch temperature and no (side-)condensing above the pinch temperature. This is consistent with the observations of Naka et al. (1980) and Agrawal and Fidkowski (1996).

The key representation proposed in this work is the composite IRS curves for complex columns with multiple feeds and side products. This article uses the novel concept of decomposition of a complex column into multiple simple columns. Ordering of multiple feeds and their appropriate locations in the column have been targeted based on the minimum reflux criterion. The minimum reflux (rather than boiling point, flow rate, composition, or thermal condition) has been shown to be a better criterion for sequencing feeds in a complex column by earlier studies (Nikolaides and Malone, 1987; Vishwanathan and Grossmann, 1993).

The energy-saving potential for different column modifications like reflux reduction, feed conditioning, and scope for side reboiler/condenser had not been addressed for complex columns by previous approaches. The composite IRS curves simultaneously allow feed sequence, feed location, and minimum energy targets to be established ahead of configuring the column. Furthermore, the composite IRS curves allow targeting for feed preconditioning (preheating/cooling).

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Notation

B = bottom product molar flow
D = distillate molar flow
F = feed molar flow
H = enthalpy
IR = invariant rectifying (curve)
IS = invariant stripping (curve)
IRS = invariant rectifying–stripping (curves)
K = vapor–liquid equilibrium ratio
L = liquid molar flow
MTC = minimum thermodynamic condition
N = number of stages
n = number of feeds
Q = heat duty
q = quantity related to feed condition
R = gas constant
SRK = Soave–Redlich–Kwong
S = slope of rectifying/stripping line
T = temperature
V = vapor molar flow
x = mole fraction in liquid
y = mole fraction in vapor
z = mole fraction in feed

Greek letters

α = relative volatility
Δ = enthalpy difference defined in Eq. 4
λ = heat of vaporization

Subscripts and Superscripts

A = active (part of IRS curves) or component A
B = bottom product or component B
c = condenser
D = distillate
F = feed
i, j = index variables
L = liquid
min = minimum
r = reboiler
R = rectifying curve
RT = rectifying curve (translated)
S = stripping curve
ST = stripping curve (translated)
t = total (number of stages)
V = vapor
* = equilibrium condition

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