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# Optimal Feed Locations and Number of Trays for Distillation Columns with Multiple Feeds

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MINLP models for finding the optimal locations for the feeds and the number of trays required for a specified separation for a distillation column with multiple feeds are presented. Systems with ideal, Soave–Redlich–Kwong equation of state and UNIQUAC thermodynamic models are considered. This rigorous procedure requires no assumptions concerning the order of the feeds—i.e., the disposition of any feed with respect to other feeds. The optimization step automatically determines the order and the locations.

## Introduction

Distillation columns with multiple feeds with different compositions occur frequently in practice. Clearly, there are economic benefits in letting the feeds enter at different locations depending on their characteristics (molar flow rates, compositions, thermal conditions, etc). Yet, so far as is known, no rigorous procedures exist for the design of such columns.

Approximate methods (e.g., Nikolaides and Malone (1987) and Van Winkle (1967)), however, have been proposed. These are very useful for preliminary designs and rapid screening of alternatives. However, the approximate methods make simplifying assumptions such as constant relative volatility and constant molal overflow, which generally do not hold in nonideal systems.

In this Research Note, an algorithmic approach for solving these design problems is presented. First, we consider the problem where the number of trays in the column are known and it is required to find the optimal locations for the feeds. Next, we consider the problem of finding simultaneously the optimal locations and the number of trays for a specified separation. No assumption concerning the disposition of any feed with respect to other feeds needs to be made—the order and the locations for the feeds are determined automatically.

In the framework adopted here, the equations and inequalities describing the thermodynamics of the system (the defining equations for fugacities, enthalpies, etc.) are included explicitly in the optimization problem—in more familiar terminology, the approach is completely equation-based (although, strictly speaking, one should say equation- and inequality-based). This means that, for example, for a system with $c$ components governed by Soave–Redlich–Kwong equation of state thermodynamics, there are $(6c + 13)$ equations and 3 inequalities and $(5c + 13)$ additional or intermediate variables to describe the phase equilibium relations on a tray—rather than $c$ equations as one would normally expect when invoking (external) procedures for computation of thermodynamic properties. The resulting system is large and sparse, and so, the full power of sparse matrix techniques can be utilized for the efficient solution of both the nonlinear program (NLP) and the mixed integer program (MIP). It should be noted, however, that this is by no means a restriction: the proposed model and the solution procedure will work equally well in the usual framework for solving distillation problems where external thermodynamic subroutines are invoked.

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This Research Note is essentially self-contained; however, the reader may find some useful additional information in Viswanathan and Grossmann (1993), where the MINLP approach for finding the number of trays for a column with a single feed is described.

## MINLP Model for Optimal Locations for a Column with Known Number of Trays

Consider a distillation column (Figure 1) with $N$ trays, including the condenser and the reboiler. The stages are numbered bottom upward so that the reboiler is the first tray and the condenser is the last ($N$th) tray. Only the total condenser and kettle-type reboiler case is considered—the other cases can be dealt with similarly. For definiteness, only two feeds are considered. The straightforward extension to three or more feeds is indicated in Remarks at the end of this section.

Let $I = \{1, 2, ..., N\}$ denote the set of trays and let $R = \{1\}$, $C = \{N\}$, and $S = \{2, 3, ..., N - 1\}$ denote subsets corresponding to the trays in the reboiler, in the condenser, and within the column, respectively.

Let $\mathcal{F}^1$ and $\mathcal{F}^2$ denote the feeds. Let $c$ denote the number of components in the feeds, and let $J = \{1, 2, ..., c\}$ denote the corresponding index set. Let $F^k$, $T_f^k$, $p_f^k$, $v_f^k$, $z_f^k$, and $h_f^k$, $k = 1,2$ denote, respectively, the molar flow rate, the temperature, the pressure, the vapor fraction, the vector of mole fractions (with components, $z_{f1}^k, z_{f2}^k, ..., z_{fc}^k$), and the molar specific enthalpy of the corresponding feeds.

Let $p_i$ denote the pressure prevailing on tray $i$. It is assumed that $p_{\rm reb} = p_1$, $p_{\rm bot} = p_2$, $p_{\rm top} = p_{N-1}$, and $p_{\rm con} = p_N$ are given, although one may treat them as variables to be determined, if desired. (In many cases, it is quite adequate to regard all of them as equal to the same value.) Then $p_1 \geq p_2 \geq ... p_{N-1} \geq p_N$, and for simplicity, let $p_f^k \geq p_{\rm bot}$, $k = 1, 2$.

Let $L_i$, $x_i$, $h_i^{\rm L}$, and $f_{ij}^{\rm L}$ denote the molar flow rate, the vector of mole fractions, the molar specific enthalpy, and the fugacity of component $j$, respectively, of the liquid leaving tray $i$. Similarly, let $V_i$, $y_i$, $h_i^{\rm V}$, and $f_{ij}^{\rm V}$ denote the corresponding quantities for the vapor. Let $T_i$ denote the temperature prevailing on tray $i$. Then

$$f_{ij}^{\rm L} = f_{ij}^{\rm L}(T_i, p_i, x_{i1}, x_{i2}, ..., x_{ic})$$

$$f_{ij}^{\rm V} = f_{ij}^{\rm V}(T_i, p_i, y_{i1}, y_{i2}, ..., y_{ic})$$

$$h_i^{\rm L} = h_i^{\rm L}(T_i, p_i, x_{i1}, x_{i2}, ..., x_{ic})$$

$$h_i^{\rm V} = h_i^{\rm V}(T_i, p_i, y_{i1}, y_{i2}, ..., y_{ic}) \qquad (1)$$

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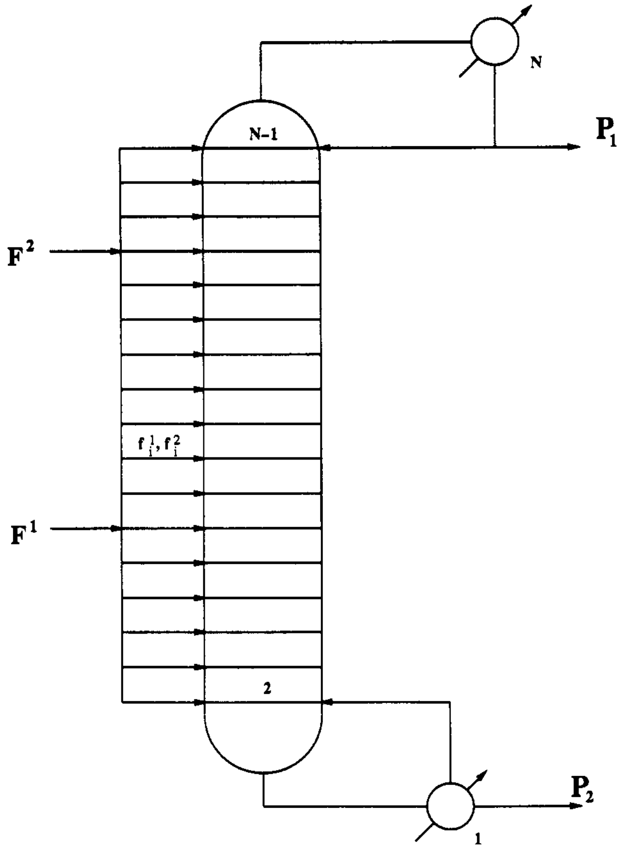


**Figure 1.** Optimal locations for feeds.

where the functions and/or procedures on the right-hand sides depend on the thermodynamic model used.

Let $P_1$ and $P_2$ denote the top and bottom product rates, respectively and let $r$ denote the reflux ratio. Let $v_{\rm lk}^{\rm c}$ and $l_{\rm hk}^{\rm r}$ denote the recoveries of the light key in the top product (liquid or vapor, depending) and the heavy key in the bottom liquid product, respectively. Let $q_{\rm reb}$ and $q_{\rm con}$ denote the reboiler and condenser duties, respectively.

Let $f_i^1$, $i \in S$, denote the amount of $\mathcal{F}^1$ entering tray $i$, i.e., $\sum_{i\in S} f_i^1 = F^1$. Similarly, for $f_i^2$, $i \in S$. Let $z_i^1$, $i \in S$ be the binary variable associated with the selection of tray $i$ for the location of the feed $\mathcal{F}^1$ i.e.; $z_i^1 = 1$ iff all of the feed $\mathcal{F}^1$ enters on tray $i$. Similarly, for $z_i^2$, $i \in S$.

The modeling equations are as follows:

Phase equilibrium relations:

$$f_{ij}^{\rm L} = f_{ij}^{\rm V} \qquad j \in J, \quad i \in I \tag{2}$$

Phase equilibrium normalizations:

$$\sum_{j\in J} x_{ij} = 1 \qquad i \in I \tag{3}$$

$$\sum_{j\in J} y_{ij} = 1 \qquad i \in I \tag{4}$$

Component material balances: $\forall\, j \in J$:

$$V_{i-1}y_{i-1,j} - (L_i + P_1)x_{ij} = 0 \qquad i \in C$$

$$L_i x_{ij} + V_i y_{ij} - L_{i+1}x_{i+1,j} - V_{i-1}y_{i-1,j} - f_i^1 z_{fj}^1 - f_i^2 z_{fj}^2 = 0 \qquad i \in S$$

$$P_2 x_{ij} + V_i y_{ij} - L_{i+1}x_{i+1,j} = 0 \qquad i \in R \tag{5}$$

Definition of reflux ratio:

$$L_N = rP_1$$

Enthalpy balances:

$$(L_i + P_1)h_i^{\rm L} - V_{i-1}h_{i-1}^{\rm V} = q_{\rm con} \qquad i \in C$$

$$L_i h_i^{\rm L} + V_i h_i^{\rm V} - L_{i+1}h_{i+1}^{\rm L} - V_{i-1}h_{i-1}^{\rm V} - -f_i^1 h_{\rm f}^1 - f_i^2 h_{\rm f}^2 = 0 \qquad i \in S$$

$$P_2 h_i^{\rm L} + V_i h_i^{\rm V} - L_{i+1}h_{i+1}^{\rm L} = q_{\rm reb} \qquad i \in R \tag{6}$$

Constraints on feeds and their locations: For $k = 1, 2$

$$f_i^k \le F^k z_i^k \qquad i \in S$$

$$\sum_{i\in S} f_i^k = F^k$$

$$\sum_{i\in S} z_i^k = 1 \tag{7}$$

Pressure profile:

$$p_N = p_{\rm con}$$

$$p_{N-1} = p_{\rm top}$$

$$p_2 = p_{\rm bot}$$

$$p_1 = p_{\rm reb}$$

$$p_{i-1} - 2p_i + p_{i+1} = 0 \qquad 3 \le i \le N-2 \tag{8}$$

*Remarks*:

1. The system of equations (8) ensure that the pressure profile is linear between top and bottom of the column.
2. In the above, the candidate locations for both the feeds are assumed to be $2 \le i \le N-1$. In some cases, the set of (contiguous) candidate locations may be smaller, e.g., $2 \le i_1 \le i \le i_2 \le N-1$. The required modifications are straightforward.
3. If there are more than two feeds, then the additional terms in (5) and (6) and the additional set of constraints similar to (7) are obvious.
4. Sometimes it may be possible to order the feeds according to the relative proportions of light and heavy components. If, for example, feed $\mathcal{F}^1$ contains a significantly higher proportion of the heavier components than $\mathcal{F}^2$, then one can impose the logical condition that $\mathcal{F}^2$ enters on or above the tray on which $\mathcal{F}^1$ enters by

$$z_i^1 - \sum_{i\le i'\le N-1} z_{i'}^2 \le 0 \qquad i \in S$$

These inequalities ensure that if $z_i^1 = 1$ for some $i \in S$, i.e., $\mathcal{F}^1$ enters on tray $i$, then, that implies $\sum_{i\le i'\le N-1} z_{i'}^2 = 1$, i.e., $\mathcal{F}^2$ enters on some tray on or above tray $i$.

5. It is quite easy to model the situation where one wants to consider the splitting of one or more of the feeds for introduction at more than one location. Suppose, for instance, we want to consider the possibility of splitting the second feed for introduction at $m$ different locations: Then, the last equation in (7) is to be changed to

$$\sum_{i\in S} z_i^2 = m$$

where $m > 1$. In case one does not know *a priori* the value

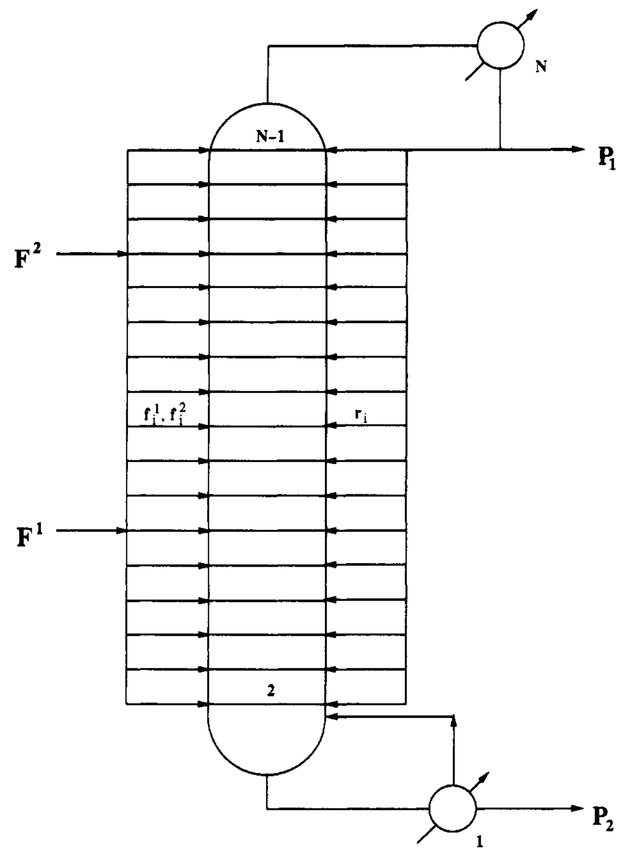


**Figure 2.** Simultaneous determination of number of trays and optimal locations for feeds.

of $m$, but has only an estimate, say $m_{\max}$, then the above equation is to be replaced by the inequalities

$$1 \leq \sum_{i \in S} z_i^2 \leq m_{\max}$$

i.e., the second feed can be split and introduced in at most $m_{\max}$ different locations. The optimization step will automatically determine the (optimal) values for the split fractions.

The MINLP problem is to minimize or maximize an objective function subject to all the above equations and inequalities (1)–(8), bounds on the variables, and specifications such as top/bottom product rates, purity, and recovery.

## MINLP Model for Finding the Number of Trays

The notation is as in the previous section. It is assumed that a reasonable estimate of the upper bound on the number of trays $N$ is available—for example, from Gilliland's correlation.

In the previous section, the location of the entering tray for reflux, i.e., $N-1$, is fixed. But now the problem is to find the optimal location for the reflux as well (Figure 2). However, the entering location of the boilup is fixed. It is worth noting that this idea could have been used even for the single-feed case considered in Viswanathan and Grossmann (1993).

Let $r_i$, $i \in S$, denote the amount of reflux entering tray $i$ and $z_i^r$, $i \in S$, be the binary variable associated with location for the reflux; i.e., $z_i^r = 1$ iff all the reflux enters on tray $i$. Let $(x_1^r, x_2^r, ..., x_c^r)$ denote the vector of mole fractions of the reflux and $h^r$ denote its molar specific enthalpy. Let $f_{\max}$ denote any reasonable estimate on the upper bound of liquid and vapor flow rates within the system. Then, the modeling equations are as follows:

Phase equilibrium relations:

$$f_{ij}^{L} = f_{ij}^{V} \qquad j \in J, \quad i \in I \tag{9}$$

Phase equilibrium normalizations:

$$\sum_{j \in J} x_{ij} = 1 \qquad i \in I \tag{10}$$

$$\sum_{j \in J} y_{ij} = 1 \qquad i \in I \tag{11}$$

Component material balances: $\forall\ j \in J$,

$$x_j^r = x_{ij} \qquad i \in C$$

$$V_{i-1} y_{i-1,j} - (r+1) P_1 x_{ij} = 0 \qquad i \in C$$

$$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} - f_i^1 z_{fj}^1 - f_i^2 z_{fj}^2 - r_i x_j^r = 0 \qquad i \in S$$

$$P_2 x_{ij} + V_i y_{ij} - L_{i+1} x_{I+1,j} = 0 \qquad i \in R \tag{12}$$

Simplification:

$$L_N = 0$$

Enthalpy balances:

$$h^r = h_i^L \qquad i \in C$$

$$(r+1) P_1 h_i^L - V_{i-1} h_{i-1}^V = q_{\text{con}} \qquad i \in C$$

$$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h_{i-1}^V - -f_i^1 h_f^1 - f_i^2 h_f^2 - r_i h^r = 0 \qquad i \in S$$

$$P_2 h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L = q_{\text{reb}} \qquad i \in R \tag{13}$$

Constraints on feeds and their locations: for $k = 1, 2$,

$$f_i^k \leq F^k z_i^k \qquad i \in S$$

$$\sum_{i \in S} f_i^k = F^k$$

$$\sum_{i \in S} z_i^k = 1 \tag{14}$$

Constraints on the amounts of reflux and their locations:

$$r_i \leq f_{\max} z_i^r \qquad i \in S$$

$$\sum_{i \in S} r_i = r P_1$$

$$\sum_{i \in S} z_i^r = 1 \tag{15}$$

Logical relations between the locations of the feeds and the reflux:

$$z_i^1 - \sum_{i < i' < N-1} z_{i'}^r \leq 0 \qquad i \in S$$

$$z_i^2 - \sum_{j < i' \leq N-1} z_{i'}^r \leq 0 \qquad i \in S \tag{16}$$

Pressure profile:

$$p_N = p_{\text{con}}$$

$$p_{N-1} = p_{\text{top}}$$

$$p_2 = p_{\text{bot}}$$

$$p_1 = p_{\text{reb}}$$

$$p_{i-1} - p_i \geq 0 \qquad 3 \leq i \leq N-1$$

$$p_{i-1} - 2p_i + p_{i+1} \leq 2(p_{\text{bot}} - p_{\text{top}})(1 - \sum_{i \leq i' \leq N-1} z_{i'}^{r}) \qquad 3 \leq i \leq N-2$$

$$p_{i-1} - 2p_i + p_{i+1} \geq 2(p_{\text{top}} - p_{\text{bot}})(1 - \sum_{i \leq i' \leq N-1} z_{i'}^{r}) \qquad 3 \leq i \leq N-2$$

$$p_i - p_{\text{top}} \leq (p_{\text{bot}} - p_{\text{top}})(1 - z_i^r) \qquad i \in S \qquad (17)$$

As before, the MINLP problem is to minimize or maximize an objective function subject to (9)–(17). Remarks similar to those at the end of the last section apply. Note also that there is no flow of liquid on the trays above

**Table I. Data for MF1**

| | |
|---|---|
| system | benzene–toluene–*o*-xylene |
| thermodynamic model | |
| vapor phase | ideal |
| liquid phase | ideal |
| source for thermodynamic data | Reid *et al.* (1987) |
| condenser type | total |
| reboiler type | kettle type |
| number of trays ($N$) | 45 |
| feed 1 | $F^1 = 50$, $z_f^1 = (0.15, 0.25, 0.60)$ $p_f^1 = 1.2$ bar, $t_f^1 = 411.459$ K, $v_f^1 = 0.1$ |
| feed 2 | $F^2 = 50$, $z_f^2 = (0.55, 0.25, 0.20)$ $p_f^2 = 1.2$ bar, $t_f^2 = 390.387$ K, $v_f^2 = 0.0$ |
| | $p_{reb} = 1.25$, $p_{bot} = 1.20$, $p_{top} = 1.10$, $p_{con} = 1.05$ bar |
| purity constraint on top product | $x_{45,1} \geq 0.999$ |
| purity constraint on bottom product | $x_{1,2} + x_{1,3} \geq 0.999$ |
| upper bound on reflux ratio | 10 |
| objective function | $2.4217 \times 10^{-5} q_{reb}$ |
| direction of optimization | minimize |

**Table II. Data for MF2**

| | |
|---|---|
| system | *n*-hexane–*n*-heptane–*n*-nonane |
| thermodynamic model | both liquid and vapor phaes are modeled by Soave–Redlich–Kwong equation of state |
| source for thermodynamic data | Reid *et al.* (1987) |
| condenser type | total |
| reboiler type | kettle type |
| number of trays ($N$) | 35 |
| feed 1 | $F^1 = 50$, $z_f^1 = (0.30, 0.10, 0.60)$ $p_f^1 = 1.4682$ bar, $t_f^1$; $= 390.506$ K, $v_f^1 = 0.0$ |
| feed 2 | $F^2 = 50$, $z_f^2 = (0.40, 0.30, 0.30)$ $p_f^2 = 1.5785$ bar, $t_f^2 = 379.441$ K, $v_f^2 = 0.0$ |
| | $p_{reb} = 1.7404$, $p_{bot} = 1.7301$, $p_{top} = 1.388$, $p_{con} = 1.3785$ bar |
| recovery constraint on top product | $P_1 x_{35,2}/(F^1 z_{f2}^1 + F^2 z_{f2}^2) \leq 0.01$ |
| recovery constraint on bottom product | $P_2 x_{1,1}/(F^1 z_{f1}^1 + F^2 z_{f1}^2) \leq 0.01$ |
| upper bound on reflux ratio | |
| objective function | $r$ |
| direction of optimization | minimize |

**Table III. Data for MF3**

| | |
|---|---|
| system | acetone–acetonitrile–water |
| thermodynamic model | |
| vapor phase | virial |
| liquid phase | UNIQUAC |
| source for thermodynamic data | Prausnitz *et al.* (1980) |
| condenser type | partial |
| reboiler type | kettle type |
| number of trays ($N$) | 30 |
| feed 1 | $F^1 = 50$, $z_f^1 = (0.05, 0.85, 0.10)$ $p_f^1 = 1.045$ bar, $t_f^1 = 350.321$ K, $v_f^1 = 0.0$ |
| feed 2 | $F^2 = 50$, $z_f^2 = (0.55, 0.25, 0.20)$ $p_f^2 = 1.045$ bar, $t_f^2 = 347.465$ K, $v_f^2 = 1.0$ |
| | $p_{reb} = 1.1$, $p_{bot} = 1.055$, $p_{top} = 1.035$, $p_{con} = 1.015$ bar |
| upper bound on reflux ratio | 25 |
| objective function | $(v_{lk}^{c} + l_{hk}^{r}) - 3.33 \times 10^{-7}(q_{reb} - q_{con})$ |
| direction of optimization | maximize |

**Table IV. Data for MF4**

| | |
|---|---|
| system | ethanol–water |
| thermodynamic model | |
| vapor phase | virial |
| liquid phase | UNIQUAC |
| source for thermodynamic data | Prausnitz *et al.* (1980) |
| condenser type | total |
| reboiler type | kettle type |
| number of trays ($N$) | 30 |
| feed 1 | $F^1 = 80$, $z_f^1 = (0.05, 0.95)$ $p_f^1 = 1.055$ bar, $t_f^1 = 364.588$ K, $v_f^1 = 0.0$ |
| feed 2 | $F^2 = 20$, $z_f^2 = (0.60, 0.40)$ $p_f^2 = 1.055$ bar, $t_f^2 = 353.529$ K, $v_f^2 = 0.5$ |
| | $p_{reb} = 1.1$, $p_{bot} = 1.055$, $p_{top} = 1.035$, $p_{con} = 1.015$ bar |
| azeotropy condition | $x_{i1} \leq y_{i1}$, $\forall\, i \in I$ |
| "purity" condition | $x_{N1} \geq y_{N1} - 0.005$ |
| recovery condition | $v_{lk}^{c} \geq 0.96(F^1 z_{f1}^1 + F^2 z_{f1}^2)$ |
| upper bound on reflux ratio | 25 |
| objective function | $r$ |
| direction of optimization | minimize |

**Table V. Data for MF5**

| | |
|---|---|
| system | methanol–water |
| thermodynamic model | |
| vapor phase | virial |
| liquid phase | UNIQUAC |
| source for thermodynamic data | Prausnitz *et al.* (1980) |
| condenser type | total |
| reboiler type | kettle type |
| number of trays ($N$) | 60 |
| feed 1 | $F^1 = 43.5$, $z_f^1 = (0.15, 0.85)$ $p_f^1 = 1.42$ bar, $t_f^1 = 365.0$ K, $v_f^1 = 0.0$ |
| feed 2 | $F^2 = 29.5$, $z_f^2 = (0.50, 0.50)$ $p_f^2 = 4.8$ bar, $t_f^2 = 392.697$ K, $v_f^2 = 0.0$ |
| feed 3 | $F^3 = 27.0$, $z_f^3 = (0.89, 0.11)$ $p_f^3 = 1.38$ bar, $t_f^3 = 347.797$ K, $v_f^3 = 0.0$ |
| | $p_{reb} = 1.4475$, $p_{bot} = 1.44064$, $p_{top} = 1.0408$, $p_{con} = 1.0340$ bar |
| purity constraint on top product | $x_{45,1} \geq 0.9999$ |
| purity constraint on bottom product | $x_{1,2} \geq 0.9999$ |
| upper bound on reflux ratio | 25 |
| objective function | $r$ |
| direction of optimization | minimize |

**Table VI. Problem Sizes and Solution Times**[a]

| problem | no. of variables: continuous | binary | total | no. of rows: nonlinear | total | no. of nonzeros: nonlinear | total | solution time |
|---|---|---|---|---|---|---|---|---|
| MF1 | 588 | 86 | 674 | 408 | 592 | 2056 | 3515 | 0.72 |
| MF2 | 1298 | 66 | 1364 | 670 | 1407 | 5205 | 8367 | 2.59 |
| MF3 | 1053 | 56 | 1109 | 813 | 1055 | 4130 | 5940 | 0.72 |
| MF4 | 787 | 56 | 843 | 543 | 792 | 2511 | 3885 | 0.27 |
| MF5 | 1621 | 174 | 1795 | 1083 | 1627 | 5031 | 8592 | 2.17 |

[a] Times reported are CPU minutes on an HP 9000/730 running HP-UX A.08.07. The NLP solver is CONOPT version 2.040–017.

**Table VII. Solution of the Relaxed NLP**

(a) Feed Locations

| problem | objective function | nonzero binary variables | nonzero feeds |
|---|---|---|---|
| MF1 | 52.149 | $z_{15}^1 = 1$, $z_{44}^1 = 7.5\text{E}{-5}$,[a] $z_{25}^2 = 1$ | $f_{15}^1 = 49.996$, $f_{44}^1 = 0.004$, $f_{25}^2 = 50.000$ |
| MF2 | 1.594 | $z_{20}^1 = 1$, $z_{34}^1 = 3.1\text{E}{-4}$, $z_{15}^2 = 1$ | $f_{20}^1 = 49.985$, $f_{34}^1 = 0.015$, $f_{15}^1 = 50.000$ |
| MF3 | 78.533 | $z_{11}^1 = 1$, $z_{20}^2 = 1$ | $f_{12}^1 = 50.0$, $f_{20}^2 = 50.0$ |
| MF4 | 3.494 | $z_1^1 = 1$, $z_4^2 = 1$ | $f_1^1 = 80.0$, $f_4^2 = 20.0$ |
| MF5 | 1.194 | $z_6^1 = 1$, $z_7^2 = 1$, $z_{13}^3 = 1$ | $f_6^1 = 43.5$, $f_7^2 = 29.5$, $f_{13}^3 = 27.0$ |

(b) Reflux Ratio and Products

| problem | reflux ratio | top product, $P_1$: flow rate | composition | bottom product, $P_2$: flow rate | composition |
|---|---|---|---|---|---|
| MF1 | 1.204 | 34.97 | (0.999, 9.92E–4, 7.9E–6) | 65.03 | (0.001, 0.384, 0.615) |
| MF2 | 1.594 | 34.85 | (0.994, 0.006, 1.36E–5) | 65.15 | (0.005, 0.304, 0.691) |
| MF3 | 14.291 | 11.86 | (0.970, 0.004, 0.026) | 88.14 | (0.011, 0.794, 0.195) |
| MF4 | 3.494 | 17.59 | (0.873, 0.127) | 82.41 | (0.008, 0.992) |
| MF5 | 1.194 | 45.30 | (0.9999, 0.0001) | 54.7 | (0.0001, 0.9999) |

[a] 7.5E–5 represents $7.5 \times 10^{-5}$, etc.

**Table VIII. Data for MT1**

| | |
|---|---|
| system | benzene–toluene–*o*-xylene |
| thermodynamic model | |
| vapor phase | ideal |
| liquid phase | ideal |
| source for thermodynamic data | Reid *et al.* (1987) |
| condenser type | total |
| reboiler type | kettle type |
| estimated maximum number of trays ($N$) | 40 |
| feed 1 | $F^1 = 50$, $z_5^1 = (0.15, 0.25, 0.60)$ $p_f^1 = 1.2$ bar, $t_f^1 = 411.459$ K, $\upsilon_f^1 = 0.1$ |
| feed 2 | $F^2 = 50$, $z_f^2 = (0.55, 0.25, 0.20)$ $p_f^2 = 1.2$ bar, $t_f^2 = 390.387$ K, $\upsilon_f^2 = 0.0$ |
| | $p_{reb} = 1.25$, $p_{bot} = 1.20$, $p_{top} = 1.10$, $p_{con} = 1.05$ bar |
| purity constraint on top product | $x_{45,1} \geq 0.999$ |
| purity constraint on bottom product | $x_{1,2} + x_{1,3} \geq 0.999$ |
| upper bound on reflux ratio | 2 |
| objective function | $r + \sum_{i \in S} ord(i) z_i^r - 1$ |
| direction of optimization | minimize |

the tray on which the reflux enters—these are "dry" trays on which there is no heat or mass transfer.

## Results on Optimal Locations

The data for five problems are presented in Tables I–V. The subset of candidate locations is all the trays in the column (i.e., $\{2, 3, ..., N - 1\}$). The objective function in problem MF1 is the reboiler duty times a cost coefficient, while in problems MF2, MF4, and MF5, it is the reflux ratio—i.e., in these problems the objective is to minimize a measure of the operating cost. The objective function for problem MF3 is due to Kumar and Lucia (1988). It represents a trade-off between reboiler and condenser duties (operating costs) and recoveries of the light and heavy keys in the top vapor and bottom liquid products (a measure of benefit or revenues), respectively.

**Table IX. Data for MT2**

| | |
|---|---|
| system | *n*-hexane–*n*-heptane–*n*-nonane |
| thermodynamic model | both liquid and vapor phases are modeled by Soave–Redlich–Kwong equation of state |
| source for thermodynamic data | Reid *et al.* (1987) |
| condenser type | total |
| reboiler type | kettle type |
| estimated maximum number of trays ($N$) | 35 |
| feed 1 | $F^1 = 50$, $z_f^1 = (0.30, 0.10, 0.60)$ $p_f^1 = 1.4682$ bar, $t_f^1 = 390.506$ K, $\upsilon_f^1 = 0.0$ |
| feed 2 | $F^2 = 50$, $z_f^2 = (0.40, 0.30, 0.30)$ $P_f^2 = 1.5785$ bar, $t_f^2 = 379.441$ K, $\upsilon_f^2 = 0.0$ |
| | $p_{reb} = 1.7404$, $p_{bot} = 1.7301$, $p_{top} = 1.388$, $p_{con} = 1.3785$ bar |
| recovery constraint on top product | $P_1 x_{35,2}/(F^1 z_{f2}^1 + F^2 z_{f2}^2) \leq 0.01$ |
| recovery constraint on bottom product | $P_2 x_{1,1}/(F^1 z_{f1}^1 + F^2 z_{f1}^2) \leq 0.01$ |
| upper bound on reflux ratio | 5 |
| objective function | $3.64 \times 10^{-6} q_{reb} + \sum_{i \in S} ord(i) z_i^r - 1$ |
| direction of optimizatino | minimize |

The models were solved using a recent version of DICOPT++ (Viswanathan and Grossmann, 1990) integrated in GAMS (version 2.25). Recall that the OA/ER/AP algorithm for MINLP begins with the solution of the NLP by treating the binary variables as continuous variables with lower bound zero and upper bound one ("relaxed NLP"). The data on problem sizes and CPU times for solutions are shown in Table VI. The solutions of the relaxed NLPs are presented in Table VIIa. It is seen that within the accuracy of numerical computations the solution is found at the relaxed NLP phase itself. This is remarkable, and it is possible that there is some thermodynamic significance for this result. Product distributions and reflux ratio from the solution of the relaxed NLP are shown in Table VIIb.

**Table X. Data for MT3**

| | |
|---|---|
| system | acetone–acetonitrile–water |
| thermodynamic model | |
| vapor phase | virial |
| liquid phase | UNIQUAC |
| source for thermodynamic data | Prausnitz *et al.* (1980) |
| condenser type | partial |
| reboiler type | kettle type |
| estimated maximum number of trays ($N$) | 35 |
| subset of candidate locations for reflux | {11, 12, ..., 34} |
| feed 1 | $F^1 = 50$, $z_f^1 = (0.05, 0.85, 0.10)$ $p_f^1 = 1.045$ bar, $t_f^1 = 350.321$ K, $v_f^1 = 0.0$ |
| feed 2 | $F^2 = 50$, $z_f^2 = (0.55, 0.25, 0.20)$ $p_f^2 = 1.045$ bar, $t_f^2 = 347.465$ K, $v_f^2 = 1.0$ |
| | $p_{reb} = 1.1$, $p_{bot} = 1.055$, $p_{top} = 1.035$, $p_{con} = 1.015$ bar |
| upper bound on reflux ratio | 30 |
| objective function | $v_{lk}^c + l_{hk}^r - 3.33 \times 10^{-7}(q_{reb} - q_{con}) - 0.08(\sum_{i\in S}\text{ord}(i)z_i^r - 1)$ |
| direction of optimization | maximize |

**Table XI. Data for MT4**

| | |
|---|---|
| system | ethanol–water |
| thermodynamic model | |
| vapor phase | virial |
| liquid phase | UNIQUAC |
| source for thermodynamic data | Prausnitz *et al.* (1980) |
| condenser type | total |
| reboiler type | kettle type |
| estimated maximum number of trays ($N$) | 30 |
| feed 1 | $F^1 = 80$, $z_f^1 = (0.05, 0.95)$ $p_f^1 = 1.055$ bar, $t_f^1 = 364.588$ K, $v_f^1 = 0.0$ |
| feed 2 | $F^2 = 20$, $z_f^2 = (0.60, 0.40)$ $p_f^2 = 1.055$ bar, $t_f^2 = 353.529$ K, $v_f^2 = 0.5$ |
| | $p_{reb} = 1.1$, $p_{bot} = 1.055$, $p_{top} = 1.035$, $p_{con} = 1.015$ bar |
| azeotropy condition | $x_{i1} \le y_{i1}$, $\forall\, i \in I$ |
| "purity" condition | $x_{N1} \ge y_{N1} - 0.005$ |
| recovery condition | $v_{lk}^c \ge 0.96(Fz_{f1})$ |
| upper bound on reflux ratio | 10 |
| objective function | $r + \sum_{i\in S}\text{ord}(i)z_i^r - 1$ |
| direction of optimization | minimize |

Problem MF2 is the same as example 1 in Nikolaides and Malone (1987). The optimal feed locations found here (tray numbers 20 and 15) are different from those (tray numbers 26 and 16) used by them. The optimal value of the reflux ratio obtained (1.594) is smaller than the value (1.728) reported in that paper. The Aspen Plus simulation program with the optimal locations found here predicts a value of 1.606 for the reflux ratio for the given recovery specifications.

The cubic equation of the Soave–Redlich–Kwong equation of state generally has one real root, but sometimes can have three real roots. For the phase (liquid or vapor) chosen, the correct root is selected by imposing the empirical criteria for isothermal compressibility factors (Poling *et al.*, 1981). (The compressibility factor, $z = Pv/RT$, should not be confounded with the isothermal compressibility factor, $\beta = (1/v)(\partial v/\partial P)_T$.) These are the three inequalities mentioned in the last-but-one paragraph of the Introduction.

It may be also pointed out that there is a slight difference in the thermodynamic model for problem MF2 and MT2 (below) in that in MF2 there are $(5c + 13)$ equations and 3 inequalities and $(4c + 13)$ additional variables to decrease the phase equilibrium relations on a tray, while for MT2

**Table XII. Data for MT5**

| | |
|---|---|
| system | methanol–water |
| thermodynamic model | |
| vapor phase | virial |
| liquid phase | UNIQUAC |
| source for thermodynamic data | Prausnitz *et al.* (1980) |
| condenser type | total |
| reboiler type | kettle type |
| estimated maximum number of trays ($N$) | 60 |
| subset of candidate locations for feed trays | {2, 3, ..., 20} |
| feed 1 | $F^1 = 43.5$, $z_f^1 = (0.15, 0.85)$ $p_f^1 = 1.42$ bar, $t_f^1 = 365.0$ K, $v_f^1 = 0.0$ |
| feed 2 | $F^2 = 29.5$, $z_f^2 = (0.50, 0.50)$ $p_f^2 = 4.8$ bar, $t_f^2 = 392.697$ K, $v_f^2 = 0.0$ |
| feed 3 | $F^3 = 27.0$, $z_f^3 = (0.89, 0.11)$ $p_f^3 = 1.38$ bar, $t_f^3 = 347.797$ K, $v_f^3 = 0.0$ |
| | $p_{reb} = 1.4475$, $p_{bot} = 1.44064$, $p_{top} = 1.0408$, $p_{con} = 1.0340$ bar |
| purity constraint on top product | $x_{60,1} \ge 0.999$ |
| purity constraint on bottom product | $x_{1,2} \ge 0.999$ |
| upper bound on reflux ratio | 20 |
| objective function | $6.3887 \times 10^{-6}q_{reb} + \sum_{i\in S}\text{ord}(i)z_i^r - 1$ |
| direction of optimization | minimize |

there are $(6c + 13)$ equations and 3 inequalities and $(5c + 13)$ variables—the additional $c$ equations and $c$ variables being the definitions of the $K$ values:

$$K_{ij} = \phi_{ij}^{L}(T_i, p_i, x_{i1}, x_{i2}, ..., x_{ic})/\phi_{ij}^{V}(T_i, p_i, y_{i1}, y_{i2}, ..., y_{ic}) \tag{18}$$

where $\phi_{ij}^V$ and $\phi_{ij}^L$ denote, respectively, the fugacity coefficient of the $j$th component in vapor and liquid leaving tray $i$. In other words, phase equilibrium was expressed in MF2 without introducing explicitly the definitions of $K$ values (see below).

## Results on Number of Trays and Optimal Locations

The data and problem sizes for five problems are presented in Tables VIII–XII. In the objective function of these problems, the symbol ord($i$) denotes the ordinal number of the indexed tray. Recall that $\sum_{i\in S}z_i^r = 1$, i.e., reflux enters exactly on one tray, and so $\sum_{i\in S}\text{ord}(i)z_i^r - 1$ is just the number of trays within the column. Thus, in these problems the objective function is a representative sum of the capital cost (number of trays) and the operating cost (reflux ratio or reboiler duty). In problem MT3, the trade-off is between recovery of key components and the sum of capital and operating costs.

The data on problem sizes are shown in Table XIII. The computational resource usages are given in Table XIV. Note the smaller subset of candidate locations for the feeds (problem MT5) and the reflux (problem MT3). In all other cases, the candidate locations were all the trays in the column. The values of the binary variables at the end of major iterations determined by the algorithm are shown in Table XVa. Paths to the solutions are shown in Table XVb. Optimal design values are shown in Table XVIa, and the distribution of products as shown in Table XVIb.

It is interesting to compare the results for problem MT2 with those for problem MF2. Although the reflux ratio

**Table XIII. Problem Sizes**

| problem | no. of variables: continuous | binary | total | no. of rows: linear | nonlinear | total | no. of nonzeros: linear | nonlinear | total |
|---|---|---|---|---|---|---|---|---|---|
| MT1 | 638 | 114 | 752 | 472 | 359 | 831 | 3761 | 2355 | 6116 |
| MT2 | 1543 | 99 | 1642 | 901 | 915 | 1816 | 5711 | 6204 | 11915 |
| MT3 | 1324 | 99 | 1423 | 515 | 948 | 1463 | 3707 | 5187 | 8894 |
| MT4 | 874 | 84 | 958 | 475 | 543 | 1018 | 3028 | 2799 | 5827 |
| MT5 | 1683 | 115 | 1798 | 836 | 1083 | 1919 | 6252 | 5619 | 11871 |

**Table XIV. Solver Times**[a]

| problem | major iterations | solver times: NLP, min | MIP, min | Total, min | NLP, % | MIP, % |
|---|---|---|---|---|---|---|
| MT1 | 3 | 1.42 | 5.47 | 6.89 | 20.6 | 79.4 |
| MT2 | 10 | 43.93 | 11.96 | 55.89 | 78.6 | 21.4 |
| MT3 | 4 | 20.97 | 17.24 | 38.21 | 54.9 | 45.1 |
| MT4 | 3 | 2.56 | 1.36 | 3.92 | 65.1 | 34.9 |
| MT5 | 7 | 52.77 | 16.65 | 69.42 | 76.0 | 24.0 |

[a] $N$ major iterations mean $N$ NLP problems (including relaxed NLP) and $(N-1)$ MIP problems. Times reported are CPU minutes on an HP 9000/730 running HP-UX A.08.07. The NLP solver is CONOPT version 2.040–017. MIPs were solved with OSL release 2.002; SOS1 conditions are not implemented in this release of GAMS/DICOPT++/OSL interface (even though they are implemented in GAMS/OSL interface for mixed integer linear programs).

**Table XV. Paths to Solutions**

(a) Nonzero Binary Variables

| problem | iteration | nonzero binary variables |
|---|---|---|
| MT1 | 1 | $z_3^r = 0.47$, $z_{31}^r = 0.226$, $z_{32}^r = 0.304$, $z_{12}^1 = 0.530$, $z_{13}^1 = 0.470$, $z_{18}^2 = 0.470$, $z_{19}^2 = 0.530$ |
| | 2 | $z_{29}^r = 1$, $z_{12}^1 = 1$, $z_{19}^2 = 1$ |
| | 3 | $z_{30}^r = 1$, $z_{12}^1 = 1$, $z_{19}^2 = 1$ |
| MT2 | 1 | $z_3^r = 0.702$, $z_{27}^r = 0.193$, $z_{28}^r = 0.103$, $z_{34}^r = 0.002$, $z_{14}^1 = 0.098$, $z_{15}^1 = 0.298$, $z_{16}^1 = 0.298$, $z_{17}^1 = 0.298$, $z_{30}^1 = 0.002$, $z_{31}^1 = 0.002$, $z_{32}^1 = 0.002$, $z_{33}^1 = 0.002$ |
| | 2 | $z_{26}^r = 1$, $z_{16}^1 = 1$, $z_{13}^2 = 1$ |
| | 3 | $z_{26}^r = 1$, $z_{15}^1 = 1$, $z_{13}^2 = 1$ |
| | 4 | $z_{26}^r = 1$, $z_{16}^1 = 1$, $z_{12}^2 = 1$ |
| | 5 | $z_{26}^r = 1$, $z_{16}^1 = 1$, $z_{14}^2 = 1$ |
| | 6 | $z_{26}^r = 1$, $z_{17}^1 = 1$, $z_{13}^2 = 1$ |
| | 7 | $z_{26}^r = 1$, $z_{15}^1 = 1$, $z_{12}^2 = 1$ |
| | 8 | $z_{26}^r = 1$, $z_{15}^1 = 1$, $z_{14}^2 = 1$ |
| | 9 | $z_{26}^r = 1$, $z_{17}^1 = 1$, $z_{12}^2 = 1$ |
| | 10 | $z_{26}^r = 1$, $z_{17}^1 = 1$, $z_{14}^2 = 1$ |
| MT3 | 1 | $z_{11}^r = 0.375$, $z_{24}^r = 0.141$, $z_{25}^r = 0.300$, $z_{26}^r = 0.183$, $z_8^1 = 1.000$, $z_{16}^2 = 0.375$, $z_{17}^2 = 0.625$ |
| | 2 | $z_{23}^r = 1$, $z_8^1 = 1$, $z_{17}^2 = 1$ |
| | 3 | $z_{24}^r = 1$, $z_8^1 = 1$, $z_{17}^2 = 1$ |
| | 4 | $z_{25}^r = 1$, $z_8^1 = 1$, $z_{17}^2 = 1$ |
| MT4 | 1 | $z_3^r = 0.901$, $z_{29}^r = 0.099$, $z_2^1 = 1.000$, $z_2^2 = 0.605$, $z_3^2 = 0.099$, $z_4^2 = 0.099$, $z_5^2 = 0.099$, $z_6^2 = 0.099$ |
| | 2 | $z_{24}^r = 1$, $z_2^1 = 1$, $z_5^2 = 1$ |
| | 3 | $z_{28}^r = 1$, $z_2^1 = 1$, $z_5^2 = 1$ |
| MT5 | 1 | $z_3^r = 0.553$, $z_{53}^r = 0.249$, $z_{54}^r = 0.199$, $z_4^1 = 1.000$, $z_6^2 = 1.000$, $z_{11}^3 = 0.015$, $z_{12}^3 = 0.447$, $z_{13}^3 = 0.447$ |
| | 2 | $z_{53}^r = 1$, $z_4^1 = 1$, $z_6^2 = 1$, $z_{12}^3 = 1$ |
| | 3 | $z_{53}^r = 1$, $z_4^1 = 1$, $z_5^2 = 1$, $z_{12}^3 = 1$ |
| | 4 | $z_{53}^r = 1$, $z_4^1 = 1$, $z_6^2 = 1$, $z_{13}^3 = 1$ |
| | 5 | $z_{53}^r = 1$, $z_5^1 = 1$, $z_6^2 = 1$, $z_{12}^3 = 1$ |
| | 6 | $z_{53}^r = 1$, $z_4^1 = 1$, $z_5^2 = 1$, $z_{13}^3 = 1$ |
| | 7 | $z_{54}^r = 1$, $z_4^1 = 1$, $z_6^2 = 1$, $z_{12}^3 = 1$ |

(b) Objective Function Values

| major iteration no. | major solution step | value of objective function for problem: MT1 | MT2 | MT3 | MT4 | MT5 |
|---|---|---|---|---|---|---|
| 1 | NLP | 18.647 | 21.0201 | 76.841 | 8.090 | 220.290 |
| 1 | MIP | 30.552 | 35.5064 | 77.369 | 28.436 | 227.924 |
| 2 | NLP | 30.646 | ∞ | 76.448 | 27.085 | ∞ |
| 2 | MIP | 31.752 | 35.5420 | 76.866 | 31.851 | 227.949 |
| 3 | NLP | 31.564 | ∞ | 76.454 | 30.583 | 253.184 |
| 3 | MIP | | 35.5535 | 76.813 | | 227.966 |
| 4 | NLP | | ∞ | 76.436 | | ∞ |
| 4 | MIP | | 35.5666 | | | 227.973 |
| 5 | NLP | | ∞ | | | 253.164 |
| 5 | MIP | | 35.5845 | | | 227.991 |
| 6 | NLP | | ∞ | | | 253.095 |
| 6 | MIP | | 35.5890 | | | 258.577 |
| 7 | NLP | | ∞ | | | 253.756 |
| 7 | MIP | | 35.6026 | | | |
| 8 | NLP | | 37.0389 | | | |
| 8 | MIP | | 35.6316 | | | |
| 9 | NLP | | ∞ | | | |
| 9 | MIP | | 35.6447 | | | |
| 10 | NLP | | 37.1228 | | | |

is higher (1.809 vs 1.594), the number of trays is smaller (27 vs 35), but the order of the feeds has changed. The Aspen Plus program with this configuration (i.e., 27 trays with feeds at the optimal locations) and pressure and recovery specifications predicts a reflux ratio of 1.826. As pointed out by Sargent and Gaminibandara (1976), the solutions of mathematical optimization problems in distillation columns often do not conform to one's intuitive understanding of the problems. Nikolaides and Malone (1987) also report several counterintuitive results.

As noted in the last paragraph of the previous section, there is a slight difference in the thermodynamic models of MF2 and MT2. Recall that in MF2 the solution was found in the relaxed NLP step itself, while in MT2, the MIP master problem has to be solved nine times—the introduction of $c$ additional equations and variables in (18) seems to have helped in finding the solutions of both the nonlinear programs and mixed integer programs.

The results of problem MT4 show that the first feed enters on tray number 2. This suggests that the reboiler could also have been considered as a candidate for the feed location. Extension to such special cases can be easily handled in this framework.

Finally, in view of the results for the first case, i.e., where the number of trays is known, one may be tempted to treat the binary variables $z_i^1$ and $z_i^2$ in the second case as just continuous variables with lower bound zero and upper bound one. This will, of course, considerably reduce the number of binary variables, but in general, this will lead to a different optimum, because the master problems set up in the OA/ER/AP algorithm are different.

## Conclusions

This short note has presented the MINLP approach for finding the optimal locations and the number of trays for a distillation column with multiple feeds. As shown with the results, even difficult problems with nonideal thermodynamics can be solved in this framework. Although the solutions cannot be guaranteed to be globally optimal, the OA/ER/AP algorithm has been shown to be a robust tool for solving these problems.

**Table XVI. Optimal Design and Solutions**

(a) Optimal Design

| problem | reflux ratio | entering tray no. for feed 1 | feed 2 | feed 3 | reflux |
|---|---|---|---|---|---|
| MT1 | 1.646 | 12 | 19 | | 30 |
| MT2 | 1.809 | 15 | 14 | | 26 |
| MT3 | 14.299 | 8 | 17 | | 24 |
| MT4 | 4.085 | 2 | 5 | | 24 |
| MT5 | 1.041 | 4 | 5 | 13 | 53 |

(b) Optimal Solutions—Products

| | top product, $P_1$ | | bottom product, $P_2$ | |
|---|---|---|---|---|
| problem | flow rate | composition | flow rate | composition |
| MT1 | 34.97 | (0.999, 0.001, 0.0) | 65.03 | (0.001, 0.384, 0.615) |
| MT2 | 34.85 | (0.994, 0.006, 0.0) | 65.15 | (0.005, 0.304, 0.691) |
| MT3 | 11.78 | (0.959, 0.009, 0.032) | 88.22 | (0.014, 0.792, 0.194) |
| MT4 | 17.59 | (0.873, 0.127) | 82.41 | (0.008, 0.992) |
| MT5 | 45.30 | (0.999, 0.001) | 54.70 | (0.001, 0.999) |

The output files of the examples presented above are being made available for sharing by anonymous ftp (file transfer protocol). The first author (J.V.) may be contacted for details.

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