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A Novel Graphical Approach for Mass Exchange Networks Using Composition Driving Force

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Raw materials are considered as a corner stone for both chemical and process industries. Raw materials efficient utilization and usage within the process saves a lot. Mass integration is the most competent path to minimize the economic and environmental losses, by minimizing both the amounts of external mass separating agents and waste disposal. Mass exchange networks or MENs is the tool used to apply this integration. This article presents a new graphical approach, based on the composition driving force, to analyse the mass integration and exchange networks. The new approach is illustrated graphically, and can be applied on existing and new mass networks. The new graphical approach is constructed based on the Pinch Analysis Principle where the lean stream compositions are plotted on the X-axis, while the composition driving forces for each exchanger are plotted on the Y-axis. The performance of MENs is evaluated and analysed in terms of the composition driving force (CDF) inside the mass exchanger. In addition to be the main motive to transfer the composition from rich stream to lean stream, composition driving force is also involved in the calculation of the number of theoretical plates, consequently affecting the cost. Each mass exchanging unit is represented in this graph as a straight line whose slope is related to the mass flow rates of both rich and lean streams and its length is related to the mass load transferred within the exchanger. The CDF is divided into five regions, based on the pinch analysis principles to analyse and perfectly locate the mass exchangers. The new graphical approach is applied to existing MENs to enhance their actual performances by minimizing wastes disposal and external separating agents and accomplish the mass targets defined by the Pinch Analysis Principles.

1. Introduction

Chemical process industries consist of multiple unit operations performed on both energy and material streams. Material streams are as important as energy streams (Friedler, 2009). Operations use material streams include chemical reactions, separation processes, product purification as well as mass integration (Smith, 2005). Mass integration defines the exchange of mass within two process streams, i.e. rich and lean streams. The main objectives of mass integration tasks are either to recover a valuable by-product or to remove a certain contaminant instead of being disposed of to the environment. The new graphical approach relies on describing the mass exchange problem on a new plot relating the difference in composition of components in rich and lean streams streams versus the equivalent composition in lean streams.

1.1 Introducing CDF new graphical approach

The new graphical approach uses the basic principles of Pinch Analysis (Linnhoff et al., 1983). The two axes are employed to describe the mass load integrated within the mass exchanging unit. For a given exchanger unit, the driving force at both ends is plotted against the corresponding equivalent composition in lean stream entering or leaving the exchanging unit (Kamel et al., 2016). The equivalent lean composition is an expression that describes the composition in the lean stream in operation with the rich stream (x) added to the minimum allowable composition difference (ϵ), that represents the minimum driving force between operating and

equilibrium lines, all multiplied by the equilibrium dependency constant (m) as expressed in Eq(1). In previous research, this term was derived so that the equilibrium relation and the lean stream composition in operation with a minimum driving force are merged and expressed in one single indicative term (Gadalla, 2015). On the CDF plot the equivalent lean composition is plotted on the x-axis. However, the y-axis on the plot represents the difference in compositions between rich stream (y) and the equivalent lean stream (x_{eqv}) that was previously described. Thus, the composition driving force is expressed in Eq(2) as follows:

$$x_{\text{eqv.}} = m(x + \varepsilon) + b \tag{1}$$

$$\Delta C = y - x_{\text{eqv.}} \tag{2}$$

1.2 Rich and lean streams representation

After defining the axis of the new graphical approach, both the rich and lean stream compositions are to be represented as in Figure 1. The lean stream lines are represented as vertical lines starting from x_{eqv} . On the X-axis, while the rich stream lines are represented as 45° inclined straight lines whose slope is -1 and intercepts at y. The rich stream lines start from $\Delta C = y$ on the Y-axis that corresponds to x_{eqv} . = zero and end at $y = x_{eqv}$. on the X-axis that corresponds to ($\Delta C =$ zero) as shown below. Moreover, the rich and lean pinch compositions are previously determined analytically or graphically from pinch diagrams or composite curves and dragged onto the new plot.



Figure 1: Graphical representation for rich and lean streams on CDF plot

1.3 Datum lines on CDF plot

The new graphical approach is restricted by two prominent indicative lines. In particular, the two datum lines, represented on the plot, demonstrate the feasible and equilibrium lines. The feasible line was previously defined to represent a constant minimum driving force between the operating and the equilibrium lines (EI-Halwagi, 1997). This implies a mass driving force between the rich and lean streams compositions corresponding to the minimum allowable composition difference (ϵ). This line is represented on the graphical approach as a horizontal line starting at ΔC = zero as shown in Figure 2. However, the second datum line exhibits the linearized equilibrium relation between y and x that implies a mass driving force between rich and lean streams equal to zero (Gadalla, 2015). Consequently, this line sets up the thermodynamic limitation for the process i.e. no exchanger line can be located below this line. The physical meaning for this line is that the composition of the lean stream leaving the mass exchanging unit is exactly equal to the equilibrium composition. Therefore, an infinite number of contacting stages is required for mass separation and to achieve the mass targets. This line is represented on the graph as a horizontal line starting at ΔC = -m ϵ as shown in Figure 2.



Figure 2: Datum lines on CDF plot

2. Features of the new graphical approach

2.1 Exchanger line

Mass flow rates for the process streams within the same exchanger are assumed to be constant. As a result, each exchanger unit is represented by a straight line extending between $(x_{eqv})^{in}$, ΔC_{lean} and $(x_{eqv})^{out}$, ΔC_{rich} as shown in Figure 3. Specifically, the lean end CDF (ΔC_{lean}) is the difference between the outlet rich stream composition (y^{out}) and the inlet lean stream equivalent composition $(x_{eqv})^{in}$. However, the rich end CDF (ΔC_{rich}) is the difference between the inlet rich stream composition (y^{in}) and the outlet lean stream equivalent composition $(x_{eqv})^{out}$ as shown below.



Figure 3: Exchanger line representation on CDF plot

2.2 Feasible design regions

The combination of pinch points together with the linearized equilibrium relation defined by the line $\Delta C_{min} = -m\epsilon$, classify the graph to identify some characteristic regions useful for MENs design as in Figure 4. The line of ΔC_{min} sets up the thermodynamic limitation as previously discussed. Thus, below this line, mass exchanger design is infeasible, i.e. no exchangers are located below ΔC_{min} , demonstrated within region 5. Yet, region 1 and region 3 lead to optimal feasible design regions that integrate mass "below rich/ below lean" and "above rich/ above lean" compositions respectively. These two regions are considered the perfect regions to locate the mass exchangers and achieve the mass targets. However, regions 2 and 4 are non-optimal design regions where mass will be only integrated across the Pinch, thus mass losses would be encountered, and the design will require an excessive amount of transfer units.



Figure 4: Feasible and infeasible design regions

2.3 The Slope of the exchanger line and its limitations

Consider a mass exchange unit transferring a mass load ΔM between rich and lean streams having flow rates G and L respectively. The inlet and outlet compositions for the rich stream are y^{in} and y^{out} , while the inlet and outlet compositions for lean stream are x^{in} and x^{out} as shown in Figure 5.



Figure 5: Mass exchange unit

Eq(3) shows a mass balance performed on the mass unit:

$$\Delta M = G \Delta y = L \Delta x \tag{3}$$

However, the x-axis represents the equivalent lean stream compositions so, Eq(3) is modified to match the new axis so as shown by Eq(4) which correlates ΔM with x_{eqv}.

$$\Delta M = G \Delta y = L' \Delta x_{eqv}. \tag{4}$$

Where L' is the lean stream flow rate (L) divided by the equilibrium dependency constant (m). The slope of the exchanger line is calculated from Eq(5).

$$S = \frac{\Delta y}{\Delta x} = \frac{\Delta y - \Delta x eqv.}{\Delta x eqv.} = \frac{\Delta y}{\Delta x eqv.} - 1$$
(5)

Merging Eq(5) with Eq(4) results in an expression for the slope of the exchanger line on the CDF plot shown by Eq(6).

$$S = \frac{L'}{G} - 1 \tag{6}$$

According to Eq(6), the line of the exchanger has three different slope scenarios. For $\frac{L'}{G} > 1$, i.e. a positive slope, the rich stream has a limited mass flow rate with respect to the lean stream. Consequently, the rich stream will reach its target composition before the lean stream, while the later will reach an intermediate composition ($x_{eqv.int.}$) between its supply and target compositions that can be directly calculated from the slope of the exchanger line, or read directly from the graph. However, for $\frac{L'}{G} < 1$, i.e. a negative slope, the mass flow rate within the process lean stream is limited and reaches its target composition first and hence the rich stream will reach an intermediate composition ($y^{int.}$) between its supply and target compositions. Finally, when the two streams have equal mass flow rates, with $\frac{L'}{G} = 1$, this indicates that both streams will reach their targeted compositions.

2.4 The length of the exchanger line

As previously mentioned, the exchanger line is represented on the new graphical approach as a straight line. Performing some simple mathematical calculations, the length of the exchanger line (Θ) was found to be so indicative, as it is directly related to the mass load transferred within the exchanger mass unit (Δ M) and the flow rates of the lean and rich streams, L and G respectively. Eq(7) shows the derived relation representing the length of the exchanger line.

$$\theta = \frac{\Delta M}{LG} \sqrt{(L - mG)^2 + (mG)^2} \tag{7}$$

As a result of all of the above, quick comprehensive decisions and evaluation could be concluded from the new graphical approach regarding the performance of an existing mass exchange network. First, the location of the exchanger indicates its design region weather it is optimal, non-optimal or infeasible design region. Second, the slope of the line can also indicate, without further calculations, the stream that would reach its target composition first as it has a sufficient mass flow rate. Finally, the length of the line indicates the amount of mass load transferred within the exchanger i.e. longer lines corresponds to greater mass load transferred and vice versa.

This is actually important to perfectly select the mass exchanger within multiple possibilities, if any, for the same match between rich and lean streams.

2.5 Theoretical and graphical representation of the number of plates

The key benefit of this approach is the exact determination of the required mass transfer units used in sizing the mass exchangers from the graph without further calculations. In the new graphical representation, the exchanger lines represent operating lines for mass exchange. On the other hand, the datum line $\Delta C_{min.} = -m\epsilon$ is equivalent to the linearized equilibrium relation between the rich and the lean streams. Thus, NTP for a mass exchanger unit can be estimated by stepping off stages between the rich end and lean ends, and the line $\Delta C_{min.} = -m\epsilon$ as in Figure 6. In case of dilute mass exchange with linear equilibrium relation between both rich and lean streams, Kremser developed a simple equation Eq(10) to calculate the NTP for an isothermal exchanger between both streams, as follows (EI-Halwagi, 2012):

$$NTP = \frac{\ln\left[\left(1 - \frac{mG}{L}\right)\left(\frac{y^{in} - mx^{in} - b}{y^{out} - mx^{in} - b}\right) + \frac{mG}{L}\right]}{\ln\left(\frac{L}{mG}\right)}$$
(10)

Eq(10) is modified to match the terms introduced for the new graphical approach as described below in Eq(11) in terms of the line slope, and composition driving force as:

$$NTP = \frac{\ln\left[\frac{1}{S+1}\left(\frac{S\,\Delta y}{\Delta C_{Lean} + m\epsilon}\right) + S + 1\right]}{\ln(S+1)} \tag{11}$$

Where S is the slope of the exchanger line on the CDF plot and ΔC_{lean} is the lean end composition driving force. As a result, the theoretical number of plates for an exchanger unit can be determined either empirically from the above derived equation or graphically from the new approach. The graphical determination of the number of transfer units is performed by moving vertically downwards from the exchanger line representing the operating relation to the datum line representing the linearized equilibrium relation and presented on the CDF plot as $\Delta C_{min.} = -m\epsilon$, then moving diagonally on the rich stream lines from the line $\Delta C_{min.} = -m\epsilon$ back to the exchanger line. These steps are carried on as long as the exchanger line is extended. Figure 6 represents the graphical determination of the actual number of transfer units.



Figure 6: Graphical determination for the number of plates

3. Case study: copolymerization plant

A copolymerization plant to produce a copolymer from two stages reactions; first catalytic reactor uses a catalytic solution (process lean stream S2) while the second stage reactor enhance the polymer properties using some additives (process lean stream S1). A gaseous waste stream (R1) is produced as a by-product contains benzene used as a solvent within the manufacturing process. The main objectives aimed from this study are: to recover the benzene from the waste stream by designing MEN, and to determine the number of stages for each exchanger to achieve the targeted compositions.

Based on the study and the network described in figure 7, mx1 is the mass exchanger to integrate mass between the rich stream and the process lean stream s1 above the pinch. However, mx3 is the mass exchanger to integrate mass between the rich stream and the external mass separating agent below the pinch. Therefore, the network consisting of mx1 and mx3 is sufficient to recover the benzene vented in the waste stream. Both are located in feasible optimal design regions.



Figure 7: MEN graphical design for the copolymerization plant

The number of plates for both mx1 and mx3 were directly counted for the network represented on the CDF plot as previously discussed in section 2.5. The actual number of plates obtained from the plot for mx1 and mx3 were 2.2 and 13 respectively. From the graph, the maximum targeted composition for the process lean stream S1 is 0.001625. The driving forces for each exchanger at any stage are taken directly from the y-axis. The process lean stream S2 was not considered for two reasons; first, S1 was sufficient to integrate mass above the pinch with the rich stream, second, the mass exchanger using S2 with the rich stream was located within the infeasible design region 5.

4. Conclusions

The new graphical approach is based on Pinch Analysis Principles and has been proposed to evaluate the performance of existing MENs and design new networks. The driving force within both ends of the mass exchanging unit is plotted on the y-axis, while the equivalent lean stream composition is represented on the xaxis. Besides counting the number of transfer units required for the process, the new graphical approach also sets up some limitations for the process mass integration to follow while designing. The CDF determines the maximum targeted compositions for both rich and lean streams. Moreover, it highlights the feasible optimal design regions to perfectly locate the exchangers with minimum mass losses and minimum cost. The CDF is considered as a comprehensive visual tool to express MEN as any point on the plot is the locus of: composition driving force, lean stream composition and rich stream composition. As previously mentioned, it gives quick decisions and impressions regarding the mass network design without further calculations from the location, length and slope of the exchanger line. Furthermore, it could determine the amount of external mass separating agent if requires as well as the exact mass load transferred within the exchanger only by reading the length. Finally, the number of transfer units that is used in sizing the mass exchanger and consequently affect the cost can be calculated either empirically or directly from the graph as was discussed before. Although this graphical approach has many advantages, it is difficult to plot manually each exchanger for large mass networks. So it is recommended to extend this representations and promising modifications on existing MENs using computer programming like MATLAB.

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