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Optimal design of complex distillation system for multicomponent zeotropic separations

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ABSTRACT

The optimal design of complex distillation system for separation of multicomponent zeotropic mixtures is studied. Super column with the ability to separate any specified products from the given feed is introduced for defining integration upper limit of design alternatives. The improved state-space (SS) superstructure incorporating all basic mass and heat transfer elements are adopted to capture all configurations in the framework of super column. Specifically, by adding stages-cascade process operator in the original representation, a series of optimal flowsheets with multiple thermal links, which have never been included within previous superstructure are easily generated. The mathematical modeling of the proposed superstructure is performed with mixed integer non-linear programming (MINLP). It advocates the use of rigorous physical model for each mass/heat transfer stage to ensure the practical reliability and optimality of the attained designs. Then the derived optimization model is solved by a modified solution procedure, in which the key item is an iterative initialization scheme. Three multicomponent zeotropic separation examples are employed to illustrate the effectiveness of the proposed approach. These optimum designs yield significant savings in total annual cost (TAC) relative to Petlyuk columns and some guidelines for distillation flowsheet retrofit based on thermodynamic analysis are proposed.

1. Introduction

Distillation is one of the most important and widespread used unit operations in the process industry, as an energy-separating-agent process, distillation accounts for a substantial portion of worldwide energy consumption, as well as investment. The economic significance of distillation separations has been a driving force for the research in design of economically optimal distillation processes. Various approaches to simple column system have been proposed over the years. The design of simple distillation column systems has progressed from the design of networks of sharp split units separating a multicomponent mixture into pure component products (Westerberg, 1985), to the design of heat integrated separation systems based on non-sharp splits producing multicomponent products (Aggarwal and Floudas, 1992; Yeomans and Grossmann, 1999). In the past 20 years, researchers have witnessed a growing interest in the optimal design of complex distillation systems because of the substantial energy savings that can be achieved through the use of complex columns instead of the more conventional simple column arrangements. It has been proved that for separating a multicomponent mixture the thermally coupled configuration reduces the total energy consumption by 10% to 50% as compared to conventional systems (Annakou and Mizsey, 1996; Dünnebier and Pantelides, 1999; Wolff and Skogestad, 1995).

The task of optimal design of complex multicomponent distillation processes is an important and challenging issue. Many methods have been proposed over the years for its solution. These methods involve heuristics, evolutionary techniques, hierarchical decomposition, explicit enumeration, thermodynamic insights and so on. With the rapid development of mathematical programming techniques and a better understanding of process design, superstructure optimization has received considerable attention since it provides a systematic basis for the evaluation and optimization of numerous alternatives. This paper adopts this optimization approach. Superstructure is defined as a network structure in which many possible flowsheets are included. From a modeling perspective, the basic elements of the superstructure have been refined constantly. In the early studies of superstructure optimization, the column is the smallest unit of system. A representative superstructure which has embedded in all possible options of splitting, mixing and bypassing of the column interconnected streams was developed by Aggarwal and Floudas (1990). However, the superstructure of mixer–unit–splitter

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(M–U–S) does not include any complex column substructure, and therefore only simple distillation column sequences are generated from this strategy. Later energy efficient complex distillation columns were incorporated into the superstructures through the use of column sections instead of simple columns. A column section is defined to be a portion of a distillation column which is not interrupted by entering or exiting streams or heat flows. The first superstructure including complex arrangements was presented by Sargent and Gaminibandara (1976), and then extended in the literature of Sargent (1998) by elaborating on the state task network (STN) representation. Agrawal (1996) proposed a satellite column superstructure which contains the sequential superstructure of Sargent and Gaminibandara as a substructure, for a sharp separation of an n-component mixture using one reboiler, one condenser and minimum number of rectifying and stripping sections (4n-6). The binary tree representation was modified by introducing bypasses and nine generalized observations were used to facilitate the task of generating schemes with 4n-6 sections. Yeomans and Grossmann (2000) proposed a generalized disjunctive programming (GDP) model for the optimal design of complex column configurations, by means of the sequential column superstructure and overcoming numerical difficulties associated with common rigorous distillation models. The GDP techniques were also used in Caballero and Grossmann (2001) for the satellite column superstructure based on STN for the generation of simple and complex column flowsheets for sharp separations of an N-component mixture and using simple shortcut distillation models. In contrast to systems with conventional columns, the number of column sections is not fixed. Therefore, the trade-off between the energy consumption and the extra number of column sections can be determined. However, it is difficult to capture all possible combination of different column sections under the framework of permanent and conditional tray. Shah and Kokossis (2002) developed a supertask representation involving parallel sequences for the synthesis of complex column sequences. The supertask is based on simple tasks that accommodate for basic sequences and the hybrid tasks account for complex columns and sloppy separation. And it is formulated as a simple MILP problem by using simple shortcut distillation models. GDP was also used to model the superstructure based on the Reversible Distillation Sequence Model (RDSM) by Barttfield et al. (2004). Due to the large size and complexity of the formulation using rigorous MESH equations, a decomposition solution strategy is proposed where discrete decisions are decomposed into two hierarchical levels within an iterative procedure. However, the superstructures based on supertask or RDSM still consist of column sections. Through the Generalized Modular Framework (GMF), an alternative approach was proposed by Proios and Pistikopoulos (2005) for the systematic synthesis of complex column sequences, while avoiding potentially limiting simplifying assumptions. Although there are mix and/or split opportunities for a stream on upper and lower auxiliary blocks, the superstructure does not provide the same opportunity in the main module. Therefore the model is incapable of evolving the connection structure between side draws and thermal coupling.

Recently, there are some remarkable contributions to automatically synthesize complex column configurations. Column profile maps (CPMs) have been developed as a useful graphical tool in distillation design by allowing the designer to set reflux ratios and net molar flows to suit the specifications of the separation. This method is completely generalized. Any configurations irrespective of complexity can be modeled and graphically understood. The most important results and applications obtained using the CPM technique had been summarized by Hildebrandt et al. (2010). CPM is a good way to find new efficient configurations which should be added in existing superstructure. As Kim, Ruiz and Linninger (2010) point out, there were no rigorous algorithms to synthesize complete separation flowsheets so far without limiting assumptions of the thermodynamic vapor–liquid equilibrium model or restrictions in its applicability like sharp splits or nondistributing species. Based on the CPMs, Linninger and co-workers (Kim and Linninger, 2010; Kim, Ruiz and Linninger, 2010) extend temperature collocation methodology with the minimum bubble point distance criterion to address current unresolved design problems such as the computer-aided design of energy-efficient complex distillation networks.

The goal of this paper is to develop a novel systematic framework for one step optimization of thermally linked complex distillation sequence, operating and design parameters with rigorous computations of mass, equilibrium, summation, and heat (MESH) equations on the basis of previous works reported in the literatures. We introduce the super column (SC) as a new methodology for the design of distillation networks and for its representation, the improved state space (SS) superstructure incorporating all thermodynamically admissible combinations of simple and complex column configurations to achieve any type of product distribution such as sharp, nonsharp, and sloppy splits, is proposed. This superstructure is modeled as an MINLP then is solved with an integrated solution strategy. Three examples are presented to illustrate the scope and advantages of the proposed approach.

2. Problem statement

The problem addressed in this paper is stated as follows: Given are a set of multicomponent feeds with known flowrate and composition (temperature and pressure could also be given or included as additional optimization variables), and given are a set of available utilities such as cooling water and steams at various pressure levels. The problem consists in determining a distillation system that separates the desired pure or mixed products at minimum utility cost or total annual cost (TAC). Cost data of feeds and utilities and all thermodynamic property models are given. This paper aims to address ideal or nearly ideal mixtures separations problem without any other additional assumptions. Both sharp and sloppy split separations are included.

3. Superstructure representation

The construction of a general superstructure for complex distillation column systems is a non-trivial problem due to the large number of alternative designs that are possible. Previous superstructures mentioned in the literatures rely on the assumption that the heating, cooling, feed, and draw of material only take place in specified locations of the column array, not in every tray. Moreover, system assumptions such as number of columns or sections, type of columns (i.e., simple or complex column) are required for superstructure based on column sections. Hence, these assumptions result in only covering a portion of the combinatorial space.

It is known that for a regular zeotropic N-component separation, $N-1$ sharp-split simple columns are needed. However, for complex distillation configurations the number of columns or sections is difficult to be determined in advance. Most of the studies have focused on sharp split of N component mixtures using $N-1$ distillation columns or $2(N-1)$ sections (Rong et al., 2001). Some papers use more or less than $N-1$ columns ($2(N-1)$ sections). All of them reduce the energy consumption and/or the capital cost, for a specified separation task in some particular cases (Agrawal, 2000; Errico et al., 2009; Kim and Wankat, 2004; Rong et al., 2003). Two important superstructure proposed for