Temperature Collocation Algorithm for Fast and Robust Distillation Design

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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. 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.

The classical Underwood method for column profile computation is restricted to mixtures of constant relative volatility. Doherty and co-workers 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 Doherty 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 condition. In general (sloppy) specifications, only column profiles unambiguously verify the feasibility of a design.

Existing approaches avoid calculating the composition profile rigorously because of the huge computational effort. This holds particularly true when several columns are being designed and optimized simultaneously (i.e., in optimum column sequencing). Orthogonal collocation on finite elements (OCFE) has been shown to reduce the problem size substantially, without significant loss in 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. 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...
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, ProII, 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\(^3,4\) 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\(^27\) or the properties of the mixture.\(^28\) 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

Pinch points delineate the extreme points of all possible column profiles for a given design specification. For a known distillate composition \(x_D\) for a \(c\)-component separation, stationary points are found without performing tray-by-tray computations by enforcing the pinch equations given by eqs 1 and 2, i.e., simultaneous compound balances and thermodynamics equilibrium.\(^29\)

\[
\text{Pinch equation for the rectifying section: } \quad r x_i - (r + 1) x_{Ki} + x_{D,i} = 0 \quad i = 1, \ldots, C \tag{1}
\]

\[
\sum x_{Ki} - 1 = 0 \tag{2}
\]

Figure 1 illustrates that the distillate, \(d\), and stable node, \(\gamma\), 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.\(^5\) Each pinch point is also associated with a specific bubble-