ANALYSIS OF THE CONNECTING ZONE BETWEEN CONSECUTIVE SECTIONS IN DISTILLATION COLUMNS COVERING multiple FEEDS, PRODUCTS AND HEAT TRANSFER STAGES

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Abstract—In the present work, we provide a systematic analysis about all the streams involved in the zone connecting two consecutive sections for the design of distillation columns with different thermal feed conditions, product extractions and heat additions or withdrawals. This analysis allows a better understanding of what happens on a feed or side draw (of mass or energy) stage, what compositions are or are not in equilibrium, and the impact on internal liquid and vapor flows.

Keywords—Distillation; Side Stream; Process Design; Heat Stages; Lateral Product.

I. INTRODUCTION

Tray by tray methods for the design of distillation columns cannot compete with computer methods, but they are essential for their conceptual design. These methods do provide a clear picture of what could be expected in an approximate way along a distillation column and facilitates the visualization and best understanding of many fundamentals and important aspects of multistage distillation, such as the interrelationship of several process variables.

In this sense, typical practical calculations for the conceptual design of a distillation column, given for instance a known recovery of the key components, can be: optimal number of trays or reflux ratio, minimum number of trays (at total reflux), detecting pinched zones (minimum reflux), excessive reflux or reboil and mislocated feed streams, identifying cases where intermediate heat exchangers are attractive, etc. Therefore most mass transfer text books in chemical engineering devote some space and effort to explain tray by tray methods, such as the McCabe-Thiele method (Seader et al., 2011; Petlyuk, 2004; Stichmair and Fair, 1998; Biegler et al., 1997; Kister, 1992; King, 1980; Treybal, 1981; Henley and Seader, 1988; Benitez, 2002; Noble and Terry, 2004). However, equations for the operating lines (OL) are always developed for columns with single or multiple feed additions but product extractions and heat additions or withdrawals are not always considered.

Furthermore, the optimum point of feed introduction, which yields the least total number of trays at a particular reflux, is generally consider as the intersection point between the operative lines of the sector above and below (FP point), in order to use always at each step, the operative line that lies farther from the equilibrium curve to obtain the maximum enrichment per stage (i.e. lowest vapor composition if we start at the top of the column). Therefore, when a mass feed stream is considered, whatever its thermal condition, such optimum feed location consideration is consequent with the assumption that the feed is introduced in bulk to a single feeding tray (stage number 2 in Fig. 1a) where it mixes with the vapor of the tray below and with the liquid of the tray above. The streams leaving this feeding stage (V₂=V₂' and L₂=L₂') are considered to be in equilibrium, as in any other theoretical stage (Fig. 1a).

However, this approach can be somewhat far from the physical reality, that does not allow to exactly locate all the streams involved in the changing zone of two consecutive sectors in the McCabe-Thiele diagram, and that can introduce some significant deviations in the equilibrium compositions obtained for the different rates of the column below each particular feed, especially in systems of high relative volatility and when the feed is a subcooled liquid, a partly vaporized mixture or a superheated vapor. Thus, it is more likely to consider that when a feed stream is introduced in the distillation column, it flashes adiabatically and spontaneously to the feed stage pressure, generating a vapor phase (V_p) that flows to the tray immediately above, and a liquid phase (L_q) that flows to the tray immediately below (Fig. 1b).

Before dealing with the general case, the differences of the classical and strict approach in the case of a single feed stream are shown in Fig. 2a-b (corresponding to the schemes presented in Fig. 1a-b), with a simplified nomenclature. With the classical approach, when the step by step construction arrives to the composition y_3=y_2' by using the upper section operative line (UOL), the liquid composition x_3 is obtained directly from the equilibrium curve. The composition of the next vapor y_3 is located in the OL of the following sector, LOL. As we can see, stream L_2=L_1+L_f presents an inconsistent behavior in the sense that its composition (x_3) is located out side the interval defined by the compositions x_1 and x_f (Fig. 2a).

In an alternative approach, what is supposed to occur is that when a feed stream is introduced between two plates in the distillation column (1 and 2 in Fig. 1b), it flashes adiabatically. The vapor fraction V_p will join the vapor coming from the stage below V_2, whereas the feed liquid fraction L_f will join the liquid coming from the plate immediately above L_1, providing two streams (V_2'' and L_1') that are not in equilibrium: V_2''=V_2'+V_L=V_f+L_f and L_1'=L_1+L_f, since they are the sum of two different streams that are in equilibrium. Figure 1b presents the feed operative line (FOL) and all the streams
involved in the changing zone correctly located: \( V_2, V'_2, L_1, L'_1, L_2 \), etc.

**Figure 1.** Scheme of the streams at the zone connecting two consecutive sections using a) the classical FP approach; b) the GFOL approach.

Thus, the objective of this paper is to point out and analyze, through a fully analytical and graphical treatment, the connecting zone between consecutive sections due to different side streams (feeds, products and/or heat removals or additions) using a Generalized Feed Operating Line (GFOL) approach. In this approach, all the streams involved in the change of sector, as well as the corresponding operating lines, are unambiguously located in the McCabe-Thiele diagram. The work complements, in this sense, the academic literature dealing with this subject (e.g. Ledanois and Olivera-Fuentes, 1984; Wankat, 2012). This analysis tackles most of the possible cases and leaves no room for doubt in any possible interpretation, allowing (with a negligible extra effort) an appropriate comprehension and understanding of what would happen in a column used for the separation of binary mixtures, in accordance with the hypothesis considered (condition of constant molar overflow, CMO) and regarding the way of introducing or extracting the mass or heat to the column.

It should be noted that the analysis proposed does not alter the procedure of calculation of the minimum reflux ratio by checking all the possible pinch points where the operative lines of each section intersect the equilibrium curve.

Finally it is interesting to remark that the tray by tray methods still present some attractive characteristic for the more effectively and optimal design of separation units such as their robustness due to the fact that the convergence for a feasible postulated separation is almost always guaranteed, and a near optimal design is obtained at each iteration. Additionally some references can be found in the literature dealing with transformation of variables, such as composition, so that the McCabe-Thiele method becomes applicable in special cases of traditional distillation, reactive distillation, absorption, liquid-liquid extraction and multicomponent mixtures (McCabe et al., 1993; Doherty and Malone, 2001; Reyes-Labarta et al., 2012; Ravi, 2008; Lee et al., 2000; Marcilla et al., 1997; 1999; Reyes et al., 2000; Johnson and Morgan, 1985). The extension of the McCabe-Thiele method can also be used to analyze quickly, the effects and drawbacks of different configurations for internal heat integration in a single distillation column (HIDiC), to obtain more suitable chemical processes (Nakaiwa et al., 2003; Shenvi et al., 2011; Huang et al., 2006; Ho et al., 2010).

**II. SYSTEMATIC ANALYSIS OF THE CHANGES OF SECTION IN THE McCabe-Thiele METHOD**

A column section can be defined as the portion of a distillation column that is not interrupted by entering or exiting streams or heat flows (Hohmann et al., 1980). Thus, two consecutive sections \( k \) and \( k+1 \) of a distillation column are separated by a generalized feed side stream, GF\(_k\). Such a generalized feed stream can be either a mass stream (M\(_{GF_k}\)) or an enthalpy stream (E\(_{GF_k}\)). Considering all these possibilities, the generalized in or out feed side stream considered and their characteristics and sign are shown in Table 1.

**Table 1.** Compilation of the different cases presented for a generalized feed stream (GF\(_k\)) and its characteristics.

<table>
<thead>
<tr>
<th>Name and flow rates</th>
<th>Thermal condition</th>
<th>Molar fraction ( V_{GFk} ) [molar fraction]</th>
<th>L(_{GFk}) [molar fraction]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed ( M_{GFk} &gt; 0 ) ( \text{or} ) ( M_{GFk} &lt; 0 ) ( \text{or} ) ( M_{GFk} = 0 ) ( \text{and} ) ( E_{GFk} &gt; 0 ) ( \text{or} ) ( E_{GFk} &lt; 0 )</td>
<td>( q_{GFk} &gt; 1 ) ( \text{or} ) ( q_{GFk} &lt; 1 ) ( \text{or} ) ( q_{GFk} = 1 ) ( \text{or} ) ( q_{GFk} = 0 ) ( \text{and} ) ( q_{GFk} &gt; 0 ) ( \text{or} ) ( q_{GFk} &lt; 0 ) ( \text{or} ) ( q_{GFk} = 0 ) ( \text{and} ) ( q_{GFk} &gt; 0 ) ( \text{or} ) ( q_{GFk} &lt; 0 )</td>
<td>( 1 ) ( \frac{1}{\text{y}_{GFk}} ) ( \text{molar fraction} )</td>
<td>( \text{molar fraction} )</td>
</tr>
<tr>
<td>Product ( M_{GFk} &lt; 0 ) ( \text{or} ) ( M_{GFk} &gt; 0 ) ( \text{and} ) ( E_{GFk} &gt; 0 ) ( \text{or} ) ( E_{GFk} &lt; 0 )</td>
<td>( q_{GFk} = 0 ) ( \text{or} ) ( q_{GFk} = 1 ) ( \text{or} ) ( q_{GFk} &gt; 0 ) ( \text{or} ) ( q_{GFk} &lt; 0 ) ( \text{or} ) ( q_{GFk} = 0 ) ( \text{and} ) ( q_{GFk} &gt; 0 ) ( \text{or} ) ( q_{GFk} &lt; 0 ) ( \text{or} ) ( q_{GFk} = 0 ) ( \text{and} ) ( q_{GFk} &gt; 0 ) ( \text{or} ) ( q_{GFk} &lt; 0 )</td>
<td>( \text{molar fraction} )</td>
<td>( \text{molar fraction} )</td>
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**Figure 2.** Changing zone in the y/x McCabe-Thiele diagram for a) the classical FP approach; b) the GFOL approach.
fraction \( L_{GFK} \) joins the liquid coming from the plate immediately above \( (L_{k+1,0} = L_{k,NT} + L_{GFK}) \) which implies that \( x_{k+1,0} \) is located between \( x_{L,NT} \) and \( x_{GFK} \). It can be observed that the segment drawn of \( GFOL_k \) covers the amplitude of an equilibrium stage in the diagram. As commented on before, this \( GFOL_k \) must be used only once in the staircase construction, the first time that the condition \( x_{L,NT} \leq x_{GFK} \leq x_{IP_k} \) is satisfied.

In the case of superheated vapor feed stream \( (q_{GFK} \leq 0) \), \( FL_k \) intercepts the equilibrium curve with a positive slope lower than unity (Fig. 3b). The vapor \( y_{GFK} \) composition is lower than the composition of the feed \( (z_{GFK}) \). Since \( V_{GFK} > M_{GFK} \), \( GFOL_k \) has a higher slope than \( OL_k \) and \( OL_{k+1} \) and it is nearer the equilibrium line, which results unfavorable for the separation. Besides, it can be observed that \( y_{k,0} \) is aligned between \( y_{k+1,1} \) and \( y_{GFK} \) but \( x_{k,0} \) is not located between \( x_{L,NT} \) and \( x_{GFK} \) since \( x_{k+1,0} \) is greater than \( x_{L,NT} \) because this addition unfavorably affects the separation at the stage of the section change.

If \( M_{GFK} \) is an undercooled liquid, \( FL_k \) intercepts the equilibrium curve with a positive slope greater than unity (Fig. 3c). Since \( L_{GFK} > M_{GFK} \), \( GFOL_k \) has a slope lower than \( OL_k \) and \( OL_{k+1} \), which is unfavorable for the separation at the specific stage of the change of curve. As expected, \( x_{k+1,0} \) is located between \( x_{L,NT} \) and \( x_{GFK} \) but \( y_{k,0} \) is lower than both \( y_{k+1,1} \) and \( y_{GFK} \).

\[
\begin{align*}
\text{FP} & \text{ coincides with IP}_k \text{ or IP}_{k+1} \text{ and any of the two approaches, the classical and the one proposed, gives the same results.}
\end{align*}
\]

\[
\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure_4}
\caption{McCabe-Thiele y/x diagrams for a generalized product feed stream \( (M_{GFK} \leq 0) \) for different thermal conditions: a) \( q_{GFK} = 1 \); b) \( q_{GFK} = 0 \).}
\end{figure}
\]

\[
\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure_5}
\caption{McCabe-Thiele y/x diagrams for a generalized heat side stream \( (E_{GFK}) \): a) Intercondenser \( (E_{GFK} < 0) \); b) Interboiler \( (E_{GFK} > 0) \).}
\end{figure}
\]

Obviously, for other types of side streams, different from mass feeds, it must be considered that the stream to be removed (when the \( GFK \) is a mass product: \( M_{GFK} < 0 \)) or to be heated or cooled (for the case of heat addition or removal: \( E_{GFK} \)) must actually exist in the column to avoid incoherent design predictions, and therefore \( z_{GFK} \) (Table 1) must coincide with \( x_{L,NT} \) or \( y_{k+1,1} \) (Fig. 4 and 5).

The extraction of a product worsens the separation in the rectifying section because the slope of \( OL_{k+1} \) is lower than \( OL_k \), consequently more stages are needed, as compared to the case of mass feed addition. Figures 4a-b show the case of a saturated liquid or saturated vapor product. In these cases, in a similar way that for saturated feed streams, the \( GFOL_k \) coincides with the corresponding operative line \( k \) or \( k+1 \). In the case of the saturated liquid product \( (L_{GFK}=M_{GFK}) \): \( z_{GFK}=x_{GFK}=x_{L,NT} \) and \( y_{k,0}=y_{k+1,1}=y_{FP} \); while in the case of the saturated vapor product \( (V_{GFK}=M_{GFK}) \): \( z_{GFK}=y_{GFK}=y_{k,0} \) and \( x_{k+1,1}=x_{FP} \).

Sometimes intermediate reboilers and/or intermediate condensers are used in distillation columns, normally to adjust an existing distillation column to new separation requirements or feeds. Thus for instance, a wide gap between the component balance line and the equilibrium curve in the stripping section or enriching indicates a potential for an interreboiler or an intercondenser, respectively. Obviously, the intermediate heat supply and/or heat removal causes changes of internal vapor and liquid flows (Table 1).

The intermediate heat addition or removal leads to different diagrams from mass feed and product situations. Streams \( V_{GFK} \) and \( L_{GFK} \) are not in equilibrium but their composition is the same (given by the same point on the diagonal: \( z_{GFK}=x_{GFK}=y_{GFK} \)). Since there is neither mass addition nor removal, in the McCabe-Thiele y/x diagram of Fig. 5a-b the operative lines \( OL_k \) and \( OL_{k+1} \) present different slopes and cut with the diagonal at the
same point, giving the FP intersection point analogous to that obtained for mass feed streams. As can be observed in Fig. 5, in this case, the transition between the two consecutive operating lines shows a discontinuity.

When a heat flow \( E_{\text{GFk}} \) is removed from a vapor of composition \( x_{\text{GFk}}\) causing the corresponding condensation (Fig. 5a), the flow \( V_{k,0} \) entering the stage above decreases by \( V_{\text{GFk}} = E_{\text{GFk}}/\lambda_{\text{GFk}} \), and consequently the liquid flow \( L_{k+1,0} \) entering the stage below increases by \( L_{\text{GFk}} = -E_{\text{GFk}}/\lambda_{\text{GFk}} \) \((E_{\text{GFk}}<0 \text{ according to Table 1})\), both streams having the same composition \( x_{\text{GFk}} = y_{\text{GFk}} \).

The coherent construction shown in the diagram allows the fulfillment of the relationship among streams occurring at the stage of change of section: \( x_{l,0} \) is located between \( x_{l,\text{NTL}} = x_{\text{PK}} \) and \( x_{\text{GFk}} \) and \( y_{\text{GFk}} = y_{l,0} = y_{k+1,1} \).

Because of the liquid flow increases, the slope of the GFOL is lower than OLk but the slope of OLk+1 is higher than that of OLk. Since OLk+1 is more separated from the equilibrium line, the effect of the heat removal in the enrichment section of a column favors the separation.

An equivalent analysis can be done if heat is added to the liquid of a tray of composition \( x_{\text{GFk}} \) causing a vaporization that implies a liquid flow decrease and the consequent vapor flow increase \((V_{\text{GFk}}=-E_{\text{GFk}}/\lambda_{\text{GFk}} \text{ and } L_{\text{GFk}}=-E_{\text{GFk}}/\lambda_{\text{CF}} \text{ with } E_{\text{GFk}}>0 \text{ according to Table 1})\). The effects of these changes are represented in Fig. 5b.

Despite the presented analysis may be considered unnecessarily complex for the applications expected from the McCabe-Thiele method, we find it interesting since it does not only evidence the relationships occurring among the streams involved at the stage of the change of section, but also between them and the rest of streams at the previous or subsequent stages.

Nevertheless, differences between the two approaches are not so considerable and they depend on the thermal condition of the feed stream, the relative volatility of the system and other parameters, such as the reflux ratio, and also the position of the feed. For saturated liquid and vapor feeds both approaches give the same results, as commented previously. For the rest of cases there are two limiting situations (minimum and maximum LD/D reflux ratios) where the results obtained are also the same. For intermediate situations between minimum and maximum LD/D reflux ratios calculated differences (always lower than one tray but that can be relevant if we consider the compositions of the following trays) depend on the column characteristics and the system equilibrium. As we can see in Fig. 6a-c, the stage number tends to rise quickly in the first case (a) but for intermediate situations (b) we can see that differences are higher (especially if the last liquid descending from the previous sector lies nearly in the middle of the FOL). For the limiting case (c) both approaches tend to the same result.

Figures 7a-b show the complete staircase construction, using the feed operative line, for two numerical examples corresponding to a single column with a partially vaporized and undercooled liquid feed stream, respectively. In addition, Fig. 8a shows the comparison of the results obtained using the classical and proposed approach for the case of a superheated vapor feed. The liquid composition profile along the column is also shown (Fig. 8b). Though the number of trays obtained is very similar by the two approaches, the composition profile may significantly differ for the trays below the generalized feeds. This fact can be magnified as the number of steps or generalized feeds increase.

**III. CONCLUSIONS**

The classical approach for the McCabe-Thiele method, using the FP point, can be unrealistic and does not allow a clear understanding of the different relationships among the streams that may be involved whenever a generalized feed is introduced into a distillation column. Thus, a complete analysis (coherent with the hypothesis considered) of what may happen when changing section in a distillation column due to generalized mass or heat feed side streams, has been presented using a Generalized Feed Operating Line approach. All the streams involved in the stages corresponding to these changes of sections, as well as the operating and changeover lines are unambiguously located in the McCabe-Thiele dia-
gram, since the understanding of the different cases is not so evident, facilitating the comprehension of the method through its coherent and strict application. The analysis of several examples reveals that significant differences in the composition of the trays below the generalized feeds may be obtained when comparing with the traditional McCabe Thiele method.

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SUPPLEMENTARY MATERIAL
A complementary analysis of particular cases where the compositions of the streams developed in the rectification column coincide with one of the vapor ($y_k^{GFk}$) or liquid ($x_k^{GFk}$) portions generated from the GF$k$ can be found in the supplementary material. A review and extension of the McCabe Thiele method and the comprehended solutions to the problem can also be found in the Open Academic Repository of the University of Alicante (http://hdl.handle.net/10045/23195).

Additionally, a website of self-learning about the McCabe-Thiele method for the design of distillation columns can be consulted: http://iq.ua.es/McCabe-V2/ (http://hdl.handle.net/10045/2283).

LIST OF SYMBOLS

- $C_{PL}$, $C_{PV}$: Specific heats of liquid and vapor phase
- $D$: Distillate stream (kmole/h)
- $E_{GFk}$: Effective heat flow (kcal/h) added or removed to the column, after section k, by an intermediate heat exchanger (reboiler or condenser that we consider having a 100% efficiency) to a liquid or a vapor stream, respectively
- $F_{Lk}$: Feed line of feed stream k
- $FOL_k$: Generalized feed that separates section k and k+1 (kmole/h)
- $G_{GFk}$: Generalized feed composition of the volatile component (mole fraction)
- $H_{GFk}$: Specific enthalpy of the generalized feed mixture stream (kcal/kmole)
- $M_{GFk}$: Mass feed or product stream that separates section k and k+1 (kmole/h)
- $OL_{k+1}$: Operating line of section k+1:

$$Y_{x,k+1} = \frac{L_{x,k+1}}{V_{x,k+1}} \cdot \frac{D \cdot x_k - \sum M_{GFk} \cdot z_{GFk}}{V_{x,k+1}} = \frac{L_0 + \sum M_{GFk} \cdot z_{GFk}}{V_0 + \sum M_{GFk}} \cdot x_0 + \frac{D \cdot x_k - \sum M_{GFk} \cdot z_{GFk}}{V_0 + \sum M_{GFk}}$$

- $Q_{GFk}$: Thermal condition of the generalized feed stream k. Enthalpy change to bring the mass feed stream from its initial condition ($H_{GFk}$) to a saturated vapor ($H_{GFk}$) divided by the molar latent heat or enthalpy of vaporization of the feed $\lambda_{GFk}$ (dew point vapor enthalpy, $H_{GFk}$ minus bubble point liquid enthalpy, $h_{GFk}$)

$$q_{GFk} = \frac{H_{GFk} - H_{GFk}}{\lambda_{GFk}} = \frac{H_{GFk} - H_{GFk}}{H_{GFk}}$$

- $T_{GFk}$: Temperature of the generalized feed stream k
- $UOL$: Upper section operating line
- $V_{GFk}$: Vapor portion of the generalized feed stream k
- $V_{k,i}$: Vapor from stage i of section k (kmole/h)
- $x_{GFk}$: Liquid feed composition of the volatile component (mole fraction)
- $x_{IPk}$: x coordinate of the point IP$k$ (=$x_{opt,k}$)
- $x_{IPk+1}$: x coordinate of the point IP$k+1$ (=$x_{GFk}$)
- $x_{k,i}$: Composition of liquid falling from stage i of section k (mole fraction)
- $x_{opt,k}$: x coordinate of the optimal location of the generalized stream k (when the staircase calculation is started from the top of the column)

$$x_{opt,k} = x_{k,i} \frac{L_{x,k,i} + D \cdot \sum M_{IPk}}{L_{x,k,i} + \sum M_{IPk}}$$

- $Y_{GFk}$: Vapor feed composition of the volatile component (mole fraction)
- $Y_{k,i}$: Composition of vapor ascending from stage i of section k (mole fraction)
- $Y_{IPk}$: y coordinate of the point IP$k$ (=$y_{GFk}$)
- $Z_{GFk}$: Generalized feed composition of the volatile component (mole fraction)

Subscripts
- i: Stage
- k: Section
- N: Number of plates of the section k

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