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NOVEL MINIMUM REFLUX CALCULATION USING EIGENVECTOR MAPS

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Abstract

Column Profile Map Eigenvectors (CPM-E) technique is introduced to determine the minimum energy demand for multicomponent feed in two-product distillation processes. The technique is a short cut, geometrical, non-iterative method and can be used to predict how the minimum reflux solution is related to the feed-component distribution for all possible operating conditions. The new method makes use of Column Profile Maps and the concept of "moving triangles" and develops co-linearity criteria based on the eigenvectors of the Jacobian of the separation vector evaluated at the feed composition. The CPM-E technique is a powerful tool that can be applied to complex column arrangements, such as Petlyuk or Kaibel Columns. The CPM-E approach is non-exclusive and can therefore be applied to any type of split, sharp or non-sharp, irrespective of the number of components. It will be shown that the CPM-E technique can be used to determine minimum reflux solutions quickly and effectively. From this, it is shown that three limiting product composition regions under minimum reflux conditions are present. The links between the CPM-E technique and the determination of minimum energy demand using Underwood's methods are explored.

Keywords: Eigenvectors, graphical, non-iterative, minimum reflux, co-linearity

1. Introduction

The continuous increasing cost of energy has made it necessary for industry to reduce its energy consumption. In addition to this, the effort to prevent climate change has caused stringent environmental regulations that have generated the need to adopt new and efficient unit operations. Intensive investigations have been undertaken to develop new and more useful models to operate distillation units as optimally as possible. Koehler et al.[1] give a review of methods for determining minimum energy requirements for conventional columns as well as complex column configurations up to 1995. They show that many of the minimum energy demand techniques are related to the methods of Underwood. Many works done by Doherty and co-workers[2-4] have proposed several techniques that produce accurate minimum reflux solutions for ideal as well as highly non-ideal azeotropic systems. The drawback of these techniques is the selection of the initial reboiler duty which indicated uncertainty whether the selected duty will produce a minimum reflux solution. The approaches adopted by Doherty and co-workers rely heavily on pinch points as well as on the interaction of vectors between the pinch points of both the rectifying and stripping sections. The focus of this manuscript is to demonstrate a novel method, called Column Profile Maps Eigenvector (CPM-E) technique, to determine the minimum energy demand in any conventional column and to show the link between CPM-E and Underwood based method such as V_{min} diagrams[5].

2. Background

2.1 Column Profile Maps

Column Profile Maps, introduced by Tapp et al.[6], is produced from the Difference Point Equation (Equation 1). These Maps are composition trajectories generated for column sections (CS) for a predefined difference point (X_{Δ}) and reflux ratio (R_{Δ}). Δ is better described as the net flow of material and is a pseudo stream flowing up or down in a column section.

$$\frac{dX}{dn} = \left(1 + \frac{1}{R_{\Delta}}\right)\left(X - Y^{*}(X)\right) + \frac{1}{R_{\Delta}}(X_{\Delta} - X) \text{ Where:} X_{\Delta} = \frac{VY_T - LX_T}{\Delta};\ \ R_{\Delta} = \frac{L}{\Delta}\ ;\ \Delta = V - L \qquad (1)$$

If the vapour flow were larger than the liquid flow in a column sectionΔ would be positive as we know it to be in a rectifying section (RS) and the direct opposite applies to the stripping section. A material balance indicates that the distillate product flow is equivalent to the positive net flow in the rectifying section. Similarly, the bottoms product flow is equal to the negative net flow in the stripping section The difference point (X_{Δ}) is the pseudo composition vector of the net flow, and is physically valid anywhere in composition space. It can be shown from mass balance that the difference point for a conventional column is equivalent to the product specifications of the column. The reflux ratio is defined as the ratio of liquid flowing down the column section to the net flow in the column section. Because of its dependence onΔ, R_{Δ} can either be positive or negative. This means flow up in a rectifying section and down in a stripping section tells us that we can only have reflux ratios that are positive in the rectifying section and negative in the stripping section. Any other direction other than specified would result in an infeasible profile intersection.

2.2 Eigenvector Maps

The eigenvectors characterize the asymptotic direction of the trajectories in the neighbourhood of the singularity. Holland et al.[7] introduced Eigenvalue and Eigenvector Maps and illustrated the usefulness of these maps for manipulating phase diagrams and therefore column profiles. The maps predict movement of the singularities based on the value of the design parameters of the difference point selected in the composition space and the reflux ratio. An eigenvector map can be obtained by plotting the eigenvectors over a range of *x* values.

3. Conditions for Minimum Reflux, transformed triangles and collinearity rule.

The boundary value method introduced by Levy et al.[2], is implemented by identifying co-linear lines drawn from the saddle node of the rectifying section through the feed and the unstable node through the feed for sharp, direct splits. By plotting the liquid profiles for each section, showing that one of the profiles ends on the other and then illustrating co-linearity of the pinched lines, minimum reflux is established. The fact that column profile maps are similar to the stage by stage methods used by Doherty and co-workers indicates that the condition for minimum reflux for either method must be the same. Tapp et al.[5] showed that the Column Profile Maps at finite reflux are simply transforms of the residue curve maps. The transform shifts the fixed points of the system in the space, maintaining (in constant relative volatility systems) the shape of the boundaries initially defined by the MBT. This has resulted in the phenomenon being referred to as “Transformed Triangles” (TT). The description of co-linearity lines (CLL) at minimum reflux conditions indicates that it will be easier to track the saddle pinch and feed pinch which supplement co-linearity by using TTs of the rectifying and stripping sections. Thus it is more convenient to solve for the stationary points that define the nodes and rather plot the straight lines between these nodes.

In Figure 1a and b, the reflux ratio is greater than the minimum; the profiles cross and continue further on. Figure 1b describes a column that is subject to less energy input for the same product specifications as it is closer to the minimum reflux condition, since the overlap of the profiles is not as great as it is in the previous Figure (Figure 1a). Therefore, the desired structure that represents minimum reflux is shown in Figure 1c where the stripping profile ends or terminates on the rectifying profile. The point on the rectifying profile and stripping profile where they intersect is the feed stage. The feed it seems is the last possible ‘point’ for the TTs to intersect. Any reflux selected above the minimum will result in an overlap of TTs and any reflux selected below the minimum will result in no overlap of the TTs and therefore no feasible intersection of profiles will occur. At specified feed conditions, distillate and bottoms compositions, the exact condition for minimum reflux is that the tangent to the saddle pinch profile at the feed pinch point is a straight line through X_F. This is true regardless of whether the mixture is ideal, non-ideal, or azeotropic[2].

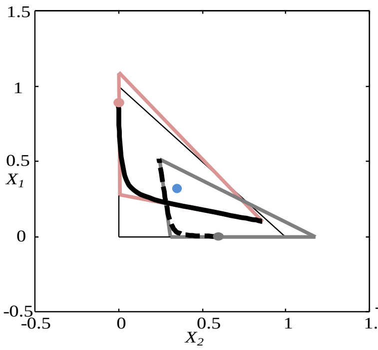

Figure 1(a). Crossing Profiles with corresponding overlapping TTs.

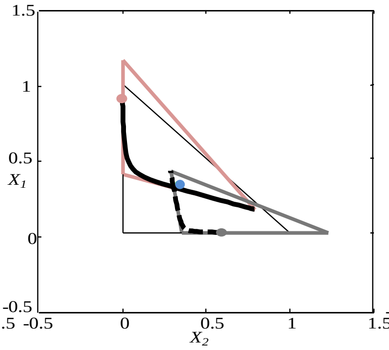

Figure 1(b). Smaller reflux, but still over refluxed system.

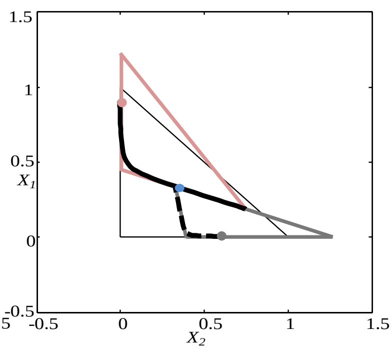

Figure 1(c). System at minimum reflux conditions.

4. CPM-E technique derivation

4.1 Eigenvector application and CPM-E technique

Holland et al.[7] demonstrated that the eigenvectors at the singularities, of constant-relative-volatility systems, always point along the direction of the TT boundaries. Because the boundaries are straight in these systems, the eigenvectors at each singularity point directly at the other singularities. Any point chosen along one of these boundaries will have eigenvectors that point directly at the same singularities, which define it. It is evident at this point that the eigenvectors evaluated on the minimum reflux TT have to be co-linear with the CLL. We can now predetermine the CLL where the minimum reflux TTs touch. Because the CLL passes through the feed composition, evaluation of the eigenvector at the feed composition show all possible CLL based on a specified feed condition. Finding these lines implies that we are a step closer to finding the stationary points where the profiles/TTs of the minimum reflux coincides. Once we find at least one stationary point associated to a profile/TT at minimum reflux conditions, finding and quantifying the minimum reflux solution would be possible.

To find the stationary points, non-specific for a thermodynamically ideal ternary system, would involve solving the right hand side of the Difference Point Equation (Equation 1) for the liquid composition when it is equivalent to zero. Taking a closer look at the terms in the Difference Point Equation, we identify two vectors. The first vector, called the separation vector is the difference between the liquid composition and the vapour composition in equilibrium with the liquid composition i.e. $\tilde{s} = (X\text{-}Y^*(X))$. The second vector is called the mixing vector and is the difference between the difference point and the liquid composition i.e. $\tilde{m} = (X_\Delta\text{-}X)$. At the stationary point this implies from a geometrical point of view that the mixing vector is co-linear with the separation vector. This is illustrated in Figure 2. The main aim is thus, to find a stationary point along the CLL. In order to determine the point, simple straight line geometrical tools are employed. The straight CLL aids with this as it passes through the stationary node. The only other line that passes through the liquid stationary point is the mixing and separation vectors co-linear line. Two unknown points arise from these points. They are the liquid pinch point and the equilibrium vapour pinch point illustrated in Figure 2. Due to the fact that the vapour composition is only a function of the constant relative volatility and liquid composition, the only unknown is the liquid composition at the stationary point. In other words, the solution to the pinch point is found by equating the gradients of the mixing vector and separation vector, and then solving for the elements of the liquid composition simultaneously with the straight line equation of the CLL. This composition would be the stationary point solution on the CLL which is one of the stationary points on the minimum reflux TT solution (Figure 2). If the transformed triangle can be found algebraically by simply specifying the R_Δ and X_Δ, then the reverse must also be true. By knowing the fixed points of a Column Profile Map or its associated TT we must be able to determine R_Δ and X_Δ. There is no need to determine the difference point as it has already been specified through the product specification. Therefore the only unknown is the reflux ratio. This very powerful result of the calculated reflux is the minimum reflux solution for a given feed. This result was found without iterations or tedious steps and is based on simple mathematics. The results of the minimum reflux are illustrated in Figure 2.

4.2 Additional CPM-E solutions

In addition to the eigenvector we have focussed on that has produced a base of solutions along our CLL, there is another eigenvector with a larger slope that we have not yet considered, but is of immense importance and produces a different set of solutions along it. We will name the co-linearity line of smaller (absolute) gradient; derived from the red eigenvector, Co-Linearity Line 1 (CLL1) and the line of larger (absolute) gradient; derived from the blue eigenvector, Co-Linearity Line 2 (CLL2).

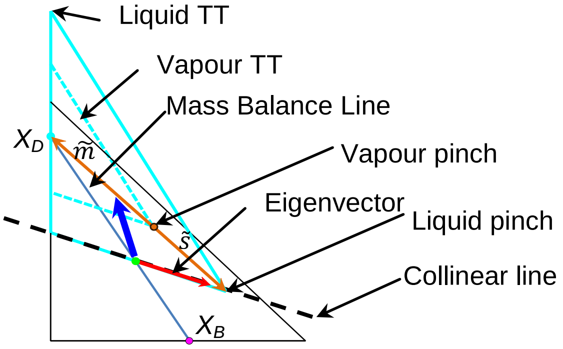

Figure 2. CLL stationary point with mixing and separation vector passing through the node of the transformed triangle for the minimum reflux solution

Additional solutions exist, other than along CLL1, which governs minimum reflux for different purities of either the distillate or bottoms product. The selection of X_D will affect the TT for each specified minimum reflux but will not affect the interaction properties of the TTs under minimum reflux conditions. Therefore, for each and every product selection, there is a specified TT that is related to a minimum reflux solution because of its association to the specified difference point placement. CLL1 and CLL2 are distinct solutions, but they can be used together under certain composition selections to produce additional solutions other than those already discussed. It is important to note that minimum reflux solutions derived from CLL1 produce TTs that interact along CLL1 (See Figure 3). Therefore, minimum reflux solutions derived from CLL2 approach along CLL2 where the distillate product has lower concentrations of light key components (See Figure 4). Increasing the impurity of the high boiler that reports to the top and solving for the minimum reflux at select points, shows a point where the solutions based on CLL1 'swap-over' to CLL2.

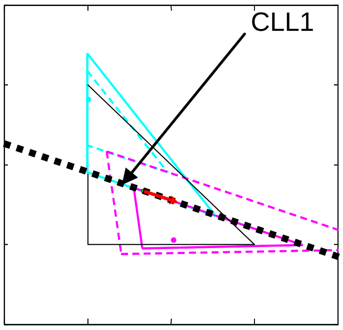

Figure 3. Minimum reflux solution along CLL1

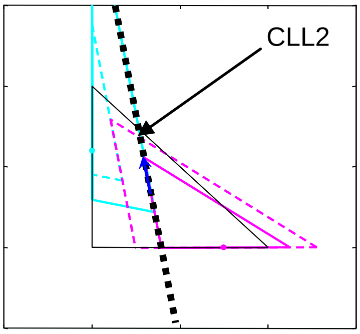

Figure 4. Minimum reflux solution along CLL2

The point where the swap-over takes place is where both eigenvectors that produce CLL1 and CLL2 are employed. This phenomenon is feed specific and is non selective to regions in the real space and is called the preferred split. This means that the feed composition at this special minimum reflux solution has become a stationary point for both the rectifying section and stripping section and therefore the preferred split will exhibit a pinch region on both sides of the feed stage and not individually as we have previously seen when either CLL1 or CLL2 are common. Selecting product compositions on the 'swap-over' point from CLL1 to CLL2 or vice versa and calculating the minimum reflux at the point for either common CLL produces the preferred split. This of course is only true if the split is sharp. If the feed is assumed to be a saturated liquid, finding the preferred split is as simple as determining the vapour composition in equilibrium with the feed composition and then extending a straight line through both points. The intersection of the line with the light intermediate axis is the preferred split. This line exhibits interesting results when product compositions are selected along it and the CPM-E technique is applied to them. Both CLLs remain common and therefore the feed composition remains a stationary point where the rectifying section's TT and stripping section's TT meet. Holland et al.[8] have described this phenomenon as “double-feed-pinches”. The “double-feed-pinch” point is phase dependent. Vapour feed columns will exhibit a vapour profile “double-feed-pinch” point - although it should be noted that both phases in both cases will pinch.

5. Minimum Reflux regions

5.1 Regions developed from CPM-E technique

The sign of the reflux in each column section is of great importance and will limit our choices of difference points in the MBT. Considering that a common CLL for a set of minimum reflux solutions remain the same, and as a result the contact boundaries of the liquid TTs and therefore the vapour TTs of the associated solutions remain the same as well, selecting difference points outside the vapour TT, but within the MBT will result in oppositely signed refluxes in the column sections.

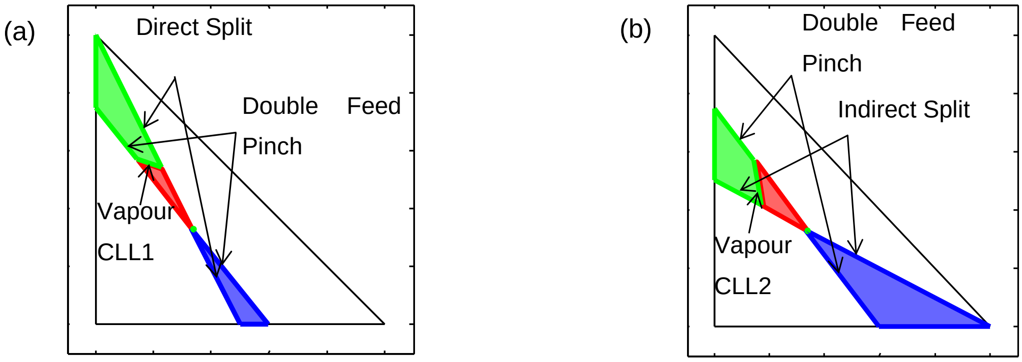

Figure 5. (a) Feasible and infeasible regions associated to common CLL1. (b) Feasible and infeasible regions associated to common CLL2.

This sets a limit for each CLL employed or feed composition selected. The vapour boundary that is associated with the coincident CLL is the last lines of possible X_D selection points. Three distinct boundaries, besides the obvious MBT, will limit our search for feasible minimum reflux solutions. They include: the double-feed-pinch, the bow-tie region and the vapour CLL depending on which column section is chosen to analyse. This means, that if a CLL is chosen to find a reflux solution based on the product selection i.e. high light key purity in distillate uses CLL1 and high heavy key in bottoms uses CLL2, then only the region that applies to the utilised CLL will produce feasible solutions and any region outside this one will not produce anything useful. By superimposing the three boundaries (double-feed-pinch, bow tie region and vapour CLL), three defining feasible regions arise (See Figure 5a-b). The interaction of the CLLs with the feed and each other is a significant aspect with regards to the number of components. Thus, if there were for example four components, more than three feasible regions would exist.

5.2 Region development associated to the V_{min} diagrams

Comparing the combination of Figure 5a-b and Figure 6, it is quite easy to see that parts of regions from each CLL solution are omitted from Figure 6. The exact minimum reflux solutions are associated to sharp split separations either in the distillate product or bottoms product, and depend purely on the CLL used. Thus the region of feasibility used in order to determine the minimum reflux solution. This means that if for instance CLL1 were to be used, not the entire green region characterised in Figure 5a produces exact minimum reflux solutions by utilising CPM-E. Only the sharp split in the distillate composition i.e. light-intermediate axis that coincides with the feasible region produces exact solutions. The remaining region is merely an approximation. The bottoms compositions undergo similar behaviour when CLL2 is utilised. The sharp split i.e. heavy-intermediate axis coinciding with the blue region in Figure 5b represents true minimum. Although CLL1 distillate region illustrated in Figure 5a is reduced to a line does not mean that the blue region associated to the bottoms composition when CLL1 is used is reduced to the sharp split criterion. Due to the fact that the stripping section profile terminates on the rectifying section profile or equivalently the TT of the stripping section means that the impurity is based on any component pertaining to the material balance can be selected within the feasible region. The opposite argument is true for CLL2s feasible region. In this way we reduce the regions depicted in Figure 5a-b to the sloppy-split minimum reflux regions shown in Figure 6. The combined exact minimum reflux solution regions are illustrated in Figure 6. Figure 7 is the V_{min} diagram that is associated to the exact minimum reflux regions produced in Figure 6. There is of course a way to find these regions based on either method, but for now, we will just mention that the eigenvectors used in the CPM-E method have a relationship to the common Underwood roots used in the V_{min} diagram[5]. The comparison of the Rmin calculated by utilising the CPM-E technique produces exactly the same results as compared to the result of the Underwood equations. Table 1 shows the comparison between the Underwood[9] method, the boundary value method (BVM) introduced by Levy et al.[2] and the CPM-E technique.

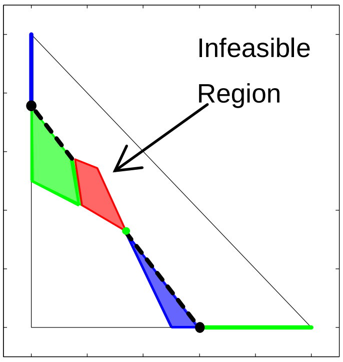

Figure 6. Minimum reflux regions associated to Underwood roots. Equimolar feed

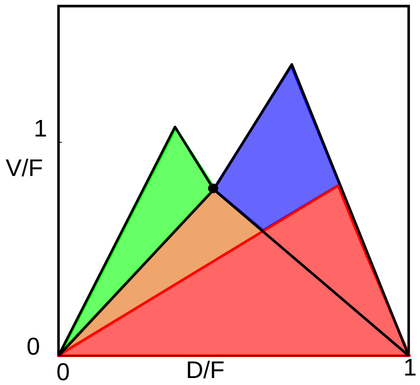

Figure 7. Vmin diagram associated to Figure 6. Equimolar feed.

Table 1. Comparison of different methods to CPM-E technique

Relative volatilities		Feed composition		Product compositions		Reflux ratio		
α_{12}	α_{13}	X_{F1}	X_{F2}	X_{D1}	X_{B1}	Underwood	BVM	CPM-E
1.25	1.5	0.3	0.3	0.95	0.01	9.08	9.1	9.08
2.37	12.67	0.3	0.3	0.999	0.001	1.52	1.54	1.52

6. Conclusion

We have illustrated a general method for calculating minimum reflux ratios, for ternary and higher order systems, through the use of Column Profile Maps and eigenvector maps, named the CPM-E technique. The method applies to ideal, non-ideal, and azeotropic distillations, becoming identical with Underwood's method for ideal mixtures. The technique makes use of eigenvectors evaluated at the feed composition in order to find a linear relationship between the saddle node and feed conditions. This line is called the co-linearity line (CLL). Three distinct solutions exist for the CPM-E technique. A solution that arises when each of the individual CLLs are common and a special solution when both CLLs are common. The simplicity of the method originates from uncomplicated mathematics combined with graphical interpretation. This is not only true for conventional columns, but for any thermally coupled systems.

Nomenclature

X : Liquid phase composition
$Y^*(X)$: Eqm vapour composition
R_Δ: Reflux ratio of column section
L :CS internal liq flowrate [*mol/s*]
V :CS internal vap flowrate [*mol/s*]

Δ:Net flow defined as $\Delta=V-L$ [*mol/s*]
X^T: Liquid composition top of CS
Y^T: Vapour composition top of CS
N is the stage number equivalent
X_Δ *is the* Difference point of a CS

Subscripts :
F:Feed Composition
D: Distillate product composition
B: Bottoms product composition
CS Is Column Section

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