

SHORT NOTE

AN ALTERNATE MINLP MODEL FOR FINDING THE NUMBER OF TRAYS REQUIRED FOR A SPECIFIED SEPARATION OBJECTIVE

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Abstract—This is a brief note on an alternate MINLP model for finding the number of trays required for a separation objective described by Viswanathan and Grossmann [*Computers chem. Engng* 14, 769-782 (1990)]. The idea is to fix the location of the feed tray and to model the problem of finding the trays on which the reflux and the boilup enter as optimum location problems for them. The resulting model is not only conceptually simple and elegant, but also results in shorter solution times. Nonideal distillation problems have also been solved by this approach.

INTRODUCTION

Traditionally, the problem of finding the number of trays for a system with product rates specified has been done by short-cut methods based on the pioneering works of Underwood, Fenske, Gilliland, Winn and others (see, e.g. Henley and Seader, 1981). These methods make simplifying assumptions such as constant molal overflow, constant relative volatility, etc. which seldom hold when the system is nonideal. These estimates are subsequently verified by rigorous tray-by-tray methods. Furthermore, it is not straightforward to extend these methods for problems with complex specifications such as those encountered in applications. As a result, a large number of simulations and optimizations must be done to arrive at a suitable design for the problem in hand.

In this paper, an MINLP model is presented that will automatically determine the number of theoretical trays required for a specified objective of separation. It is a simplification of the model proposed in Viswanathan and Grossmann (1990). In that model, a binary variable is associated with each tray to indicate its existence. Here, the problem is viewed as that of determining the optimal locations for the reflux and boilup. Thus, in some ways it is similar to the problem of optimum feed location. However, the important difference is that unlike that problem, generally nothing is known explicitly about the flowrate, composition and temperature of either the reflux or the boilup. The model is computationally more efficient: even difficult, nonideal distillation problems can be solved, as will be seen later.

MINLP MODEL

Consider a distillation column (Fig. 1) with N trays, including the condenser and the reboiler. The stages are numbered bottom upwards (like the floors of a building) so that the reboiler is the first tray and the condenser is the last (N th) tray. (For definiteness, only the total condenser and kettle-type reboiler case is considered—the other cases can be dealt with similarly.)

Let $I = \{1, 2, \dots, N\}$ denote the set of trays and let $R = \{1\}$, $C = \{N\}$ and $COL = \{2, 3, \dots, N-1\}$ denote subsets corresponding to the trays in the reboiler, the condenser and those within the column, respectively. The value of N is decided from reasonable estimates (such as those given by Gilliland correlation) of the upper bounds on the number of trays in the rectifying and stripping sections.

Let i_{feed} denote the location of the feed. Then, the set of candidate locations for the reflux are $\{i_{\text{feed}} + 1, i_{\text{feed}} + 2, \dots, (N-1)\}$. However, in some cases, it may be known that a certain minimum number of trays are required in the rectifying section. So, more generally, let i_{min} denote the lowermost location for the entering tray for reflux (see Fig. 1). Then:

$$(i_{\text{feed}} + 1) \leq i_{\text{min}}$$

and the subset of contiguous candidate locations for the reflux is:

$$REF = \{i_{\text{min}}, i_{\text{min}} + 1, \dots, N-1\}$$

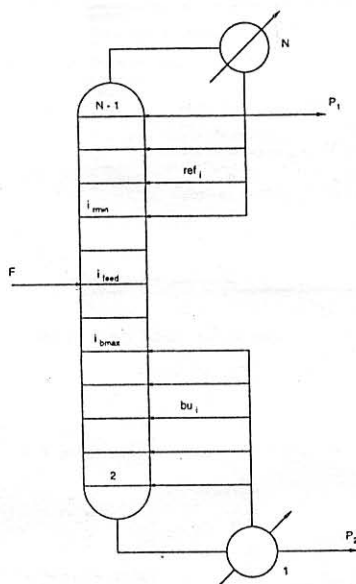


Fig. 1. Determination of minimum number of trays for specified separation objective.

Similarly, let i_{bmax} denote the uppermost location for the entering tray for boilup. Then:

$$i_{bmax} \leq (i_{feed} - 1)$$

and the subset of contiguous candidate locations for boilup is:

$$BU = \{2, 3, \dots, i_{bmax} - 1, i_{bmax}\}.$$

For later use, let

$$FLOC = \{i_{feed}\}$$

$$AF = \{i \mid i_{feed} < i \leq (N - 1)\},$$

$$BF = \{i \mid 2 \leq i < i_{feed}\}.$$

Then

$$REF \subseteq AF, BU \subseteq BF$$

and

$$COL = BF \cup FLOC \cup AF.$$

Let c denote the number of components in the feed and let $J = \{1, 2, \dots, c\}$ denote the corresponding index set. Let F , T_i , p_i , z_i and h_i denote, respectively, the molar flowrate, temperature, pressure, the vector of mole-fractions (with components, $z_{i1}, z_{i2}, \dots, z_{ic}$) and the molar specific enthalpy of the feed.

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

Let L_i , x_i , h_i^L and f_i^L denote the molar flowrate, 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^V and f_i^V denote the corresponding quantities for the vapor. Let T_i denote the temperature prevailing on tray i . Then:

$$f_i^L = f_j^L(T_i, p_i, x_{i1}, x_{i2}, \dots, x_{ic})$$

$$f_i^V = f_j^V(T_i, p_i, y_{i1}, y_{i2}, \dots, y_{ic})$$

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

$$h_i^V = h_j^V(T_i, p_i, y_{i1}, y_{i2}, \dots, y_{ic}) \quad (1)$$

where the functions 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 f_{max} denote any reasonable estimate on the upper bound of liquid and vapor flowrates within the system.

Let v_{ik}^L and h_{ik}^L 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_{reb} and q_{con} denote the reboiler and condenser duties, respectively. Finally, let ref_i , $i \in REF$ denote the amount of reflux entering on tray i and let z_i^{ref} be the binary variable associated with the selection of tray i for the location of the reflux, i.e. $z_i^{ref} = 1$ iff all the reflux enters on tray i . Similarly, for bu_i and z_i^{bu} .

The modeling equations are as follows:

- Phase equilibrium relations:

$$f_i^L = f_j^V \quad j \in J, i \in I. \quad (2)$$

- Phase equilibrium error:

$$\sum_{j \in J} x_{ij} - \sum_{j \in J} y_{ij} = 0, \quad i \in I. \quad (3)$$

- Total material balances:

$$V_{i-1} - \left(\sum_{i \in REF} ref_i + L_i + P_1 \right) = 0, \quad i \in C,$$

$$L_i + V_i - L_{i+1} - V_{i-1} - ref_i = 0, \quad i \in REF,$$

$$L_i + V_i - L_{i+1} - V_{i-1} = 0, \quad i \in AF \setminus REF,$$

$$L_i + V_i - L_{i+1} - V_{i-1} - F = 0, \quad i \in FLOC,$$

$$L_i + V_i - L_{i+1} - V_{i-1} = 0, \quad i \in BF \setminus BU$$

Table 1. Data for Ternary1

| | |
|---|--|
| System | Benzene-toluene- <i>o</i> -xylene |
| Thermodynamic model | vapor phase: ideal liquid phase: ideal |
| Source for thermodynamic data | Reid <i>et al.</i> (1987) |
| Condenser type | Total |
| Reboiler type | Kettle type |
| Estimated maximum number of trays (N) | 30 |
| Feed location (i_{feed}) | 17 |
| Lowermost location for reflux (i_{min}) | 20 |
| Uppermost location for boilup (i_{max}) | 14 |
| $F = 100$, $z_i = (0.15, 0.25, 0.60)$ | |
| $p_t = 1.2$ bar, $t_f = 391.172$ K | |
| $p_{\text{reb}} = 1.25$, $p_{\text{bot}} = 1.20$, $p_{\text{top}} = 1.10$, $p_{\text{con}} = 1.05$ bar | |
| Top product rate, P_1 | 40 |
| Purity constraint on bottom product | $x_{1,j} \geq 0.995$ |
| Upper bound on reflux ratio | $r \leq 15$ |
| Objective function | $5r + \sum_{i \in \text{REF}} \text{ord}(i); z_i^{\text{ref}} - \sum_{i \in \text{BU}} \text{ord}(i); z_i^{\text{bu}} + 1$ |
| Direction of optimization | Minimize |

$$L_i + V_i - L_{i+1} - V_{i-1} - bu_i = 0, \quad i \in BU,$$

$$L_i + V_i + \sum_{i \in BU} bu_i - L_{i+1} = 0, \quad i \in R,$$

$$L_i = P_2,$$

$$V_i = 0,$$

$$\sum_{i \in \text{REF}} \text{ref}_i = rP_1,$$

$$L_N = 0. \quad (4)$$

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

$$V_{i-1}y_{i-1,j} - \left(\sum_{i \in \text{REF}} \text{ref}_i + L_i + P_1 \right) x_{ij} = 0, \quad i \in C,$$

$$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} - \text{ref}_i x_{ij} = 0, \quad i \in \text{REF},$$

$$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} = 0, \quad i \in \text{AF} \setminus \text{REF},$$

$$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} - Fz_{ij} = 0, \quad i \in \text{FLOC},$$

$$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} = 0,$$

$$i \in \text{BF} \setminus \text{BU},$$

$$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j}$$

$$- bu_i x_{ij} = 0, \quad i \in \text{BU},$$

$$L_i x_{ij} + \left(V_i + \sum_{i \in \text{BU}} bu_i \right) y_{ij} - L_{i+1} x_{i+1,j} = 0, \quad i \in R. \quad (5)$$

- Enthalpy balances:

$$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h_{i-1}^V - \text{ref}_i h_N^L = 0, \quad i \in \text{REF},$$

$$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h_{i-1}^V = 0, \quad i \in \text{AF} \setminus \text{REF},$$

$$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h_{i-1}^V = 0, \quad i \in \text{FLOC},$$

$$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h_{i-1}^V = 0, \quad i \in \text{BF} \setminus \text{BU},$$

$$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h_{i-1}^V - bu_i h_i^L = 0, \quad i \in \text{BU}. \quad (6)$$

Table 2. Data for Ternary2

| | |
|---|--|
| System | Benzene-toluene- <i>o</i> -xylene |
| Thermodynamic model | vapor phase: ideal liquid phase: ideal |
| Source for thermodynamic data | Reid <i>et al.</i> (1987) |
| Condenser type | Total |
| Reboiler type | Kettle type |
| Estimated maximum number of trays (N) | 30 |
| Feed location (i_{feed}) | 16 |
| Lowermost location of reflux (i_{min}) | 20 |
| Uppermost location for boilup (i_{max}) | 12 |
| $F = 100$, $z_i = (0.15, 0.25, 0.60)$ | |
| $p_t = 1.2$ bar, $t_f = 391.172$ K | |
| $p_{\text{reb}} = 1.25$, $p_{\text{bot}} = 1.20$, $p_{\text{top}} = 1.10$, $p_{\text{con}} = 1.05$ bar | |
| Top product rate, P_1 | 15 |
| Purity constraint on top product | $x_{30,1} \geq 0.995$ |
| Upper bound on reflux ratio | $r \leq 20$ |
| Objective function | $5r + \sum_{i \in \text{REF}} \text{ord}(i); z_i^{\text{ref}} - \sum_{i \in \text{BU}} \text{ord}(i); z_i^{\text{bu}} + 1$ |
| Direction of optimization | Minimize |

Table 3. Data for unit

| | |
|---|--|
| System | Acetone-acetonitrile-water |
| Thermodynamic model | vapor phase: virial liquid phase: UNIQUAC |
| Source for thermodynamic data | Prausnitz <i>et al.</i> (1980) |
| Condenser type | Partial |
| Reboiler type | Kettle type |
| Estimated maximum number of trays (N) | 25 |
| Feed location (i_{feed}) | 10 |
| Lowermost location of reflux (i_{min}) | 11 |
| Uppermost location for boilup (i_{bmax}) | 9 |
| $F = 100$, $z_i = (0.1, 0.75, 0.15)$ | |
| $p_r = 1.055$ bar, $t_r = 348.675$ K | |
| $p_{reb} = 1.1$, $p_{bot} = 1.055$, $p_{top} = 1.035$, $p_{con} = 1.015$ bar | |
| Upper bound on reflux ratio | $r \leq 50$ |
| Objective function | $(v_{ik}^s + l_{ik}^s) - 3.33 \times 10^{-7}(q_{reb} - q_{con})$ $- 0.1 \left[\sum_{i \in REF} ord(i)z_i^{ref} - \sum_{i \in BU} ord(i)z_i^{bu} + 1 \right]$ |
| Direction of optimization | Maximize |

- Reflux enters exactly on one tray:

$$\begin{aligned} ref_i &\leq f_{max} z_i^{ref}, \\ \sum_{i \in REF} z_i^{ref} &= 1. \end{aligned} \quad (7)$$

- Reboiled vapor enters exactly on one tray:

$$\begin{aligned} bu_i &\leq f_{max} z_i^{bu}, \\ \sum_{i \in BU} z_i^{bu} &= 1. \end{aligned} \quad (8)$$

- Pressure profile:

$$p_N = p_{con},$$

$$p_{N-1} = p_{top},$$

$$p_2 = p_{bot},$$

$$p_1 = p_{reb},$$

$$p_i \leq p_{i-1}, \quad i \in COL,$$

$$p_{i-1} - 2p_i + p_{i+1} \leq 2(p_{bot} - p_{top})z_i^{ref}, \quad i \in REF,$$

$$p_{i-1} - 2p_i + p_{i+1} \geq 2(p_{top} - p_{bot})z_i^{ref}, \quad i \in REF,$$

$$p_i - p_{top} \leq (1 - z_i^{ref})(p_{bot} - p_{top}), \quad i \in REF,$$

$$p_{i-1} - 2p_i + p_{i+1} = 0,$$

$$i \in (AF \setminus REF) \cup FLOC \cup (BF \setminus BU),$$

$$p_{i-1} - 2p_i + p_{i+1} \leq 2(p_{bot} - p_{top})z_i^{bu}, \quad i \in BU,$$

$$p_{i-1} - 2p_i + p_{i+1} \geq 2(p_{top} - p_{bot})z_i^{bu}, \quad i \in BU,$$

$$p_i - p_{bot} \geq (1 - z_i^{bu})(p_{top} - p_{bot}), \quad i \in BU. \quad (9)$$

The above equations and inequalities are quite self-explanatory. If i_{ref} and i_{bu} denote respectively, the tray on which the reflux and the reboiled vapor enters, then in the above, the system corresponding to pressure profile ensures that the profile is flat between 2 and i_{bu} (i.e. $p_i = p_{bot}$ for $2 \leq i \leq i_{bu}$), linear between i_{bu} and i_{ref} , and again flat between i_{ref} and $N - 1$ (i.e. $p_i = p_{top}$ for $i_{ref} \leq i \leq N - 1$).

The MINLP problem is to minimize or maximize an objective function subject to all the above equations and inequalities (1-9), bounds on the variables, and specifications such as top/bottom product rates, purity, recovery, etc.

It is perhaps worth pointing out that using component molar flowrates instead of mole-fractions in

Table 4. Data for ethanol

| | |
|---|---|
| System | Ethanol-water |
| Thermodynamic model | vapor phase: virial liquid phase: UNIQUAC |
| Source for thermodynamic data | Prausnitz <i>et al.</i> (1980) |
| Condenser type | Total |
| Reboiler type | Kettle type |
| Estimated maximum number of trays (N) | 25 |
| Feed location (i_{feed}) | 4 |
| Lowermost location of reflux (i_{min}) | 7 |
| Uppermost location for boilup (i_{bmax}) | 3 |
| $F = 100$, $z_i = (0.05, 0.95)$ | |
| $p_r = 1.055$ bar, $t_r = 364.588$ K | |
| $p_{reb} = 1.1$, $p_{bot} = 1.055$, $p_{top} = 1.035$, $p_{con} = 1.015$ bar | |
| Azeotropy condition | $x_{i1} \leq y_{i1}, \forall i \in I$ |
| "Purity" condition | $x_{N1} \geq y_{N1} - 0.005$ |
| Recovery condition | $v_{ik}^s \geq 0.96 (Fz_{i1})$ |
| Bounds on reflux ratio | $4 \leq r \leq 6$ |
| Objective function | $r + \sum_{i \in REF} ord(i)z_i^{ref} - \sum_{i \in BU} ord(i)z_i^{bu} + 1$ |
| Direction of optimization | Minimize |

Table 5. Problem sizes

| Problem | No. of variables | | | No. of rows | | | No. of nonzeros | | |
|----------|------------------|--------|-------|-------------|-----------|-------|-----------------|-----------|-------|
| | Continuous | Binary | Total | Linear | Nonlinear | Total | Linear | Nonlinear | Total |
| Ternary1 | 398 | 23 | 421 | 269 | 203 | 472 | 672 | 1715 | 2387 |
| Ternary2 | 396 | 21 | 417 | 269 | 197 | 466 | 648 | 1699 | 2347 |
| Unit | 891 | 22 | 913 | 279 | 678 | 957 | 1501 | 3741 | 5242 |
| Ethanol | 662 | 20 | 682 | 298 | 453 | 751 | 1198 | 2311 | 3509 |

the modeling equations would be inappropriate in the present context. To see this, let i_{ref} denote the tray on which reflux enters. Then:

$$L_i = 0 \quad \text{for } i = i_{ref} + 1, i_{ref} + 2, \dots, (N - 1).$$

i.e. there is no flow of liquid on these trays. Nevertheless, the mole-fractions:

$$x_{ij}, \quad j \in J, \quad i = i_{ref} + 1, \quad i_{ref} + 2, \dots, (N - 1),$$

are not zero. In fact,

$$x_{ij} = x_{ref,j}, \quad j \in J, \quad i = i_{ref} + 2, \dots, (N - 1).$$

Were one to use component flows, then ratios of the form $0/0$ have to be dealt with.

RESULTS

The data and problem size for four cases (two ideal, two nonideal) are presented in Tables 1-5. The models were solved using a recent version of *DI-COPT* ++ (Viswanathan and Grossmann, 1990) integrated in GAMS (Version 2.25). The computational resource usages are given in Table 6. The values of the binary variables at the end of major iterations determined by the AP/OA/ER algorithm are shown in Table 7. 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 the lower bound zero and upper bound one "relaxed NLP". The algorithm terminates when no further improvement takes place in the solution of NLP subproblems. Optimal solutions are shown in Table 8.

Table 6. Solver times

| Problem | Major iterations | Solver times | | | | |
|----------|------------------|--------------|-----------|-------------|---------|---------|
| | | NLP (min) | MIP (min) | Total (min) | NLP (%) | MLP (%) |
| Ternary1 | 3 | 2.81 | 4.31 | 7.12 | 39.5 | 60.5 |
| Ternary2 | 6 | 3.22 | 13.41 | 16.63 | 19.36 | 80.64 |
| Unit | 5 | 14.54 | 25.80 | 40.34 | 36.1 | 63.9 |
| Ethanol | 3 | 1.17 | 1.46 | 2.63 | 44.9 | 55.1 |

Notes: N major iterations mean N NLP problems (including relaxed NLP) and $(N - 1)$ MIP problems. Times reported are CPU min on an IBM RS 6000 running AIX 3.1. Relaxed NLPs were solved using CONOPT; other NLPs with MINOS 5.3 in GAMS 2.25 for Ternary1 and Ternary2 and with CONOPT for unit and ethanol. MIPs were solved with OSL release 2.001; SOS1 conditions are not implemented in this release of GAMS/DICOPT ++/OSL interface (even though they are implemented in GAMS/OSL interface for MILPs).

Although optimization provides a better framework for studying nonideal distillation problems, finding the right set of constraints and a suitable objective function is not always a trivial task. For problems Ternary1, Ternary2 and Ethanol (Examples 1, 2 and 4), the objective function is a trade-off between number of trays (capital cost) and reflux ratio (operating cost). For the problem unit in Example 3, the form of the objective function was suggested in Kumar and Lucia (1988). It represents a trade-off between number of trays, reboiler and condenser duties and recoveries of the light and heavy keys in the top vapor and bottom liquid products, respectively.

As is well-known, the ethanol-water system of Example 4 forms an azeotrope. At 1,013 bar, the UNIQUAC model predicts the azeotrope temperature to be 351.03 K with the ethanol mole-fraction at 0.913. The usual specifications like product rate and purity do not seem to work for this system, and so the following "purity" and recovery constraints were used:

$$x_{vi} \leq y_{vi}, \quad \forall i \in I$$

$$x_{vi} \geq y_{vi} - \epsilon,$$

$$v_{lk}^0 \geq R(F_{z_i}),$$

where ϵ specifies the closeness of the liquid and vapor compositions in the condensate and R is the recovery factor for ethanol. The values used were $\epsilon = 0.005$ and $R = 0.96$.

To appreciate the significance of the optimum design presented in Table 8a, note, for example, that for Ternary1, with $|REF| = 10$ and $|BU| = 13$, there are 130 possible combinations. The OA/ER/AP algorithm required the solution of just 3 NLP problems and the solution of 2 MIP master problems.

Computationally, the solution of the relaxed NLP proves to be the most difficult, especially for nonideal systems. For the nonlinear programs (NLPs), both codes CONOPT and MINOS were used. CONOPT is based on the Generalized Reduced Gradient (GRG) algorithm together with many refinements (Drud, 1992), while MINOS is based on a projected Lagrangean method (Murtagh and Saunders, 1982). For the nonideal systems, CONOPT was able to find

Table 7a. Paths to solutions—nonzero binary variables

| Problem | Iteration | Nonzero binary variables | |
|----------|-----------|--|------------|
| | | z_i^{bu} | z_i^{bf} |
| Ternary1 | 1 | $z_1^{bu} = 0.068, z_{14}^{bu} = 0.932$ | |
| | | $z_{23}^{bf} = 0.888, z_{25}^{bf} = 0.002, z_{26}^{bf} = 0.023$ | |
| | | $z_{27}^{bf} = 0.036, z_{28}^{bf} = 0.042, z_{29}^{bf} = 0.009$ | |
| | 2 | $z_2^{bu} = 1, z_{28}^{bf} = 1$ | |
| | 3 | $z_3^{bu} = 1, z_{28}^{bf} = 1$ | |
| Ternary2 | 1 | $z_1^{bu} = 0.089, z_{10}^{bu} = 0.911$ | |
| | | $z_{20}^{bf} = 0.767, z_{26}^{bf} = 0.063, z_{27}^{bf} = 0.102, z_{28}^{bf} = 0.067$ | |
| | 2 | $z_2^{bu} = 1, z_{26}^{bf} = 1$ | |
| | 3 | $z_3^{bu} = 1, z_{26}^{bf} = 1$ | |
| | 4 | $z_4^{bu} = 1, z_{27}^{bf} = 1$ | |
| | 5 | $z_5^{bu} = 1, z_{27}^{bf} = 1$ | |
| | 6 | $z_6^{bu} = 1, z_{28}^{bf} = 1$ | |
| Unit | 1 | $z_1^{bu} = 0.037, z_{10}^{bu} = 0.963$ | |
| | | $z_{11}^{bf} = 0.963, z_{22}^{bf} = 0.037$ | |
| | 2 | $z_2^{bu} = 1, z_{11}^{bf} = 1$ | |
| | 3 | $z_3^{bu} = 1, z_{11}^{bf} = 1$ | |
| | 4 | $z_4^{bu} = 1, z_{22}^{bf} = 1$ | |
| | 5 | $z_5^{bu} = 1, z_{22}^{bf} = 1$ | |
| Ethanol | 1 | $z_1^{bu} = 0.176, z_{10}^{bu} = 0.824$ | |
| | | $z_{11}^{bf} = 0.963, z_{24}^{bf} = 0.161$ | |
| | 2 | $z_2^{bu} = 1, z_{22}^{bf} = 1$ | |
| | 3 | $z_3^{bu} = 1, z_{24}^{bf} = 1$ | |

Table 7b. Paths to solutions—objective function values

| Major iteration number | Major solution step | Value of the objective function for problem | | | |
|------------------------|---------------------|---|------------|---------|---------|
| | | Ternary1 | Ternary2 | Unit | Ethanol |
| 1 | NLP | 23.5323 | 55.9066 | 80.2360 | 12.5172 |
| 1 | MIP | 33.5674 | 60.9648 | 80.2366 | 25.6597 |
| 2 | NLP | 39.3286 | 105.075 | 74.4537 | 25.5789 |
| 2 | MIP | 41.5647 | 1139.13 | 71.3057 | 27.9694 |
| 3 | NLP | 41.0322 | infeasible | 77.5925 | 27.5952 |
| 3 | MIP | | 1201.77 | 66.9491 | |
| 4 | NLP | | 70.4454 | 78.4552 | |
| 4 | MIP | | 21278.9 | 58.2258 | |
| 5 | NLP | | 70.0608 | 77.6466 | |
| 5 | MIP | | 34130.2 | | |
| 6 | NLP | | 72.1965 | | |

the optimum for the relaxed NLP, while MINOS with default settings could not.

For the mixed integer programs (MIPs) the Optimization Subroutine Library (OSL) of IBM was used.

It should also be noted that the computational requirements for the MIP master problems will decrease significantly with the implementation of the SOS1 structure of the model, (7) and (8).

Table 8a. Optimal solutions—column design

| Problem | Objective function | Reflux ratio | Entering tray number for | |
|----------|--------------------|--------------|--------------------------|--------|
| | | | Reboiled vapor | Reflux |
| Ternary1 | 39.33 | 3.07 | 3 | 26 |
| Ternary2 | 70.06 | 9.01 | 3 | 27 |
| Unit | 78.46 | 16.54 | 2 | 22 |
| Ethanol | 25.58 | 5.58 | 3 | 22 |

Table 8b. Optimal solutions—products

| Problem | Top product, P_1 | | Bottom product, P_2 | |
|----------|--------------------|-----------------------|-----------------------|-----------------------|
| | Flowrate | Composition | Flowrate | Composition |
| Ternary1 | 40.0 | (0.375, 0.617, 0.007) | 60.0 | (0.000, 0.005, 0.995) |
| Ternary2 | 15.0 | (0.995, 0.005, 0.000) | 85.0 | (0.001, 0.293, 0.706) |
| Unit | 8.951 | (0.964, 0.007, 0.029) | 91.049 | (0.015, 0.823, 0.162) |
| Ethanol | 5.497 | (0.873, 0.127) | 94.503 | (0.002, 0.998) |

CONCLUSIONS

This work has presented simple MINLP model for finding the number of trays for a separation objective. The location of the feed tray is fixed and the problem is viewed as one of finding optimum locations for the reflux and the boilup. As shown in the results, even difficult, nonideal distillation problems can be solved with the OA/ER/AP algorithm.

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