Industry-wide energy saving by complex separation networks

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A B S T R A C T

Different column configurations in a distillation network can achieve the same ultimate products, with different amounts of energy to do so. Only recently, methods have been discovered for the systematic generation and evaluation of all possible complex column configurations for the separation of multicomponent mixtures. However, there is a lack of methods for the globally optimal design of complex column sequences. This presentation reviews recent advances to tackle the challenges of synthesizing complex column networks with computer-aided design algorithms. An automatic procedure to generate optimal column sequences based on thermodynamic problem transformation called temperature collocation is discussed and its current capabilities and limitations illustrated with the help of two realistic case studies.

1. Introduction

Separation processes make up 40–70% of capital and operating costs of chemical manufacturing. Distillation accounts for more than 60% of the total process energy for the manufacture of commodity chemicals (DOE, 2005). Optimal complex column configuration is estimated to harness energy savings up to 70% (Engelien & Skogestad, 2005). Therefore, distillation trains are a meaningful target for energy improvement on an industry-wide scale. The current world-wide increase for fuel demand should fuel research for more energy efficient separations. Despite intensive research, a closed solution for identifying the most energy efficient separation networks for a given separation task is elusive. The gap is especially wide when dealing with many species forming highly non-ideal mixtures or the design of fully heat integrated complex column configurations.

The most famous complex column configuration may be the Petlyuk column; with full thermocoupling this column configuration earned energy savings up to 40%. However, complex column synthesis entails structural and physical interaction between countercurrent vapor and liquid flows. The next two major challenges hamper the development of a general algorithmic solution for complex column networks. Numerous arrangements and internal connections of complex column networks increase the problem’s combinatorial complexity. It would be desirable to explore only configurations that might be optimal, while pruning suboptimal configurations expanding without major computational effort.

The second reason is that the inverse or column design problem for the best minimum distillation configurations for given product targets suffers from numerical difficulty at the pure ends of the column profile computations, in which small changes in the design parameters may cause large changes in column performance; these are the characteristics of a recalcitrant—if not chaotic problem. There are many significant contributions from the systems community towards the solution of the separation synthesis problem: Heuristic methods, explicit enumeration (Chavez, Seader, & Wayburn, 1986), a systematic column sequencing (Andrecovich & Westerberg, 1985), state task network methods (Sargent, 1998; Sargent & Gaminibandara, 1976; Shah & Kokossis, 2002). Doherty, Malone and coworkers (Fidkowski, Doherty, & Malone, 1991; Fidkowski, Doherty, & Malone, 1993a; Fidkowski, Malone, & Doherty, 1993b; Julka & Doherty, 1990, 1993; Levy, Van Dongen, & Doherty, 1985) introduced the boundary value and zero volume methods to compute the minimum energy requirement for non-ideal and azeotropic mixtures. Grossmann formulated a generalized disjunctive programming (GDP) for complex column to overcome numerical difficulties related with rigorous tray-by-tray distillation models (Barttfeld, Aguirre Pio, & Grossmann, 2004; Grossmann, Aguirre Pio, & Barttfeld, 2005). The Imperial group (Dunnebier & Panteleides, 1999; Ismail, Pistikopoulos, & Papalexandri, 1999; Ismail, Proios, & Pistikopoulos, 2001; Papalexandri & Pistikopoulos, 1996) recently proposed a generalized modular framework with MINLP techniques and the use of rigorous distillation models.

The rise in energy demand as well as environmental concerns heightens the importance of engineering low-energy distillation configurations by revamping existing infrastructure. Additional
structures for global optimality problems for each network (Bausa, Watzdorf, & Marquardt, 1998; feed stream to be separated and leads to independent optimization

2 is a strong function of thermodynamics and composition of the networks for any mixture of the same number of components. Step 2 is a strong function of thermodynamics and composition of the feed stream to be separated and leads to independent optimization problems for each network (Bausa, Watzdorf, & Marquardt, 1998; Giridhar & Agrawal, 2007; Giridhar et al., 2006).

Their observations dramatically reduce the search space of the optimal complex column network. Details can be found in elsewhere (Giridhar & Agrawal, 2007; Giridhar et al., 2006). They systematically evaluated the energy consumption of column sequences and the energy savings that can potentially be achieved through thermal coupling. Recently, they came up with a novel integer programming formulation for generating all possible complex configurations. They found that so-called basic configurations were always more efficient than any network belonging to the group of non-basic configurations. Examples of possible basic configurations for separating zeotropic quaternary mixtures are shown in Fig. 1. Their observations dramatically reduce the search space of the distillation synthesis. Their integer program provides a closed mathematical formulation to synthesize all meaningful candidate solutions for an optimal complex column network. Details can be found in elsewhere (Giridhar & Agrawal, 2007; Giridhar et al., 2006).

Their mathematical programming formulation could constitute the key element of a complete column network synthesis solution at least from mixtures without azeotropes as follows:

Step 1: Generic structure synthesis: Generate all possible network configurations.

Step 2: Specific Separation Task Optimization: Rigorously explore structures for global optimality.

Step 1 uses only structural information thus yielding identical networks for any mixture of the same number of components. Step 2 is a strong function of thermodynamics and composition of the feed stream to be separated and leads to independent optimization problems for each network (Bausa, Watzdorf, & Marquardt, 1998; Giridhar & Agrawal, 2007; Giridhar et al., 2006). It could be performed with existing short-cut or rigorous algorithms which take the column network structure as input. An even more advanced method would already account for thermodynamic and product purity targets for the specific separation task to further discriminate sub-optimal solutions in step 1, or perhaps implicitly in combination with step 2 without the need for profile computation of each and every structure. Further research might show that such an implicit pruning criterion does not exist. If it is true, Agrawal’s structural solution would be the best that can be done; and his contribution be declared the most advanced element of the general solution to the separation synthesis problem.

2.2. Topological maps

Doherty and Malone (2001) have compared graphical and topological methods to analyze distillative separation problems systematically. Recently, Tapp et al. (2004a, 2004b) generalized difference point equation concepts to produce column profile maps (CPMs). At infinite reflux, their CPMs are identical to the residue curve maps. The CPMs have the same number of relative constellation of singular points as the RCMs, but their position is moved relative to the composition triangle as shown in Fig. 2. For finite reflux, the column profile maps teach that the composition triangle merely shifts inside a relatively constant topological space. Their maps enable graphical assessment of thermodynamic features such as pinch point loci, displacement of separation boundaries with respect to a shifting composition triangle. Rather myopic analysis within the narrow window of composition triangles, topological features like shifts of singular points, appearance, or disappearance of separatrices or distillation boundaries can be studied in the generalized thermodynamics space defined by the composition simplex. They also propose to assemble separation complex networks by connecting generic column sections. A column section is defined as a sequence of equilibrium trays terminated on either end by the addition and/or removal of material and/or energy. They also presented a generalized difference point equations for the evolution of the liquid composition profiles for a generic column section as in Eq. (1).

\[
\begin{align*}
\frac{dx_i}{dn} &= (1 + \frac{1}{R_i}) \left( x_i - y_i \right) + \frac{1}{R_i} \left( X_{i-1} - x_i \right) & \text{with } R_i = L_i / \Delta, \\
x_i &= V_i - L_i / \Delta & \Delta = V - L 
\end{align*}
\]

(1)

where \( x_i \) is the liquid composition, \( y_i \) is the vapor composition, \( n \) is the number of stages, \( R_i \) is the generalized reflux ratio, \( X_{i-1} \) is the difference point, \( c \) is the number of components, \( L_i \) is the liquid flowrate, \( V_i \) is the vapor flowrate, \( \Delta \) is the net flow. Their method has a vast potential, but has not yet been extended to multi-component separation tasks with optimal energy or cost performance. Nevertheless, generalized column sections and column profile maps are expected to contribute significantly to a general separation network solution.

2.3. Shortest column profile optimization

Lucia, Amale, and Taylor (2006) introduced an interesting shortest stripping profile idea. They observed that residue curves with infinite energy requirement have the longest connecting path between stationary product nodes. The converse of their proposition suggests that the shortest liquid equilibrium column profile should yield the separation with minimum energy. Lucia and Feng (2004) also offer a global terrain method to rigorously compute shortest liquid profiles independent of the non-linearity or extrema.
Their new approach finds minimum energy requirements for distillations with feed pinch, saddle pinch, and tangent pinch points. The method can also produce non-pinched minimum energy solutions. The solution to the system (2) with the global terrain method renders the liquid profile with the minimum boil-up ratio as shown in Fig. 3. Their results show that the separation multiplicity in the composition space as in (2).

\[
\begin{align*}
\min \ D &= \sum_{j=1}^{N} \|x_j'\| = \|x_{j+1} - x_j\| \\
\text{s.t.} \\
x_j' &= x_{j+1} - x_j = \frac{s}{s+1} y_j - x_j + \frac{1}{s+1} x_B \\
x_1 &= x_B \\
r &= (s - q + 1) \frac{B}{D} - q \\
x_j' &= x_{j+1} - x_j = \frac{r + 1}{r} y_j - x_j - \frac{1}{r} x_D \\
D_{D,\text{low}} &\leq x_D \leq D_{D,\text{high}}
\end{align*}
\]
3. Towards generalized separation synthesis

The general separation network synthesis problem can be stated as follows: Given the thermodynamic pure and mixture properties of a multi-component mixture, find the network of separation units and the operating conditions that satisfy desired purity limits at minimum cost. We adopt a product-oriented view of setting purity limits as opposed to the customary fractional recoveries. The deterministic version of the separation synthesis problem considers feed composition and thermodynamics properties as precise; methods to account for uncertainty in the vapor-liquid models or operational uncertainty causing feed composition variation are discussed elsewhere (Chakraborty & Linninger, 2003). We also advocate to aim for realizable solutions with finite reflux and tray numbers, a goal referred to as non-pinched solutions by several researchers, instead of basing design decisions exclusively on idealizations such as the Underwood method which is limited by the strong restriction of constant relative volatility as well as unattainable product purities.

An algorithmic approach to distillation synthesis should ideally guarantee rigorous column profiles. The main reason in support of this argument is not necessary mathematical rigor or accuracy, but due to the paramount importance of validation with industrially accepted simulation software. A converged solution to a separation synthesis problems should accordingly render the following results: cost for separation as the best trade-off between capital and operating cost as specified in the design objective function, the network configuration composed of a complex interconnected network of generic column sections including their operating conditions like tray numbers, condenser and reboiler duties, as well as the liquid and vapor profiles for all columns and column sections. It should cost little extra effort to validate such solutions with commercial flowsheet simulators for synthesis solutions to be valuable for the industry. Validation with separation solutions based only on idealized methods are therefore cumbersome to validate in flowsheet simulators and are in the opinion of this author a partial solution at best.

Recent research efforts shift from optimizing single columns to gain small efficiency improvements towards completely rethinking separations as the complex network synthesis problem by taking best decisions for the network structure simultaneously with setting optimal operating condition decisions. The successful Petlyuk configuration is an example that justifies our belief in solutions of huge energy savings potentially achievable when redesigning entire separation trains in the chemical manufacturing industry. Our approach towards a general solution of the separation task has three major components: (i) thermodynamics, (ii) systematic network generation and (iii) advanced algorithm engineering. Fundamentally thermodynamic transformation like temperature collocation in combination with profile mathematical models drastically reduces the combinatorial burden to make rigorous separation synthesis tractable for numerical algorithms.

The second element is systematic network generation. Until recently, there were no algorithms to generate a complete set of meaningful complex column configurations. Novel formulations such as Agrawal’s basic configurations rigorously synthesize complex networks without missing significant structures. The third element advanced algorithm engineering combines the advantages of deterministic and stochastic search techniques to tackle open design problems with structural and parametric degrees of freedom appearing in separation network synthesis.

3.1. Generalized separation network synthesis method

3.1.1. Bubble point temperature collocation for complex separation networks

Temperature collocation has at its core a thermodynamically motivated problem transformation of the rigorous column profile equations. Its derivation departs from the continuous column profile equations proposed by Doherty. These equations are rigorous for packed columns and were shown to be given profiles closely matching rigorous tray-by-tray MESH models. These equations also apply to any mixture model including highly non-ideal mixtures with azeotropes. In temperature collocation we replace the column height or equilibrium stages as an independent variable with the bubble point temperature of the liquid mixture on a given equilibrium tray. The composition trajectories are expressed as functions in the independent variable, \( T \), instead of the height \( z \) of the column sections. Temperature collocation, Eq. (3) describes the composition profiles, \( x_i \), as function of the temperature-dependent equilibrium constant, \( K_i \), column section difference points, \( x_{2i} \), and generalizes column section reflux, \( R \). This transformation has been found to approximate column profiles for various solution models very accurately (Zhang & Linninger, 2004). The liquid profile equations in terms of temperature can be conveniently solved with finite element methods of orthogonal polynomials. In effect, this transformation constitutes an affine mapping of the column height into a dimensionless bubble point temperature, \( T \). This thermodynamic transformation of separation problem offers several key advantages: (i) massive problem size reduction and (ii) meaningful thermodynamic design coordinate. A detailed derivation can be...
found elsewhere (Zhang & Linninger, 2004).

\[
\frac{\partial K_i}{\partial T} = - \left( \sum_{i=1}^{c} \frac{1}{R_{Ai}} \right) \left(x_i - y_i\right) + \frac{1}{R_A} \left(x_{Ai} - x_i\right) 
\sum_{i=1}^{c} \left( \frac{1}{R_{Ai}} \right) \left(x_i - y_i\right) + \frac{1}{R_A} \left(x_{Ai} - x_i\right) K_i 
\]

(3)

Massive problem size reduction. The reduction of problem size to approximate the results of rigorous column profile computations is massive. First, it overcomes problems with infinite tray numbers near pinch or stationary points. Even when infinite tray numbers are needed to traverse pinched regions, temperature collocation – by virtue of monotonically increasing bubble point temperatures typically penetrates them without numerical problems. Independent of equilibrium trays needed for a column section, its entire profile can be calculated with two or three elements of two to three internal nodes. Even problems otherwise requiring many stages near saddle pinches or due to high purity separations can be tackled with fewer elements. Thus, temperature collocation massively reduced the number of state variables for the rigorous column profile computations. For given product specification and energy supply determined by the reflux or reboil ratios, realizability of simple or complex networks can be formulated rigorously as bubble point distance minimization problem (Zhang & Linninger, 2004).

3.1.2. Meaningful thermodynamic design coordinate

In addition, bubble point temperature is a meaningful thermodynamic coordinate for separation design, while tray numbers are not. In addition to being bounded a priori by the desired purity targets, the bubble point temperatures corresponding to products and pinch points offer thermodynamic criteria for the detection of difficulty of separation that the column height cannot provide. For example, column sections whose pinch bubble point temperatures do not overlap can never make a realizable column. Temperature also helps to eliminate unattainable product target based only to the relative temperature coordinate of products and associated pinch points. The attainable temperature window criteria is illustrated in Fig. 4. There is evidence that the inclusion of meaningful thermodynamic coordinates will soon provide further pruning criteria to tame the combinatorial complexity. Consider now Fig. 5b depicting the one-to-one thermodynamic transformation into a rectangular space of dimensionless temperatures and residue curve (ρ) coordinates. We have observed and believe it to be true in general – the bubble point profiles become monotonically both in temperature and residue curve coordinates. Monotonicity or other geometrical properties still hidden in the thermodynamic state space have the potential to further simplify separation problems. On the other hand, simplifications are more difficult to realize in the insightful space of trays and compositions predominantly used in traditional design methods. Temperature is also a suitable variable for heat integration, because it is ideal for identifying potential matching streams in complex separation trains.

3.2. Stochastic optimization for complex column synthesis

We successfully incorporated temperature collocation into a computer-aided design methodology for synthesizing multi-component distillation networks. We solved the mixed-integer non-linear programming using a hybrid method using a stochastic genetic algorithm with rigorous finite element collocation of column profiles (Leboreiro & Acevedo, 2004; Zhang & Linninger, 2004).

Fig. 5. Visualization of the same separation column profiles in different problem domains. Frame (a) shows column profiles in the composition triangle. The new thermodynamic coordinates bubble point temperature, T, and residue curve coordinate, ρ, used in Frame (b) are also indicted. Frame (b) shows the transformation of the composition triangle into a rectangular space with the help of thermodynamics coordinates bubble point temperature, and residual curve coordinate. In contrast to the column profile’s characteristic with rise and descent, the transformed profiles are strictly monotonic decreasing from the bottom to the distilled as we go along the column height. Rectangular thermodynamic profile spaces may hold the key for better search strategies for separation network synthesis.
imum number of degrees of freedom for all possible networks. The DOF minimum set enables the genetic algorithm to search a drastically reduce search space. The assessment of realizability and feasibility of complex column is delegated to a feasibility test between two neighboring column sections. It ensures the satisfaction of rigorous tray equilibria and component balances in a dimensionless bubble point space thus eliminating the need for the equality constraints in (4).

\[
\min_{d,x} \alpha \text{ Opt} + \beta \text{ Cap}
\]

s.t.

Tray balances and connections between sections
Feasibility between two column sections
Product purities

The high-level GA constructs different candidate separation configurations by varying the structural as well as key design variables such as different product sequences and operating conditions like reflux ratio, bottoms and distillate purities respectively. In each iteration, crossover produces new candidate solutions by a mathematical recombination process of their parents with the same structure. Mutations randomize the search. Repeated loops improve the whole population’s performance at least in a statistical sense thus solving the original optimization problem without ever computing gradient information. More implementation details can be found in Zhang and Linninger (2006).

3.3. Advances in algorithm engineering—hybrid algorithms

We have adopted hybrid algorithms to combine advantages of Newton-type technique with stochastic search techniques. Newton methods are particularly useful to satisfy constraints such as a large set of state variables. Open design variable especially structural decisions change the problem topology and equations are better suited for stochastic methods. We use a stochastic search in the discontinuous but drastically reduced design space. The massive number of state variable, however, is solved extremely efficiently by the orthogonal temperature collocation method. Combination of stochastic search with rigorous quadratic convergent Newton-type method allows us to solve minimum reflux ratio for five or six components for ideal mixture, constant alpha mixture, non-ideal mixture including azeotropic mixture and determine a range of operating condition including minimum reflux ratio, maximum reflux ratio which is possible in particular splits. It is working for sharp split as well as sloppy split, pinch or non-pinch solution.

3.3.1. Parallelization

A hybrid method is also ideal for massive parallelization, in which rigorous column profile evaluation are delegated to different computer clusters. The global solution is maintained by master computer which schedules the task and keeps the track of overall algorithm. Fig. 6 shows two layers algorithm for synthesizing complex column network, outer layer searches the reduced design space; inner layer deploys Newton type solver to converge the feasibility test base on column profile equations. The temperature collocation brings about a massive problem size reduction typically compressing hundreds of equilibrium stage equations into a few elements with two nodes.

4. Applications and case studies

This section demonstrates two examples of synthesis problem our methods is capable of solving. The first case study seeks a cheapest solution for ternary separation task. For various trade-offs between energy and capital cost specified by the design engineer, we wish to determine the globally optimal solution without excluding any viable combination of simple as well as complex sec-

Fig. 6. Hybrid genetic algorithm for synthesizing the complex column network.

Fig. 7. Column profiles of the best direct separation sequence in ternary mixture.
4. Global solution of ternary separation problem

The separation of an ideal ternary mixture elucidates the current capabilities of the proposed design procedure. The task consists in finding the minimum total annualized cost distillation sequence for separating an ideal mixture of three alkanes: pentane, hexane and heptane. The product purity of the recovered species needs to be above 99%. For each optimal solution, the hybrid algorithm described in previous section is deployed with 100 generations and population size of 200. The column separation is discretized with four elements with two nodes; the total number of state variables for ternary complex column network is 288. Fig. 7 plots the actual tray composition profiles of the best direct sequence with the optimal trade-off between capital and operating cost. The intersection of the column profiles confirms that the columns are realizable. For additional validation of the computational results, we solved the same problem again but considered only operating cost in the objective. Accordingly, the optimal solution should encompass two pinched columns operating at minimum reflux. Fig. 7 shows the GA solution with an intersection at the stripping pinch confirming the minimum reflux operation as expected.

We also expanded this case study to admit complex column configurations. Fig. 8 plots the actual composition profiles of the complex column with the optimal trade-off between capital and operating cost for complex column configuration.

Table 1 compares the optimal trade-off of direct split, indirect split and complex column configurations. For separation tasks with even amount of species in the feed, complex column configurations appear to always outperform the best networks using only simple columns. The best complex column has 28.58% lower total capital and operating cost than the best direct split network. The total required minimum vapor rate which is a measure of the overall energy efficiency of the network is only half the energy needed for the best direct split configuration! This example underscores significant energy savings realizable with better separation designs.

4.2. Initialization of a commercial flowsheet simulator and validation of results

The column profiles, product recovery and feed compositions, column refluxes and tray numbers of the optimal solutions to the solvent recovery problem were used to initialize a previous Hysys flowsheet simulator. Each column simulation converged immediately and the columns profiles agreed with the temperature

![Fig. 8. Optimal network of complex column profiles for separating an ideal ternary mixture.](image)

![Table 1](image)

![Fig. 9. Complete solution map of optimal column sequences for separating ternary mixtures with different feed compositions. Cost contours, A, B, C, ..., J, indicate optimal minimum cost-for-separation for specific feed.](image)
Implementing and optimizing a flowsheet solution of an entirely new separation design problem with unknown columns specifications and intermediate feeds is worth several days of work by an experienced engineer. We initialized each column section of the simple and/or complex network using tray numbers, reflux and reboil ratios, product purities and profiles what were computed with temperature collocation. Hysys using these results converged within a
few iterations. This combination of design with validated commercial separation codes is very important for industrial applications.

We also compared the algorithm’s performance to a study for separating the same feed mixtures into products of similar purity (Grossmann et al., 2005). The complex column configuration and composition profiles are similar and the optimal design of complex column network coincides. Unfortunately, the authors do not specify the vapor rate for comparison of energy performance. The CPU time for our method was 17 min independent of the initial conditions. This value reported in the reference was 14.37 min for runs made with a pre-processing procedure. These results demonstrate that achieved size reductions due to temperature collocation made even CPU performance competitive with deterministic methods.

4.3. Complete solution maps with complex column configuration

The speed and robustness of the proposed method enables design engineers to address problems previously not amenable to numerical analysis. Consider the problem of finding the best distillation network for separating any possible feed or for varying feed compositions in a ternary mixture. For feeds lying in some region of the composition triangle, a direct split may be optimal. In the other region, the indirect split may be superior, yet close to the pure component side, a single column may be sufficient. In the center region of around equimolar feeds, complex column may be the best option. It would be desirable to calculate the “cost-for-separation” for any possible feed composition. A global separation solution map specific for the given thermodynamics of the mixture as well as the desired purity target features the globally optimal cost contours and could delineate regions for which particular column configurations are the best choice. Such a diagram summarize the complete solution spectrum and for cost-for-separation for a particular ternary mixture. We demonstrate the current status of our proposed method towards the generation of such a global solution map. Samples of feed mixtures in the composition space were generated. A structured mesh pattern was used to cover the entire space and make visualization easier. For each possible realization of feed composition, separate synthesis problems were run on separate computer nodes inside a parallel PC cluster. The pure component thermodynamics was an ideal solution model and Antoine equations for the pure component vapor pressure model. Non-ideal solution models require no special modifications and are merely included in the computational burden. The product targets in terms of product purities with respect to A, B, and C were considered fixed and enforced in each global sub-optimization problem. The objective function in (4) defined trade-off between operating energy and capital cost (equipment, column). For each feed scenario, the globally optimal structure including simplified as well as complex column configurations were determined. For the optimal solutions operating conditions, section tray numbers, tray vapor and liquid column section profiles were computed rigorously. The novel hybrid algorithm with massive parallelization produces optimal solutions for each subprocess separately in typically 10 iterations. We also checked that the embedded temperature collocation algorithm ran robustly without convergence problems.

A complete solution map delineating the optimal achievable separation emerges as depicted in Fig. 9. Complete solution maps also make complex trade-offs involved in separation synthesis transparent. Each point in that space represents the global solution for the associated feed scenario. The complex column configuration is the optimal choice for feed compositions located in middle of composition triangle as region I. Feeds in region II are separated cheaper by indirect split near the top of the triangle. Direct split with simple column is the optimal choice for feed located in the bottom region III. Feed compositions in region IV, V, VI require only one column to separate binary mixture and do not constitute a ternary separation problem, but were indicated for completeness. Surprisingly, cost contour C, D, E are lowest, which the total cost of separation increases toward node, β along AB as well as towards node α along contours F–J. It also appears that cost contours trace bubble point curves.

Fig. 10 gives three examples for the best column networks for feeds lying in three different regions of the composition triangle. The feed composition located in region II shows to favor the indirect split as depicted in Fig. 10a. The mixture is separated to product AB and C in first column. Intersection of column section profiles S1 and S2 confirms the feasibility of the first column. The top product mixture, AB, is further separated as a binary mixture. Column profiles, S3 and S4, meet on the edge of composition triangle.

When feed composition located in the bottom of composition space (Region II), our algorithm finds the direct sequence of simple columns to be optimal configuration, as reported in Fig. 10b. The composition profiles of column sections S1 and S2 intersect each other and bottom product of S2 is further purified into pure products, B and C.

A network of complex columns is best on the feed composition in the middle of composition triangle. The fractionation column helps implement the more thermodynamic efficient separation. The product A, B and C are split in a single complex column. Column section profiles S3, S4, S5 and S6 make up the complex column profile.

For each global solution and algorithm, it reports column profiles, feed tray location and tray numbers which can be used a perfect initial guesses for validation with a commercial solution algorithm. We found that solutions reported with our temperature collocation method required but 2–5 iterations to converge with Hysys. The solution profile is very close, but cannot be expected to be identical as collocations does a continuous problem representation, while flowsheet simulators deploy discrete state-by-stage options. Practicing engineering may find the robust initialization step for complex column configurations of great value in practice.

5. Conclusions

In this article, recent progresses for synthesizing energy efficient distillation network are reviewed. Several milestones relating challenges and possible solutions are proposed and discussed. The backbone of a novel generalized column section approach towards a generalized solution of the separation synthesis problem is presented. Difference point equations with temperature as an independent variable instead of tray number are employed to complex column computation for column section. The feasibility of complex column can be formulated rigorously as a continuous sequence of column section profiles. A novel hybrid genetic algorithm deploying stochastic search in a reduced design space and Newton-methods to satisfy state equations were shown to solve optimal structure and design variables simultaneously. Two case studies show the global solution of a ternary sequence with cost function arbitrary trade-off of capital and energy cost. We also demonstrated the capability of the proposed approach to generate complete solution maps which encode the cost and states of global solutions in the entire thermodynamics composition space.

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