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The importance of the sequential synthesis methodology in the optimal distillation sequences design

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ABSTRACT

The sequential design method is presented as a complementary tool of the systematical synthesis procedure that allows to define a clear connection among the different types of distillation column sequences. In particular, the connection with the simple column subspace is considered, since this subspace represents the comparison reference for all the alternatives considered. The sequential design procedure, based on the correspondence between the functionality of the column's section among the simple columns and the derived sequences, is compared with a mathematical based optimization algorithm. The separations of a four-component near ideal mixture and the azeotropic ethanol–water mixture are considered as case studies and the designs obtained applying both methods have been compared. The results confirmed that the sequential design method is a fast and reliable tool in the optimal design of the column sequence.

1. Introduction

The definition of a searching space that includes all or most of the possible alternatives for the separation of a multicomponent mixture, is the first step in the identification of the optimal flowsheet. Once the most suitable separation method is identified, the problem becomes how to generate the alternatives to be included in the searching space. The most suitable separation method is usually selected by using appropriate indexes. When the relative volatility between the key components is higher than 1.05, distillation can be considered as a feasible separation method (Seader & Westerberg, 1977). Focusing on distillation, the well known simple column sequences are the first class of configurations explored. They represent the simplest solution since are composed by columns with a single feed, one top and one bottom product. Anyway their design simplicity is counterbalanced by the high energy consumption and high capital costs.

The high energy consumption is related to thermodynamic inefficiencies like the irreversible mixing of non-identical streams (feed mismatching) or the energy lost when a middle component is initially separated and then mixed again with the other components (remixing effect). The capital costs are mainly associated to the number of columns and auxiliary equipments. For a N-component mixture, if N product streams are required, it is necessary a sequence composed by $N-1$ columns.

The number of simple column sequences can be predicted using the formula (Thompson & King, 1972):

$$S_N = \frac{[2(N-1)]!}{[N!(N-1)!]} \qquad (1)$$

Among all the simple column sequences the most promising one/s, identified by means of predefined criteria, is/are utilized as reference case to compare the performances of all the other alternatives included in the searching space. A complete searching space could theoretically include sequences with more than $N-1$, exactly $N-1$ and less than $N-1$ columns.

The convenience to include in the searching space configurations with less than $N-1$ columns has been explored by Kim and Wankat (2004) for different four-component mixtures. For each feed composition case, the corresponding five simple column

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Nomenclature

Az.	azeotropic mixture
b_i	molar availability function of the output stream i [kJ mol^{-1}]
b_l	molar availability function of the input stream l [kJ mol^{-1}]
C	column
G_{max}	maximum number of generations
h	molar enthalpy [kJ mol^{-1}]
LW	lost work [kJ h^{-1}]
N	number of feed components
n_i	molar flowrate of the output stream i [mol/h]
n_l	molar flowrate of the input stream l [mol/h]
PS	population size
Q_j	heat flow j out the system [kJ h^{-1}]
Q_m	heat flow m in the system [kJ h^{-1}]
s	molar entropy [kJ K^{-1} mol^{-1}]
S_N	number of possible simple column sequences
TAC	total annual cost [k$ yr^{-1}]
T_0	temperature of surroundings [K]
$T_{s,j}$	temperature of the reservoir for the heat flow j out the system [K]
$T_{s,m}$	temperature of the reservoir for the heat flow m in the system [K]
vap.	vapor phase
W_{min}	minimum work of separation [kJ h^{-1}]
W_{min}	shaft work k produced by the system [kJ h^{-1}]
$W_{s,k}$	shaft work n fed to the system [kJ h^{-1}]
ΔS_{irr}	irreversible entropy production [kJ K^{-1} h^{-1}]
η	thermodynamic efficiency

sequences were considered and compared to the eleven alternative sequences proposed. Among all the alternatives, ten are composed by two columns and one alternative includes only one column with two side streams. Among the ten column sequences, two of them have a product side stream connecting the columns. All the alternative sequences were defined considering the possibility to have a side stream above or below the column's feed, in liquid or vapor phase. The authors considered the synthesis and the design as sub sequential steps. It means that once all the alternatives were identified, their design was done independently since no connection between the simple column sequences and the configurations included in the searching space was evidenced.

Caballero and Grossmann (2004) introduced a superstructure optimization approach able to generate a very complete set of distillation sequences that constitutes the searching space used by the authors to identify the configuration with the lowest cost. Simple column sequences, fully thermally coupled sequences, all the possible partially thermally coupled sequences and even the thermodynamic equivalent sequences were considered. An appropriate design method was selected to define the design parameters used in the cost evaluation. Once a feed composition case has been defined, the design calculation was performed for all the feasible sequences generated.

Shenvi, Shah, Zeller, and Agrawal (2012) completed the previous work of Shah and Agrawal (2010) introducing a eight-step matrix-based method able to include in the searching space also the configurations with less than $N-1$ columns. The matrix-based method proposed, includes both sharp and non-sharp splits and generates simple and thermally coupled configurations. The authors proved the validity of their methodology by means of a case study of a four-component normal paraffin mixture. All the configurations were first screened using a short-cut method, and

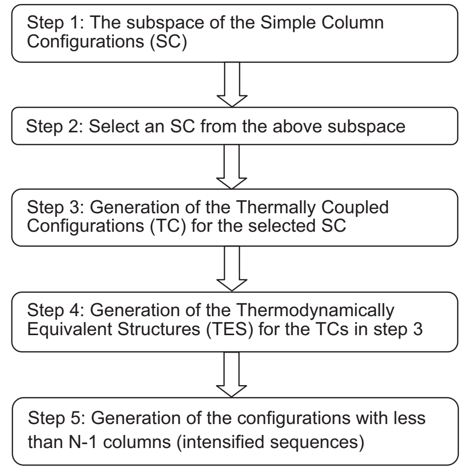

Fig. 1. The simplified systematic procedure for the sequential distillation sequence synthesis.

then the most promising ones were simulated again through a rigorous method. Since each class of configurations was developed individually, the design was done independently.

It is clear that all the authors approached the necessity to generate a complete searching space following different mathematical tools; anyway the simple column sequences are always considered as a basis for the comparison with the alternative sequences proposed.

The aim of this work is to analyze the benefits in the design procedure when the searching space generation method is able to keep a strict connection between the different sequences. Two case studies have been presented to prove the validity of the methodology. The first case regards the separation of a four-component hydrocarbon mixture; the second one is the well known ethanol–water azeotropic separation. For the same cases a hybrid multi-objective optimization algorithm is used to obtain the optimal design parameters. The results are then compared and commented.

2. The sequential design method

In our previous works (Errico & Rong, 2012a; Errico, Rong, Tola, & Turunen, 2009; Rong & Errico, 2012) the synthesis of alternative configurations was realized following a sequential method that allows to establish a clear connection between all the sequences. Fig. 1 reports a simplified five-step procedure that guides the designers from the simple to the complex configurations. The introduction of one or more thermal couplings is used to move from step 2 to step 3, then by the column section recombination the step 4 can be completed. The configurations included in the last step 5 are obtained by replacing one or more single column sections with a product side stream or an interconnecting column stream (intensified sequences).

Considering as an example the separation of a four component mixture, where the components are listed in decreasing order of relative volatility, the indirect-direct configuration reported in Fig. 2(a) was chosen among all the simple column configurations. The corresponding thermally coupled configurations can be obtained by replacing a condenser, a reboiler, or both, associated to non-product streams, with two interconnecting vapor and liquid streams between the columns. In the case considered three alternatives are possible, but only the one obtained by substitution of the condenser corresponding to the ABC submixture is reported in Fig. 2(b). The column sections, defined according to Hohmann, Sander, and Dunford (1982), are enumerated in each sequence. The thermodynamically equivalent configuration can be obtained for