Designing Multicomponent Distillation Columns Based On Geometric Pinch Analysis

Frank Z. Hu, Stanislaw K. Wasylkiewicz and Hiren K. Shethna
Hyprotech Ltd.
Suite 800, 707 - 8th Avenue SW, Calgary, Alberta, Canada T2P 1H5

Abstract

A design approach for multicomponent distillation columns is presented. Based on a geometric analysis of pinch point solutions of composition profiles, the approach provides a suite of accurate and efficient methods for determining minimum reflux, the number of stages and the optimum feed-tray location. Tangent pinches are taken into account in the design. The approach applies to ideal, nonideal and azeotropic mixtures with no restrictions on the number of components. It is demonstrated with applications to column design and column sequencing for multicomponent azeotropic distillation.

Introduction

Commercial process simulators are widely used by process engineers in their routine jobs. These simulators are a natural and, most likely, the best choice for rating purposes. However, it is usually neither effective nor efficient to use them directly for solving design problems of multicomponent distillation columns from scratch. This simulation-based design approach requires repeated performance simulations by trial and error with various design parameters. For highly nonideal systems, the simulators often need good initial estimates of column profiles (temperature and compositions) to converge the columns. In addition, feasibility of the desired separation can further reduce the chances of success. One may have performed extensive and lengthy simulations only to find out that the specified separation is inherently infeasible.

We need shortcut methods to figure out the design parameters and, perferably, the associated column profiles. They should complement the simulators by eliminating most of unnecessary simulations. The Fenske-Underwood-Gilliland method can be used for this purpose for ideal mixtures. The boundary-value design method applies to nonideal and azeotropic ternary mixtures (Doherty and Malone, 2001). But it can not be generalized for multicomponent systems because of sensitivities of the profiles to nonkey components in products.

In this article, we present an alternative design approach and its implementation in a software tool that complements the simulators in process design. It is an extension to previous work by Bausa et al. (1998) and Julka and Doherty (1993). We demonstrate the approach with applications to column design and column sequencing for multicomponent azeotropic distillation.

Composition Profiles and Pinch Points

The equilibrium-stage model of a distillation column consists of material and energy balances and phase equilibrium. Mathematically, it can be viewed as an implicit recurrence of compositions of the liquid (and vapor) streams leaving successive stages in the column, with the distillate or bottoms product composition and the reflux or reboil ratio at each end of the column as parameters. Analogous to the construction of McCabe-Thiele diagrams for binary systems, composition profiles in each section of a multicomponent column can be determined when the product compositions and the reflux and reboil ratios are fixed at both ends of the column. The liquid phase compositions on each stage are calculated successively from stage to stage by solving the material and energy balances along with the phase equilibrium. A nonlinear analysis of the implicit recurrence indicates that the compositions will not change from stage to stage when the recursion approaches an infinite number of stages. This corresponds to a zone of constant composition in a column section. These points in the composition space are called fixed points or pinch points.

The number and location of the pinch points is a function of the product composition and reflux (or reboil) ratio at the end of the column section. With the product composition fixed, all branches of the pinch points in the section can be computed by an arc length continuation in the reflux (or reboil) ratio. The pinch points on each branch can be either nodes (stable or unstable) or saddles in terms of stability. Their stability characteristics are determined by a set of eigenvectors associated with each pinch point. The stability of the pinch point governs local geometric structure of the composition profiles in the vincinity of the pinch point (Bausa et al., 1998).

For a feasible column, the rectifying and stripping composition profiles must intersect at the feed stage in the composition space. A geometric property of the profiles is that they are highly sensitive to the trace amount of nonkey components in the products (Julka and Doherty, 1993). Small variations in the product composition will result in a sizable manifold of the profile for the section. On the other hand, the pinch points are insensitive to the small variations in the product composition. We use a linear combination of selected pinch points in each section to construct a geometric plane or body. The plane or body approximately represents an envelope of the profile manifold. Instead of checking the profiles for intersection, either bodies from the rectifying and stripping sections are checked against each other or the profile of one section is checked against the plane of the other section. So we circumvent the difficulty caused by the high sensitivity of the profiles to the product compositions. These goemetric ideas form the basis for the following design procedure for multicomponent distillation columns.

Minimum Reflux

Minimum reflux calculations are based on the rectification body method proposed by Bausa et al. (1998). First, all possible paths of the composition profiles are identified for each column section . They start from the distillate or bottoms product, follow the pinch points of strictly increasing stabilities (i.e., number of stable eigenvectors) and end at a stable node. Geometric (rectification) bodies are constructed around each path. Each body is a simplex in the composition space, with its vertices being all the points contained in the path. The bodies from the rectifying and stripping sections are checked against each other for intersection. The minimum reflux ratio Rmin is the result from a one-dimensional search in the reflux ratio. Prior to the search, all pinch point branches are already computed for all possible values of the reflux (or reboil) ratio. At each iteration during the search, pinch points are calculated for specific reflux ratio by interpolation between points on each of the pinch point branches. If the bodies do not intersect at current iteration, the reflux ratio is increased for next iteration. If there is any intersection between the bodies, the reflux ratio is reduced. The iteration continues until the minimum reflux ratio is found.

A thermodynamic consistency check is used to exclude infeasible paths, which will tight the envelopes (bounds) on the manifolds of the composition profiles. If any path does not have a positive and increasing entropy production through all the points on the path, the path is infeasible and excluded from the minimum reflux calculations.

Tangent Pinches

Tangent pinches often occur in the separation of nonideal binary mixtures as well as multicomponent systems. They may or may not control minimum reflux. The above procedure for determing minimum reflux needs a special treatment to deal with the tangent pinches. We illustrate the problem with the tangent pinches and the solution in the following example.

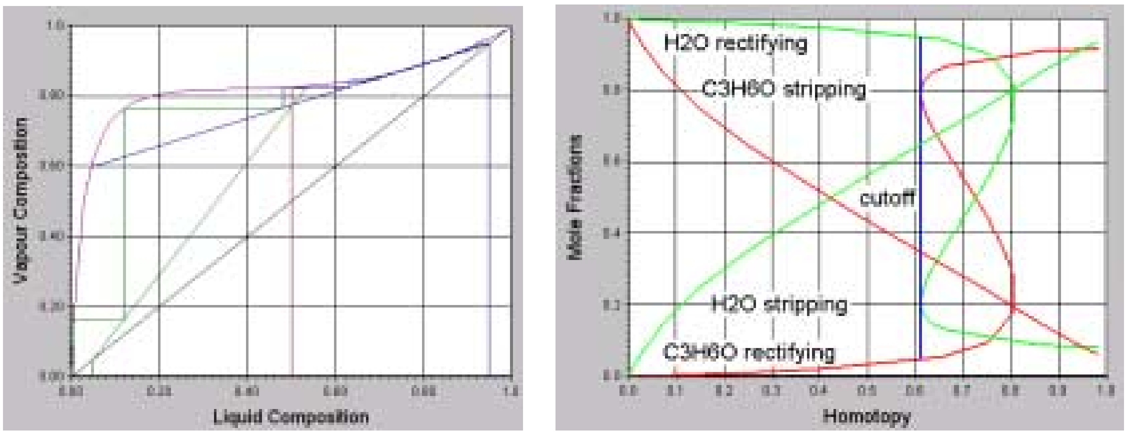

Figure 1. McCabe-Thiele diagram at minimum reflux (a) and bifurcation diagram of pinch composition versus homotopy with branch cutoff (b) for Example 1.

Example 1: a binary mixture with a tangent pinch

Consider the separation of an equimolar saturated liquid feed of the acetone-water mixture, to give a distillate containing 95 mol% acetone and a bottoms product containing 95 mol% water. Figure 1a shows a McCabe-Thiele diagram for a column operating at the minimum reflux ratio of 0.6329, which corresponds to a tangent pinch in the rectifying section. The equilibrium curve in the diagram is calculated using the Margules-ideal gas model. All pinch point branches are computed for the rectifying and stripping sections and represented on a bifurcation diagram of the pinch composition of the two components versus a homotopy parameter, as shown in Figure 1b. The homotopy parameter is defined as the reverse of the reflux (reboil) ratio plus 1 for the rectifying (stripping) section. Both branches of the rectifying section have an S-shaped section with two turning points. It is an indication that a tangent pinch is present in the rectifying section (Fidkowski et al., 1991). If we follow the above procedure for minimum reflux, we will get 0.2393 for the minimum reflux ratio. Notice that this value of the reflux ratio corresponds to the turning point with the higher homotopy value in Figure 1b. The minimum reflux ratio is underestimated because the procedure is trapped into the physically unattainable region between the two turning points, when the tangent pinch controls the minimum reflux. In order to avoid this problem, we cut off the S-shaped section at the other turning point with the lower homotopy value (i.e. the higher reflux ratio), and replace it with the vertical line in Figure 1b. The procedure then gives 0.6328 as the minimum reflux ratio. The value ends up exactly at the cutoff location. It also agrees very well with the result from the McCabe-Thiele diagram.

As a general rule, we cut off any S-shaped sections found on any branches whether tangent pinches control minimum reflux or not. The tangent pinches do not control if the turning points appear at a reflux ratio lower or higher than Rmin. In this case, the cutoff does not hinder the procedure from determing Rmin. This cutoff treatment applies to binary as well as multicomponent tangent pinches, as will be demonstrated in Example 2.

Number of Stages and Feed Stage Location

An initial-value method is employed to determine the number of theoretical stages required and the optimum feed stage location at a specified reflux ratio greater than the minimum value. The method is based on previous work by Julka and Doherty (1993). It also makes use of the pinch point solutions of the composition profiles.

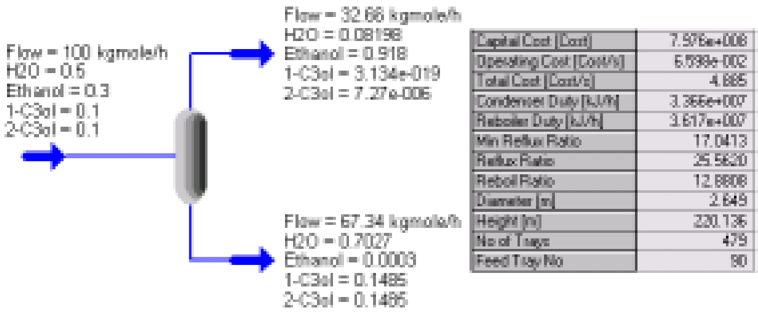

Figure 2. Design specifications and results for Example 2.

For direct splits, the rectifying profile is sensitive to small variations in the distillate composition while the stripping profile is not. A hyperplane is constructed by a linear combination of pinch points for the rectifying section. These pinch points are selected from within the continuous distillation region where the split is located (Wasylkiewicz and Castillo, 2000). The hyperplane is to approximate the manifold of the rectifying profile for the variations in the distillate composition. The stripping profile is calculated from the bottoms composition up to the stable node. If the profile intersects the hyperplane, the intersecting point and the node define bounds on feasible feed stage locations. The optimum location is searched for over the profile segment between the two points. Starting from different feed stage compositions, the rectifying profile is calculated up the column until the required distillate purity is reached. The optimum feed stage location is obtained when the total number of stages in the rectifying and stripping sections is minimized. The design procedure for indirect splits is analogous to that for the direct splits. The above geometric design methods for minimum reflux and number of stages have been implemented in DISTIL v5.0, a software tool for conceptual process design (Hyprotech, 2001).

Example 2: a quaternary mixture with tangent pinches

Figure 2 shows a distillation column that separates an ethanol-water azeotrope from a four-component mixture of ethanol, *n*-propanol, *iso*-propanol and water. This is a direct split. The vapor-liquid equilibrium for this mixture can be described by the NRTL-ideal gas model. The mixture has three azeotropes, all binary between the alcohols and water. There is a distillation boundary that separates the composition space into two regions. These two basic distillation regions can be further divided into four continuous distillation regions. The split specified in Figure 2 is performed within a continuous region that has the three azeotropes and water as its stationary points.

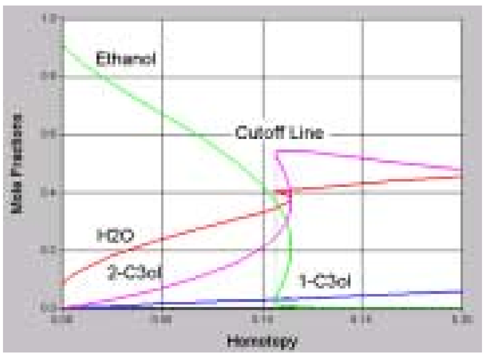

Figure 3. S-shaped branch with cutoff in the stripping section for Example 2.

Pinch point branches are computed for the rectifying and stripping section, each starting from one of the stationary points. There is an S-shaped section in two of the branches. One starts from the *iso*-propanol-water azeotrope (saddle) in the rectifying section, while the other starts from the ethanol-water azeotrope (stable node) in the stripping section as shown in Figure 3. The tangent pinch in the stripping section controls minimum reflux and Rmin is 17.0413 as shown in Figure 2. At a reflux ratio of 1.5 times Rmin, the number of stages and the optimum feed stage location are calculated and shown in Figure 2, too. Note that a large number of stages are required for the stripping section because of the controlling tangent pinch in the section.

Example 3: application to column sequencing

The goemetric methods presented in this paper can be used to design individual columns generated in column sequencing. Consider the separation of an equimolar mixture of acetic acid-water-ethyl acetate-ethanol. This mixture was discussed by Julka and Doherty (1993) and is modeled using the Wilson equation for the liquid phase and dimerization of acetic acid in the vapor phase. The mixture has three binary saddle azeotropes and a minimum boiling ternary azeotrope. Although there is no distillation boundary, the single basic distillation region actually contains six continuous distillation regions. This is a very restrictive system. As shown in Figure 4, only two column sequences can be generated using direct and indirect splits. Each individual column in the sequences is designed by the geometric methods. A reflux ratio is specified to be 1.5 times Rmin for the column. Results from DISTIL are listed in Table 1. These column designs are verified by rigorous simulations in HYSYS version 2.4.2. Table 2 compares the design and simulation results for the first columns in both sequences, which perform direct and indirect splits on the quaternary mixture, respectively. The results agree very well with each other.

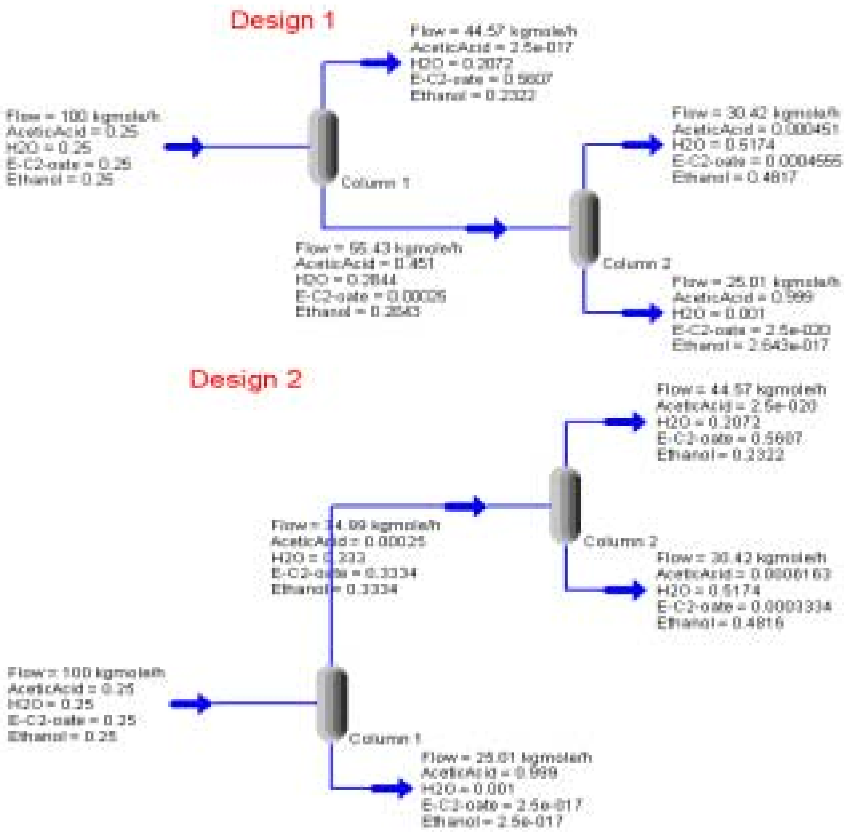

Figure 4. Two column sequences generated using direct and indirect splits for Example 3.

Table 1. Design results for the columns in the two sequences of Example 3

Column Sequencing: Design 1

Name	Column 1	Column 2
Pressure [kPa]	101.3	101.3
Feed	Stream 1	Stream 3
Top Product	Stream 2	Stream 5
Bottom Product	Stream 3	Stream 4
Capital Cost [Cost]	6.224e+005	4.927e+005
Operating Cost [Cost/s]	2.206e-002	4.653e-003
Total Cost [Cost/s]	2.582e-002	7.630e-003
Condenser Duty [kJ/h]	1.150e+007	3.396e+006
Reboiler Duty [kJ/h]	1.196e+007	1.952e+006
Min Reflux Ratio	4.0859	1.1641
Reflux Ratio	6.1289	1.7461
Reboil Ratio	5.7310	3.3403
Diameter [m]	1.583	0.915
Height [m]	18.544	15.582
No of Trays	38	32
Feed Tray No	13	17

Streams | Columns | Notes

Column Sequencing: Design 2

Name	Column 1	Column 2
Pressure [kPa]	101.3	101.3
Feed	Stream 1	Stream 3
Top Product	Stream 3	Stream 4
Bottom Product	Stream 2	Stream 5
Capital Cost [Cost]	4.451e+005	8.670e+005
Operating Cost [Cost/s]	6.081e-003	0.1555
Total Cost [Cost/s]	8.770e-003	0.1607
Condenser Duty [kJ/h]	4.313e+006	7.812e+007
Reboiler Duty [kJ/h]	2.625e+006	8.595e+007
Min Reflux Ratio	0.3320	31.6020
Reflux Ratio	0.4980	47.4030
Reboil Ratio	4.4926	70.9157
Diameter [m]	1.058	4.067
Height [m]	13.270	11.019
No of Trays	27	22
Feed Tray No	12	7

Streams | Columns | Notes

Table 2. Comparison of design and simulation results for Example 3

Split	Component	Distillate Mole Fractions		Bottoms Mole Fractions	
		Design	Simulation	Design	Simulation
Direct	Acetic Acid	7.68E-10	4.97E-11	0.4510	0.4510
	Water	0.2022	0.2040	0.2844	0.2869
	Ethyl Acetate	0.5546	0.5557	2.50E-4	4.18E-3
	Ethanol	0.2432	0.2401	0.2643	0.2579
Indirect	Acetic Acid	2.50E-4	2.55E-4	0.9970	0.9988
	Water	0.3330	0.3330	2.82E-3	1.07E-3
	Ethyl Acetate	0.3334	0.3334	4.32E-6	2.26E-6
	Ethanol	0.3334	0.3333	1.36E-4	8.71E-5

Conclusions

We have developed a design approach to multicomponent distillation columns and implemented in a software tool that complements simulators in process design. Based on a geometric analysis of pinch point solutions of composition profiles, the approach provides a suite of accurate and efficient methods for determining minimum reflux, the number of stages and the optimum feed-tray location. These design parameters can readily be transferred along with associated temperature and composition profiles to the simulators for a rigorous and detailed simulation. Tangent pinches are identified and taken into account in the design. The approach applies to ideal, nonideal and azeotropic mixtures with no restrictions on the number of components. We have demonstrated the approach with applications to column design and column sequencing for multicomponent azeotropic distillation.

References

Bausa, J., R.v. Watzdorf and W. Marquardt, 1998, Shortcut methods for nonideal multicomponent distillation: 1. Simple columns, *AIChE J.*, 44, 2181-2198.

Doherty, M.F. and M.F. Malone, 2001, Conceptual Design of Distillation Systems, McGraw-Hill, New York.

Fidkowski, Z.T., M.F. Malone and M.F. Doherty, 1991, Nonideal multicomponent distillation: Use of bifurcation theory for design, *AIChE J.*, 37, 1761-1779.

Hyprotech Ltd., 2001, DISTIL v5.0, www.hyprotech.com.

Julka, V. and M.F. Doherty, 1993, Geometric nonlinear analysis of multicomponent nonideal distillation: A simple computer-aided design procedure, *Chem. Eng. Sci.*, 48, 1367-1391.

Wasylkiewicz, S.K. and F.J.L. Castillo, 2000, Solvent recovery by distillation, Paper 233u, AIChE Annual Meeting, Los Angeles.