# ANALYSIS OF MINIMUM VAPOR FLOWRATE REQUIREMENTS FOR THE FULLY THERMALLY COUPLED DISTILLATION SYSTEM WITH POSTFRACTIONATOR

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Abstract

In recent years, thermally coupled distillation schemes, especially the fully thermally coupled distillation system (Petlyuk column), have been studied because of their important energy savings with respect to the conventional distillation sequences. A disadvantage of the Petlyuk column is that the savings decrease when a high purity of the middle component is required. A Petlyuk column with postfractionator has been recently proposed, which can correct the differences between the interlinking trays to increase the thermodynamic efficiency.

However, because of the extra recycle streams, design and simulation of this new system is not trivial. This work presents a degrees of freedom analysis and a set of suggested design variables for this system. Then, as a basis for a shortcut design method, Underwood´s equation is developed to calculate the minimum vapor flowrate.

One important problem for the solution of Underwood's equation is the selection of values for the flowrates and compositions for the postfractionator interlinking streams. We show an alternative solution for this problem using a graphical McCabe-Thiele analysis.

## 1. Introduction

Energy saving has been the focus of many studies in distillation systems. In recent years, thermally coupled distillation schemes, especially the fully thermally coupled distillation system (Petlyuk column), have been studied because of their potential energy savings with respect to the conventional distillation sequences (Tedder and Rudd, 1978, Glinos and Malone, 1985, Fidkowski y Krolikowski, 1986, 1987 and 1990, Triantafyllou and Smith, 1992, Wolff and Skogestad,1995 Halvorsen and Skogestad, 2004). Petlyuk columns are known to have the lowest energy demand for the separation of ternary mixtures, although for certain values of relative volatilities and feed compositions, they can show considerably lower values of thermodynamic efficiencies than the thermally coupled and conventional configurations (Agrawal and Fidkowski, 1998). A disadvantage of the Petlyuk column is that the energy savings decrease when a high purity of the intermediate component is required.

Degrees of freedom for Petlyuk columns have been reported (Chavez-Contreras, 1985; Fidkowski and Krolikowski, 1986). If one assumes adiabatic stages and constant pressure, there exist C+9 degrees of freedom. Chavez-Contreras (1985) established two possible sets of variables that can meet the Petlyuk columns' degrees of freedom.

Shortcut methods have been proposed for the design of Petlyuk and Kaibel columns (Triantafyllou and Smith, 1992, Muralikrishna et. al., 2002). Shortcut methods can be used to quickly evaluate the applicability of a Peltyuk system for a given problem (Halvorsen and Skogestad, 2004). Underwood's equation (Underwood, 1948) has also been used to compare energy requirements of Petlyuk arrangements with other coupled and non coupled distillation systems (Fidkowski and Agrawal, 2001; Agrawal and Fidkowski, 1999).

The thermodynamic efficiency of conventional distillation systems is affected by the remixing of the middle component (Triantafyllou and Smith,1992). For a Petlyuk column, the mismatch between the feed stream and feed tray composition, and between the interlinking streams and interlinking trays compositions are the main reasons for the reduction of its thermodynamic efficiency (Kim, 2002a). The composition differences at the interlinking trays for a Kaibel column have also been studied for quaternary systems (Kim, 2002b).

A new thermally coupled distillation column with postfractionator (FTCDCP) was proposed by Kim (2006). The main purpose of the postfractionator is to solve the mismatch in composition in the interlinking trays of the Petlyuk column, therefore raising its thermodynamic efficiency. Petlyuk and FTCDCP designs have been made using Fenske's equation to calculate the minimum stages in each section, and then using twice that value for a practical column. The interlinking trays between the prefractionactor and the main column are selected so that the compositions match as close as possible. The postfractionator is taken from the middle section of the main column, which has a high composition of intermediate component.

This work presents a degrees of freedom (DOF) analysis for the FTCDCP. A set of design variables is proposed, and Underwood´s equation is developed to calculate the minimum vapor flowrate for FTCDCP. Finally, a McCabe-Thiele analysis is used to fix the values for the flowrates and compositions for the postfractionator interlinking streams.

## 2. Degrees of Freedom Analysis

The analysis of DOF for the FTCDCP system was made using a similar methodology as the one used by Chavez-Contreras (1985) for the Petlyuk column. FTCDCP can be divided into subsystems (prefractionator, main column and postfrationator), which are formed by basic elements (stages, condenser, reboiler, etc), Figure 1. DOF of each subsystem is computed adding the DOF for its basic elements, and then subtracting (C+2) DOF for each redundant stream. Finally, the DOF for the FTCDCP system is obtained adding the DOF for each subsystem and then subtracting the DOF of the corresponding interlinking streams.

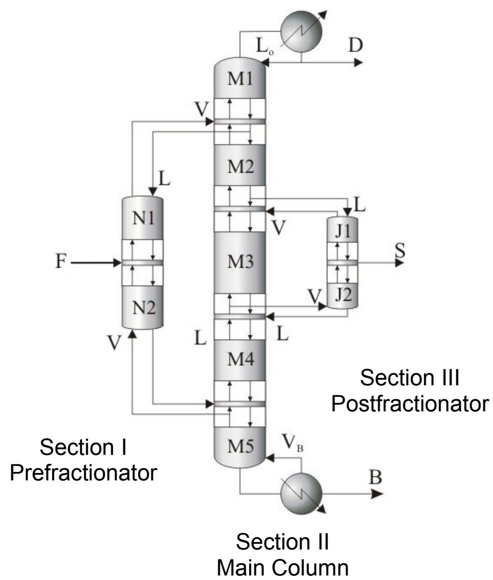



**Figure 1.** Subsystems of FTCDCP column

A summary of the DOF computation is shown in Table 1. All stages are considered non-adiabatic; feed stage and interlinking stages are included. The DOF for Section I are 2N+3C+8, which are the same as those obtained by Chavez-Contreras (1985). Section II has 2M + 4C + 20 DOF. This section has 2C+3 additional DOF than the Petlyuk main column because of the two additional feeds at the interlinking stages with postfrationator and the flow rates of side streams of the interlinking stages. Finally, the overall system has 2(N + M + J) + C + 19 DOF.

**Table 1.** DOF of the FTCDCP system

| SUBSYSTEM | DOF |
|---|---|
| SECTION I | **2N + 3C + 8** |
| SECTION II | **2M + 4C + 20** |
| SECTION III | **2J + 2C + 7** |
| Sum | 2(N + M + J) + 9C + 35 |
| Redundant streams= 8(C+2) | -8C – 16 |
| **FTCDCP's DOF** | **2(N + M + J) + C + 19** |

Two convenient initial sets of specified variables are shown in Table 2. The first 2(N+M+J)+C+3 variables are quite common. Sixteen additional degrees of freedom remain. Case I of Table 2 is to be used for design problems, and Case II for simulation cases.

**Table 2.** Proposed set of specified variables

| | | | |
|---|---|---|---|
| Heat transfer to/from all stages, including divider and excluding condenser and reboiler | | | M+N+J-1 |
| Pressure of each equilibrium stage, including condenser, reboiler and divider | | | M+N+J+1 |
| Condenser degree of subcooling | | | 1 |
| Feed stream completely specified | | | C+2 |
| **Sub Total** | | | **2(N + M + J) + C + 3** |
| **CASE I Component recoveries specified** | | **CASE II Number of equilibrium stages specified** | |
| Total flow rate of two product streams | 2 | Number of stages of each column | 3 |
| Reflux ratio (> minimum) of main column | 1 | Feed location | 1 |
| Recovery of light, middle and heavy key component in distillate, sidestream and bottom respectively | 3 | Location of the interlinking stage and stage with sidestream | 5 |
| Purity of light or heavy key in sidestream | 1 | External reflux ratio | 1 |
| Recovery of light and heavy component in section I | 2 | Flow rate of the interlinking vapor streams | 2 |
| Reflux ratio (L/V > minimum) of section I | 1 | Flow rate of the interlinking liquid strems | 2 |
| Net flow rate from main column to section VI or two interlinking flow rates | 2 | Total flow rate of two product streams | 2 |

3. Minimum flows of FTCDCP

Underwood`s equation is developed to obtain the minimum vapor flowrate for the FTCDCP system, which is divided as shown in Figure 2.

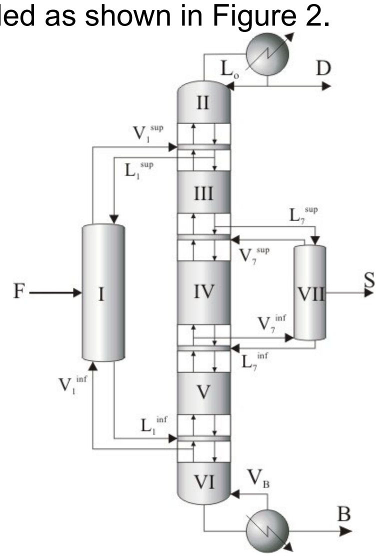



**Figure 2.** Sections of Thermally Coupled Distillation System for Underwood’s procedure

Section I

Section I can be treated as a conventional column, with a given distribution of the middle component in the top and bottoms products; the minimum vapor flowrate is determined using a conventional Underwood's procedure (Triantafyllou and Smith, 1992, Muralikrishna et. al., 2002).

Sections II, III, IV, V and VI

The main column of FTCDCP is divided into 5 sections, Figure 4. Each of these sections must operate above minimum flow rate conditions, and we must estimate which one of them is the controlling section. Minimum vapor flow rates for complex columns arrangements (as the main column of FTCDCP) can be determined from extensions of Underwood´s equation (Kister, 1992; Nikolaides and Malone, 1987). Equations 1-4 show the minimum flow rate required for each Section of the main column.

$$V_{2\min} = \sum_{i=1}^{3} \frac{\alpha_i \left( Dx_{Di} - L_1^{\sup} x_{1i}^{\sup} \right)}{\alpha_i - \phi^{II}} \tag{1}$$

$$V_{3\min} = \sum_{i=1}^{3} \frac{\alpha_i (Dx_{Di} - D^1 x_{Di}^1)}{\alpha_i - \phi^{III}} \tag{2}$$

$$V_{4\min} = \sum_{i=1}^{3} \frac{\alpha_i (Dx_{Di} - D^1 x_{Di}^1 + D^7 x_{Di}^7)}{\alpha_i - \phi^{IV}} \tag{3}$$

$$V_{5\min} = \sum_{i=1}^{3} \frac{\alpha_i (Dx_{Di} - D^1 x_{Di}^1 + D^7 x_{Di}^7 + B^7 x_{Bi}^7)}{\alpha_i - \phi^{V}} \tag{4}$$

The postfractionator can be divided into two sections, as shown in Figure 3; the upper section is taken as a stripping section, while the lower section is considered as a rectifying section. Side stream flow rate, S, will be the sum of bottoms flow rate S1 and distillate flow rate S2.

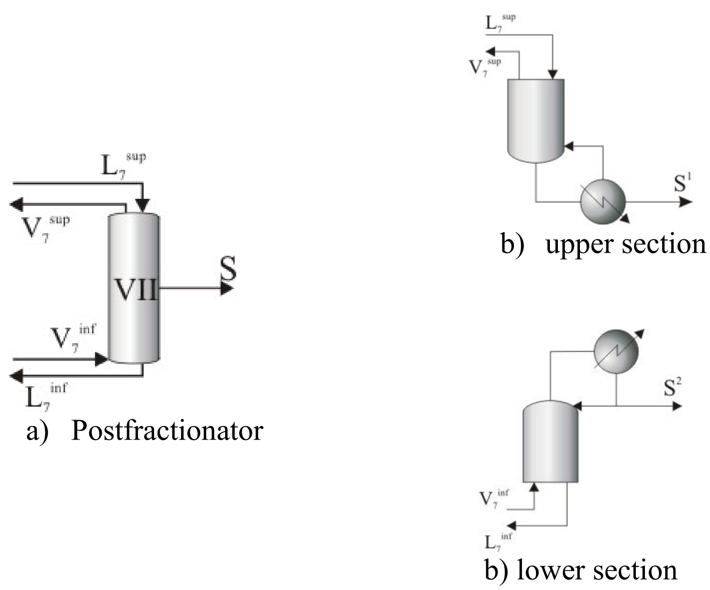


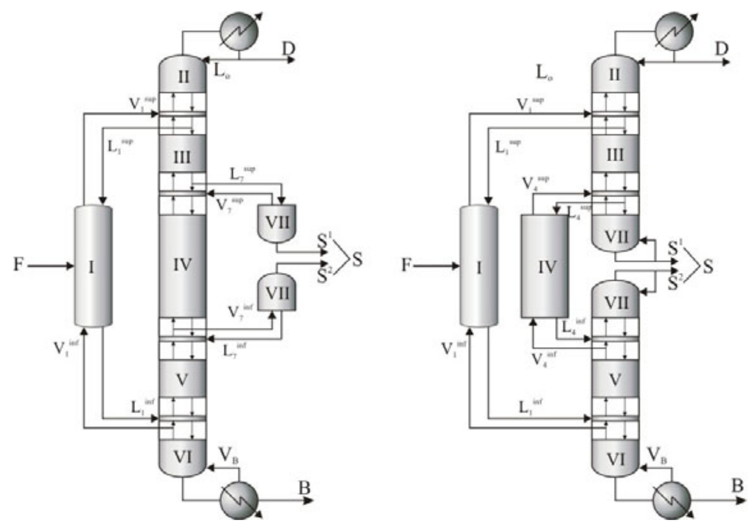

**Figure 3.** Postfraccionador system

Equation 5 estimates the upper section minimum flow rate, while Equation 6 estimates the lower section minimum flow rate.

$$-\frac{V_7^{\sup}}{S^1} = \sum_{i=1}^{3} \frac{\alpha_i x_{Si}^1}{\alpha_i - \phi_{\sup}^{VII}} \tag{5}$$

$$\frac{V_7^{\inf}}{S^2} = \sum_{i=1}^{3} \frac{\alpha_i x_{Si}^2}{\alpha_i - \phi_{\inf}^{VII}} \tag{6}$$

At this point, minimum vapor flow rates for each section of FTCDCP could be determined if all the values of $\phi$ were known. However, the interlinking feed stage of section III-IV is the same that for the upper section of the postfractionator; these sections therefore have the same minimum vapor flow rate and the same absorption factor ($\phi^{III} = \phi_{\inf}^{VII}$). A similar analysis can be done with the interlinking feed stage of sections IV-V and the lower section of the postfractionator. Section IV should be a simultaneous rectifying and stripping section. If this observation holds, the structure could be rearranged as shown in Figure 4, with section IV operating at total reflux. In the modified structure, the minimum flow rate in section IV is not calculated, and flow rates of sections VII (upper and lower) are set equal. In addition, we need to find the optimum values of liquid and vapor interlinking streams for the postfractionator.




a) Initial Structure b) Modified Structure

**Figure 4.** Thermally coupled distillation system with post-fractionator

The Underwood's equations for the modified structure are:

<u>Section between D – S[1]</u>

$$R_{II\min} = \sum_{i=1}^{3} \frac{\alpha_i x_{Di}}{\alpha_i - \phi^{II}} - 1 \quad where \quad R_{II\min} = \frac{L_{II\min}}{D}$$

$$\phi^{II} \text{ is determined by equation: } \sum_{i=1}^{3} \frac{\alpha_i x_D^1}{\alpha_i - \phi^{II}} = 1 + \frac{L_1^{\sup}}{D^1} \tag{7}$$

$$R_{3\min} = \frac{1}{\left(L_1^{\sup} + D\right)} \left[ \sum_{i=1}^{3} \frac{\alpha_i (D x_{Di} - D^1 x_{Di}^1)}{\alpha_i - \phi^{III}} + D^1 - D \right] \quad where \quad R_{3\min} = \frac{L_{3\min}^{\sup}}{L_1^{\sup} + D}$$

$$\phi^{II} \text{ is determined by equation: } \sum_{i=1}^{3} \frac{\alpha_i x_{4i}^{\sup}}{\alpha_i - \phi^{III}} = 0 \tag{8}$$

$$R_{3\min} = \frac{1}{\left(L_1^{\sup} + D\right)}\left[\sum_{i=1}^{3}\frac{\alpha_i\,(Dx_{Di} - D^1 x_{Di}^1)}{\alpha_i - \phi^{III}} + D^1 - D\right] \quad where \quad R_{3\min} = \frac{L_{3\min}^{\sup}}{L_1^{\sup} + D} \tag{9}$$

$$\phi^{II} \text{ is determined by equation: } \sum_{i=1}^{3}\frac{\alpha_i y_{4i}^{\sup}}{\alpha_i - \phi^{III}} = 1$$

One should notice that the value of $D_4$ is 0 because section IV operates at total reflux conditions (the absorption factor is infinite). Once the reflux ratios for the top zone have been calculated, we establish the dominant reflux as follows.

$$R_{\min}^{up} = \max\begin{cases}\dfrac{L_{2\min}^{\sup}}{D} \\[2ex] R_{3\min} + \dfrac{L_1^{\sup}}{D}\left(R_{3\min} + 1\right) + \dfrac{L_4^{\sup}}{D} \\[2ex] R_{3\min} + \dfrac{L_1^{\sup}}{D}\left(R_{3\min} + 1\right) + \dfrac{L_4^{\sup}}{D}\end{cases} \tag{10}$$

<u>Section between $S^2$-B</u>

$$R_{7\inf\min} = \sum_{i=1}^{3}\frac{\alpha_i x_{Si}^2}{\alpha_i - \phi^{VII\inf}} - 1 \quad where \quad R_{7\inf\min} = \frac{L_{7\inf\min}^{\sup}}{S^2} \tag{11}$$

$$\phi^{VII} \text{ is determined by equation: } \sum_{i=1}^{3}\frac{\alpha_i y_{4i}^{\inf}}{\alpha_i - \phi^{VII\inf}} = 1$$

$$R_{7\inf\min} = \sum_{i=1}^{3}\frac{\alpha_i x_{Si}^2}{\alpha_i - \phi^{VII\inf}} - 1 \quad where \quad R_{7\inf\min} = \frac{L_{7\inf\min}^{\sup}}{S^2} \tag{12}$$

$$\phi^{VII} \text{ is determined by equation: } \sum_{i=1}^{3}\frac{\alpha_i x_{4i}^{\inf}}{\alpha_i - \phi^{VII\inf}} = 0$$

$$R_{5\min} = \sum_{i=1}^{3}\frac{\alpha_i x_{Si}^2}{\alpha_i - \phi^{V}} - 1 \quad donde \quad R_{5\min} = \frac{L_{5\min}^{\sup}}{S^2} \tag{13}$$

$$\phi^{V} \text{ is determined by equation: } \sum_{i=1}^{3}\frac{\alpha_i x_{Bi}^1}{\alpha_i - \phi^{V}} = 1 - \frac{L_1^{\inf}}{B^1}$$

The net flow rate B4 is also 0 because section IV operates at total reflux conditions. The absorption factor has to be calculated with the compositions the interlingking streams. The controlling minimum reflux is calculated using Equation 14.

$$R_{\min}^{low} = \max\begin{cases}\dfrac{L_{7\inf\min}^{\sup}}{S^2} \\[2ex] R_{5\min} - \dfrac{L_4^{\inf}}{S^2} \\[2ex] R_{5\min} + \dfrac{L_4^{\inf}}{S^2}\end{cases} \tag{14}$$

Finally, the minimum reflux ratio for the whole system can be set as the highest value from each section.

4. McCabe-Thiele analysis

In the FTCDCP arrangement for ternary mixtures, sections II, III and VII can be viewed as a column that separates a binary mixture (AB) if the amount of the heavy component (C) is low. The same can be said for sections VII, V and VI, which practically separate the binary mixture BC if the amount of A is not significant. McCabe-Thiele diagrams for both cases are shown in Figures 5 and 6.

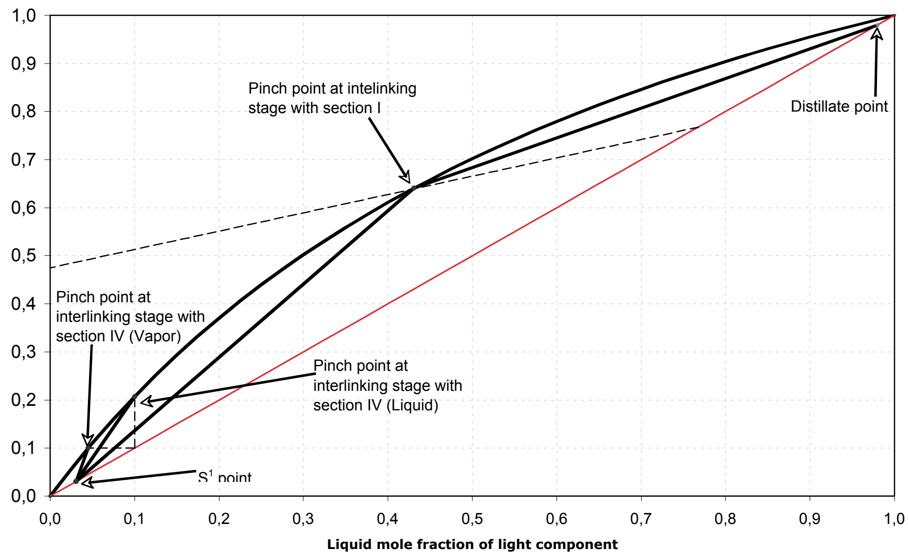
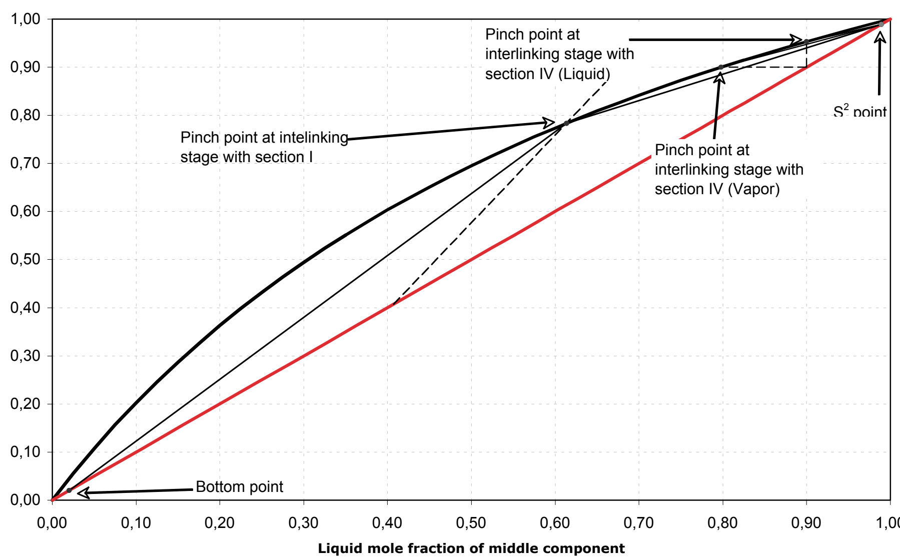



**Figure 5.** McCabe-Thiele diagram (minimum conditions) of the binary column that represents Sections II, III and




VII

**Figure 6.** McCabe-Thiele diagram (minimum conditions) of the binary column that represents Sections VII, V and VI

Pinch points, which are equivalent to Equations 7, 8 and 9 (Figure 5) and Equations 11, 12 and 13 (Figure 6), are shown in both figures. Also, one can find the compositions of the interlinking stages (at minimum reflux conditions). Compositions of interlinking streams between sections IV and VII are part of the specifications (Table 2). Therefore, pinch points compositions at interlinking stages with section VII are a consequence of those specifications. On the other hand, compositions of the interlinking stream between sections I and II, and I and VI, which are not specified, can be obtained directly with a McCabe-Thiele diagram. Interlinking streams can be represented by an equivalent net flow with a superheated or subcooled thermal condition (Glinos and Malone, 1985); therefore, distillate and bottom lines of section I can be easily drawn on the McCabe-Thiele diagram.

A limiting case occurs if the interlinking flow rate between Sections IV and VII is cero. In this case, the operating lines of the postfractionator and the main column overlap each other; the FTCDCP becomes equivalent to a Petlyuk column, and only pinch points with Section I can exist.

## 5. Conclusions

Degrees of freedom have been determined for the FTCDCP system, and a set of design variables have been proposed to meet those degrees of freedom. Underwood's equation was developed to find the minimum flow rate for this complex arrangement. There are several variables (interlinking streams between the Prefractionator and the main column, interlinking streams between the Postfractionator and the main column, and compositions or recoveries of such interlinking streams) that can be part to an optimization problem for this distillation system.

## 6. Nomenclature

| | |
|---|---|
| *q* | Feed thermal condition |
| *B* | Bottom flow rate of FTCDCP, Kg-mol/hr |
| *D* | Distillate flow rate of FTCDCP, Kg-mol/hr |
| S | Sidestream flow rate of FTCDCP, Kg-mol/hr |
| *F* | Feed flow rate of FTCDCP, Kg-mol/hr |
| *L* | Liquid flow rate above feed, Kg-mol/hr |
| *L'* | Liquid flow rate below feed, Kg-mol/hr |
| *R* | Reflux ratio |
| *V* | Vapor flow rate above feed, Kg-mol/hr |
| *V´* | Vapor flow rate below feed, Kg-mol/hr |
| *x* | Mole fraction |
| **Greek symbols** | |
| $\alpha$ | Relative volatilities |
| $\phi$ | Underwood`s equation roots |
| **subindices** | |
| *B* | Refers to Bottom of column |
| *D* | Refers to Dome of column |
| S | Refers to Sidestream of column |
| *F* | Refers to Feed |
| *i* | Refers to the *i* component |
| *min* | Minimum |
| *(1,2,3,4,5,6,7)* | Refers to the section number of FTCDCP |
| *(I,II,III)* | Refers to the section number of FTCDCP to obtain the DOF |
| **superindices** | |
| *inf* | Inferior |
| *min* | Minimum |
| sup | Superior |
| *(1,7)* | Sección del sistema acoplado térmicamente con postfraccionador |

## 7. References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