A crude distillation unit model suitable for online applications

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Received 1 June 2000; received in revised form 1 February 2001; accepted 1 April 2001

Abstract

A steady state, multicomponent distillation model particularly suited for fractionation of crude oil has been developed based on equilibrium stage relations. For a mixture of C components, the present formulation uses $C + 3$ iteration variables namely the mole fractions of the components, temperature, total liquid and total vapor flow rates on each stage. This choice of variables makes the present model numerically stable and robust rendering a separate initial guess computation unnecessary. An improved scheme of numbering the equilibrium stages when side strippers are present, was found to be advantageous with respect to computation time. Selected example problems have been included from literature as well as industry to demonstrate the efficacy and usefulness of the method. The accuracy of predictions and speed of solution of the model equations are particularly suited for online applications such as online optimization. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Multicomponent distillation model; Crude oil; Online applications

1. Introduction

The petroleum refining industry is one of the largest users of distillation technology. The crude distillation unit is one of the most important refinery operations fractionating preheated crude oil into respective product fractions like Heavy Naphtha (HN), Kerosene

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0378-3820/01/$ - see front matter © 2001 Elsevier Science B.V. All rights reserved.
PII: S0378-3820(01)00195-3
(SK), Aviation Turbine Fuel (ATF), Light Gas Oil (LGO), Heavy Gas Oil (HGO), Reduced Crude Oil (RCO), etc. Therefore, it becomes extremely important to model the crude distillation unit to predict the composition of products from various crudes, which are processed under different operating conditions. The model thereby acts as an essential tool for production planning and scheduling, economic optimization and real-time online control and performance optimization. Additionally, such a model is also an essential prerequisite for a project engineer attempting either design of new units or rating of existing units.

2. The model

The model equations for an ordinary equilibrium stage of a simple distillation column, commonly known as Mass balance, Equilibrium, Summation and Enthalpy balance (MESH) equations, have been given by several workers [1–7]. These fundamental material and energy balance equations are available in literature in terms of different nomenclatures and variable definitions to facilitate numerical stability and ease of convergence. For a general equilibrium stage (see Fig. 1), we present one set of these equations in Table 1.

Before proceeding any further, it must be stated that from a practical viewpoint, it is not possible to represent the feed crude oil or its distillation products in terms of actual component flow rates or mole fractions since crude oil is a mixture of several hundred constituents which are not easy to analyze. A generally accepted practice is to express composition of crude in terms of a finite number of pseudocomponents. Each pseudocomponent, which is treated as a single component, is in fact a complex mixture of hydrocarbons with a range of boiling points within a narrow region say 25 °C wide. Each pseudocomponent is characterized by an average boiling point and an average specific gravity.

Fig. 1. Schematic diagram of an equilibrium stage.
Table 1
Model equations for multicomponent, multistage distillation

(1) Component material balance equation on ith stage

\[ v_{i,j} = l_{i,j} + D^y_j + D^z_j \] [Partial Condenser]

\[ v_{i,j} = l_{i,j} + D^y_j \] [Total Condenser] \[ i = 1; j = 1, \ldots, C \]

\[ (l_i - l_{i-1} + l_{i+1}) + (v_{i+1,j} + v_{i,j}) - (v_{i,j} + w_i^y) - (v_{i,j} + w_i^y) + f_{i,j} = 0 \]
\[ i = 2, \ldots, N; j = 1, \ldots, C \]

(1)

\( f_{i,j} \) may be liquid \( (f_{i,j}^L) \) or vapor \( (f_{i,j}^V) \) feed or a mixture of both. The liquid feed enters above the feed stage and vapor feed enters below it.

(2) Liquid summation equation

\[ L_i = \sum_{j=1}^{C} l_{i,j} \] \[ i = 1, \ldots, N \]

(2)

(3) Vapor summation equation

\[ V_i = (L_i / RR)[\text{Total Condenser}] \] \[ i = 1 \]

\[ V_i = \sum_{j=1}^{C} v_{i,j} \] \[ i = 2, \ldots, N \text{ if Total Condenser else } i = 1, \ldots, N \]

(3)

(4) Enthalpy balance equation

\[ \sum_{j=1}^{C} l_{i-1,j} h_{i-1,j} + \sum_{j=1}^{C} l_{i,j} h_{i,j} + \sum_{j=1}^{C} v_{i+1,j} h_{i+1,j} + \sum_{j=1}^{C} v_{i,j} h_{i,j} - \sum_{j=1}^{C} (l_{i,j} + w_i^y) h_{i,j} - \sum_{j=1}^{C} (v_{i,j} + w_i^y) h_{i,j} + \sum_{j=1}^{C} f_{i,j} h_{i,j} \pm Q_i = 0 \] \[ i = 2, \ldots, N-1 \]

\[ \sum_{j=1}^{C} l_{N-1,j} h_{N-1,j} = \sum_{j=1}^{C} v_{N,j} h_{N,j} + \sum_{j=1}^{C} l_{N,j} h_{N,j} \] \[ i = N \]

(4)

(5) Equilibrium relation

\[ y_{i,j} = K_{i,j} x_{i,j} \] \[ i = 1, \ldots, N; j = 1, \ldots, C \]

(5)

(In case of total condenser \( i = 2, \ldots, N \) with

\[ x_{i,j} = \frac{l_{i,j}}{L_i} \]

and

\[ y_{i,j} = \frac{v_{i,j}}{V_i} \]
There are several ways of grouping the variables for numerical solution of the set of nonlinear algebraic equations. For a simple column, Naphtali and Sandholm [1] arranged the equations so as to yield a block-tridiagonal matrix structure. This type of grouping reduced the required data storage capacity by taking advantage of the tri-diagonal structure of the resultant Jacobian matrix. The authors replaced mole fractions \(2NC\) variables and total flow rate \(2N\) variables by component flow rates to reduce the number of variables. Thus, \(N(2C + 1)\) stage variables were reduced to \(N(2C + 1)\). For complex columns with pumparounds and side strippers, off diagonal elements appear apart from the tri-diagonal structure. Hofeling and Seader [3] used a modified Thomas algorithm to solve the model equations for complex columns using the Naphtali and Sandholm formulation.

To reduce the matrix size, there are other types of formulations [2,6,8] with different variable groupings of \((C + 2)\) and \((C + 3)\) variables per stage. In these methods, the remaining variables are calculated explicitly. A list of independent variables, explicitly calculated variables and model equations to be used in different formulations are presented in Table 2.

In the Naphtali–Sandholm method, variables are grouped component-wise and the entire equation set is solved simultaneously. Tomich used stage-wise grouping of variables and solved the problem in two stages. In the outer computation loop the \(V_j\) and \(T_j\) are upgraded in each iteration, whereas an inner loop solves for \(I_{ij}\). While Tomich method has been found to be more suited for columns with fewer stages, Naphtali–Sandholm works better for columns having fewer components. The inside-out algorithm of Boston [5] which was latter modified by Russel [6] is considered to be suitable for problems where both number of stages as well as components are large such as in crude fractionation. It, however, uses three levels of convergence to solve the problem. The present method is simultaneous implying all model equations are solved simultaneously allowing all variables to be upgraded at the same time, which makes this method more robust and efficient.

### 2.1. Numbering of stages

The crude distillation units have pumparound streams and side strippers, which result in off-diagonal elements in the Jacobian matrix. The location of the off-diagonal

### Table 2

<table>
<thead>
<tr>
<th>No. of variables</th>
<th>Independent variables</th>
<th>Explicitly defined variables</th>
<th>Model equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N(2C + 1)) [1]</td>
<td>(l_{ij}, v_{ij}, I_i)</td>
<td>(L_i = \sum j_{ij}, V_i = \sum v_{ij})</td>
<td>Eqs. (1), (4) and (5)</td>
</tr>
<tr>
<td>(N(C + 2)) [2]</td>
<td>(l_{ij}, V_j, T_j)</td>
<td>(x_{ij} = l_{ij}/L_i, y_{ij} = v_{ij}/V_i)</td>
<td>Eqs. (1), (3) and (4)</td>
</tr>
<tr>
<td>(N(C + 3)) [6]</td>
<td>(l_{ij}, L_i, V_j, T_i)</td>
<td>(x_{ij} = l_{ij}/L_i, y_{ij} = K_{ij} x_{ij})</td>
<td>Eqs. (1), (2), (3) and (4)</td>
</tr>
<tr>
<td>(N(C + 3)) Present work</td>
<td>(x_{ij}, L_i, V_j, T_i)</td>
<td>(y_{ij} = K_{ij} x_{ij})</td>
<td>Eqs. (1), (2), (3) and (4)</td>
</tr>
</tbody>
</table>
elements with respect to the main tridiagonal band has been found to influence the convergence path and CPU time considerably during the present study. Conventionally, the stages in the main distillation column are numbered from top to bottom and then the side stripper trays are numbered in a sequence. This nomenclature generates off-diagonal elements far removed from the main tridiagonal band resulting in a very large computational effort. Actually, farther an element is positioned with respect to the band, larger will be computational load. The stages were, therefore, renumbered from top down in such a way that when connection with a side-stripper was reached, the stages of that side-stripper were numbered in succession, returning to the main column and continuing further. This scheme of numbering ensured that the off-diagonal terms were as close to the diagonal as possible thus reducing computation time as compared to the conventional scheme of numbering.

2.2. Solution procedure

The method of solution involves solving simultaneously the system of nonlinear equations representing component mass conservation, energy conservation and the summation equations for each stage of the distillation column. Traditionally, a set of nonlinear algebraic equations is solved using the Newton–Raphson method. In this method, the nonlinear equations are linearized at every iteration and because of which the procedure is known to diverge for highly nonlinear equations when the initial guess is far removed from the final solution. If the number of nonlinear equations is large then the resultant Jacobian matrix may become ill-conditioned leading to slow convergence or even at times to non-convergence. Several modifications have been suggested to overcome the convergence problems [9,10]. Rogoza and Gorodetskaya [11] suggested a multilevel solution method in which the equation set is decomposed into subproblems leading to substantial reduction in computation times. Hu [12] discussed an algorithm in which a sparse large nonlinear system of equations is solved using parallel processing computations. Martin and Rivera [13] presented a parallel algorithm based on an asynchronous scheme, which permitted high performance when the Jacobian matrix was sparse. Shahadat Hossian and Steihaug [14] discussed an efficient method for estimation of large sparse Jacobian matrix employing forward and reverse mode of automatic differentiation. Homotopy methods have been applied to difficult-to-solve distillation column problems [15,16] in which a homotopy curve is tracked to force the convergence to the desired solution. Recently, He [17] described an algorithm in which the conventional perturbation method was coupled with a homotopy technique for improved efficiency. In the present study, the correct choice of independent variables set reduced the nonlinearity of the model equations allowing conventional Newton–Raphson method to converge even from far away initial guess. A sparse matrix method further enhanced the efficiency of solution. We demonstrate the stability and efficiency of the technique here.

2.2.1. Solving a system of nonlinear equations

Let \( f(x): \Omega \to \mathbb{R}^n \) be a system of nonlinear equations, where \( \Omega \subseteq \mathbb{R}^n, \quad x \in \Omega, \)
\( x^T = (x_1, x_2, \ldots, x_n), \quad f(x)^T = (f_1(x), f_2(x), \ldots, f_n(x)) \) and \( f_i(x): \mathbb{R} \to \mathbb{R}^n \) is continu-
ousely differentiable with respect to each component of \( x \) for \( i = 1,2,\ldots,n \). Let us assume that there exists \( x^* \in \Omega \) such that \( f(x^*) = 0 \). Let \( x \) be an estimate for \( x^* \). To calculate the correction \( \Delta x \), such that \( f(x + \Delta x) = 0 \) Taylor series expansion is employed.

\[
f(x + \Delta x) = f(x) + f'(x) \Delta x + \in (x,\Delta x),
\]
where \( \in (x,\Delta x) \) is the error in the linear approximation. From Eq. (6)

\[
\Delta x = -f'(x)^{-1}f(x) - f'(x)^{-1} \in (x,\Delta x).
\]

Since \( \in (x,\Delta x) \) is not known and depends upon \( \Delta x \), hence \( \Delta x \) is estimated as

\[
\Delta x = -f'(x)^{-1}f(x).
\]

The correction \( \Delta x \) is applied repeatedly to the new estimate of \( x^* \) to obtain the final estimate of \( x^* \). From Eq. (7), we can conclude that a formulation \( f(x) \) of a problem which results in a relatively lower error of linear approximation for a given \( \Delta x \) and equivalent estimates of \( x^* \) will converge in less number of iterations and its dependence on the choice of initial estimate will also decrease. This is the reason for the convergence of a system of linear equations in one iteration starting from any initial estimate [18,19] as there is no error of linearization for linear equations.

2.2.2. Model equations

For the \( i \)th stage of a multicomponent distillation problem for a simple column, the \( C+3 \) formulation uses \( x_{i,j} \), \( L_i \), \( V_i \) and \( T_i \) as independent variables to write the following equations.

**Mass balance**

\[
DC_{i,j} = V_{i+1}K_{i+1,j}x_{i+1,j} + L_{i-1}x_{i-1,j} - L_{i}x_{i,j} - V_{i}K_{i,j}x_{i,j}
\]

**Energy balance**

\[
DH_i = V_{i+1}\sum K_{i+1,j}x_{i+1,j}H_{i+1,j} + L_{i-1}\sum x_{i-1,j}h_{i-1,j} - L_{i}\sum x_{i,j}h_{i,j}
\]

\[
- V_{i}\sum K_{i,j}x_{i,j}H_{i,j}
\]

**Summation equation**

\[
DV_i = V_i - V_i\sum K_{i,j}x_{i,j}
\]

\[
DL_i = L_i - L_i\sum x_{i,j}
\]

Here \( DC_{i,j} \), \( DH_i \), \( DV_i \) and \( DL_i \) are the discrepancies in the model equations which vanish at the solution.

The above formulation is referred to as \( C+3 \) formulation, since there are \( C+3 \) equations in the model and as many variables to be calculated.

2.2.3. Comparison of \( C+2 \) and \( C+3 \) formulations

\( C+3 \) formulation is a modification of \( C+2 \) formulation [2]. The modification has been suggested by the need to minimize the inflationary tendency of the error of linear approximation.
The variables of \( C + 2 \) formulations are \( l_{ij}, V_i \) and \( T_i \).

Mass balance

\[
DC_{i,j} = \frac{V_{i+1}K_{i+1,j}l_{i+1,j} + l_{i-1,j} - l_{i,j}}{\sum_{k=1}^{c} l_{i,k}}
\]

Energy balance

\[
DH_i = \frac{V_{i+1}}{\sum_{k=1}^{c} l_{i+1,k}} \sum_{j=1}^{c} K_{i+1,j}l_{i+1,j}h_{i+1,j} + \sum_{j=1}^{c} l_{i-1,j}h_{i-1,j}
\]

\[
- \sum_{j=1}^{c} l_{i,j}h_{i,j} - \frac{V_i}{\sum_{k=1}^{c} l_{i,k}} \sum_{j=1}^{c} K_{i,j}l_{i,j}h_{i,j}
\]

Summation equation

\[
DV_i = V_i - \frac{V_i}{\sum_{k=1}^{c} l_{i,k}} \sum_{j=1}^{c} K_{i,j}l_{i,j}
\]

The reason for multiplying the summation equations in \( C + 3 \) and \( C + 2 \) formulations by the respective total molar flow rates is that their order of magnitude become comparable to the mass and energy balance discrepancies.

We now show that the error of linearization in \( C + 2 \) formulation has a greater tendency to inflate as compared to the \( C + 3 \) formulation. For this comparison, let us consider a single stage distillation problem. A two component feed with \( F_1 \) moles of component 1 and \( F_2 \) moles of component 2 is fed to this stage which is being kept at temperature \( T \). Since the temperature is known, energy balance discrepancy is not required.

The \( C + 2 \) formulation of this problem is

\[
DC_{11} = F_1 - l_{11} - V_1K_{11}l_{11}/(l_{11} + l_{12})
\]

\[
DC_{12} = F_2 - l_{12} - V_1K_{12}l_{12}/(l_{11} + l_{12})
\]

\[
DV_i = V_i - V_i(K_{11}l_{11} + K_{12}l_{12})/(l_{11} + l_{12})
\]

The discrepancies of the above problem in \( C + 3 \) formulation are as follows.

\[
DC_{11} = F_1 - L_1x_{11} - V_1K_{11}x_{11}
\]

\[
DC_{12} = F_2 - L_1x_{12} - V_1K_{12}x_{12}
\]

\[
DV_i = V_i - V_i(K_{11}x_{11} + K_{12}x_{12})
\]

\[
DL_i = L_i - L_i(x_{11} + x_{12})
\]
It is clear that in $C_q^3$ formulation the discrepancies are linear with respect to the independent variables $x_{i1}$, $x_{i2}$, $V_i$, $L_i$ and, therefore, the error of linear approximation will be zero and hence the problem will converge starting from any initial estimate. This decrease in the nonlinearity of the system by choosing the correct set of independent variables is the major gain of $C_q^3$ formulation over $C_q^2$ formulation which makes it converge faster and the dependence on initial estimate also decreases. This stability of $C_q^3$ formulation has been tested with a number of practical problems. The component liquid flow rate appears in the denominators of the equations of the $C_q^2$ formulation. This makes the error of linearization inflate if all the liquid component flows on a tray take on small values during any iteration. These remarks apply to all those methods which use $l_{i,j}$ as iteration variables as distinguished from $x_{i,j}$ which has been used in the present case. Russel’s method [6] which, although uses $C_q^3$ variables, suffers from the same error of inflation as $C_q^2$ formulation of Tomich [2] as it too uses $l_{i,j}$ as iteration variables.

2.2.4. Solution of model equations

The independent variables which are iterated upon in $C_q^3$ formulation for the $i$th stage are $x_{i,j}$, $V_i$, $L_i$, $T_i$. Let $x^k$ be the present estimate of the solution then the next estimate is calculated as

$$x^{k+1} = x^k - \beta f'(x^k)^{-1} f(x^k),$$

where $\beta$ is the step length and is calculated by minimizing

$$\min_{\beta} f(x^{k+1})^T f(x^{k+1}).$$

For nonlinear problems, it is well known that the choice of an initial guess plays a very important role in finding the solution. If the initial guess is far from the final solution, an algorithm may either not converge or take large computation time. This is because of the error of linearization, which is likely to be substantial if the initial guess is far away. Any effort in reducing the error of linearization is, therefore, expected to make the algorithm more robust and stable. Most existing algorithms for distillation column modeling solve model equations approximately or solve a simplified model to obtain an initial guess for component flow rates or mole fractions before embarking on actual solution procedure. This is unnecessary in the present case and feed composition serves as a satisfactory initial guess for the iterated variables, $x_{i,j}$.

The major computational effort in solving Eq. (9) is in calculating $f'(x^k)^{-1} f(x^k)$ which is obtained by solving the system of linear equation

$$f'(x^k) \Delta x = f(x^k).$$

Suppose a distillation problem has 80 stages with 25 components, then the system of linear equations is of dimension $80(25 + 3) = 2240$ equations. This implies that the Jacobian of such a large system is of dimension $2240 \times 2240$. To store such a large matrix in single precision, it requires at least 40MB of memory, which is available even
in personal computers these days. Hence storage of such large a matrix in computer memory is no longer a problem. The only problem is the computation time in solving such a large system. To reduce the computation time advantage is taken of the sparsity of the Jacobian matrix \( f'(x^k) \). Usually not more than 5% of the elements of the Jacobian are nonzero. The fundamental algorithm for solving the system of linear Eq. (10) is Gaussian elimination with partial pivoting which has been modified to take advantage of the sparsity of the Jacobian.

3. Thermodynamics

Crude characterization is commonly based on the method proposed by Miquel and Castells [20,21] for petroleum fractions, which requires the true boiling point (TBP) curve along with the average specific gravity for the fraction. For breaking the crude into pseudocomponents, the given TBP data are regressed in a piece-wise manner using splines. Using an iterative procedure as given by Miquel and Castells, the values of \( T_{g1} \) and \( S_j \) are obtained for each pseudocomponent. Thermodynamic quantities like critical temperature \( T_c \), critical pressure \( P_c \) and acentric factor \( w_c \) can then be calculated using suitable correlations like those proposed by Riazi and Daubert [22] and Edmister and Lee [23].

For a distillation column simulator, computation of equilibrium constants \( K_{ij} \) of various components present and enthalpies of different streams as functions of temperature and composition are essential. Since petroleum fractions are complex mixtures of hydrocarbons, single pure component thermodynamics is not applicable. In estimation of these thermodynamic properties, the use of empirical or semi-empirical correlations is quite popular. Some of the commonly used techniques are based on the cubic equation of state proposed by Peng–Robinson [24], Redlich–Kwong [25] and Soave [26].

Thermodynamic properties of vapor–liquid mixtures are generally predicted by calculating deviations from ideality of both the vapor and liquid phases by using any of the above mentioned equations of state. In a second method, the equation of state is applied only to the vapor phase while liquid phase deviations from ideal solution behavior are calculated using thermodynamic excess functions [27–29]. For a rigorous crude distillation simulator, it is important to use prediction models for the thermodynamic properties, which are continuous functions, and are applicable in the entire range of temperature (say 0–500 °C) for the lighter as well as the heavier components. Additionally, to ensure smooth convergence, there should not be any discontinuity of real roots for the equations of state in the entire domain of operation of the crude distillation unit. While, it is still possible to use an equation of state or a combination of some of the above methods to cover the entire boiling point range, the computational effort required in this approach is prohibitive as the thermodynamic properties are required to be calculated repeatedly for each iteration. For online usage, the computation time is of utmost concern and hence, equation of state approach is not convenient to use.

In view of above, a correlation was developed in the present work using data obtained from Peng–Robinson equation for the lighter hydrocarbons and those from
Fig. 2. Comparison of equilibrium constants calculated by various methods for a low boiling pseudo-component ($T_s = 292.18$ K).

Fig. 3. Comparison of equilibrium constants calculated by various methods for a middle range boiling pseudo-component ($T_s = 442.93$ K).
Braun-K$_{10}$ (BK10) for both medium and heavier fractions in the temperature range 0–500 °C and pressure near one atmosphere. The equation has the form [30]

$$\ln\left(\frac{P^*}{P_c}\right) = (1 + w)f(T_c),$$

(11)
where \( f(T_r) \) is a function of reduced temperature. Using Eq. (11), \( K \)-value for \( j \)th component can be calculated from

\[
K_j = \frac{P_j^0}{P} = \frac{P_{cj}}{P} \exp\left[\left(1 + w_j\right)f(T_r)\right].
\]  

(12)

Figs. 2–4 show the comparison of \( K \)-values predicted by various methods for lighter, intermediate and heavier fractions of a crude oil. Fig. 5 presents a parity plot of all the data available with predictions from the proposed thermodynamic model.

Enthalpies for the liquid and the vapor phases can be obtained from Kesler and Lee [31] modification of Johnson–Grayson [32] charts.

4. Prediction of petroleum product properties

The petroleum products coming out of the crude distillation column are blended with products from various processing units and are rated based on certain product properties like RVP, flash point, pour point, specific gravity, recovery at 366 \(^\circ\)C, etc. To quantify these properties before the blending operations and validate the simulator, product properties of run down streams were experimentally measured. The distillation column simulator, which predicts product TBP, was coupled with a property estimation package developed in-house [33,34]. These predicted properties have been compared with the experimentally measured ones in Table 6.

5. Case studies

The crude fractionation unit model developed during the present work was tested on a variety of problems collected both from literature as well as the industry. Some representative samples are being presented here.
Case 1. A pipestill problem from literature [4], which consists of four side strippers and one pumparound configuration. The input specifications for this problem are available in Ref. [4]. The crude distillation model presented in this paper was run using the input specifications of this problem. The converged results are presented in Figs. 6 and 7. Fig. 6 shows a comparison of the temperature profile obtained from the model with the results of Hess and Holland. Also included in this figure are the results obtained using a commercial simulator (Aspen Plus, Aspen Tech., USA) for the same input data. Fig. 7
Table 3
Feed TBP for Case 2
The average specific gravity of the feed oil is 0.8445.

<table>
<thead>
<tr>
<th>Cumulative volume (%)</th>
<th>Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>12</td>
</tr>
<tr>
<td>5</td>
<td>52</td>
</tr>
<tr>
<td>10</td>
<td>85</td>
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<td>30</td>
<td>205</td>
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<tr>
<td>50</td>
<td>335</td>
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<tr>
<td>70</td>
<td>440</td>
</tr>
<tr>
<td>90</td>
<td>610</td>
</tr>
<tr>
<td>95</td>
<td>703</td>
</tr>
<tr>
<td>100</td>
<td>796</td>
</tr>
</tbody>
</table>

shows a comparison of the product compositions reported in literature with those predicted using the present model and the commercial simulator. It is evident from the curves that the proposed model is found to have good match with the data published in literature as well as given by the commercial simulator. The calculated vapor and liquid
profiles in the column showed similar agreements but have not been included here. An excellent overall match with the published results confirmed that the present formulation is satisfactory.

Table 5
Input specification of operating conditions for Case 3

<table>
<thead>
<tr>
<th>Feed flowrate (m³/h)</th>
<th>1228.200</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coil outlet temperature (°C)</td>
<td>328.350</td>
</tr>
<tr>
<td>Reflux flow rate (m³/h)</td>
<td>250.000</td>
</tr>
<tr>
<td>Condenser temperature (°C)</td>
<td>89.195</td>
</tr>
<tr>
<td>Reflux temperature (°C)</td>
<td>39.100</td>
</tr>
<tr>
<td>Water reflux rate (ton/h)</td>
<td>0.2</td>
</tr>
<tr>
<td>Bottom steam rate (ton/h)</td>
<td>8.380</td>
</tr>
<tr>
<td>Steam temperature (°C)</td>
<td>330.000</td>
</tr>
<tr>
<td>HN flow rate (m³/h)</td>
<td>72.400</td>
</tr>
<tr>
<td>KERO flow rate (m³/h)</td>
<td>224.250</td>
</tr>
<tr>
<td>LGO flow rate (m³/h)</td>
<td>181.810</td>
</tr>
<tr>
<td>HGO flow rate (m³/h)</td>
<td>38.070</td>
</tr>
<tr>
<td>Steam rate for HN Stripper (ton/h)</td>
<td>1.5900</td>
</tr>
<tr>
<td>Steam rate for KERO Stripper (ton/h)</td>
<td>2.6969</td>
</tr>
<tr>
<td>Steam rate for LGO Stripper (ton/h)</td>
<td>0.6666</td>
</tr>
<tr>
<td>Steam rate for HGO Stripper (ton/h)</td>
<td>0.7800</td>
</tr>
<tr>
<td>HN pump-around flow rate (m³/h)</td>
<td>685.620</td>
</tr>
<tr>
<td>KERO pump-around flow rate (m³/h)</td>
<td>408.800</td>
</tr>
<tr>
<td>LGO pump-around flow rate (m³/h)</td>
<td>416.340</td>
</tr>
<tr>
<td>HN pump-around return temperature (°C)</td>
<td>125.510</td>
</tr>
<tr>
<td>KERO pump-around return temperature (°C)</td>
<td>115.840</td>
</tr>
<tr>
<td>LGO pump-around return temperature (°C)</td>
<td>163.100</td>
</tr>
<tr>
<td>Column pressure (kg/cm²) gage</td>
<td>3.073</td>
</tr>
</tbody>
</table>
Case 2. This example consists of a 25-stage petroleum distillation column with two side strippers and three pumparound flows. The side strippers with two stages each draw from stages 8 and 17 and return to stage 7 and 15, respectively, of the main column. The pumparound flows are from stages 3, 9 and 17 to stages 2, 8, 15 of the main column, respectively. A feed of 70,000 bbl/day at 339 °C and 32 atm enters above stage no. 21 of the main column. The column overhead is subcooled to 40 °C in a condenser giving both vapor and liquid products. The column operates at a pressure of about 40 psi. The rundown from the two side strippers are 7200 and 9000 bbl/day, respectively. The pumparound circulation rates are 47.7, 133.9 and 226.25 m³/h, respectively, with return temperatures of 90 °C, 130 °C and 220 °C. The feed oil assay is given in Table 3.

Table 6
Comparison of calculated parameters and properties with the measured values

<table>
<thead>
<tr>
<th>Column parameters and product properties</th>
<th>Model generated values</th>
<th>Measured (plant) values</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Simulated results</td>
<td>With efficiencies and reconciliation</td>
</tr>
<tr>
<td>Top plate temperature (°C)</td>
<td>115.000</td>
<td>124.700</td>
</tr>
<tr>
<td>HN pump-around temperature (°C)</td>
<td>159.719</td>
<td>160.846</td>
</tr>
<tr>
<td>HN column draw temperature (°C)</td>
<td>150.860</td>
<td>154.033</td>
</tr>
<tr>
<td>HN product temperature (°C)</td>
<td>133.000</td>
<td>142.767</td>
</tr>
<tr>
<td>KERO pump-around temperature (°C)</td>
<td>223.730</td>
<td>220.788</td>
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<tr>
<td>KERO column draw temperature (°C)</td>
<td>194.230</td>
<td>204.170</td>
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<tr>
<td>KERO product temperature (°C)</td>
<td>181.160</td>
<td>191.522</td>
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<tr>
<td>LGO pump-around temperature (°C)</td>
<td>277.770</td>
<td>267.560</td>
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<tr>
<td>LGO column draw temperature (°C)</td>
<td>277.770</td>
<td>267.560</td>
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<tr>
<td>LGO product temperature (°C)</td>
<td>270.400</td>
<td>264.217</td>
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<td>HGO column draw temperature (°C)</td>
<td>302.850</td>
<td>312.790</td>
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<tr>
<td>HGO product temperature (°C)</td>
<td>287.610</td>
<td>294.695</td>
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<tr>
<td>Bottom plate temperature (°C)</td>
<td>315.750</td>
<td>311.931</td>
</tr>
<tr>
<td>Top distillate flow rate (m³/h)</td>
<td>187.853</td>
<td>247.335</td>
</tr>
<tr>
<td>Top distillate mass flow rate (ton/h)</td>
<td>135.742</td>
<td>180.814</td>
</tr>
<tr>
<td>RCO flow rate (m³/h)</td>
<td>506.719</td>
<td>447.243</td>
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<tr>
<td>Top distillate density (g/cm³)</td>
<td>0.6977</td>
<td>0.7060</td>
</tr>
<tr>
<td>Top distillate RVP (atm)</td>
<td>0.6394</td>
<td>0.5378</td>
</tr>
<tr>
<td>HN density (g/cm³)</td>
<td>0.7402</td>
<td>0.7540</td>
</tr>
<tr>
<td>HN RVP (atm)</td>
<td>0.0930</td>
<td>0.0379</td>
</tr>
<tr>
<td>HN Flash Point (°C)</td>
<td>1.500</td>
<td>9.540</td>
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<tr>
<td>Kero density (g/cm³)</td>
<td>0.7736</td>
<td>0.7862</td>
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<tr>
<td>Kero Flash Point (°C)</td>
<td>28.86</td>
<td>40.15</td>
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<tr>
<td>LGO density (g/cm³)</td>
<td>0.8188</td>
<td>0.8301</td>
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<tr>
<td>LGO Flash Point (°C)</td>
<td>69.71</td>
<td>87.65</td>
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<tr>
<td>LGO Pour Point (°C)</td>
<td>-17.83</td>
<td>-10.28</td>
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<tr>
<td>HGO density (g/cm³)</td>
<td>0.8433</td>
<td>0.8530</td>
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<tr>
<td>HGO Flash Point (°C)</td>
<td>87.63</td>
<td>100.03</td>
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<tr>
<td>HGO Recovery @ 366 °C (%)</td>
<td>100.00</td>
<td>90.42</td>
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<tr>
<td>RCO density (g/cm³)</td>
<td>0.9117</td>
<td>0.9182</td>
</tr>
<tr>
<td>RCO Recovery @ 366 °C (%)</td>
<td>30.84</td>
<td>27.72</td>
</tr>
</tbody>
</table>

1 For straight run naphtha; NR: not reported.
This problem was taken from the commercial simulator itself (Aspen Plus) where it was presented as an illustration. The crude TBP was split into 40, 30 and 25 pseudocomponents and the problem was solved using the present model. The liquid, vapor and temperature profiles were identical in all the cases. Using 25 components, the calculated product TBPs are compared with those from the commercial simulator (see Fig. 8) and again the match is quite good.

**Case 3.** Data were collected from an operating crude distillation unit in a refinery having four side strippers and three pumparound flows. A theoretical analog of the unit consists

![Fig. 9. Product TBP curves (Cases 3 and 4).](image-url)
of 34 stages with crude entering above the fourth stage from the bottom at a flow rate of 1200 m$^3$/h at 330 °C and 271 kPa. The column has a partial condenser with both liquid and vapor distillate products. The side strippers consisted of two theoretical stages each. The crude (from an Indian source) TBP data are given in Table 4 and the other input specifications are included in Table 5. The calculated column profiles for temperature, vapor and liquid flows are not included since no measured profiles were available for comparison. However, measured values of some of the parameters were available at specific locations in the plant and those have been compared with the model predictions in Table 6. Fig. 9 shows a comparison of calculated product TBPs with the measured values. The model results appear to generally match well with the plant data except at a few points. There can be two possible reasons for the mismatch observed in some column parameters and the product TBPs. The theoretical analog is not perfect and stage efficiencies are required to be introduced to better match the column parameters. The second reason is that the TBP used in the simulator is not representative of the crude being processed at that time. The actual crude TBP has been found to deviate somewhat from that measured in the laboratory during crude assay on account of spatial variations in the oil reservoir and also because of stratification in the storage tank. In the next case study, these two discrepancy sources have been accounted for.

**Case 4.** The crude distillation unit as well as the feed crude were same as in Case 3. Stage efficiencies were incorporated in the equilibrium relations as $y_{ij} = \eta_{ij} K_{ij} x_{ij}$ where $\eta_{ij}$ are the efficiencies for $j$th component on $i$th stage. The feed TBP curve was also reconciled. For the details of efficiencies, calculation and TBP reconciliation, the reader is referred to Basak [35].

Using these, the model predictions matched very well with measured values for both column parameters (see Table 6) and product TBPs (Fig. 9). Fig. 10 shows that the
crude being processed has a slightly different composition in comparison to its standard TBP. In Table 6, columns 3 and 4 show a comparison of column parameters and product properties before and after TBP reconciliation. An improved match with the measured data after reconciliation brings out the importance of feed TBP curve reconciliation. Similarly, the importance of stage efficiencies can be viewed by comparing columns 2 and 3 in Table 6.

6. Conclusions

A transport phenomena model based simulator has been developed successfully for an industrial crude oil distillation column. The choice of independent variables made the model more stable and robust and facilitated quicker convergence even from a far off initial guess. Numbering of equilibrium stages in a specific order further led to the reduction in computation time. It has been observed that equilibrium constants and enthalpy prediction using an equation of state approach increases the computational time to a large extent. Use of empirical correlations significantly reduced computation time and also led to a closer match between the results of the simulator and the actual plant data. Additionally, results of such a simulator gives complete TBP curves for all the products that can be used to predict other product properties such as RVP, flash point, pour point, etc. Comparison of the results of the present simulator with those from literature as well as from actual plant indicates that the predictions based on present simulator are reasonably good. An efficient equation-solving algorithm has been used which utilizes sparsity of the Jacobian matrix and further reduces computation time. The CPU time required was reduced to about 5–8 s on a Pentium 266 MHz machine making the model suitable for online process monitoring and/or supervisory online optimization.

Nomenclature

\( B_j \) bottom flow rate for \( j \)th component
\( C \) total number of pseudocomponents in the feed
\( D \) total distillate flow rate
\( D^L \) liquid distillate flow rate
\( D^V \) vapor distillate flow rate
\( D^V_j \) vapor distillate flow rate for \( j \)th component
\( f^L_i \) liquid feed flow rate for \( j \)th component to \( i \)th stage
\( f^V_i \) vapor feed flow rate for \( j \)th component to \( i \)th stage
\( H^D \) enthalpy of \( j \)th component in vapor distillate
\( H^F_i \) vapor enthalpy of \( j \)th component in the feed to \( i \)th stage
\( h \) liquid enthalpy for \( j \)th component on \( i \)th stage
\( h^F_i \) liquid enthalpy of \( j \)th component in the feed to \( i \)th stage
\( K_{ij} \) phase equilibrium constant of \( j \)th component on \( i \)th stage
\( L_i \) reflux flow rate
\( L' \) total liquid flow rate from \( i \)th stage
\( I_{ij} \) liquid flow rate of \( j \)th component from \( i \)th stage
\( N \) total number of stages in the column
\( P_{c} \) critical pressure of \( j \)th component
\( P_{v} \) vapor pressure of \( j \)th component
\( Q_B \) heat duty of the bottom stage reboiler
\( Q_C \) condenser heat duty
\( RR \) reflux ratio \((L/D)\)
\( S \) specific gravity of crude oil
\( S_j \) specific gravity of \( j \)th pseudo-component
\( T_{avg} \) mean average boiling point of \( j \)th pseudocomponent
\( T_{c} \) critical temperature of \( j \)th component
\( T_i \) temperature of \( i \)th stage
\( T_r \) reduced temperature
\( V_i \) total vapor flow rate from the \( i \)th stage
\( v_{ij} \) vapor flow rate of \( j \)th component from \( i \)th stage
\( w_j \) acentric factor of \( j \)th component
\( w_{Lij} \) liquid side stream of \( j \)th component from \( i \)th stage
\( w_{Vij} \) vapor side stream of \( j \)th component from \( i \)th stage
\( x_{ij} \) mole fraction of \( j \)th component in liquid phase on \( i \)th stage
\( y_{ij} \) mole fraction of \( j \)th component in vapor phase on \( i \)th stage
\( \eta \) efficiency factor of \( j \)th component on \( i \)th stage

Subscripts

M bottom plate of main column and side stripper
p pump around liquid stream from stage \( p \)
q side stripper vapor stream from stage \( q \)

Superscript

L refers to liquid phase
V refers to vapor phase

Acknowledgements

The financial grant received from the Center for High Technology, New Delhi is gratefully acknowledged.

References