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Synthesis of distillation configurations. II: A search formulation for basic configurations

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ABSTRACT

It is known that there exist a combinatorially large number of multicomponent distillation column configurations for a given feed and given product specifications. In the accompanying part I of the paper, we classified configurations into basic configurations (those that use $(n-1)$ columns for an n-component feed mixture) and non-basic configurations (those that use more than $(n-1)$ columns for the same feed). As n exceeds four, the number of non-basic configurations greatly exceeds the number of basic configurations and have a huge impact on the size of the search space. However, through extensive calculations for a four-component feed, we have found that a non-basic configuration never has a lower heat duty than the lowest heat duty basic configuration. While prior researchers have proposed a mathematical formulation that could be used to generate only the set of basic configurations, we present an alternative supernetwork model to achieve this goal. We show how the supernetwork can be reduced to a binary integer program (BIP), and how all feasible configurations can be drawn for a given application using a suitable solver. We present different solution techniques, including parallel algorithms based on the fact that the evaluation of the performance for each configuration is independent of any other configuration. Through such a procedure, all applicable basic configurations can be rank listed for a given application according to a chosen criterion. We also extend the supernetwork formulation to a unified non-convex MINLP that can be used in a flexible way to find the best candidate configurations for a given application. We show the power of our search formulation in accommodating general separation techniques other than distillation, such as membranes, adsorption, etc.

1. Introduction

The synthesis of separation networks for multicomponent feed mixtures has been a challenging problem in process design for several decades. Distillation configurations in particular have been the focus of several research efforts due to their widespread use in the process industries. The problem of finding the best configuration of distillation columns (with associated reboilers, condensers, piping, and control systems) that should separate a given multicomponent feed into individual components is usually a difficult one. This is due to two main reasons: the set of distinct feasible distillation configurations is often ill-defined, and grows combinatorially fast with the number of components that need to be separated; and, the fitness measure of a given configuration is usually a highly non-linear function of the given parameters, causing computational challenges.

Due to the industrial importance of multicomponent distillation network synthesis, the problem has been examined by several researchers in the literature (Doherty & Malone, 2001). Many early results were restricted to the case of sharp splits alone, where each column has exactly two product streams (distillate and bottom), and these two streams have no common intermediate component distributing in appreciable quantities. Thompson and King (1972) and King (1980) have examined such configurations. Heuristics for the synthesis have been proposed based on physical insights by Rathore, van Wormer, and Powers (1974), Seader and Westerberg (1977) and Douglas (1988).

A need for systematic solution methods in process synthesis has long been recognized (Westerberg, 2004), and there is a need to provide some assurance that a design that has been synthesized is at least locally optimal, if not globally. Being able to provide such an assurance is not a trivial undertaking in the case of distillation synthesis, due to the highly non-linear and non-convex search space and objective functions commonly used. The broad goal of arriving at solutions which one knows to be good may be achieved in the long-term through two complementary approaches. A better search method is the first weapon, one that makes it easier to find good locally optimal solutions than before. A tighter search space formulation may also be used independently of the search method, to aid the search by filtering out solutions that may not be desirable, or by

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providing a representation that makes it easier to locate regions that are likely to have optimal solutions. In this paper, we describe such a formulation and describe computational search methods that we have found to be useful in the synthesis of configurations with low heat duty requirement.

2. Prior work

Generally, the problem of distillation configuration synthesis has been attacked by various researchers using two broad approaches. The first is an additive approach, involving the listing of a few configurations by hand through a discovery process, then building rules to essentially interpolate or extrapolate the discovered structures to obtain more configurations. Building configurations sequentially using heuristics is an additive approach: we are assured that the final configuration will be feasible, but it is easy to miss some configurations if the rules are not complete. The second is a subtractive approach, involving the formulation of a search space that embeds various configurations, and eliminating sections of the space that do not correspond to feasible configurations, arriving at a reduced space where every point represents some feasible configuration, including those not discovered by hand. Using a mathematical superstructure is a subtractive approach, which can potentially ensure completeness of the search space, but which can also potentially generate configurations that may not be desirable from a practical viewpoint and should preferentially be removed using constraints.

Several authors have examined the concept of a superstructure, which seeks to embed all possible configurations, and which can be used to systematically explore and evaluate the space of all configurations. An early superstructure was proposed by Sargent and Gaminibandara (1976), and allowed non-sharp splits to exist through splitters, mixers and flow control. An extended space was proposed by Agrawal (1996) to include satellite configurations that were not embedded in the Sargent and Gaminibandara superstructure. Agrawal (2003) also provided a systematic rule-based method whereby individual basic configurations can be created by starting at the product end in a network and then marching towards the feed end by making several decision regarding reboilers, condensers and transfer streams. Rong, Kraslawski, and Turunen (2003), and Fidkowski (2006) published the exhaustive space for multicomponent feeds, generated through a combination of individual split possibilities. Hu and Rippin (1991) presented a method for embedding various multicomponent configurations in a single unified framework. A state task network formulation was proposed by Sargent (1998), and extended by Yeomans and Grossmann (1999).

Caballero and Grossmann (2001, 2004) have proposed an elegant mathematical generalized disjunctive model for synthesis of multicomponent distillation networks, building on the observations suggested by Agrawal (1996) and the state task network of Sargent (1998). In their formulation, the separation tasks involving pseudo-columns and heat exchangers (reboilers and condensers) are considered independently. Then a set of logical relationships are used to ensure feasibility of the sequence of tasks. In this approach, the heat exchangers are not directly connected with the set of tasks. For example, in the two-step optimization procedure, all the internal heat exchangers associated with mixtures are initially taken to be absent and the resulting configurations with varying degree of thermal coupling are solved to identify an 'optimal' configuration. This is then followed with cost and energy tradeoff calculations by adding internal heat exchangers to the identified optimal configuration to further increase the optimality of the solution. This two-step procedure, while being useful in providing an optimal solution, cannot guarantee optimality. It presumes that post-assignment of the internal heat exchangers to a configuration found to be initially optimum with the constraint of no internal heat exchangers, will result in the overall optimum configuration.

There is a need for a framework that will directly allow the generation and optimization of $(n-1)$ column configurations with any degree of thermal coupling. This goal of our work is to introduce a set of logical constraints that can first create and enumerate all the $(n-1)$ column configurations without any thermal coupling (which we refer to as basic configurations), and use these constraints to find the basic configuration with the lowest heat duty. In a subsequent paper, we will demonstrate its extension to include any desired level of thermal coupling. It should be noted that there have been earlier successful attempts to elucidate basic-only configurations for n-component mixtures (Agrawal, 2003; Caballero & Grossmann, 2006). In this work, our mathematical description of the physical structures of the distillation configurations has some similarities with the prior work in the literature. However, especially when compared to Caballero and Grossmann (2006), our method does differ in modeling the component and stream flows in the distillation configuration, and in the computational methods used to find the configuration with the lowest heat duty.

When an n-component feed is separated in n product streams each enriched in one component, the number of configurations increases rapidly when enumerated exhaustively. Moreover, for an n-component mixture, the set not only includes $(n-1)$ column basic configurations, but also non-basic configurations containing more than $(n-1)$ columns. In the accompanying paper we showed an example of a non-basic configuration containing nine distillation columns for a six-component feed. These additional columns in a non-basic configuration add cost not only due to additional columns, but also the associated hardware such as reboilers and condensers along with their utility supply systems. For a four-component feed, through extensive calculations for various feed conditions, we found in the companion paper that the six non-basic configurations having four distillation columns never have lower heat duty than the 18 basic configurations with three columns. Furthermore, as the number of components rises beyond four, the subset of non-basic configurations grows much more quickly than the subset of basic configurations. For example, in the case of a six-component mixture, the exhaustive method leads to over four million configurations of which only 4373 are basic and the rest non-basic. This problem of large search space is further exacerbated by orders of magnitude when thermal coupling between distillation columns is considered. In order to make the problem of search space manageable and in the light of heat duty result through extensive calculations for the four-component feed mixtures and the anticipated increased capital cost due to additional columns for the non-basic configurations, we include only basic configurations in a problem formulation for finding an optimal configuration.

The reduced search space of basic-only configurations provides other associated benefits. For example, when the search space is reduced in size, it is easier to enumerate several alternative configurations individually and optimize their stream flows to minimize heat duty. This ability to rank list alternative configurations according to a chosen criterion can be quite useful for a practicing engineer to assess benefits of the parameters that cannot be easily represented in mathematical form. For example, for a five or six-component feed, all the configurations within some *x*% of the lowest heat duty may be rank listed and then a process engineer can pick the desired configuration based on other parameters such as control and operability, manufacturability, shipability of columns, etc., using their experience and knowledge. Such an exercise can also be beneficial in identifying retrofittable configurations for debottlenecking of an existing distillation train.

From a computational point of view, a search space that embeds only basic configurations can be used to exhaustively generate all feasible structures (configurations), with each then being subjected