

NEW METHOD FOR DESIGNING DISTILLATION COLUMNS OF MULTICOMPONENT MIXTURES

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Abstract

This paper presents a series of calculation procedures for computer design of ternary distillation columns overcoming the iterative equilibrium calculations necessary in these kind of problems and, thus, reducing the calculation time. The proposed procedures include interpolation and intersection methods to solve the equilibrium equations and the mass and energy balances. The calculation programs proposed also include the possibility of rigorous solution of mass and energy balances and equilibrium relations.

1.Introduction

The initial research covering the theoretical aspects of distillation date from 1893 (Sorel, 1893). The remarkable feature in the development of these calculations was the publication of the first graphical methods (Ponchon, 1921 and McCabe and Thièle, 1925). Later, in the 50's, the development of computers allowed the appearance of several convergence procedures based on the Newton-Raphson method (i.e., Nielsen, 1957; Greenstad *et al.*, 1958). The constant development of computers has allowed more exact solutions for both, steady and non-steady state problems (i.e., Gallun and Holland, 1980 and 1982).

The time required for applying such methods is usually long, and various procedures have been developed in order to accelerate the calculations (i.e., Broyden, 1965; Vickery and Taylor, 1986).

The methods developed to simulate the operation of distillation

columns are aimed at finding the separation which can be obtained from a given feed, operation conditions and column configuration (i.e., for a given number of trays and specified location of the feeds and side streams). On the other hand, the design methods focus on the determination of the best column configuration for a specified separation. Both problems require different approaches to find the solution. Simulation problems can be solved by any kind of approximated or rigorous method whereas the design problems involve more difficulties, such as finding approximate solutions from the minimum number of trays and minimum reflux (Underwood, 1932) or empirical correlations between tray number and reflux (Erbar and Maddox, 1961). Rigorous tray to tray methods often show convergence problems whereas the successive approximation methods are not directly applicable (Ricker and Greens, 1974).

In modern distillation practice, rigorous methods are the primary design and optimization tools and the role of shortcut calculations is restricted to eliminating the least desirable design options. In very common situations, the product composition requirements are fixed and the optimum design is that which minimizes the cost of achieving this requirements. Kister (1992) presented a design procedure that optimizes the product purity versus the distillation cost, where the ideal feed point can be determined by graphical, shortcut or rigorous techniques. Small variations are introduced to the feed point, and their effect on the top and bottom compositions is estimated by a rigorous or shortcut method. The results are substituted into the objective function, and the next test begins with the feed entering a stage for which the objective function is lower.

The rigorous methods generally involve the following steps:

1. Specification of variables
2. Initialization of MESH variables
3. Actual calculation
4. Test of solution
5. Exit and engineering evaluation

The existing calculation methods differ in their selection of independent and dependent variables and in the procedure used to solve the MESH equations (usually tridiagonal matrix or Newton-Raphson methods). In this work, different tray to tray calculation methods are suggested for distillation columns, that combine original approximate and rigorous procedures to solve the mass and energy balances and

the equilibrium relations, avoiding the iterations necessary for equilibrium calculations and optimising the feed tray location.

The calculation procedure suggested is based on a extension of the graphical method of Ponchon-Savarit for complex columns and for multicomponent mixtures proposed by Marcilla *et al.* (1995). The methods proposed in this work are design methods in the sense that knowing the product compositions and reflux calculate the number of stages and the optimum feed stage location.

The proposed procedures have been applied to two ternary mixtures, both ideal and non-ideal respectively, and the results obtained have been compared with those provided by a conventional rigorous method, showing a very good agreement. The effect of the different calculation and interpolation methods suggested has been analysed.

2. Calculation procedure

An extension of The Ponchon-Savarit method to solve the problem of the separation of a binary mixture in a complex column was proposed by Marcilla *et al.* (1995). The extension of this procedure to multicomponent mixtures can be easily made if explicit functions for the saturated vapor enthalpy, saturated liquid enthalpy and saturated liquid composition of the type $H=H(y^i, T, P)$, $h=h(x^i, T, P)$ and $x^i=x(y^i, T, P)$ are available. In the other case, approximate methods are necessary. In this work, we have generated these enthalpy functions from fittings of the

equilibrium data in all the composition range to polynomial functions. These functions have been combined with different suggested interpolation methods in order to obtain the equilibrium compositions at each stage.

Figure 1 shows a sketch of the location of the net flow points (Δ_j) and the graphical solution of a simple column for a ternary system, as in the classical Ponchon-Savarit method for binary mixtures. Obviously, systems with more than three components (and ternary systems with great difficulties) cannot be graphically represented and the problem must be solved by the use of computational methods. Nevertheless, these methods are still based on the same geometrical concepts as those used for the binaries in combination with the algorithms that involve the corresponding equations for the equilibrium conditions and mass and enthalpy balances. Equations (1) and (2) show the composition (δ_k) and enthalpy (M_k), respectively, of the net flow (Δ_k) in the section k of the column of Figure 2, in the Ponchon Savarit diagram:

$$\delta_k^{(j)} = \frac{\sum_k P_k \cdot z_{p,k}^{(j)} + D \cdot x_D^{(j)} - \sum_k A_k \cdot z_{A,k}^{(j)}}{\sum_k P_k + D - \sum_k A_k} \quad (1)$$

$$M_k = \frac{\sum_k P_k \cdot H_{p,k} + D \cdot H_D + Q_D}{\sum_k P_k + D - \sum_k A_k} - \frac{\sum_k A_k \cdot H_{A,k} + \sum_k Q_{E,k} - \sum_k Q_{A,k}}{\sum_k P_k + D - \sum_k A_k}$$

where Eqn. (3) represents the operative line in the enthalpy-composition diagram.

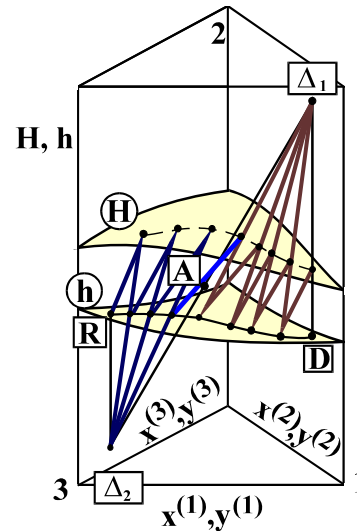


Figure 1. Graphical representation of the Ponchon-Savarit method for a ternary mixture.

$$\frac{L_{k,i+1}}{V_{k,i}} = \frac{(y_{k,i}^{(1)} - x_k^{(1)})}{(x_{k,i+1}^{(1)} - x_k^{(1)})} = \dots \quad (3)$$

$$\dots = \frac{(y_{k,i}^{(c)} - x_k^{(c)})}{(x_{k,i+1}^{(c)} - x_k^{(c)})} = \frac{(H_{k,i} - M_k)}{(h_{k,i+1} - M_k)}$$

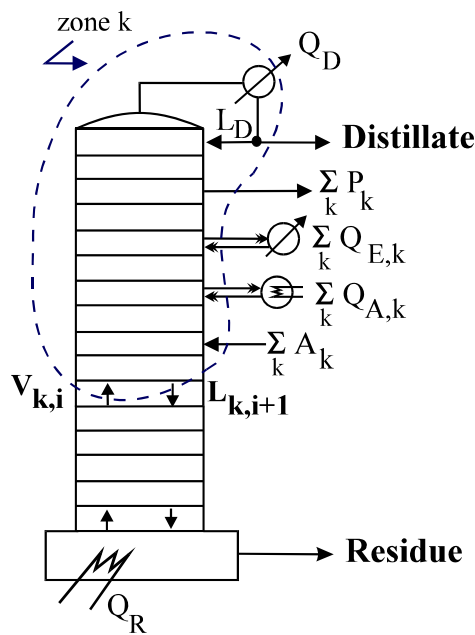


Figure 2. Generalized distillation column.

To find the analytical solution to the problem, two problems must be solved:

a) Establish a procedure to calculate, the vapor-liquid equilibrium and to obtain the liquid phase in equilibrium with a given vapor phase (or viceversa) in each tray, and b) to set a procedure to obtain the intersection point between the operative line and the enthalpy-composition surface (in the enthalpy/composition n-dimensional space).

2.1. Procedures to calculate the vapor-liquid equilibrium

The methods proposed in this work fall into two categories:

a) the rigorous method, where the equilibrium data have been obtained using the NRTL model and the procedure proposed by Renon *et al.* (1971). This method obviously involves

an iterative calculation method wherever an equilibrium composition is required.

b) the approximate methods suggested, where the equilibrium data in all the composition range are generated at once by the previous rigorous procedure forming two ordered lattices of equilibrium points. The data obtained in such a way, are used in combination with any of the interpolation methods suggested allowing (without any iterative calculation) the determination of the composition in equilibrium with any given phase in equilibrium.

The interpolation procedures proposed in this work are the following:

2.1.1. Simple interpolation with distances

This procedure was suggested and applied elsewhere (Ruiz *et al.*, 1986) to a liquid-liquid extraction problem. This method involves the following steps:

a) in the network corresponding to the phase containing the point whose equilibrium composition is to be calculated (P_0 , with composition $x_o^{(i)}$), to find the three nearest points, P_1 , P_2 and P_3 (with compositions $x_p^{(i)}$) and to calculate their distances, d_p , from point P_0 in the composition space, according to the following equation:

$$d_p = \sqrt{\sum_i (x_o^{(i)} - x_p^{(i)})^2} \quad (4)$$

The coordinates of the interpolated point (P'_0) in the conjugated phase are obtained from points P'_1 , P'_2 and P'_3 , in equilibrium with P_1 , P_2 and P_3 ,

applying Eqn. (5) which considers the contribution of each point inversely to its distance to P_0 .

$$y_o^{(i)} = \frac{\sum_p \frac{y_p^{(i)}}{d_p}}{\sum_p \frac{1}{d_p}} \quad (5)$$

This is a very simple method, but yields results which are not very accurate except for very dense networks, because the vapor-liquid equilibrium produces a distorsion in the conjugated equilibrium space which is not considered by this method. A diagram of this procedure is shown in Figure 3.

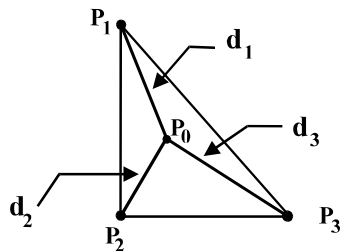


Figure 3. Simple interpolation with distances

2.1.2. Interpolation by intercepting lines from the three or four nearest points.

These two methods do consider the equilibrium network distorsion and relate the composition of the point to be interpolated, not only with those of the (three/four) nearest points, but also their relative positions in the equilibrium lattice. The calculation method has been prepared to operate with the nearest three or four points, and because both

methods are very similar, only the second procedure based on the four nearest points is described.

This procedure of interpolation involves the following steps:

- a) to find the four nearest points, P_1 , P_2 , P_3 and P_4 , to point P_0 to be interpolated,
- b) to calculate the respective distances, d_p , to P_0 ,
- c) to obtain the intersection points between the following straight lines:
 P_5P_6 and P_1P_2
 P_5P_6 and P_3P_4
 P_7P_8 and P_1P_3
 P_7P_8 and P_2P_4
as shown in Figure 4,

d) calculate the distances d_5 , d_6 , d_7 and d_8 , also described in Figure 4, and the corresponding distances d'_5 , d'_6 , d'_7 and d'_8 in the conjugated phase, as indicated in Figure 5, and according to Eqn. (6), which allows the situation of points P'_5 , P'_6 , P'_7 and P'_8 to be fixed.

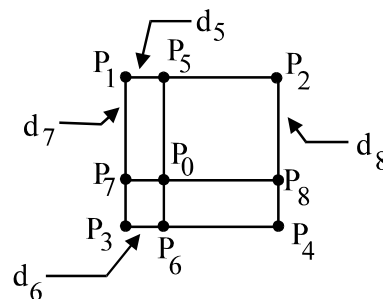


Figure 4. Intercepting lines for interpolation with four points. Localization of point of interpolation.

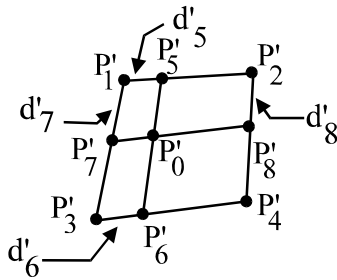


Figure 5. Intercepting lines for interpolation with four points. Localization of interpolated point.

$$\begin{aligned}
 d'_5 &= d_5 \cdot \frac{[P'_1 P'_2]}{[P_1 P_2]} & d'_6 &= d_6 \cdot \frac{[P'_3 P'_4]}{[P_3 P_4]} \\
 d'_7 &= d_7 \cdot \frac{[P'_1 P'_3]}{[P_1 P_3]} & d'_8 &= d_8 \cdot \frac{[P'_2 P'_4]}{[P_2 P_4]}
 \end{aligned}
 \tag{6}$$

e) the interpolated point, P'_0 , is obtained from the intersection between the straight lines P_5P_6 and P_7P_8 .

The calculation procedure for the interpolation method from intercepting straight lines with three points can be easily understood from the diagram shown in Figure 6.

The results obtained by these methods are better than those from the simple interpolation method.

2.1.3. Interpolation from linear fitting of compositions

This method is based on expressing the composition of point P_0 as a linear combination of the compositions of the three nearest points, P_1, P_2, P_3 :

$$P_0 = a \cdot P_1 + b \cdot P_2 + c \cdot P_3 \tag{7}$$

Because the three points P_i are defined by their composition and by their enthalpy, there are two possibilities for the interpolation, depending on the three coordinates chosen to define the equilibrium:

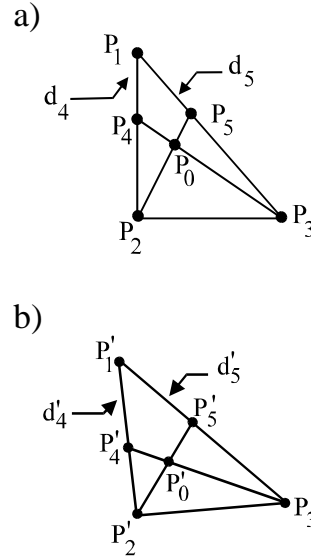


Figure 6. Intercepting lines for interpolation with three points. Localization of point of interpolation (a) and interpolated point (b).

- a) interpolation using linear fitting of compositions or,
- b) interpolation using linear fitting of compositions and enthalpies.

When these coordinates are defined:

$$P_k = \left(x_k^{(1)}, x_k^{(2)}, \dots, x_k^{(c)} \right)$$

the solution of the system of equations shown in Eqn. (8) allows the calculation of the coefficients a, b and c:

$$X_0 = X \cdot A$$

$$X_0 = \left(x_0^{(1)}, x_0^{(2)}, \dots, x_0^{(c)} \right)^T$$

$$A = (a, b, c)^T \quad (8)$$

$$X = \begin{pmatrix} x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(c)} \\ x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(c)} \\ x_3^{(1)} & x_3^{(2)} & \dots & x_3^{(c)} \end{pmatrix}$$

a, b and c can be used to find the point P'0, from points P'1, P'2 and P'3, in equilibrium with P1, P2 and P3.

This method is similar to the simple interpolation method and, does not consider the distortion of the conjugated lattice produced by de vapor-liquid equilibrium either.

2.2. Procedures to calculate the mass and energy balances

In the Ponchon-Savarit method, the mass and energy balances connect two consecutive trays through the net flow, Δ_k , intersection between the operative line shown in Eqn. (3) (that connects points Δ_k and $L_{k,j+1}$) with the surface defined by the points representing the saturated vapor (Figure 1). The procedures proposed in this work to solve this intersection are of two types: i.e., approximate and rigorous methods.

2.2.1. Approximate methods

The approximate procedures proposed in this work require a fitting of the equilibrium points in each phase to the corresponding enthalpy-composition polynomial functions, as shown in Eqn. (9):

$$a \cdot (z^{(1)})^2 + b \cdot (z^{(2)})^2 + c \cdot z^{(1)} + d \cdot z^{(2)} + e \cdot H = 1 \quad (9)$$

where z can be x or y and H can be h or H depending on the phase. This equation represents parabolic surfaces, and its intersection with the operative lines (Eqn. 3) allows the mass and energy balances to be solved using a simple method.

This method involves very short calculation times and yields very good results.

The solution for the enthalpy of this intersection point is of the type shown in Eqn. (10):

$$A \cdot h^2 + B \cdot h + C = 0 \quad (10)$$

and there are two possible solutions, but only one with a physical sense. The correct solution is selected by comparison with the average value of equilibrium enthalpy.

Another procedure that allows better results than that previously described is to find the three nearest points from the intersection point and afterwards obtain a linear fitting of their enthalpies versus their compositions (Eqn. 11):

$$h = c_1 \cdot x^{(1)} + c_2 \cdot x^{(2)} + c_3 \cdot x^{(3)} \quad (11)$$

the coefficients of this fitting, in combination with the composition of the intersection point previously calculated, allow the obtention of a new enthalpy value, that once substituted in the Eqn. (3) of the operative line, allows a better new composition. This composition can be considered as definitive, or used in Eqn. (11) in an iterative process to find

the best value of the intersection. Generally, after two or three iterations, the values are very stable.

2.2.2. Rigorous method

This method is based on an iterative process that calculates, in a rigorous way, the intersection between the enthalpy/composition function and the operative lines, by solving the following system of equations:

$$\begin{aligned}
 y^{(i)} &= K^{(i)} \cdot x^{(i)} \\
 \frac{L_{k,i+1}}{V_{k,i}} &= \frac{\left(y_{k,i}^{(1)} - \delta_k^{(1)} \right)}{\left(x_{k,i+1}^{(1)} - \delta_k^{(1)} \right)} = \dots \\
 \dots &= \frac{\left(y_{k,i}^{(c)} - \delta_k^{(c)} \right)}{\left(x_{k,i+1}^{(c)} - \delta_k^{(c)} \right)} = \frac{\left(H_{k,i} - M_k \right)}{\left(h_{k,i+1} - M_k \right)}
 \end{aligned}
 \tag{12}$$

The expressions for the equilibrium constants, $K^{(i)}$, are very complex and non-linear. Consequently, Eqn. (12) must be solved by an iterative procedure. In this case the problem has been solved by the procedure shown in Figure 7: calculation begins at an equilibrium point P_1 , near to intersection point; its enthalpy h_1 allows the calculation of (by Eqn. 3) the composition of a point P_2 , with the same enthalpy as P_1 , but not in the equilibrium surface. A rigorous calculation with the composition of P_2 , allows P_3 to be obtained, on the equilibrium surface with the same composition but different enthalpy. This point is used for the next iteration. This process continues until the difference

between the two consecutive values of enthalpy is less than a small quantity previously fixed.

This procedure is, obviously slower than the approximate methods, but yields the most accurate results.

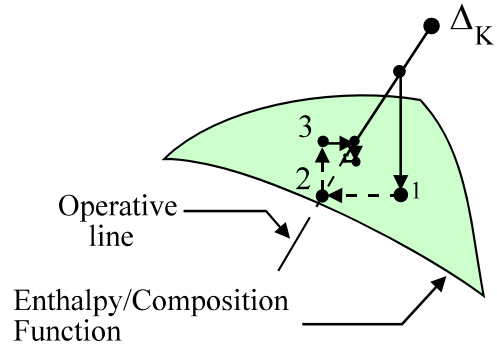


Figure 7. Sketch of the iterative calculation to determine the intersection point between an operative line and the enthalpy-composition surface

3. Description of proposed procedure

The proposed procedures for designing a rectifier of ternary mixtures are based on the Ponchon-Savarit method and includes various combinations of rigorous or approximate methods. Figure 8 shows the general flowsheet corresponding to the algorithm of calculation used in this work.

There are three categories of calculation programs:

rigorous program, that rigorously solve the mass and energy balances and the equilibrium equations, *semi-rigorous programs*, that rigorously solve the equilibrium equations but only approximately the enthalpy balances and

approximate programs, that approximately solve both enthalpy balances and equilibrium equations.

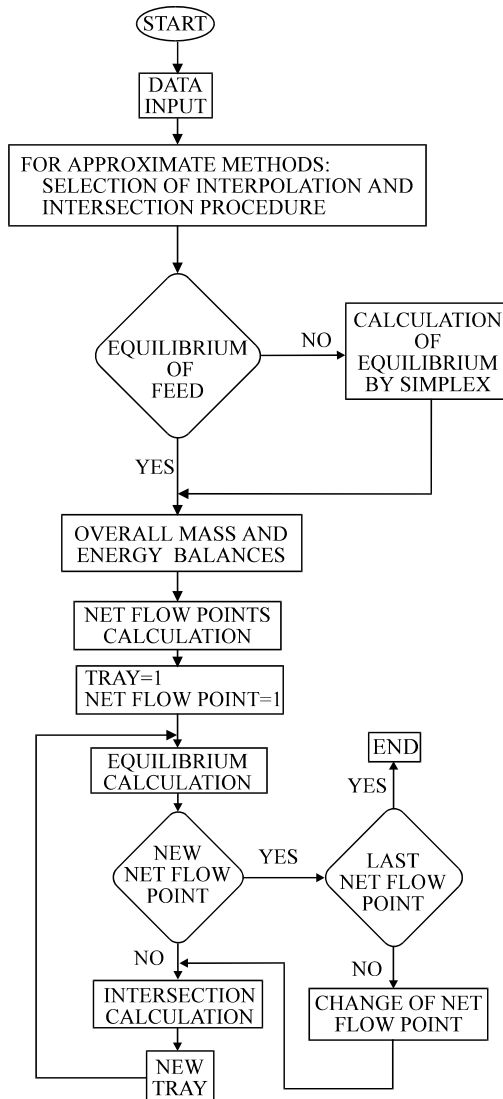


Figure 8. Flowsheet of proposed program for calculation of a rectification column.

All programs start with the input of required data:

- * Percentage of separation desired
- * Net flow of distillate
- * Reflux (L_D/D)
- * Characteristics of side streams (feeds, side products or heat additions or removals): flow, composition, enthalpy

and code indicating a mass stream or a heat stream. The sign of flow indicates a feed or a side product.

* Thermodynamic data for the components of the system

* A file containing the lattice of equilibrium points and the coefficients of their fittings to polynomial functions. After the data input, the calculation procedure which can be summarized in the following steps, begins:

* Solve the equations for overall mass and energy balances

* Locate the net flows, Δ_k

* Start the tray to tray calculations

The equations for overall mass and energy balances are shown elsewhere (Marcilla *et al.*, 1995) and the equilibrium is calculated using the NRTL model (Renon *et al.*, 1971).

The tray to tray calculation procedure starts at the top of column, from the distillate composition, which is the same as that of the vapor from the first tray, and calculating the liquid in equilibrium with this vapor. To pass to the next tray, it is necessary to solve the mass and energy balances. This can be done by connecting the point representative of the liquid with the point representative of the net flow of the corresponding sector of the column (operative line, Eqn. 3) and calculating the intersection of this straight line with the equilibrium surface corresponding to the saturated vapor: the intersection point is the vapor leaving the next tray. This procedure is repeated until the tray where a side stream (feed or product in its optimum location) is reached, and

where the change of sector (and of course of net flow point, Δ_k) is required.

The following criterion has been used to test if this condition has been reached: - the last tray in a sector is that which verifies Eqn. (14):

$$\frac{x_{k,i}^{(1)} / x_{A,i}^{(1)}}{x_{k,i}^{(3)} / x_{A,i}^{(3)}} \leq 1 \quad (13)$$

where the subindex A refers to the side stream separating sectors k and k+1. The procedure continues, using the same criterion until the residue composition calculated from the overall mass balance is reached or exceeded.

4. Results

In order to test the validity of the proposed methods, BASIC programs were prepared, according to the previous procedures. The programs were applied to two ternary mixtures, and the results compared with those obtained by the rigorous method described by Renon *et al.* (1971). Table 1 shows the characteristics of each problem considered. Both distillation columns analysed are simple, with only one liquid feed at the bubble point, and with a total condenser that produces the distillate (D) and the reflux (L_D) streams, both at the bubble points. The components of the mixture in column 1 are considered to form an ideal system in the vapor phase, whereas those in column 2 form a heavy non-ideal system

in the vapor phase. Several equilibrium lattices have been calculated for both systems, at varying composition increments (Table 2). These lattices have been used to test the influence of the composition increment in the lattice (i.e., the number of equilibrium points in the lattice) on the accuracy of the different interpolation methods, as well as on the intersection of the operating lines with vapor surface.

Table 1. Characteristics of distillation columns

	Feed of column 1	Feed of column 2
Flow(mol/h)	100	100
Composition (molar fraction)	Benzene: 0.600 Cyclohexane: 0.006 Toluene: 0.394	Methanol: 0.55 Acetone: 0.15 Water: 0.30
Distillate flow (mol/h)	60	69
Reflux ratio (L_D/D)	2	2
% Separation of key component 1	97.3072	96.9187
% Separation of key component 2	97.39858	97.6606

Table 2. Lattices for vapor-liquid equilibrium points

Composition increment	Number of points
0.001	5151
0.025	861
0.05	231
0.1	66

Figures 9 and 10 compare the results obtained from the rigorous method presented in this work and the results from Renon *et al.* (1971). As can be seen, the results are exactly the same, as expected since both are rigorous methods. It should be noted that the proposed procedure presents several advantages over other methods found in literature, such as the short calculation time required and its theoretical simplicity as it is based on the same geometrical concepts as the Ponchon and Savarit method.

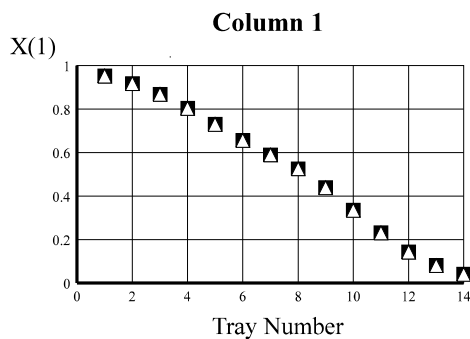


Figure 9. Comparison between the rigorous method proposed in this work (⊕) and those from Renon *et al.* (1971) (Δ), for column 1

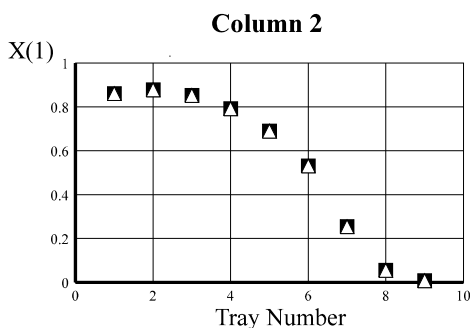


Figure 10. Comparison between the rigorous method proposed in this work (⊕) and those from Renon *et al.* (1971) (Δ), for column 2.

For the next discussion, the results obtained by the rigorous method proposed are used to test the validity of approximate and semi-rigorous methods.

Figure 11 shows the comparison between the results obtained for column 1 by the approximate methods, using a network with 231 points and varying the interpolation procedure (to solve the equilibrium eqns.) and the intersection procedure (to solve the mass and energy balances) selected as compared to the results obtained by the rigorous method. Interpolation 1 refers to simple interpolation, interpolation 2 and 3, to those with intercepting lines from the four or three nearest points respectively and interpolations 4 and 5 are those based on linear fitting of compositions or compositions and enthalpies, respectively. Intersection 1 refers to normal intersection described in section 2.2.1 of this paper and intersection 2 is that with linear fitting of enthalpies.

As can be seen in Figure 11, interpolation 1 yields the poorest results, as was expected, since this method does not take into account the distortion of the vapor-liquid equilibrium network. Interpolation 2 and 4 allow very coincident results: it can be concluded that there are two different ways (one geometrical and the other arithmetical) of expressing the same concepts. Logically, interpolation 5 is very close to interpolation 4 because the only difference is the type of coordinates used. In general it can be said that the best results are those obtained by

interpolation 3, by intercepting lines from the nearest four points.

With regard to the two types of intersection proposed, intersection 2 yields the best results.

The results obtained for column 2 lead to similar conclusions.

As an example, Figure 12 shows the comparison between the results obtained for column 1 by the approximate methods, using lattices with different number of points (increment in composition in mole fraction of 0.1, 0.05 and 0.025, corresponding to lattices with 66, 231 and 861 points, respectively) using the best approximate option (interpolation 3 and intersection 2). When a comparison between all options is made, it can be concluded that from an increment in the composition of 0.05 (in mole fraction) all methods yield excellent results and that the results are improved when increasing the number of points of the lattice. This is an important conclusion because it allows a multicomponent complex distillation column to be calculated in short time, as with shortcut methods, but with an accuracy close to that provided by rigorous methods.

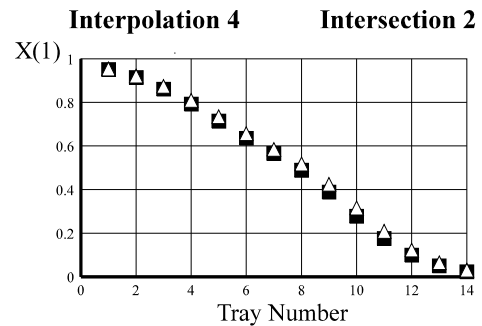
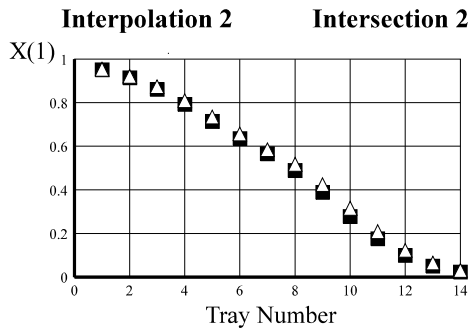
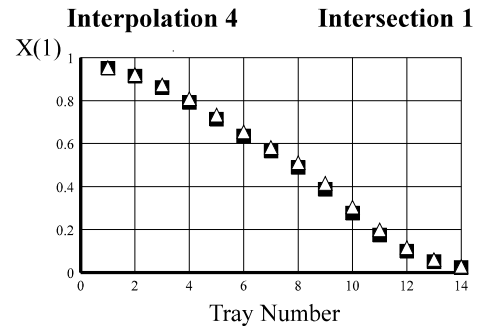
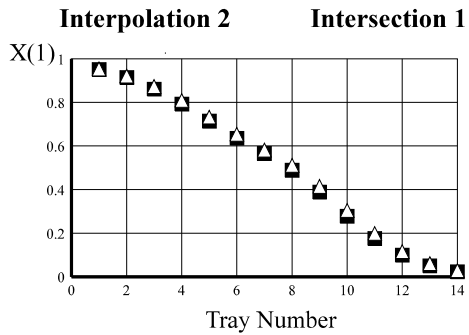
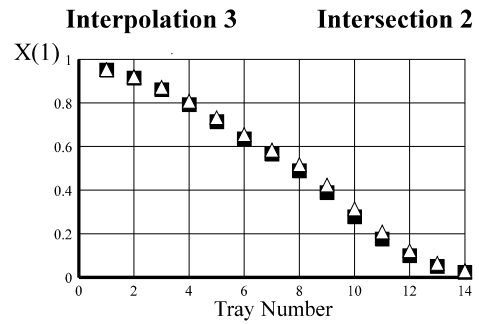
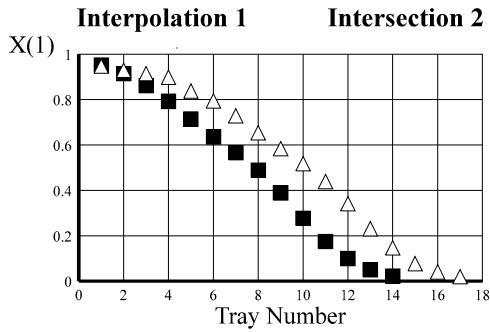
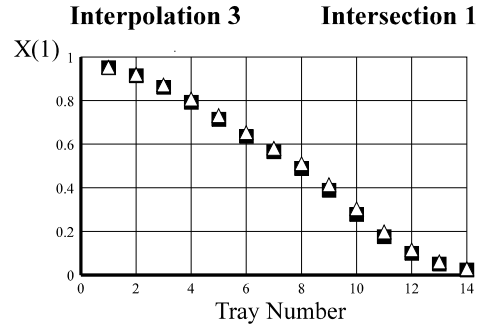
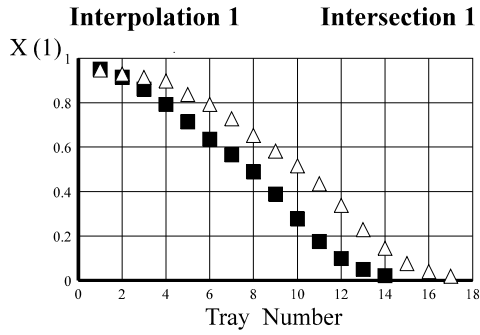
The results obtained by the application of semirigorous methods to the two examples show the same influence of the spacing of the network: accuracy is greater when the number of points increases. Figures 13 and 14 show results for column 1 and column 2, respectively, when comparing the semirigorous methods (with intersection 1 and 2) and the rigorous method, for lattices with 231 points. Semi-rigorous

methods lead to very good results, especially when using the intersection with fitting of enthalpies. This fact is very important since it allows lattices with a smaller number of points to be used.

5. Conclusions

In this work, several methods for multicomponent distillation complex column calculations are proposed. These procedures range from the approximate methods to a rigorous method, and are based on very simple geometrical concepts. Results obtained are very close to the rigorous methods but use highly reduced calculation times.

Approximate methods yield good results, even for lattices with a relatively small number of points. Results greatly depend on the type of interpolation used. The simple interpolation method is the one yielding the worse results and the interpolation with intercepting straight lines with four points, is the one yielding the better results. In all cases, a remarkable improvement of the results can be noted when increasing the number of points in the lattice. Obviously, with a saturating type behaviour. Semi-rigorous methods lead to very good results, especially when using the intersection with fitting of enthalpies. This fact allows lattices with a smaller number of points to be used. As expected, the rigorous method leads to the same results as other rigorous methods proposed in literature.



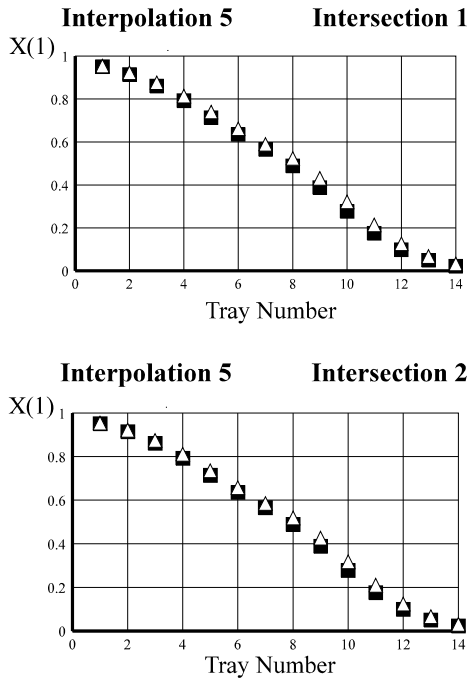


Figure 11. Comparison between approximate (Δ) and rigorous methods (\bullet), for column 1 using a lattice with 231 points (increment in the composition in mole fraction of 0.05).

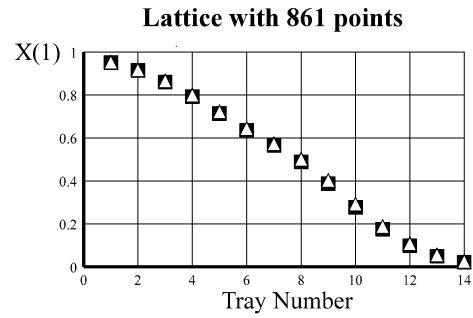
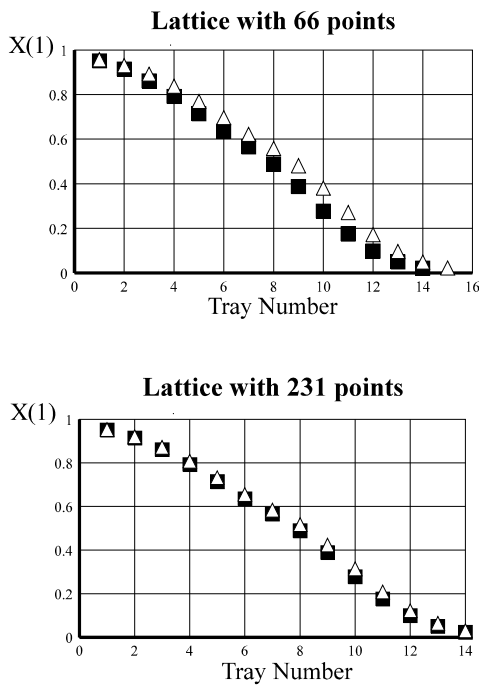


Figure 12. Comparison between rigorous (\bullet), and approximate methods (Δ), using lattices with different number of points

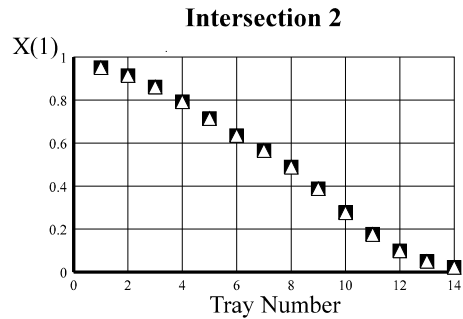
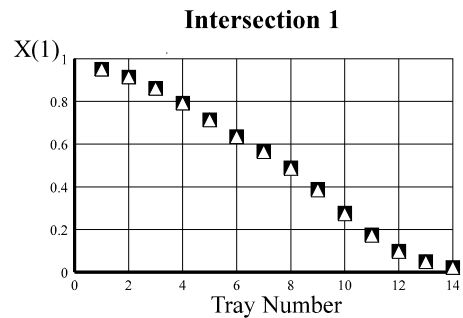
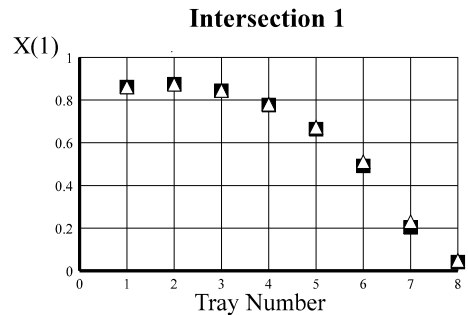


Figure 13. Comparison between semirigorous (Δ) and rigorous methods (\bullet), for column 1, using a lattice with 231 points.



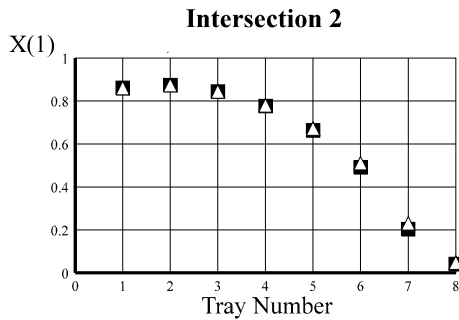


Figure 14. Comparison between semirigorous (Δ) and rigorous methods (\otimes), for column 2, using a lattice with 231 points.

List of symbols

A_k : Feed flow rate number k .

A, B, C y a, b, c, d, e: adjust coefficients.

D: Distillate flow rate.

d_i : Distance between P_i and P_0 .

H: Enthalpy of the vapor phase.

H_D : Enthalpy of the vapor from top of column.

h: Enthalpy of the liquid phase.

h_D : Distillate enthalpy.

$H_{A,k}$: Enthalpy of feed number k .

$H_{P,k}$: Enthalpy of side stream number k .

$K^{(i)}$: Equilibrium constant for component number i .

L_D : Reflux mass flow.

$L_{k,i}$: Flow rate of the liquid from stage i in sector k .

M_k : Enthalpy of the net flow in zone k .

P_i : Points for interpolation.

P'_i : Points in equilibrium with P_i .

P_k : Side-product flow rate number k .

$Q_{A,k}$: Heat added in the interboiler number k .

Q_D : Heat eliminated in the top condenser.

$Q_{E,k}$: Heat eliminated in an intercondenser or heat losses in zone k .

Q_R : Heat added in the reboiler.

R: Residue mass flow.

$V_{k,i}$: Mass flow of the vapor stream from stage i in zone k .

x^i : Mole fraction of component i in phase liquid.

$x_D^{(j)}$: Composition of the distillate stream.

$x_{k,i}^{(j)}$: Composition of the liquid stream from stage i in zone k .

$x_R^{(j)}$: Composition of the residue stream.

y^i : Mole fraction of component i in phase vapor.

$y_{k,i}^{(j)}$: Composition of the vapor stream from stage i in zone k .

$z_{A,k}^{(j)}$: Composition of the feed stream number k .

$z_{P,k}^{(j)}$: Composition of the side-product stream number k .

$\Delta_{C,k}$: Net mass flow in the zone between the upper and lower stages of the feed number k .

Δ_D : Net mass flow in the rectifying sector of a simple column.

Δ_k : Net mass flow in sector k .

Δ_R : Net mass flow in the stripping sector of a simple column.

$\delta_k^{(i)}$: Composition of the net mass flow point k .

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