

## MULTICOMPONENT RECTIFICATION: A NEW METHOD OF CALCULATION

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**This poster 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.**

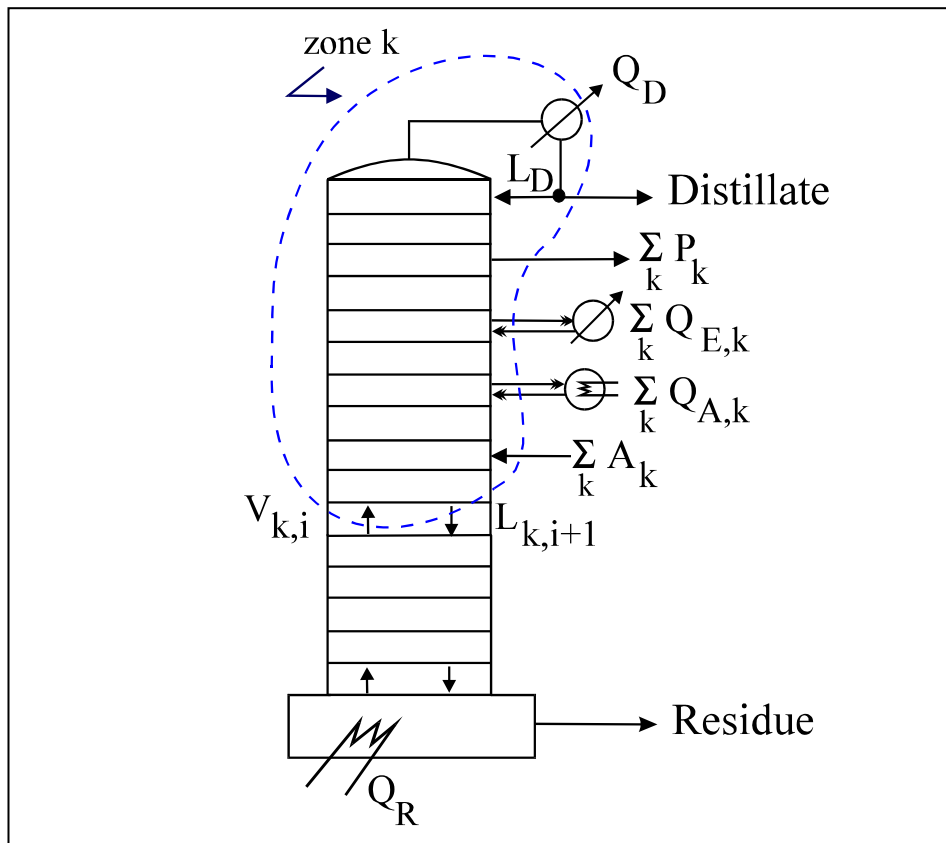
In 1995 Marcilla *et al.* proposed an extension of The Ponchon-Savarit method to solve the problem of the separation of a binary mixture in a complex column as those of the Fig. 1. The equations are the following:

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

$$M_k = \frac{\sum_k P_k \cdot H_{p,k} + D \cdot H_D + Q_D - \sum_k A_k \cdot H_{A,k} - \sum_k Q_{E,k} + \sum_k Q_{A,k}}{\sum_k P_k + D - \sum_k A_k} \quad (2)$$

$$\frac{L_{k,i+1}}{V_{k,i}} = \frac{\left( y_{k,i}^{(1)} - x_k^{(1)} \right)}{\left( x_{k,i+1}^{(1)} - x_k^{(1)} \right)} = \frac{\left( y_{k,i}^{(c)} - x_k^{(c)} \right)}{\left( x_{k,i+1}^{(c)} - x_k^{(c)} \right)} = \frac{\left( H_{k,i} - M_k \right)}{\left( h_{k,i+1} - M_k \right)} \quad (3)$$

Equations (1) and (2) show the composition ( $\delta_k$ ) and enthalpy ( $M_k$ ), respectively, of the net flow ( $\Delta_k$ ) in the section  $k$  of the column of Figure 1 in the Ponchon Savarit diagram and Eqn. (3) represents a operative line in the enthalpy-composition diagram.



**Figure 1. Generalized distillation column.**

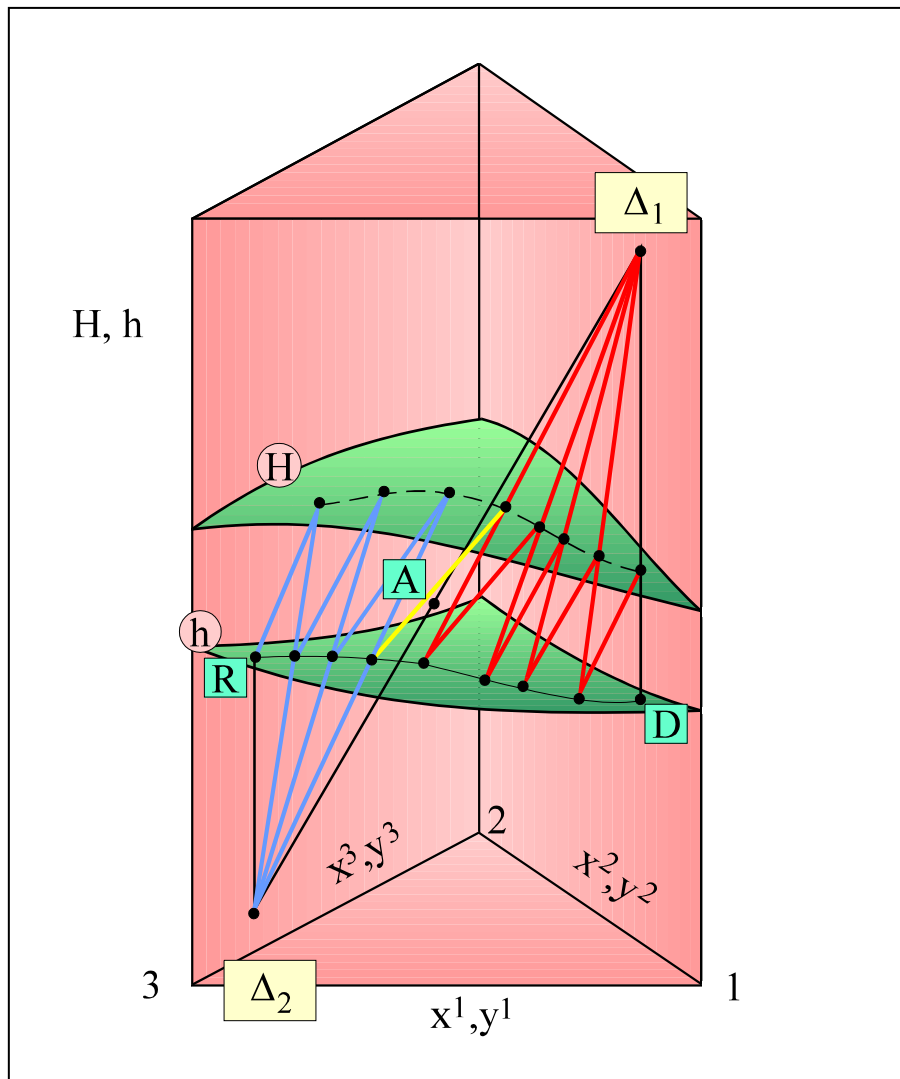
Figure 2 shows a sketch of the location of the net flow points ( $\Delta_j$ ) and the graphical solution of a simple column for a ternary system, as in the classical Ponchon-Savarit method for binary mixtures. Obviously, systems with more than three components (and ternary systems with great difficulties) cannot be graphically represented and the problem must be solved by the use of computational methods.

The extension of this procedure to multicomponent mixtures proposed by Marcilla et al. (1995) 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.

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

- 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,

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).



**Figure 2. Graphical representation of the Ponchon-Savarit method for a ternary mixture.**

## PROCEDURES TO CALCULATE THE VAPOR-LIQUID EQUILIBRIUM

The methods proposed in this work fall into two categories:

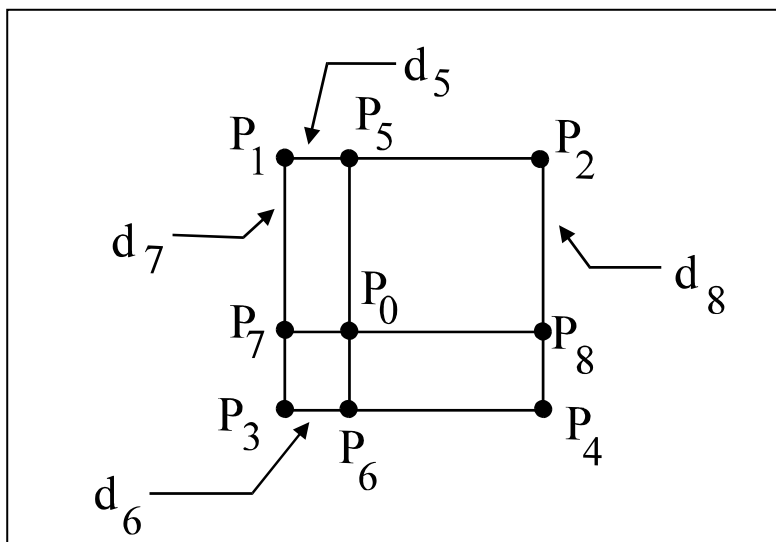
a) the rigorous method, where the equilibrium data have been obtained using the NRTL model and the procedure proposed by Renon *et al.* (1971) (this method obviously involves an iterative calculation method wherever an equilibrium composition is required).

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 based in the following steps:**

- 1) In the network corresponding to the phase containing the point whose equilibrium composition is to be calculated ( $P_0$ ) to find the three nearest points ( $P_i$ ,  $i \neq 0$ ) and to calculate their distances,  $d_i$ , from point  $P_0$  in the composition space.
- 2) To find the points  $P'_i$  in equilibrium with  $P_i$  in the network corresponding to the conjugated phase.
- 3) To establish an appropriate relation between  $P_0$  and  $P_i$ .
- 4) Translate the previous relation to the other phase for pass from  $P'_i$  to  $P'_0$ .

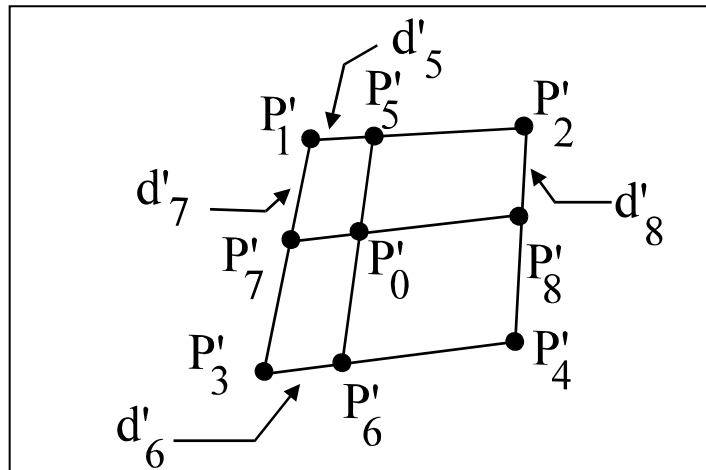
Figures 3 and 4 shows one of this procedures proposed with the existing relation between the corresponding points.



**Figure 3. Intercepting lines for interpolation with four points. Localization of point of interpolation.**

The interpolated point,  $P'_0$ , is obtained from the intersection between the straight lines  $P_5'P_6'$  and  $P_7'P_8'$  (Fig. 4).

$$\begin{aligned}
 d_5' &= d_5 \cdot \frac{[P_1'P_2']}{[P_1P_2]} & d_6' &= d_6 \cdot \frac{[P_3'P_4']}{[P_3P_4]} \\
 d_7' &= d_7 \cdot \frac{[P_1'P_3']}{[P_1P_3]} & d_8' &= d_8 \cdot \frac{[P_2'P_4']}{[P_2P_4]}
 \end{aligned}
 \tag{4}$$



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

An **Interpolation from linear fitting of compositions** is also proposed, based on expressing the composition of point  $P_0$  as a linear combination of the compositions of the three nearest points,  $P_1, P_2, P_3$ :

$$P_0 = a \cdot P_1 + b \cdot P_2 + c \cdot P_3 \tag{5}$$

When these coordinates are defined:

$$P_k = \left( x_k^{(1)}, x_k^{(2)}, \dots, x_k^{(c)} \right) \tag{6}$$

the solution of the system of equations shown in Eqn. (7) allows the calculation of the coefficients  $a, b$  and  $c$ :

$$X_0 = X \cdot A$$

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

$$A = (a, b, c)^T \tag{7}$$

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

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.

## PROCEDURES TO CALCULATE THE MASS AND ENERGY BALANCES

### i) Approximate methods

The approximate procedure 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. (8):

$$a \cdot (z^{(1)})^2 + b \cdot (z^{(2)})^2 + c \cdot z^{(1)} + d \cdot z^{(2)} + e \cdot H = 1 \tag{8}$$

where  $z$  can be  $x$  or  $y$  and  $H$  can be  $h$  or  $H$  depending on the phase. This equation represents parabolic surfaces, and their 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 time, yields very good results and can be improved by updating the fitting of the enthalpies using the nearest points to the intersection point versus their compositions.

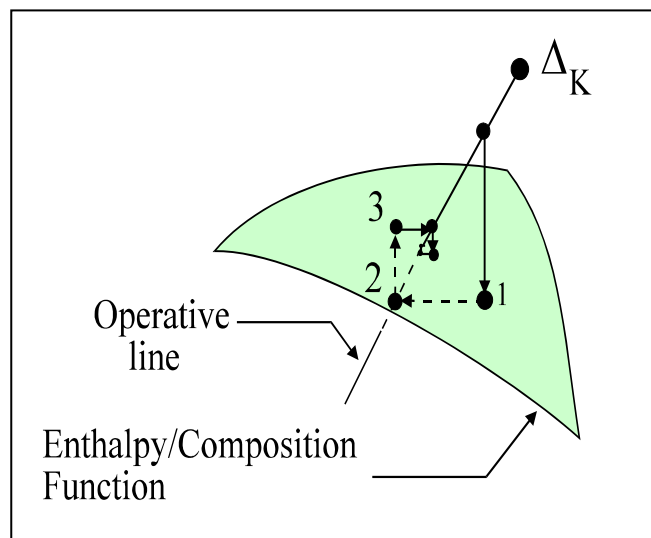
### ii) Rigorous method

The problem has been solved by the procedure shown in Figure 5: calculation begins at an equilibrium point P1, near to the intersection point; its enthalpy  $h_1$  allows the calculation of the composition of a point P2 (by Eqn. 3), with the same enthalpy as P1, but not in the equilibrium surface. A rigorous calculation with the composition of P2, allows P3 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.

Figure 6 shows the general flowsheet corresponding to the algorithm of calculation used in this work and Eqn (9) shows the criterion has been used to test if the condition for the change of sector (and of  $\Delta k$ ) has been reached: - the last tray in a sector is that which verifies Eqn. (9), where the subindex A refers to the side stream separating sectors k and k+1.

$$\frac{x_{k,i}^{(1)} / x_{k,i}^{(3)}}{x_{A,i}^{(1)} / x_{A,i}^{(3)}} \leq 1 \quad (9)$$



**Figure 5. Sketch of the iterative calculation to determine the intersection point between an operative line and the enthalpy-composition surface.**

## RESULTS

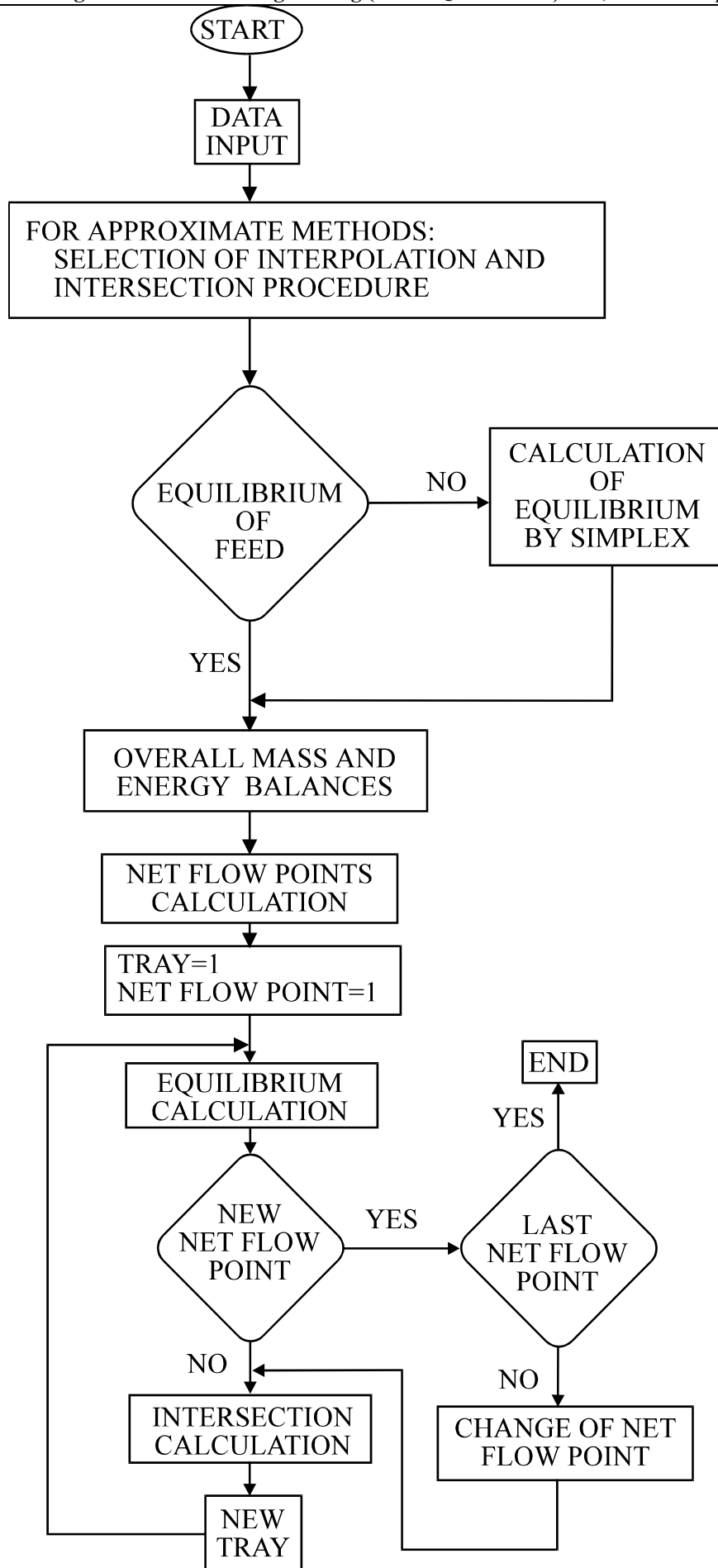
As an example, Figure 6 shows the comparison between the results obtained for a column with the characteristics of the table 1 by the approximate methods, using a

network with 231 points and varying the interpolation procedure to solve the equilibrium and compared to the results obtained by the rigorous method. Figure 7 compares the results obtained from the rigorous method presented in this work and the results from Renon *et al.* (1971).

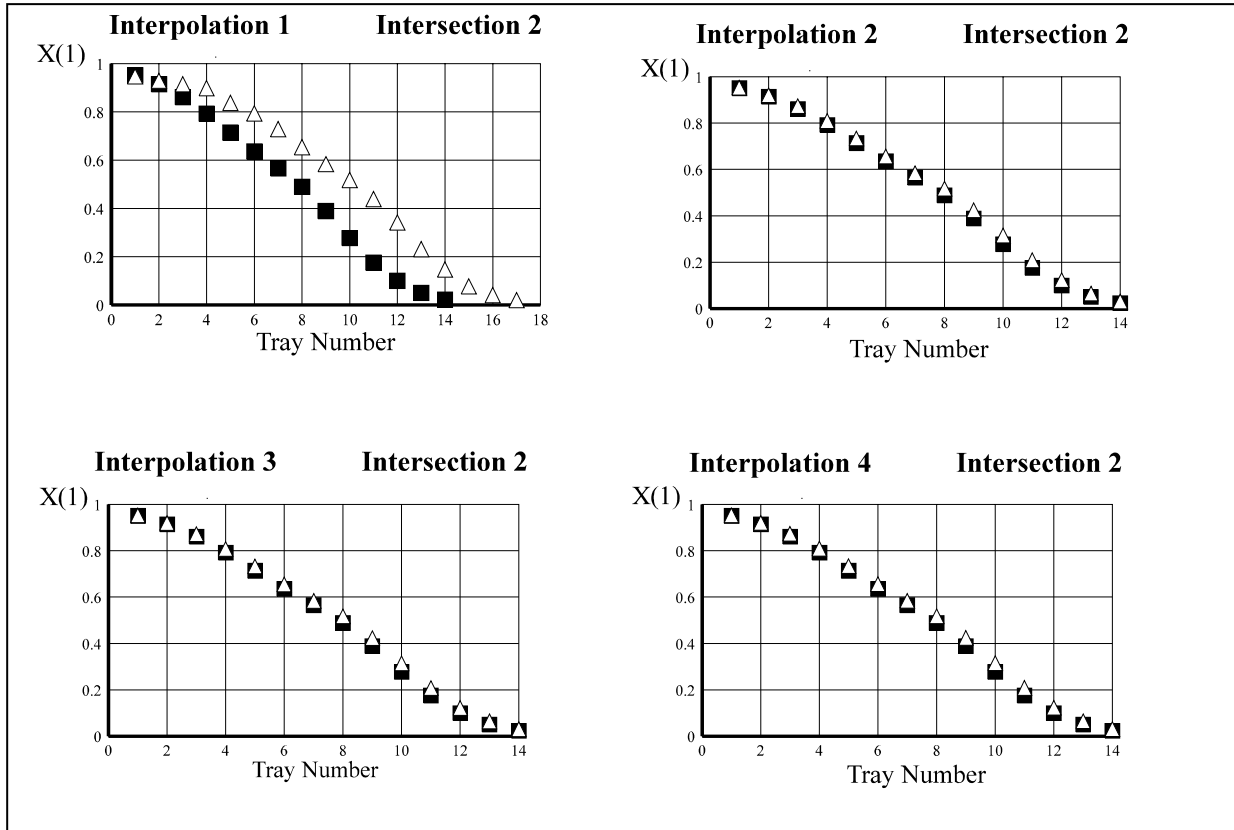
**Table 1. Characteristics of distillation column**

|                                   |  |
|-----------------------------------|--|
| Feed Flow rate (mol/h)            | 100  |
| Feed Composition (molar fraction) | Benzene: 0.600<br>Cyclohexane:0.006<br>Toluene:0.394 |
| Distillate flow rate (mol/h)      | 60   |
| Reflux ratio (LD/D)               | 2  |
| % Separation of key component 1   | 97.3072  |
| % Separation of key component 3   | 97.39858   |

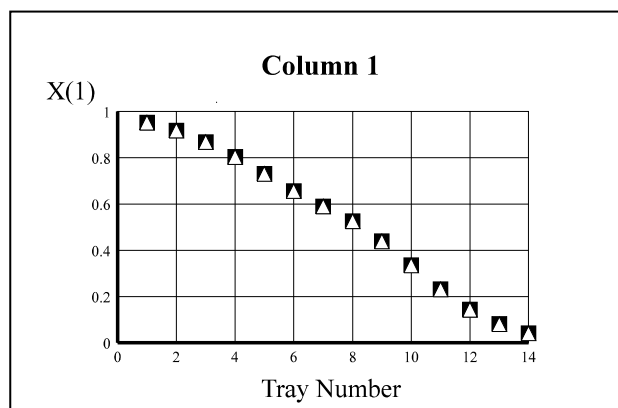




**Figure 6. Flowsheet of proposed program for calculation of a rectification column.**



**Figure 6. Comparison between approximate ( $\Delta$ ) and rigorous methods ( $\ominus$ ), for column of table 1 using a lattice with 231 points (increment in the composition in mole fraction of 0.05). Interpolation 1, 2, 3 and 4 refers to interpolation methods showed in figures 3, 4 an 6 and to interpolation method based in linera fitting of compositions, respectively.**



**Figure 7. Comparison between the rigorous method proposed in this work (★) and those from Renon et al. (1971) (Δ), for column 1**

## CONCLUSIONS

- The results obtained by the methods for multicomponent distillation complex column calculations proposed are very close to those obtained by the rigorous methods, using 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. A simple interpolation method is the one yielding the worse results and the interpolation with intercepting straight lines with four points shown in figures 3 and 4, is the one yielding the better results. In all cases studied, a remarkable improvement of the results can be noted when increasing the number of points in the lattice.
- Semirigorous methods, using a rigorous calculation of vapor-liquid equilibrium and the intersection procedure proposed to solve the balances in the column lead to very good results.
- Rigorous method using the rigorous calculation of the vapor-liquid equilibrium and the procedure showed in figure 5 to solve the balances in the column allow the same results as the rigorous methods found in the bibliography (Renon *et al.*, 1971).

## References

- Marcilla, A., Ruiz, F. and Gómez, A., "Graphically find trays and minimum reflux for complex binary distillation for real systems", *Latin American Applied Research*, 25, 87 (1995).
- Renon, H., Asselineau, L., Cohen, G. et Raimbault, C., "Calcul sur ordinateur des équilibres liquide-vapeur et liquide-liquide", *Publications de l'Institut Français du Pétrole, Collection "Science et Technique du Pétrole"*, n° 17 (1971).