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Logic hybrid simulation-optimization algorithm for distillation design

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ABSTRACT

In this paper, we propose a novel algorithm for the rigorous design of distillation columns that integrates a process simulator in a generalized disjunctive programming formulation. The optimal distillation column, or column sequence, is obtained by selecting, for each column section, among a set of column sections with different number of theoretical trays. The selection of thermodynamic models, properties estimation, etc. is all in the simulation environment. All the numerical issues related to the convergence of distillation columns (or column sections) are also maintained in the simulation environment. The model is formulated as a Generalized Disjunctive Programming (GDP) problem and solved using the logic based outer approximation algorithm without MINLP reformulation. Some examples involving from a single column to thermally coupled sequence or extractive distillation shows the performance of the new algorithm.

1. Introduction

The general separation problem was defined more than 40 years ago by Rudd and Watson (1968) as the transformation of several source mixtures into several product mixtures. More than 40 years later we can say that this general problem has not been completely solved. We will focus, in this work, in the more restricted problem of separating a single source mixture into several products using only distillation columns.

Distillation is likely the most important separation and purification operation in chemical process industries. Typically more than half of the process heat distributed to a plant is dedicated to supply heat in the reboilers of distillation columns (Kunesh et al., 1995). However, the energy is provided to the bottom of the column and approximately the same amount of energy removed in the top, although at lower temperature, which yields an inefficient process, but still one of the most effective for homogeneous mixtures separations. To get an idea of the importance of distillation, Humphrey (1995) estimated that distillation handles more than 90% of all the separations and purifications. Soave and Feliu (2002), using data by Mix et al. (1978) estimated that distillation accounts about 3% of the total United States energy consumption. This is equivalent to 2.87×10^{18} J per year (91 GW or 54 million tons of crude oil). The capital investment for these distillation systems was estimated to be around 8 billion US$.

The optimization of distillation columns involves the selection of the number of trays, the feed location and the operating conditions to minimize a performance function, usually the total annualized cost that involves investment and operating costs. Discrete decisions are related to the calculation of the number of trays and feed and products location, and continuous decisions are related to the operation conditions. Due to the discrete-continuous nature of the problem and to the complex equations involved, it is common use shortcut or aggregated models together with some rules of thumb that under some assumptions have proved to produce good results, at least in the first stages of design where a rigorous design is neither necessary nor convenient due to the large computational effort needed. Some of the most successful shortcut methods are:

Fenske – Underwood – Gilliland (*FUG*). (Fenske, 1932; Gilliland, 1940; Underwood, 1948). The FUG method assumes a constant molar overflow and constant relative volatilities in all the trays of the distillation column. This method considers two extreme ideal situations. (a) The distillation column operates at total reflux (no feed is entering or exiting from the column), which allows calculating the minimum number of trays for a given separation of two key components, and (b) when the column operates at pinch conditions, (infinite number of trays), which allows calculating the minimum reflux. The optimal situation is in some point in between these two extreme cases. *Group methods* (GM) (Edmister, 1943; Kamath et al., 2010; Kremser, 1930). GMs use approximate calculations to relate the outlet stream properties to the inlet stream specifications and number of equilibrium trays. They provide only an overall treatment of the stages in the cascade without

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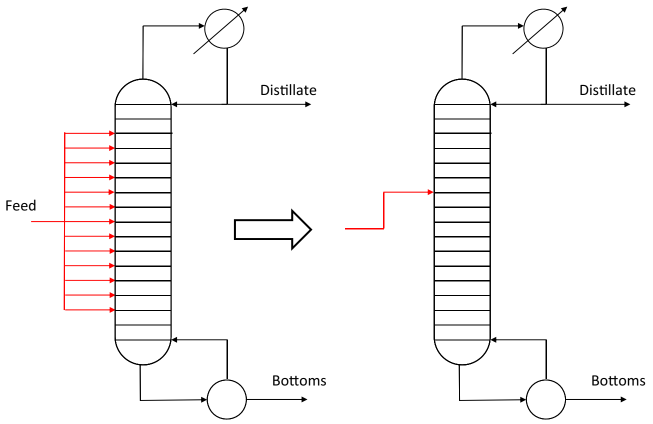

Fig. 1. Superstructure by Sargent and Gaminibandara (left) and a possible solution (right).

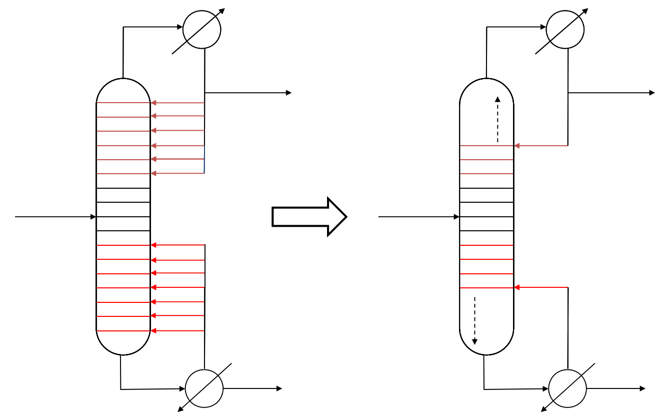

Fig. 2. Superstructure by Viswanathan and Grossmann (left) and a possible solution (right).

considering detailed changes in the temperature and composition of individual stages. However, they are much easier to solve because they involve fewer variables and constraints. *Aggregated models* (AG) (Bagajewicz and Manousiouthakis, 1992; Caballero and Grossmann, 1999). AG models are similar to group methods, they are based on mass balances and equilibrium feasibility, expressed in terms of flows, inlet concentrations, and recoveries. The *Boundary Value Method* (BVM) (Barbosa and Doherty, 1988; Fidkowski et al., 1993, 1991; Julka and Doherty, 1990; Levy and Doherty, 1986; Levy et al., 1985). BVM can be used to determine the minimum reflux ratio and feasible design parameters for a column separating a ternary mixture. It allows to obtain the number of trays, composition profiles, etc. The *Rectification Body Method* (RBM) (Bausa et al., 1998; von Watzdorf et al., 1999). RBM is used for the determination of minimum energy requirements for a specified separation. The method approximates rectification bodies by straight lines. The intersection of the rectification bodies of two sections indicates its feasibility. *Driving Force Method* (DFM) (Gani and Bek-Pedersen, 2000). The DFM is a graphical method. Its authors proved that the minimum energy requirements correspond to a maximum in the driving force. The *Shortest Stripping Line* (SSL) (Lucia et al., 2008; Lucia and McCallum, 2010; Lucia and Taylor, 2006) Authors showed that the longest residue curve is related with the highest energy consumption for a given separation. Then the shortest curve should produce the minimum energy required for the same separation.

Some of the previous methods have been automated, although not all of them can be directly used with an optimization algorithm. In any case, they are valuable tools for obtaining precise initial values or reliable bounds for the rigorous optimization of distillation columns.

2. Overview of rigorous tray-by-tray optimization models

As commented in Section 1, the economic optimization of a distillation column involves continuous decisions, related to the operational conditions and energy involved in the separation, and discrete decisions related to the total number of trays, and the tray positions of each feed and product streams. A major challenge is to perform the optimization using tray-by-tray models that assume phase equilibrium.

The first approach to solve the above commented problem was due to Sargent and Gaminibandara (1976). In this case, the authors assumed a fixed number of trays, and the goal was to select the optimal feed location. To that end, the feed is split into as many streams as trays have the column (condenser and reboiler are excluded). Fig. 1 shows the superstructure. The model can be written as a Mixed Integer Nonlinear Programming (MINLP) problem by considering the MESH equations (Mass balances, Equilibrium equations, molar fraction Summation equals one in all phases, and Enthalpy balances). However, computational experience shows that this problem is usually solved as a relaxed NLP.

The first model that considers both, the feed tray position optimization and the total number of trays was due to Viswanathan and Grossmann (1993). The authors used a superstructure that involves a variable reflux location as shown in Fig. 2. The superstructure considers a fixed feed tray and a column formed by a large enough number of trays above and below the feed. The reflux (reboil) is returned to all the trays above (below) the feed. The model takes the form of a MINLP and relies also on MESH equations. A major difficulty with this model is related to the non-existing trays. In these trays, there is a zero liquid flow (rectifying section) or a zero vapor flow (stripping section), which can produce numerical problems due to the convergence of equilibrium equations with a zero value in the flow of one of the phases.

To avoid the numerical problems in MINLP models Yeomans and Grossmann (2000a, 2000b) proposed a Generalized Disjunctive Programming model by allowing the bypass of those trays that are not selected. Fig. 3 shows the column representation for this approach. For each existing tray the mass transfer task is accounted for and modeled with the MESH equations. For a non-existing or inactive tray the task considered is simply an input-output operation with no mass transfer. Because the MESH equations include the solution for trivial mass and energy balances, the only difference between existing and non-existing trays is the application of the equilibrium equations. As for the permanent trays, all the equations for an existing tray apply. The advantage of the disjunctive modeling approach is that the MESH equations of the non-existing trays do not have to be converged, and no flows in the column are required to take values of zero, making the convergence of the optimization procedure more reliable. Also, by using Generalized Disjunctive Programming (GDP) as the modeling tool, the computational expense of solving the problem can be reduced. Barttfeld et al., (2003) considered different representations for the GDP model. Numerical results studies for separation of ternary mixtures in a single column suggests that the GDP formulation requires less solution time but is more sensitive toward local optima than MINLP formulations. Even though, GDP seems to be more reliable than MINLP models both require good initial values and bounds to converge. Barttfeld and Aguirre (2002, 2003) propose to use a reversible distillation model that involves the minimum reflux conditions as well as minimum entropy production to provide a feasible initial design, and good initial values for the rigorous optimization. Their method is mainly limited by the drawbacks of this so-called “preferred separation”, because, for azeotropic mixtures,