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A graphical method for designing reactive distillation columns I. The Ponchon–Savarit method

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We show how to construct a Ponchon–Savarit diagram for a binary reactive distillation column, illustrating it specifically for isomerization and decomposition reactions. We first show the properties needed for points to lie on a straight line in composition/enthalpy space. Then, for the isomerization reaction, we show how to step off the stages using a reactive cascade difference point. In the Ponchon–Savarit diagram, the reactive cascade difference point has two elements. One is the composition coordinate formed as a linear combination of stoichiometric coefficient vectors and the top product composition. The other is the enthalpy coordinate formed by combining the top product molar enthalpy, the condenser molar duty and the molar heat of reaction. Finally, and in a similar manner, we construct the Ponchon–Savarit diagram for a decomposition reaction.

Keywords: Ponchon–Savarit method; reactive distillation; reactive cascade difference point

1. Introduction

Reactive distillation is a promising technology that integrates the functions of reaction and separation. In special cases (DeGarmo *et al*. 1992; Siirola 1995), this integrated unit can reduce investment and operating costs dramatically. As yet, there are few design methods for reactive distillation. Barbosa & Doherty (1988*a*,*b*) introduced single- and double-feed distillation columns under the assumptions of constant molal overflow (CMO) and reaction equilibrium in a column. Okasinski & Doherty (1998) proposed a design method for a reactive distillation column considering the heat effect from reaction and the reaction residence time in terms of the vapour-to-feed ratio and the Damköhler number. In terms of graphical methods, Espinosa *et al*. (1993) developed Ponchon–Savarit diagrams in a transformed enthalpy-composition space, and Perez-Cisneros (1997) proposed McCabe–Thiele diagrams for designing reactive distillation columns based on the element balance approach. However, until now, there have been no easy graphical methods for designing reactive distillation such as Ponchon–Savarit and McCabe–Thiele diagrams in terms of untransformed mole fraction coordinates.

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The Ponchon–Savarit diagram (Ponchon 1921; Savarit 1922) for binary distillation allows one to account for enthalpy effects that cause a varying molar overflow when stepping off stages graphically. It is a diagram that plots vapour and liquid enthalpy curves versus composition. Through the use of tie-lines to express vapour/liquid equilibrium, one can step off the stages required in a binary column as a function of product purities, feed quality and condenser duty. It, like the McCabe–Thiele diagram (McCabe & Thiele 1925), provides very powerful visualization of the behaviour of binary distillation columns. Our goal is to extend these visualizations to reactive distillation. In this paper we show how to formulate and then construct a reactive cascade difference point, which is a useful concept to extend into higher dimensions such as ternary and quaternary mixtures (Lee *et al*. 2000; Hauan *et al*. 1999, 2000), to reflect the reaction effect in terms of energy and material balances on a Ponchon–Savarit diagram. We employ two types of reaction—when there is no net change in the number of moles caused by the reaction, as for an isomerization reaction, and when there is a net change, as for a decomposition reaction.

2. Theory and implications

The lever rule is ubiquitous in chemical engineering. It states that, if we have two multi-component mixtures M_1 and M_2, then the composition resulting from mixing M_1 with M_2 to form M_3 must lie on the straight line connecting the compositions of M_1 and M_2. Furthermore, it says that the lengths of the lines connecting the composition of M_1 to M_3 and connecting the composition of M_2 to M_3 are proportional to the amounts of M_2 and M_1, respectively. Hauan *et al*. (2000) present a very concise proof of this rule. We show here that this rule is readily extended and that the Ponchon–Savarit diagram is a special case of this extension.

Suppose we can relate three vectors, $\boldsymbol{v}_1$, $\boldsymbol{v}_2$, $\boldsymbol{v}_3$, with the following linear relationship, where a_i $(i = 1, 2, 3)$ are scalars:

$$a_3\boldsymbol{v}_3 = a_1\boldsymbol{v}_1 + a_2\boldsymbol{v}_2. \tag{2.1}$$

If the components of each $\boldsymbol{v}_j$ add to a constant b, then, when we plot the points corresponding to $\boldsymbol{v}_1$, $\boldsymbol{v}_2$ and $\boldsymbol{v}_3$ in the space spanned by them, these points will lie on a straight line. The proof, based on that in Hauan *et al*. (2000), is as follows. Add all relationships with each element in each $\boldsymbol{v}_j$ on the right- and left-hand sides of the above equation to get the following:

$$a_3 b = a_1 b + a_2 b \quad \text{or} \quad a_3 = a_1 + a_2. \tag{2.2}$$

Substituting for a_3 in (2.1) and rearranging, we get

$$\boldsymbol{v}_3 = \alpha\boldsymbol{v}_1 + (1 - \alpha)\boldsymbol{v}_2, \tag{2.3}$$

where $\alpha = a_1/(a_1 + a_2)$. This last equation says that $\boldsymbol{v}_3$ is the stated linear combination of $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ with the properties claimed.

We can generalize this result as follows. Suppose we can write another equation with the same constants a_1, a_2, a_3,

$$a_3 z_3 = a_1 z_1 + a_2 z_2. \tag{2.4}$$

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Then we can extend the space spanned by $\boldsymbol{v}_1$, $\boldsymbol{v}_2$, $\boldsymbol{v}_3$ by adding to each vector the components z_1, z_2, z_3, respectively, and, in this augmented space, the points will still lie on a straight line. In other words, we form the vectors

$$\boldsymbol{v}_j'^{\mathrm{T}} = [\boldsymbol{v}_j^{\mathrm{T}}, z_j] \tag{2.5}$$

for each $\boldsymbol{v}_j'^{\mathrm{T}}$, where each has one additional element z_j in it. The proof is simple: equation (2.3) still holds for this augmented vector.

What we see is that, as long as any *subset* of the components of a set of vectors satisfying (2.1) sums to a constant, then the points represented by these vectors will lie on a straight line in the space spanned by those vectors. For the Ponchon–Saravit diagram, as we show momentarily, we write material balances around the top of a non-reactive distillation column,

$$V_{n+1}\boldsymbol{y}_{n+1} = L_n\boldsymbol{x}_n + D\boldsymbol{x}_{\mathrm{D}}. \tag{2.6}$$

Here, the composition vectors have terms that always add to unity. Thus, these composition vectors are on a straight line in composition space. We can also write an energy balance around a non-reactive rectifying section,

$$V_{n+1}H_{n+1} = L_nh_n + D(h_{\mathrm{D}} + Q_{\mathrm{C}}/D). \tag{2.7}$$

Thus we can augment the composition vector with these three enthalpies, H_{n+1}, h_n and $h_{\mathrm{D}} + Q_{\mathrm{C}}/D$, where H_{n+1}, h_n, h_{D} and Q_{C} are the vapour enthalpy at stage $(n+1)$, the liquid enthalpy at stage n, the distillate enthalpy and the condenser duty, respectively, and find that these points also lie on a straight line, which is the basis for construction of the Ponchon–Savarit diagram.

To construct Ponchon–Savarit diagrams for reactive distillation in composition/enthalpy space, we will consider reactive distillation columns in which isomerization and decomposition reactions take place within a reaction zone above the feed stage in figure 1.

(*a*) *Isomerization reaction*

Here, we consider the isomerization reaction regardless of the reaction phase in (2.8) between R1 and P1 components, where R1 is assumed to be less volatile than P1. The reaction takes place in the rectifying section of a staged distillation column with a partial reboiler and a total condenser. The unconverted R1 exits at the bottom of the column and the product P1 exits at the top through a total condenser. If we take the total and component-wise material balance equations around the rectifying section, including the reaction zone in figure 1, we have the following equations (2.9) and (2.10). An energy balance around the rectifying section yields (2.11), as follows:

$$\mathrm{R1} \Leftrightarrow \mathrm{P1}, \tag{2.8}$$

$$V_{n+1} = L_n + D - \nu_{\mathrm{T}}\xi_n, \tag{2.9}$$

$$V_{n+1}\boldsymbol{y}_{n+1} = L_n\boldsymbol{x}_n + D\boldsymbol{x}_{\mathrm{D}} - \boldsymbol{\nu}\xi_n, \tag{2.10}$$

$$V_{n+1}H_{n+1} = L_nh_n + Dh_{\mathrm{D}} + Q_{\mathrm{C}} + \Delta h_{\mathrm{R}}\xi_n. \tag{2.11}$$

In (2.9), the total sum of stoichiometric coefficients, ν_{T}, is zero for the isomerization reaction (2.8). Because we can think of ξ_n as a flowrate in units of, for example,

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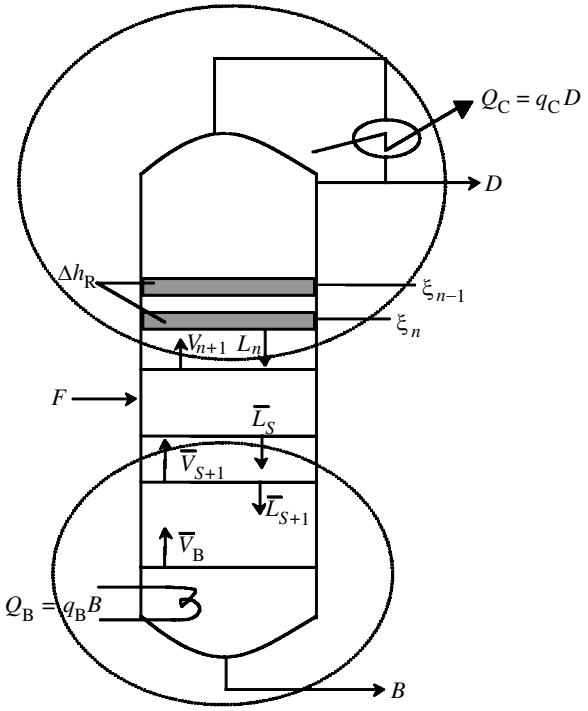


Figure 1. A schematic of a reactive distillation column.

mol s^{-1}, we shall call ξ_n a molar turnover flowrate of reaction. It is the *sum* of the reaction turnovers occurring on stages n and above. (ξ_n is often termed an extent of reaction.) If the reaction always proceeds in the forward direction from a reactant to a product on each reacting stage, then ξ_n is a sum of positive numbers or zero and will thus be monotone increasing as one moves down the column. $\boldsymbol{\nu}$ is the stoichiometric coefficient vector $[-1, 1]^{\mathrm{T}}$ and can be written as the difference between the product coefficient vector $\boldsymbol{c}_{\mathrm{P}} = [0, 1]^{\mathrm{T}}$ and the reactant coefficient vector $\boldsymbol{c}_{\mathrm{R}} = [1, 0]^{\mathrm{T}}$ in (2.10). In (2.11), Q_{C} is the condenser duty and Δh_{R} is the heat of reaction, which is negative for an exothermic reaction and positive for an endothermic reaction. We will illustrate for an exothermic reaction here. We can rearrange (2.9)–(2.11) as follows:

$$V_{n+1} - L_n = D, \tag{2.12}$$

$$V_{n+1}\boldsymbol{y}_{n+1} - L_n\boldsymbol{x}_n = D\boldsymbol{x}_{\mathrm{D}} - \boldsymbol{c}_{\mathrm{P}}\xi_n + \boldsymbol{c}_{\mathrm{R}}\xi_n = D\delta^{\mathrm{r}}_{\mathrm{R},n}, \tag{2.13}$$

$$V_{n+1}H_{n+1} - L_n h_n = Dh^{\mathrm{r}}_{\mathrm{R},n}, \tag{2.14}$$

where

$$\delta^{\mathrm{r}}_{\mathrm{R},n} = (D\boldsymbol{x}_{\mathrm{D}} - \boldsymbol{c}_{\mathrm{P}}\xi_n + \boldsymbol{c}_{\mathrm{R}}\xi_n)/D, \tag{2.15}$$

$$h^{\mathrm{r}}_{\mathrm{R},n} = (h_{\mathrm{D}} + q_{\mathrm{C}} + \Delta h_{\mathrm{R}}\xi_n/D), \tag{2.16}$$

$$q_{\mathrm{C}} = Q_{\mathrm{C}}/D. \tag{2.17}$$

Equations (2.12)–(2.14) have the same forms as (2.1), (2.2) and (2.4). Hence these will produce straight lines for material and energy balances in composition/enthalpy

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space. We call $\delta^{\mathrm{r}}_{\mathrm{R},n}$ the composition coordinate and $h^{\mathrm{r}}_{\mathrm{R},n}$ the enthalpy coordinate for the reactive cascade difference point $(\delta^{\mathrm{r}}_{\mathrm{R},n}, h^{\mathrm{r}}_{\mathrm{R},n})$ in the rectifying section. We can step off stages on a Ponchon–Savarit diagram using this difference point for a reactive cascade. Note that the Ponchon–Savarit diagram plots enthalpy versus the composition of only one of the two species, generally the more volatile one. Thus, while (2.13) and (2.15) are actually two equations each, we use only the first equation for each in constructing this plot.

We assume reaction only proceeds in the forward direction, so the reaction molar turnover flowrate ξ_n increases as we go down the column. Thus the composition coordinate $(\delta^{\mathrm{r}}_{\mathrm{R},n})$ in (2.15) will move from the distillate composition toward the reactant coefficient vector $(\boldsymbol{c}_{\mathrm{R}})$. For an exothermic reaction, the enthalpy coordinate $(h^{\mathrm{r}}_{\mathrm{R},n})$ in (2.16) will decrease. Thus the reactive cascade difference point $(\delta^{\mathrm{r}}_{\mathrm{R},n}, h^{\mathrm{r}}_{\mathrm{R},n})$ will move toward the reactant and downward as we go down the column.

With no reaction in the stripping section, the material and energy balances are as follows:

$$\bar{V}_{s+1} - \bar{L}_s = -B, \tag{2.18}$$

$$\bar{V}_{s+1}\boldsymbol{y}_{s+1} - \bar{L}_s\boldsymbol{x}_s = -B\boldsymbol{x}_{\mathrm{B}}, \tag{2.19}$$

$$\bar{V}_{s+1}H_{s+1} - \bar{L}_s h_s = -B(h_{\mathrm{B}} - q_{\mathrm{B}}), \tag{2.20}$$

$$q_{\mathrm{B}} = Q_{\mathrm{B}}/B. \tag{2.21}$$

Here, Q_{B} is reboiler duty. Thus the construction of straight lines in the stripping section is the same as for an ordinary distillation column (reproduced in King 1980; Henley & Seader 1981).

Figure 2 illustrates how to step off stages in both the reactive rectifying and the non-reactive stripping sections. First, we fix the top difference point $(h_{\mathrm{D}} + q_{\mathrm{C}}, x_{\mathrm{D}})$ and bottom difference point $(h_{\mathrm{B}} - q_{\mathrm{B}}, x_{\mathrm{B}})$. Arbitrarily here, we shall assume that stages 1 and 2 from the top are non-reactive (no catalyst present). Thus we step off the stages until stage 3 by alternating between using the operating lines emanating from the top difference point and equilibrium tie lines. This stepping off of stages is exactly as we would do for a non-reactive column. We assume an arbitrary but realistic extent of reaction on stage 3, which will move the reactive cascade difference point $(\delta^{\mathrm{r}}_{\mathrm{R},3}, h^{\mathrm{r}}_{\mathrm{R},3})$ toward the left (i.e. toward the reactant) and downward (for an exothermic reaction). The vapour composition at stage 4 (y_4) lies at the intersection of the vapour enthalpy line and the straight line connecting the reactive cascade difference point $(\delta^{\mathrm{r}}_{\mathrm{R},3}, h^{\mathrm{r}}_{\mathrm{R},3})$ to the liquid composition at stage 3 (x_3). We follow the phase equilibrium tie line from y_4 to find the liquid composition (x_4) of stage 4. Assuming more reaction occurs on stage 4, we obtain the vapour composition at stage 5 from the operating line connecting the reactive cascade difference point $(\delta^{\mathrm{r}}_{\mathrm{R},4}, h^{\mathrm{r}}_{\mathrm{R},4})$ and the liquid composition at stage 4. The liquid composition at stage 5 (x_5) is also available on the other end of the equilibrium tie line.

Assume the reaction turns off at stage 5. Thus the final reactive cascade difference point of the rectifying section is $(\delta^{\mathrm{r}}_{\mathrm{R},4}, h^{\mathrm{r}}_{\mathrm{R},4})$. We would continue to use this difference point for all subsequent stages above the feed stage when stepping down the column. Using the bottom difference point, we step up the stages from the bottom in the same way as in non-reactive distillation, since there is no reaction in the stripping section. The feed stage can be stage 4 through stage 6, as we cannot move below stage 6 from the final reactive difference point of the rectifying section $(\delta^{\mathrm{r}}_{\mathrm{R},4}, h^{\mathrm{r}}_{\mathrm{R},4})$ and cannot

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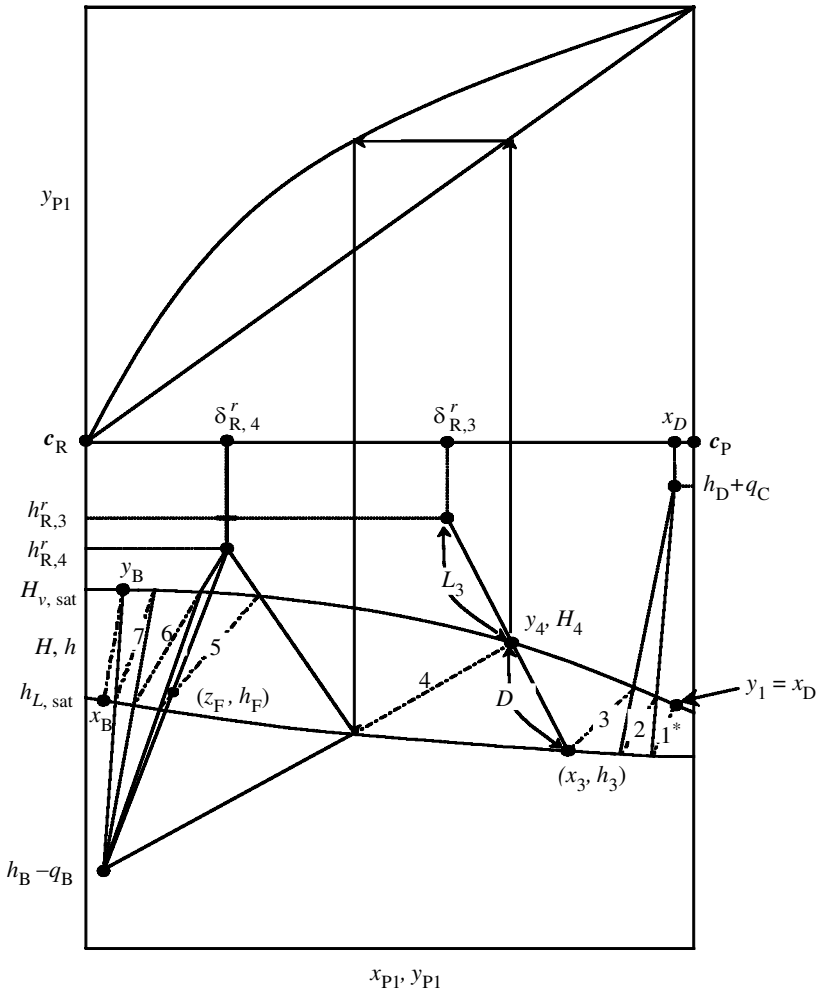


Figure 2. A Ponchon–Savarit diagram for reactive distillation when an isomerization reaction occurs. Dot-dash line, equilibrium tie line; solid line, balance line; arrow, construction line for the V/L equilibrium relationship; asterisk, stage number.

move up from stage 4 using the bottom difference point. We find in each of these cases that the operating lines coincide with the equilibrium tie lines, creating pinch points.

We determine the optimal feed stage in the same way as in non-reactive distillation (Henley & Seader 1981). Connecting the bottom difference point and the final difference point of the rectifying section by a straight line to satisfy total material and energy balances, we obtain the intersection point of the total balance line and an equilibrium tie line, as seen in figure 2. Below this line, we use the bottom difference point and above the top difference points, which makes stage 5 the optimal feed stage. The intersection point is the feed point with its composition and the enthalpy.

We can construct equilibrium tie lines by using a y–x equilibrium diagram placed above the H, x diagram, as shown in figure 2 (Wankat 1988). As shown, the flow of liquid leaving the third stage L_3 relates to the distance from $(\delta^r_{R,3}, h^r_{R,3})$ to (y_4, H_4) and the distillate flow D to the distance from (y_4, H_4) to (x_3, h_3) in terms of a lever rule.

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We note, in this example, that reaction changes the slopes of the balance lines in reactive stages 3 and 4. With the amount of reaction we show occurring, the slopes have even become negative. In this way, reactive distillation may allow us to step across an azeotropic composition or a pinch point. Also, the reaction turnover we used here has significantly reduced the number of stages in the column.

(*b*) *Decomposition reaction*

Here, R1 decomposes to form P1. We assume R1 and P1 form an ideal mixture, and R1 is less volatile than P1. In a reactive distillation column, unconverted reactant R1 exits at the bottom, and we recover product P1 at the top. If we take the following decomposition reaction, the material and energy balance equations around the rectifying section are the same as (2.9)–(2.11), except here the sum of the stoichiometric coefficients, ν_{T}, is 1 rather than zero for reaction (2.22). Thus we introduce the reaction difference point, $\boldsymbol{\delta}_{\mathrm{R}}$ equal to $\boldsymbol{\nu}/\nu_{\mathrm{T}}$, $[-1,2]^{\mathrm{T}}$ for R1 and P1 (instead of decomposing the stoichiometric coefficient vector as in the previous section to avoid the infinite reaction difference point (Lee *et al.* 2000)). While the composition elements of the reaction difference point add to one, this point lies on the right extension of the pure P1 and outside a conventional composition space, as shown in figure 3. We rearrange (2.9)–(2.11) to give the following equations (the material and energy balance equations for the stripping section are the same as (2.18)–(2.21)):

$$\mathrm{R1} \Leftrightarrow 2\mathrm{P1}, \tag{2.22}$$

$$V_{n+1} - L_n = D - \nu_{\mathrm{T}}\xi_n = \Delta^{\mathrm{r}}_{\mathrm{R},n}, \tag{2.23}$$

$$V_{n+1}\boldsymbol{y}_{n+1} - L_n\boldsymbol{x}_n = D\boldsymbol{x}_{\mathrm{D}} - \nu_{\mathrm{T}}\xi_n\boldsymbol{\delta}_{\mathrm{R}} = \Delta^{\mathrm{r}}_{\mathrm{R},n}\delta^{\mathrm{r}}_{\mathrm{R},n}, \tag{2.24}$$

$$V_{n+1}H_{n+1} - L_nh_n = D(h_{\mathrm{D}} + q_{\mathrm{C}}) + \Delta h_{\mathrm{R}}\xi_n = \Delta^{\mathrm{r}}_{\mathrm{R},n}h^{\mathrm{r}}_{\mathrm{R},n}, \tag{2.25}$$

$$\Delta^{\mathrm{r}}_{\mathrm{R},n} = D - \nu_{\mathrm{T}}\xi_n, \tag{2.26}$$

$$\delta^{\mathrm{r}}_{\mathrm{R},n} = (D\boldsymbol{x}_{\mathrm{D}} - \nu_{\mathrm{T}}\xi_n\boldsymbol{\delta}_{\mathrm{R}})/\Delta^{\mathrm{r}}_{\mathrm{R},n}, \tag{2.27}$$

$$h^{\mathrm{r}}_{\mathrm{R},n} = [D(h_{\mathrm{D}} + q_{\mathrm{C}}) + \Delta h_{\mathrm{R}}\xi_n]/\Delta^{\mathrm{r}}_{\mathrm{R},n}. \tag{2.28}$$

Here, $\Delta^{\mathrm{r}}_{\mathrm{R},n}$ is the difference in the vapour and liquid flowrates between stages $(n+1)$ and n in the rectifying section. $\delta^{\mathrm{r}}_{\mathrm{R},n}$ is the composition coordinate and $h^{\mathrm{r}}_{\mathrm{R},n}$ the enthalpy coordinate for the reactive cascade difference point in the rectifying section. $\nu_{\mathrm{T}}\xi_n$ is a flowrate of new moles produced by reaction. Here, it has a maximum value in the system equal to the flowrate of species R1 in the feed, since each mole of R1 converted produces one additional mole of material handled by the column. If we recover in the distillate more than half of the product P1 produced and if the reaction only proceeds in the forward direction anywhere in the column, then the distillate flowrate D must be larger than $\nu_{\mathrm{T}}\xi_n$. We shall arbitrarily assume reaction occurs only on stage 2. As shown in figure 3, the composition coordinate of the reactive cascade difference point starts at x_{D}. $\delta^{\mathrm{r}}_{\mathrm{R},2}$ moves to the left of the distillate composition away from the reaction difference point, since ξ_2 is positive. If our decomposition reaction is exothermic, the enthalpy difference point also goes down. We draw a balance line for reactive stage 2 in figure 3 using the reactive difference point $(\delta^{\mathrm{r}}_{\mathrm{R},2}, h^{\mathrm{r}}_{\mathrm{R},2})$. The length of the line between $(\delta^{\mathrm{r}}_{\mathrm{R},2}, h^{\mathrm{r}}_{\mathrm{R},2})$ and (y_3, H_3) is denoted by L_2 and the length from (y_3, H_3) to (x_2, h_2) is represented by $\Delta^{\mathrm{r}}_{\mathrm{R},2}$, in the sense of a lever rule. We can easily complete tray-by-tray calculations in the same way as in the previous case of

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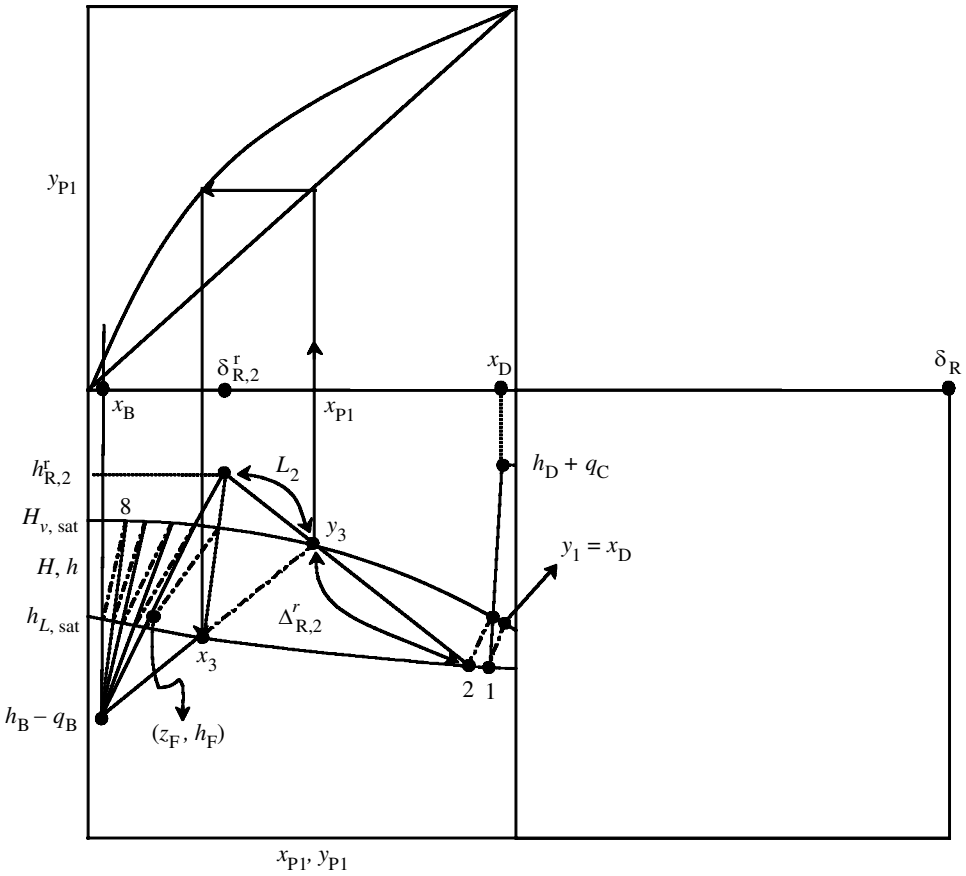


Figure 3. A Ponchon–Savarit diagram for reactive distillation when the decomposition reaction takes place.

figure 2. The feed stage can be any of stages 3 through 5, but the optimal location is stage 4, as the total balance line connecting $(\delta^{r}_{R,2}, h^{r}_{R,2})$ and $(x_B, h_B - q_B)$ intersects with the equilibrium tie line of stage 4. We require eight stages, including a partial reboiler, to obtain the desired top and bottom products with only one reactive stage, as shown in figure 3.

(*c*) *Alternative way to construct a Ponchon–Savarit diagram*

If we want to relate D and L_n geometrically, and to obviate a reactive cascade difference $\Delta^{r}_{R,n}$ with a zero value (in which case the composition coordinates for the corresponding reactive cascade difference point is at infinity due to the low recovery of the product at the top), we can reformulate (2.24) and (2.25) using the following equations:

$$V_{n+1} - (L_n + D) = -\nu_T \xi_n, \tag{2.29}$$

$$V_{n+1}\boldsymbol{y}_{n+1} - (L_n \boldsymbol{x}_n + D\boldsymbol{x}_D) = -\nu_T \xi_n \boldsymbol{\delta}_R, \tag{2.30}$$

$$V_{n+1}H_{n+1} - [L_n h_n + D(h_D + q_C)] = -\nu_T \xi_n(-\Delta h_R/\nu_T). \tag{2.31}$$

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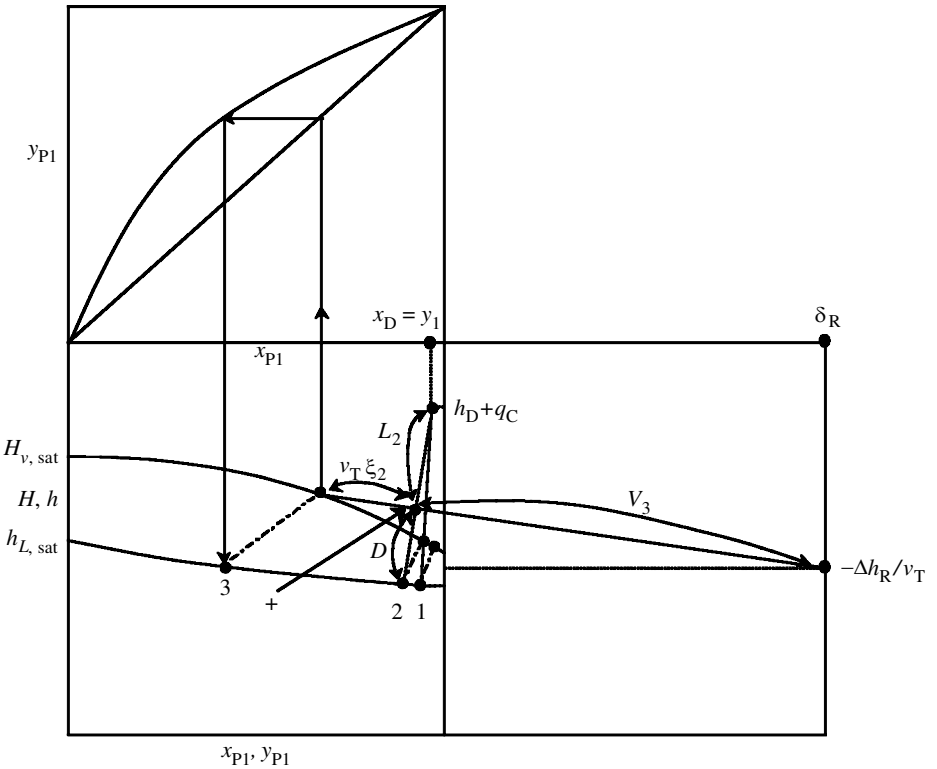


Figure 4. A Ponchon–Savarit diagram for reactive distillation when we take a different linear combination in the decomposition reaction. +, Linear combination of (x_2, h_2) and $(x_D, h_D + q_C)$.

Here, we take stage 2 as a reactive tray for the decomposition reaction. For decomposition in a reactive distillation column, we first draw a straight line between $(\boldsymbol{x}_D, h_D + q_C)$ and $(\boldsymbol{x}_2, h_2)$, as we illustrate in figure 4. Since we know $(\boldsymbol{x}_2, h_2)$ from the equilibrium relationship with $(\boldsymbol{y}_2, H_2)$ (as indicated in the construction of the line for equilibrium by the arrow lines in figure 4), we can determine the combined point (+). The lengths of $(\boldsymbol{x}_D, h_D + q_C)$ and $(\boldsymbol{x}_2, h_2)$ from the combined point (+) reflect the relative amounts of L_2 and D, respectively. At the second step, we construct a straight line connecting $(\boldsymbol{y}_3, H_3)$, the combined point (+) and $(\boldsymbol{\delta}_R, -\Delta h_R/\nu_T)$. The distance between $(\boldsymbol{y}_3, H_3)$ and the combined point (+) denotes the relative amount of $\nu_T\xi_2$, and the length from the combined point (+) to $(\boldsymbol{\delta}_R, -\Delta h_R/\nu_T)$ that of V_3.

3. Conclusions

In this work, we illustrate how to construct a Ponchon–Savarit diagram for binary reactive distillation. One important point is that the number of stages and the feed stage location strongly depend on the extent of reaction in a reactive distillation column. The Ponchon–Savarit method will provide an accurate description of a reactive distillation column if enthalpy data and the heat of reaction are correct. We can also obtain many design implications, such as the proper reaction distribution within a column and the determination of optimal feed stage location, using the proposed diagram. Historically, the Ponchon–Savarit method (Ponchon 1921; Savarit

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1922) preceded the McCabe–Thiele method (McCabe & Thiele 1925). We also developed the Ponchon–Savarit diagram for a reactive distillation column earlier than the McCabe–Thiele method. Thus subsequent papers will deal with McCabe–Thiele diagrams for reactive distillation columns and apply these two graphical methods to actual processes.

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Nomenclature

a_1, a_2, a_3, b	vector coefficient or constant
B	bottom product molar flowrate (mol s^{-1})
$\boldsymbol{c}_{\mathrm{P}}$	product coefficient vector
$\boldsymbol{c}_{\mathrm{R}}$	reactant coefficient vector
D	top product (distillate) molar flowrate (mol s^{-1})
H_{n+1}	saturated vapour molar enthalpy at stage $n+1$ of the rectifying section (J mol^{-1})
H_{s+1}	saturated vapour molar enthalpy at stage $s+1$ of the stripping section (J mol^{-1})
h_{B}	bottom product molar enthalpy (J mol^{-1})
h_{D}	top product molar enthalpy (J mol^{-1})
h_{F}	feed molar enthalpy (J mol^{-1})
h_n	saturated liquid molar enthalpy at stage n of the rectifying section (J mol^{-1})
h_s	saturated liquid molar enthalpy at stage s of the stripping section (J mol^{-1})
$h^{\mathrm{r}}_{\mathrm{R},n}$	enthalpy coordinate at stage n of the rectifying section in equations (2.16) and (2.28) (J mol^{-1})
L_n	liquid molar flowrate at stage n of rectifying section (mol s^{-1})
$\bar{L}_s$	liquid molar flowrate at stage s of stripping section (mol s^{-1})
R1, P1	a reactant and a product
Q_{B}	reboiler heat duty (J s^{-1})
q_{B}	reboiler molar heat duty (J mol^{-1})
Q_{C}	condenser heat duty (J s^{-1})
q_{C}	condenser molar heat duty (J mol^{-1})
V_{n+1}	vapour molar flowrate at stage $n+1$ of the rectifying section (mol s^{-1})
$\bar{V}_{s+1}$	vapour molar flowrate at stage $s+1$ of the stripping section (mol s^{-1})
$\boldsymbol{v}_1$, $\boldsymbol{v}_2$, $\boldsymbol{v}_3$	vectors
$\boldsymbol{v}'_j$	augmented vector
$\boldsymbol{x}_{\mathrm{B}}$	bottom product molar composition vector
$\boldsymbol{x}_{\mathrm{D}}$	top product molar composition vector
$\boldsymbol{x}_n$	liquid molar composition vector at stage n of the rectifying section
$\boldsymbol{x}_s$	liquid molar composition vector at stage s of the stripping section

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$\boldsymbol{y}_{n+1}$	vapour molar composition vector at stage $n+1$ of the rectifying section
$\boldsymbol{y}_{s+1}$	vapour molar composition vector at stage $s+1$ of the stripping section
z_1, z_2, z_3	elements of a vector
$\boldsymbol{z}_{\mathrm{F}}$	feed molar composition vector

Greek letters

α	parameter used in equation (2.3)
$\Delta^{\mathrm{r}}_{\mathrm{R},n}$	difference flow in vapour and liquid flowrates in equation (2.23) (mol s^{-1})
$\boldsymbol{\delta}_{\mathrm{R}}$	reaction difference point
$\delta^{\mathrm{r}}_{\mathrm{R},n}$	composition coordinate for a reactive cascade difference point in equations (2.15) and (2.27)
Δh_{R}	molar heat of reaction, negative for exothermic and positive for endothermic (J mol^{-1})
$\boldsymbol{\nu}$	stoichiometric coefficient vector
ν_{T}	sum of stoichiometric coefficients
ξ_n	sum of reaction molar turnover flowrate or extent of reaction (mol s^{-1}) from the top to stage n

Definition

$(\delta^{\mathrm{r}}_{\mathrm{R},n}, h^{\mathrm{r}}_{\mathrm{R},n})$	reactive cascade difference point at stage n in Ponchon–Savarit diagram (subscript 'R' denotes 'reaction' and superscript 'r' represents rectifying section)

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