Temperature Collocation Algorithm for Fast and Robust Distillation Design

Libin Zhang and Andreas A. Linninger*

Laboratory for Product and Process Design, Department of Chemical Engineering, University of Illinois at Chicago, Chicago, Illinois 60607

In this paper, we describe a new minimum bubble-point distance (MIDI) algorithm for assessing the feasibility of a desired distillation specification. The algorithm computes the rectifying and stripping temperature profiles by temperature collocation on finite elements with orthogonal polynomials. We discovered the beneficial use of a dimensionless equilibrium tray temperature as an independent variable. This novel choice is bounded between 0 and 1, improves the numerical quality of the design problem formulation, and is well-behaved even in the vicinity of pinch regions. It also employs the fixed points of column sections as collocation points. Adaptive-element boundary placement at saddle temperatures can effectively overcome problems with numerical instability near pinch regions. Extensions of our MIDI algorithm to the calculation of the minimum and maximum refluxes are also introduced. We show the application of this algorithm in the separation of quaternary mixtures and provide an outlook of the methodology for optimal column sequencing. Cases studies demonstrate the algorithm’s robustness and reliability.

1. Introduction

Distillative separation is among the least expensive methods for separating mixtures that exhibit suitable volatility differences.1 Hence, continuous distillation columns, along with their optimal operation and heat integration, constitute a major engineering activity in refineries and bulk commodity manufacturing. The common practice for distillation design often involves numerous trial-and-error experiments by means of state-of-the-art process flowsheet simulators. However, this time-consuming practice does not guarantee the production of successful designs; it might not provide any information about the feasibility of a particular specification in cases when the efforts do not converge. When the design-by-simulation approach is used, infeasibilities are often discovered only after extensive simulation studies.2

The classical Underwood method for column profile computation is restricted to mixtures of constant relative volatility.3,4 Doherty and co-workers5,6 introduced the boundary value method (BVM), which examines the intersection of rectifying and stripping profiles graphically. However, the BVM is inconvenient for mixtures with more than four components because of the lack of graphical representations for composition trajectories in higher dimensions. Julka and Doherty7,8 extended this methodology to multicomponent systems, employing a geometric theory based on topological concepts. They demonstrated that the feed point and C-1 pinch points lie in one hyperplane satisfying a zero-volume formula at minimum reflux. The rectification body (RB) method9 employed pinch points of the top and bottom sections to approximate the space of reachable column profiles. If the rectification bodies for the rectifying and stripping sections just touch each other, the authors conjectured that the minimum reflux ratio is obtained. However, these methods are only accurate for high-purity splits in which the composition profiles approach saddle pinches. They break down for sloppy separations in which the intersection of hyperspaces spanned by the pinch point is a necessary but not a sufficient feasibility condition. In general, specifications to ensure high accuracy close to the columns' end sections when using collocation.

Despite the attention devoted to continuous distillation simulations, less work has been aimed at developing algorithms to determine whether a given specification, sloppy or sharp, is feasible or not. In this research, we propose a minimum bubble-point distance (MIDI) algorithm for ascertaining the feasibility of any arbitrary design specification for simple continuous distillation columns. Our research objective targets the development of an efficient and reliable computational algorithm for establishing the feasibility or infeasibility of specifications for sharp or sloppy separations of any number of species. The availability of a fast and globally convergent feasibility test would introduce an essential element for automatic computer-aided distillative separation synthesis.26 This work constitutes an important intermediate milestone toward that long-term objective.

Outline. A theoretical basis for the novel robust feasibility test algorithm is developed in section 2. Fundamental concepts pertinent to the new approach...
such as the attainable temperature window (ATW) and the bubble-point distance (BPD) are introduced. A temperature finite-element collocation method capable of overcoming stationary points in the composition profile is presented. The methodology section also includes numerical results and implementation issues. Section 3 demonstrates the robustness and performance characteristics of our approach for constant relative volatility mixtures, ideal mixtures, and nonideal mixtures with three or four components. Section 4 extends our methodology to ascertain the boundaries of feasible operation, i.e., it describes the robust computation of minimum and maximum reflux ratios. Section 5 addresses problematic design tasks such as the separation of mixtures with tangent pinches and provides suggestions toward novel computational solution options for structural design problems such as optimal column sequencing. The paper closes with conclusions and an outlook for future research.

2. Methodology

A performance problem predicting expected distillate and bottoms compositions given the feed and column parameters for an existing column always has a solution that is readily attainable with commercial flowsheet packages (e.g., AspenPlus, HYSYS, ProfII, etc.). On the other hand, the inverse design problem seeking the column operation and parameters to achieve desired separation targets might not have a solution even for a consistent set of design specifications. In this paper, we shall, without loss of generality, assume given feed compositions and column pressure. A simple column configuration has four design degrees of freedom, typically three product-purity specifications and a desired reflux value, for example.

Unfortunately, no generally applicable, globally convergent algorithm exists for determining the feasibility of a given design specification. The classical Underwood method converges only for feasible designs; it is of limited use in the synthesis of distillation trains because of its extremely nonlinear behavior. Other design methodologies are restricted in either the number of species or the properties of the mixture. To the best of our knowledge, no algorithm is robust enough for structural flowsheet optimizations, which typically lead to large-scale mixed integer nonlinear mathematical programming (MINLP) problems.

Critical numerical difficulties in the design problem stem from singularities in the composition profiles near stationary pinch and saddle points that naturally occur even in ideal mixtures. To overcome the existing shortcomings, we propose a combination of two simple but very effective concepts: (1) transformation of column profiles into the space of dimensionless bubble-point temperatures; (2) minimization of a bubble-point distance function between stationary profile nodes in the bubble-point temperature space.

This novel approach reduces the dimensionality of the design problem; eliminates singularities encountered in the tray-by-tray approach; extends to any number of species with customary vapor-liquid equilibrium solution models, including constant-relative-volatility, ideal, and nonideal mixtures; and applies to both sharp and sloppy splits. In effect, the column design problem becomes more tractable from a computational point of view. Before the introduction of our new methodology, a discussion of reachable product compositions is in order.

2.1. Reachable Compositions and Their Equilibrium Temperatures

Figure 1 illustrates that the distillate, d, and stable node, ç, span all possible rectifying profiles for a given specification. Rectifying composition profiles start at the distillate and terminate in the stationary pinch point. For high-purity separations, the profiles approach a saddle point dividing the composition profile into two branches that can be reached only after an infinite number of equilibrium trays have been traversed. Each pinch point is also associated with a specific bubble-
point temperature as illustrated in Figure 1b. Consequently, realizable rectifying sections exhibit tray equilibrium temperatures within the interval delimited by the temperatures of the distillate, T\(_D\), and the stationary pinch point, T\(_P\). Correspondingly, the bubble points of the bottoms, T\(_B\), and the stationary stripping pinch, T\(_P\), bracket the temperature range for all possible stripping sections. For a simple column configuration (i.e., with no side trays or multiple feeds), the stripping and rectifying profiles must intersect at the liquid tray composition of the feed plate. Hence, the temperature interval between \(\min(T_P, T_B)\) and \(\max(T_P, T_D)\) constitutes the attainable temperature window (ATW) for the given column design specification. The ATW marks all possible equilibrium tray temperatures that can be reached by the column sections, as illustrated in Figure 2 (i.e., boiling points of mixtures on an equilibrium tray).

If the ATW associated with a design specification is empty (i.e., \(T_{P_1} < T_{P_2}\)), then one can conclude unequivocally that the specification is infeasible (e.g., Figure 2b). By comparing the temperature ranges in the stripping and rectifying sections, we can already exclude many design specifications without actually performing tray-by-tray computations as expressed in remark 1. This property can also be very valuable in assessing the separability of mixtures with azerotropes.

**Remark 1. Attainable Temperature Windows.** If the attainable temperature window (ATW) of the rectifying and stripping section is empty, the given design specification is infeasible.

2.2. Bubble-Point Distance (BPD). In cases of overlapping ATWs, more detailed quantitative analysis is required. Numbers of trays or column heights are unsuitable independent variables in numerical computations because of their indefinite value range, namely, \([0, \infty[. We propose an affine mapping of the column height into a dimensionless bubble-point temperature, \(\Theta\). The mapping establishes a bijective relationship between height and bubble-point temperature. We also convert the tray-by-tray difference equations into ordinary differential equations as proposed by Doherty. The composition trajectories expressed as functions of the independent variable, \(\Theta\), do not approach infinity hampering the traditional tray-by-tray methods. Using the dimensionless temperature instead of the column height, we arrive at a system of differential-algebraic equations. Equations 3 determine the composition profiles, \(x_i(\Theta)\), as a function of the equilibrium constant, \(K_i\); the distillate specification, \(x_{D_i}\); and the reflux, \(r\). The new temperature transformation reduces the nonlinearity of the profile equations significantly, because the use of temperature as an independent variable makes temperature-dependent expressions explicit. Equation 4 represents the stripping profile in terms of the bottoms composition, \(x_{B_i}\), and the reboiler ratio, \(s\). The detailed derivations of continuous rectifying and stripping profiles as well as the total derivative of the equilibrium constant, \(dk_i/d\Theta\), in terms of temperature and composition for a general nonideal mixture model are provided in the appendices.

Continuous rectifying profile equations

\[
dx^R_i = -\left(\frac{R_{1}}{R}x^R_i - \frac{1}{R}y^R_i + \frac{1}{R}x^S_{B_i}\right)\sum_{j=1}^{c}\left(\frac{dK_{j}}{d\Theta}x^R_j\right)
\]

Continuous stripping profile equations

\[
dx^S_i = -\left(\frac{S}{S+1}x^S_i - \frac{1}{S+1}x^S_{B_i}\right)\sum_{j=1}^{c}\left(\frac{dK_{j}}{d\Theta}x^S_j\right)
\]

The bubble-point distance (BPD) is defined as the Euclidean distance between two equilibrium compositions belonging to the stripping and rectifying profiles with the same bubble-point temperature. Figure 3 depicts two instances of bubble-point distances, \(d_{P1}\) and \(d_{P2}\), for two discrete bubble-point temperatures (T\(_A\) and T\(_B\), respectively), as well as the traces of the bubble-point surfaces in a nonideal ternary mixture. For a...