



# Design and optimization of modified non-sharp column configurations for quaternary distillations

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## ABSTRACT

The possible structural changes of a non-sharp quaternary distillation configuration are considered. For the reference configuration composed of four columns, different alternatives are generated following the process intensification principle to reduce the number of equipment units. The intensified systems with three or two columns are obtained, including the dividing wall columns. Simulator Aspen Plus V8.0 was used to design and simulate all the systems for a hydrocarbon mixture. The intensified structures showed relevant energy savings compared to the reference case. The most promising alternatives were optimized by means of the differential evolution (DE) method minimizing the total annual cost (TAC). It was observed that the intensified systems were able to reduce both the energy consumption and the number of equipment units. The best intensified system has a TAC of 11.98% lower than the optimized reference case.

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## 1. Introduction

Distillation is one of the most used separation methods in the process engineering and at the same time is responsible of high energy consumptions. According to the U.S. Department of Energy, there are more than 40,000 distillation columns in North America only, and they consume about 40% of the total energy used to operate refining and bulk chemical industries (White, 2012). Then, the improvement of the energy efficiency of this unit operation represents an important tool for the overall plant economy.

In many industrial separation tasks, the feedstocks usually involve multiple components and several distillation columns are required. Therefore, research on process synthesis aimed to find intensified distillation systems with the potential to significantly reduce both energy consumption and capital investment, represents an issue of utmost importance. Among the different energy-efficient configurations for multicomponent distillation, the thermally coupled configurations have received considerable efforts in the last five decades. Especially, the thermally coupled

configurations for ternary distillations have been studied extensively in the earlier works.

For ternary mixtures, the earlier studied thermally coupled schemes include the side-rectifier, the side stripper and the fully thermally coupled configuration (so-called Petlyuk column, Petlyuk et al., 1965). Their performance has been compared with the conventional configurations (Tedder and Rudd, 1978; Glinos and Malone, 1988). Subsequently, a considerable effort has been given on the design and optimization of these ternary thermally coupled schemes (Fidkowski and Królikowski, 1986; Carlberg and Westerberg, 1989a,b; Triantafyllou and Smith, 1992; Finn, 1993; Hernández and Jiménez, 1996, 1999a,b, to name a few). The possible structural changes for ternary thermally coupled schemes were also explored by either considering vapor-transfer direction (Agrawal and Fidkowski, 1998, 1999) or adding additional column sections (Agrawal, 2000). Subsequently, design and analysis works were performed for the modified ternary schemes (Jiménez et al., 2003; Ramírez and Jiménez, 2004). The extension of the design methods for thermally coupled configurations to four or more component mixtures were also investigated (Rong et al., 2001; Blancarte-Palacios et al., 2003).

Notice that the various configurations for ternary mixtures have been coming into light gradually in a somewhat chaotic, evolutionary process (Fidkowski, 2006). For example, the two more

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## Nomenclature

$B$ [kmol/h]	bottom flowrate
$C_i$ ( $i = 1, 2, 3, \dots$ )	column number
$C_r$	crossover probability
$C_j$ ( $j = \alpha, \beta, \gamma, \dots$ )	column section of DWC
$D$ [kmol/h <sup>-1</sup> ]	distillate flowrate
DE	differential evolution
DWC	dividing wall column
DWC-IS	dividing wall column intensified sequence
$F$	mutation factor
$G$	number of generations
SIS	simple intensified sequence
$N_F$	feed stage
$N_p$	size of population
$N_k$ ( $k = a, b, c, \dots$ )	side stream stage
TCS	thermally coupled sequence
$P_c$ [bar]	column pressure
$P_F$ [bar]	feed pressure
$P(\bar{x}_{var})$	penalty function of the $x_{var}$ vector
$Q$	feed condition
$Q_c$ [kW]	condenser duty
$Q_r$ [kW]	reboiler duty
RR	reflux ratio
RCS	remaining column section
SS [kmol/h]	side stream flowrate
SPLIT	splitter of internal flows (liquid and vapor) for the DWC sequences
TAC [k\$/yr]	total annual cost
TES	thermodynamically equivalent sequence
TS	transport section
$x_F$	feed molar fraction
$x_{var}$	variable decision
$u_o$	trial vector
$\Phi$ [m]	column diameter
RefSC	reference simple column sequence

operable configurations (Agrawal and Fidkowski, 1998) that are thermodynamically equivalent to the one by Petlyuk et al. (1965) seems to have been drawn through inventive activity rather than a systematic procedure (Agrawal, 2000).

Synthesis of thermally coupled configurations for four or more component mixtures has also achieved significant progress in the last decade. The method for synthesis of the thermally coupled configurations for the space of the simple column configurations with sharp splits was first developed by Rong and Kraslawski (2002, 2003) for the five-component mixtures. Unlike ternary mixtures, there are a large number of possible distillation configurations for four or more component mixtures. In the literature, there are different synthesis methods presented to synthesize multicomponent distillation configurations (four or more component). Agrawal (2003) presented a method to draw distillation configurations with  $N - 1$  columns through modifying a network-superstructure for a multicomponent mixture, the principles of the method are simple, but the details are somewhat overwhelming (Fidkowski, 2006). Caballero and Grossmann (2004) presented a state-task-network superstructure method to mathematically formulate the alternatives space of multicomponent distillation configurations. Rong et al. (2003a) presented a method which can synthesize all possible distillation configurations with equal to  $N - 1$  or more than  $N - 1$  columns for an  $N$ -component mixture. This method was based on formulating all the feasible distinct separation sequences for an  $N$ -component mixture a priori, which consisted of both sharp and nonsharp sequences.

Notice that there are only three feasible separation sequences for ternary mixtures, two sharp sequences and one nonsharp sequence. Notice also that the fully thermally coupled scheme of the Petlyuk column (Petlyuk et al., 1965) was based on the one nonsharp sequence. This fully thermally coupled Petlyuk column was proved to require the minimum energy consumption for ternary distillations (Fidkowski and Królikowski, 1987). The underlying fundamental is that the nonsharp split can intrinsically improve the thermodynamic efficiency by reducing the process irreversibility (Petlyuk et al., 1965).

Therefore, it is very important that all nonsharp separation sequences are considered during the synthesis of all distillation configurations for a multicomponent mixture. When considering all distinct separation sequences for synthesis of multicomponent distillation configurations, there were obtained the following three types distinct thermally coupled configurations (Rong et al., 2003a,b):

- Type 1: thermally coupled configurations with  $N - 1$  columns from all the sharp sequences.
- Type 2: thermally coupled configurations with  $N - 1$  columns from nonsharp sequences.
- Type 3: thermally coupled configurations with more than  $N - 1$  columns from nonsharp sequences.

It is obvious that a distillation configuration from type 3 with more than  $N - 1$  columns is disadvantageous compared to those with  $N - 1$  columns for an  $N$ -component distillation. However, recently, we have presented a method to derive the possible distillation configurations with less than  $N - 1$  columns for the sharp sequences, there it was demonstrated that each sharp sequence can produce a certain number of intensified configurations with less than  $N - 1$  columns (Errico et al., 2009). Recently, we have also presented a method to derive the possible dividing-wall column (DWC) configurations with less than  $N - 1$  columns for the sharp sequences, there it was also demonstrated that each sharp sequence can produce a certain number of intensified DWC configurations with less than  $N - 1$  columns (Rong, 2011). Such distillation configurations with less than  $N - 1$  columns for an  $N$ -component separation are considered as intensified distillation systems which have the potential to reduce both energy and capital costs.

The purpose and novelty of this work is focusing on the intensification of the nonsharp distillation configuration with more than  $N - 1$  columns (Type 3, Rong et al., 2003a,b). The objective here is twofold: first, the synthesis of the possible intensified schemes with  $N - 1$  or less than  $N - 1$  columns is presented, which include the sidestream columns and DWC columns. Second, the design and optimization for all the versions of the considered schemes are implemented for the evaluation of their potential savings in energy and capital costs.

## 2. The structural synthesis of non-sharp configurations

In the present work the introduction of thermal couplings together with the possibility of column section recombination were used as a tool to generate the alternative configurations. It was already proved that this method is able to generate the complete subspace of intensified systems for the sharp sequences (Errico et al., 2009). In this work a very specific subspace of alternatives is considered which consists of the nonsharp configurations with more than  $N - 1$  columns. The reference configuration is reported in Fig. 1, which was first obtained as the feasible distillation configurations with more than  $N - 1$  columns in the complete space for an  $N$ -component mixture by Rong et al. (2003a). Considering only the possibility to introduce one or two thermal couplings in the first

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