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Production Zone Method: a New Non-ideal Shortcut Method for Distillation Column Design

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Abstract

This work describes a new non-ideal shortcut method for distillation design and includes a graphical representation. Based on the operation leaves of Castillo et al. (1998) the method uses production segment rather than completely specified product which eliminates any sensitivity to the composition of the minor products. It has two aims. The first is to determine if a specified separation respects the mass balance and the thermodynamic feasibility. The second one is to find the minimum reflux ratio and a preliminary design of the column. The following mixtures are investigated: an ideal mixture of ethanol, n-propanol, and n-butanol; a non-ideal mixture of acetone, water, and acetic acid; and an azeotropic mixture of acetone, isopropanol, and water. Designs obtained with this new method lead to purity and recovery rate close to specifications which is sometimes impossible with conventional ideal shortcut like the well-known Fenske-Underwood-Gilliland shortcut.

Keywords: Distillation – Shortcut Method – Non-ideal Mixture

1. Introduction

Distillation is one of the most important fields in process engineering and attracts an important attention as reported by Yildirim et al. (2011). Several distillation shortcut methods already exist including methods with graphical tools, but the latter have two major inconveniences. The first is that many are sensitive to product composition like the Boundary Value Method (Levy et al., 1985) or the Zero-Volume Criterion (Julka and Doherty, 1990). The second is that if composition areas are defined, most of the time the boundaries are straight lines which take not in good account the thermodynamic behavior of the systems. This is for example the case with the Rectification Body Method (Bausa et al., 1996) and another method developed by Thong and Jobson (2001). Based on the operation leaves of Castillo et al. (1998), the aim of the presented method called Production Zone Method (PZ method), concerns the feasibility of the separation in the acquisition of a column pre-design. The method uses production segment rather than product with completely specified composition which avoid being sensitive to the composition of the minor product. Concerning phase equilibria, no restrictive assumptions are made.

2. Description of the Method

The PZ method is based on the use of operation leaves. Each leaf is the area of all reachable compositions in a single column section. Figure 1 presents three operation leaf. It is defined by two curves: the distillation line (Stichlmair, 1987), which represents the liquid composition profile at total reflux and the pinch-point curve (Wahnschafft et al., 1992), which represents the liquid composition profile for an infinite number of stages. All composition points between these two curves can be reached depending of the choose reflux or reboiling ratio. Operation leaf advantage is the thermodynamic meaning of its boundaries. However, it is very sensitive to the product composition.

To overcome this constraint, PZ method requires only one specification for each product stream instead of both complete defined products. Graphically, for a ternary mixture, this is equivalent to defining a production segment. In Figure 2, a production segment is defined for a composition of 70 % in A at the distillate and 80 % in C at the residue. Both distillate and residue segments must respect the masse balance feasibility represented by the two dotted lines and also the thermodynamic feasibility of the separation. The latter, shown in Figure 1, corresponds to the overlap of the distillate and the residue leaves which provides an intersection between both section liquid profiles. Once the feasibility of the separation is established the method can be used to find which specific mass balance provides the smallest minimum reflux. This parameter is interesting to obtain an energy-optimized preliminary design. To do that, the method scans the production segments and determines the minimum reflux for each couple of distillate and residue points. The minimum reflux is the smallest reflux which provides an intersection of both liquid profiles – calculated with stage to stage calculation and equilibrium stages model - and the respect of the relation between r, the reflux ratio, s, the reboil ratio, q, the feed thermal condition and the feed (zF), the distillate (xD) and the residue (xW) composition presented in Eq.(1). Then an actual reflux ratio R=a.Rmin is chosen. In this study the common value of a=1.3 is used. Thus, using Eq.(1), the associated reboil ratio is found and the corresponding profiles are calculated. The number of stages in each column section is then the number of calculated points on each profile between the product and the intersection point. The feed stage corresponds to the latter.

$$z_F^i = \frac{1-q+s}{r+s+1} x_D^i - \frac{q+r}{r+s+1} x_W^i \quad (1)$$

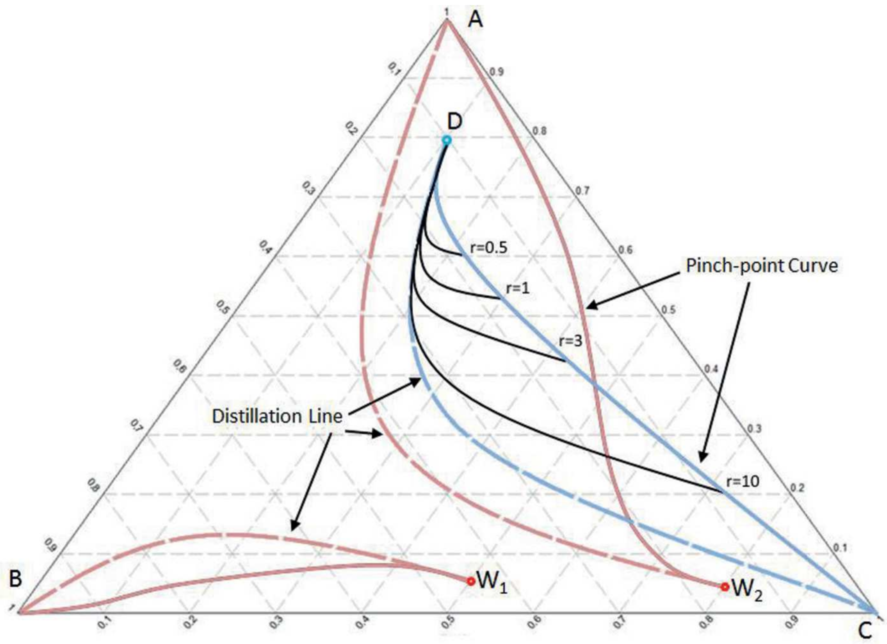

Figure 1. Operation leaves in a A (light), B and C (heavy) ternary diagram - Separation of D and W1 is unfeasible whereas separation of D and W2 is feasible. Operation leaf of D shows some liquid composition profiles for some values of the reflux ratio

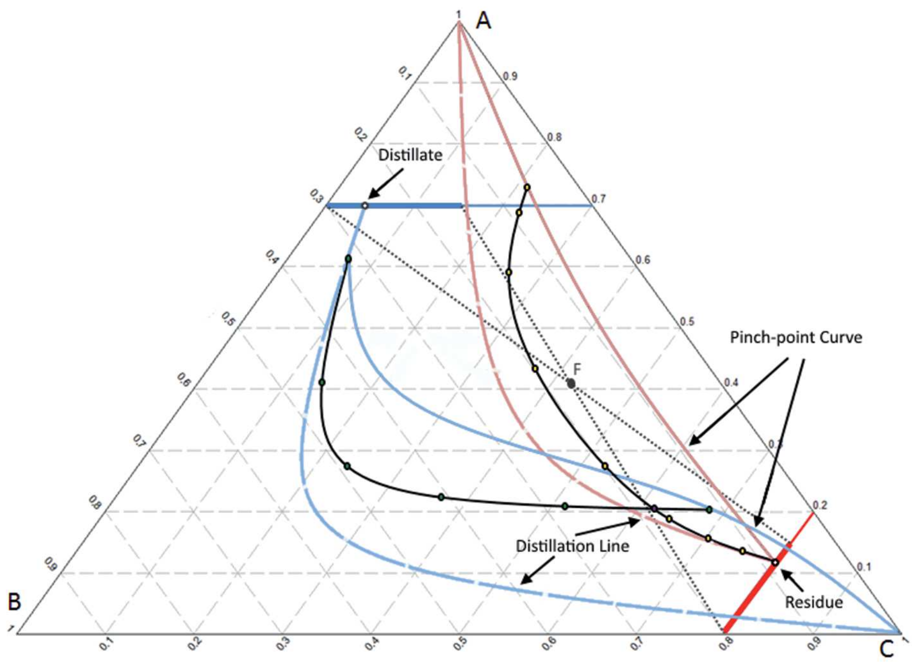

Figure 2. Theoretical number of stages: 5 stages in the rectifying section, 3 stages in the stripping section and the feed plate at the intersection which makes a total of 9 stages plus one total condenser and one reboiler

3. Case studies

The proposed method was compared with the well-known FUG shortcut. The reflux ratio, the distillate flowrate, the feed stage and the number of theoretical stages obtained by both shortcut are used to initialize rigorous simulations in ProsimPlus software. Results are shown in Figure 3, 4, 5 and 6. Three mixtures were studied: an ideal mixture of Ethanol / n-Propanol / n-Butanol, a non-ideal mixture of Acetone / Water / Acetic Acid and an azeotropic mixture of Acetone / Isopropanol / Water. For each case, xF, the respective feed compositions, can be found in Figure 4, 5 and 6 as well as q, the feed thermal condition, and xD/xW, the distillate/residue specifications. The feed flowrate is 100 mol/s for all cases.

3.1. Relative gap study for the specifications

In this first study, rigorous simulations were made without specification on the product compositions: the outlet compositions of each case are then different depending of the shortcut method used. Figure 3 highlights six cases that are representative of the whole results. The figure shows the relative gap between the distillate light key composition results of the simulation and the input distillate specification of the shortcut. The relative gap is usually smaller than 1 % in absolute value when the simulation was initialized with PZ method whereas, in several cases, the gap is higher than 5 % in absolute value when the simulation was initialized with FUG shortcut. Relative gaps for the residue specification and the recovery specifications follow the same trend. These results show that the compositions and the recovery ratios are close to their input values with the PZ column design and the relative gaps are of the same order of magnitude. With the FUG column design, relative gap sizes varied considerably from case to case. PZ method seems to be more precise and reliable than FUG shortcut.

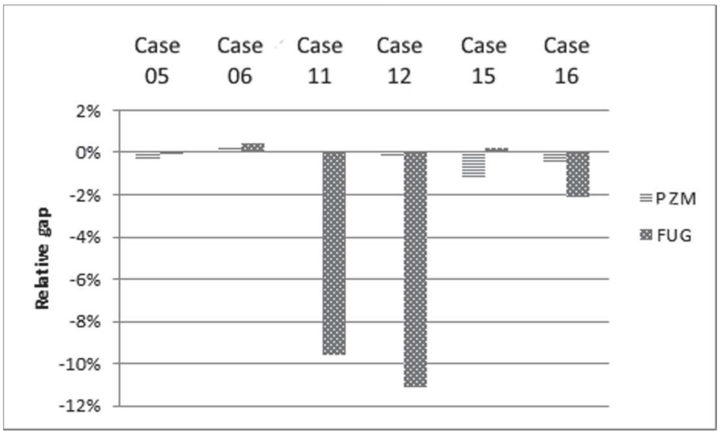

Figure 3. Relative gap between the distillate composition results of the simulation and the desired distillate specification

3.2. Cost study

In this second rigorous simulation study, the energy consumption and the total annual cost (TAC) of each designed column are compared more specifically. TAC calculations are based on the equations and the recommended values of Kiss (2013) and the packing properties are those of Mellapack 250Y. In these simulations, the feed stage and the number of theoretical plates are fixed while the reflux ratio and the reboil duty are adjusted to obtain the product specifications. Results in Figure 4, 5 and 6 show that PZ designs provide always the smallest TAC compared with FUG designs except for cases 09 and 10. In some case, like case 11, TAC of the FUG design is almost the double of

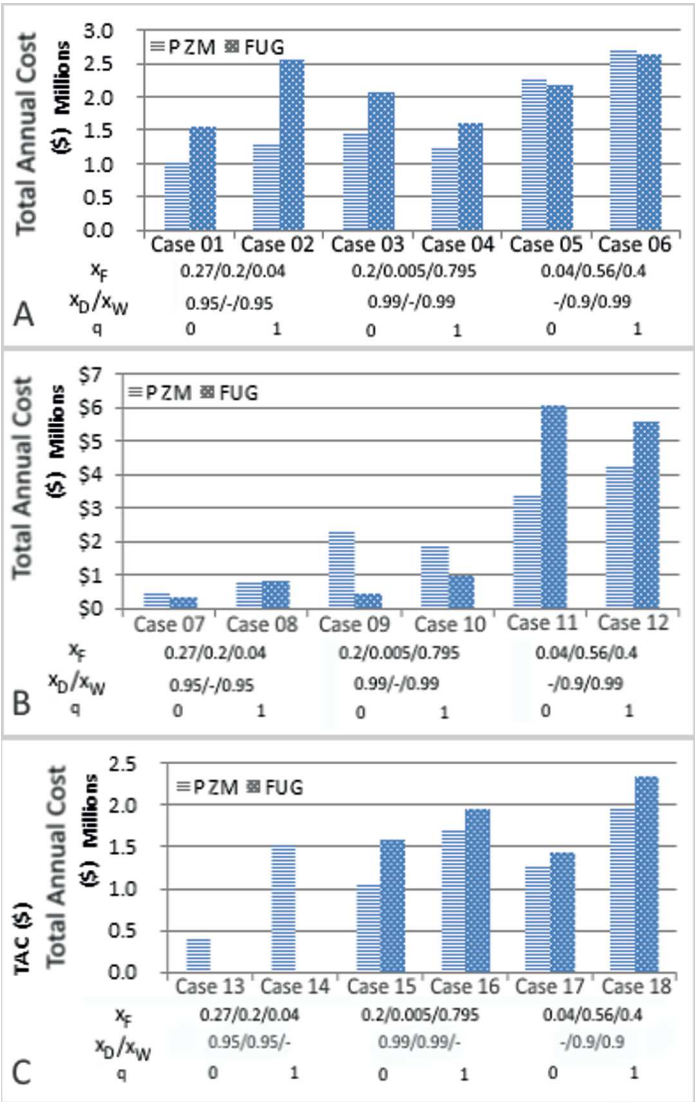

Figure 4. Total annual costs ($) A: an ideal mixture of Ethanol / n-Propanol / n-Butanol - B: a non-ideal mixture of Acetone / Water / Acetic Acid - C: an azeotropic mixture of Acetone / Isopropanol / Water

the TAC of the PZ design. In case 13 and 14, non-convergence can be found with the FUG design. However, cases 09 and 10 show the limits at the moment of the method: in some configuration, the imprecision due to the resolution of the code in Matlab becomes significant.

4. Conclusion

A new shortcut method for distillation has been developed. This method provides the knowledge of the mass balance and thermodynamic feasibility of the separation and determines the minimum reflux ratio when the separation is possible. From the minimum reflux ratio, a first design can be obtained and used to initialize a rigorous simulation. Results show that the method gives a good approximation of the rigorous results and is more precise and reliable than the FUG shortcut. Moreover designs proposed by the method are more efficient than those proposed by the FUG shortcut in terms of economic. Required data for the method are the composition, the thermal condition and the flowrate of the feed and one specification for each outlet stream. These data were chosen because they will be obtained easier than others possible data: it will be easier to use it for industrial and engineering purposes. Future work will be the adaptation of this method to unconventional column design and the first one which will be investigated will be the design of a dividing wall column.

References

J. Bausa, R.V. Watzdorf, W. Marquardt, 1996, Minimum energy demand for nonideal multicomponent distillations in complex columns, Comput. Chem. Eng., 20, S55–S60

F.J.L. Castillo, D.Y.C. Thong, G.P. Towler, 1998, Homogeneous azeotropic distillation 1. Design procedure for single-feed columns at non-total reflux, Ind. Eng. Chem. Res., 37, 3, 987–997

V. Julka, M.F. Doherty, 1990, Geometric behavior and minimum flows for nonideal multicomponent distillation, Chem. Eng. Sci., 45, 7, 1801–1822

A.A. Kiss, 2013, Design, control and economics of distillation, Advanced distillation technologies: design, control and applications, Chichester, UK: John Wiley & Sons, Ltd, 55-63

S.G. Levy, D.B. Van Dongen, Michael F. Doherty, 1985, Design and synthesis of homogeneous azeotropic distillations 1. Problem formulation for a single column, Ind. Eng. Chem. Fundam., 24, 4, 454–463

J. Stichlmair. 1987, Distillation and rectification, Ullmann's Encyclopedia of Industrial Chemistry, 4.1-4.94

D.Y.C. Thong, M. Jobson, 2001, Multicomponent homogeneous azeotropic distillation 2. Column design, Chem. Eng. Sci., 56, 14, 4393–4416

O.M. Wahnschafft, J.W. Koehler, E. Blass, A.W. Westerberg, 1992, The product composition regions of single-feed azeotropic distillation columns, Ind. Eng. Chem. Res. 31, 10, 2345–2362

Ö. Yildirim, A.A. Kiss, E.Y. Kenig, 2011, Dividing wall columns in chemical process industry: A review on current activities, Sep. Purif. Technol., 80, 3, 403–417