



## A new design method and operation of fully thermally coupled distillation column



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### ABSTRACT

From economic point of view, the fully thermally coupled distillation columns have shown benefits in terms of energy and capital cost savings when compared with conventional distillation columns. However, the design of such column systems is a topic of ongoing research because there are more degrees of freedom to deal with during the design phase. In this paper, a design method is presented and used to determine the structures of conventional two-product and Petlyuk columns, and the results show that the proposed design method works well. The steady state models are developed using HYSYS software, and the results show that the proposed design method provides good initial values for rigorous simulation. According to controllability analysis, the steady state models present better theoretical control properties; consistent with controllability results, when the steady state model is studied under closed-loop using PI controllers good dynamic responses for load rejection are obtained.

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### 1. Introduction

Distillation, a commonly used method for purifying liquids and separating liquids mixtures of chemical components, is the most mature operation among the industrial processes and a very energy-intensive technique. For separation of more than two components, continuous distillation has traditionally been accomplished by arranging columns in series, several alternative configurations exist, notably the direct and indirect sequences (where light or heavy components are removed first, respectively) [1]. To improve the energy performance of distillation systems, various strategies have been suggested which lead to the use of nonconventional sequences. Nonconventional distillation sequences involve the use of thermal couplings in which heat transfer is accomplished by a direct contact of material flows between columns of the system, fully thermally coupled distillation column (FTCDC) is an example of nonconventional distillation column (Fig. 1a), which is often materialized as divided wall column (DWC) (Fig. 1b) [2].

With the use of thermally coupled distillation columns, cost savings between 10 and 50% have been reported compared to the case where simple columns are employed in series to achieve the

desired product purities [3–8]. The salient features of fully thermally coupled distillation column lie in the use of the prefractionator column whereby non-sharp split of light, medium and heavy components into two products occurs. Mainly, the top product of prefractionator contains light and medium components while bottom product contains medium and heavy components. The thereof product mixtures are introduced into main column by thermal coupling arrangements of the top and bottom of prefractionator; finally components into product mixtures introduced into main column are completely separated into three distinct products [9].

Cost and energy saving features associated with thermally coupled distillation columns have seduced many researchers; consequently, in these last few decades an important effort has been dedicated to the development of thermally coupled distillation models. The main focus was on developing methods for optimization, design and control of specific configurations usually constrained to three component mixtures [7,9–18]. Different researchers have presented a set of interesting papers focusing on rigorous design of some specific configurations for three, four or five components mixtures; we may name Kim and co-workers [19–24], Hernandez and Jimenez [25], Hernandez et al. [26], Blancarte-Palacios et al. [27], Calzon-McConville [28], Chu et al. [29], Sun and Bi [30], Uwitonze et al. [31,32], Zapiain-Salinas et al. [33]. Caballero and Grossmann, based mainly on Agrawal's work, have developed a set of logical rules that can be expressed in terms

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## Nomenclature

$a$	Absorption factor
$A$	Light component
$B$	Middle component
$c_1$	Propane composition into distillate
$c_2$	$n$ -Butane composition into side product
$c_3$	$n$ -Hexane composition into bottoms
$C$	Heavy component
$D$	Overhead product
$D_1$	Prefractionator top product
DSV	Distillate flow rate, side flow rate, vapor boilup flow rate
DWC	Divided wall column
FT	Feed tray number
$K$	Equilibrium constant
LIT	Lower interlinking tray
$L_P$	Prefractionator liquid flow rate (kg-mol/h)
LSV	Reflux flow rate, side flow rate, vapor boilup flow rate
$m_{1a}$	Reflux flow rate
$m_{1b}$	Distillate flow rate
$m_2$	Side product flow rate
$m_3$	Reboiler duty
$m_i$	Total number of tray of section $i$
NT	Number of tray in main column
$NT_P$	Number of tray in prefractionator
RGA	Relative gain array
$s$	Stripping factor
$S$	Side product (kg-mol/h)
SDT	Side product draw tray
UIT	Upper interlinking
$V$	Vapor flow rate (kg-mol/h)
$V_P$	Prefractionator vapor flow rate (kg-mol/h)
$W$	Bottom flow product (kg-mol/h)
$W_1$	Prefractionator bottom net flow (kg-mol/h)
$x$	Liquid composition (mole fraction)
$y$	Vapor composition (mole fraction)

## Subscripts

$A$	Component A
$B$	Component B
$B$	Column bottom section
$C$	Component C
$D_1$	Prefractionator to product
$H$	Heavy component
$i$	Component
$j$	Component
$L$	Light component
$P$	Prefractionator
RS	Rectifying section
SS	Stripping section
$T$	Column top section
$W$	Bottom flow product
$W_1$	Prefractionator bottom net flow

of Boolean or binary variables, which ensure basic configurations, and introduced them in an optimization based environment for generating an optimal column sequence covering from conventional to fully thermally coupled distillation sequences [34–37].

For the aspect of column system operability, interesting papers have been presented. Wolff and Skogestad [8] reported a steady state study and operability analysis on a three-product Petlyuk

column and concluded by stating that simultaneous specification of both impurities into side-product is generally infeasible. Mutalib et al. [38] reported experimental studies conducted on a pilot plant and recommended a two point control of system. Christiansen and Skogestad [39], Halvorsen and Skogestad [40] proposed a use of liquid split to control key impurity into least pure end of prefractionator. Ling and Luyben [41] explained that liquid split valve must be manipulated and proposed a control structure of four composition loops with liquid split controlling heavy key at the top stage of prefractionator. Ling et al. [42] suggested a control structure to avoid remixing of the intermediate component for optimal operation. Kiss and Rewagad [43], Rewagad and Kiss [44] suggested that controlling heavy key at the top of prefractionator together with three composition loops of main column may be sufficient to yield high-purity products and implicitly minimize energy usage. Other different works on suitability of model predictive control (MPC) for dividing-wall columns have also been reported [44–46].

Different works about the design of Petlyuk-type columns have been reported; however, some design methods are tedious while others yield infeasible solutions (poor quality output streams) when applied to different mixture types. In this present work, a design method for structural design of thermally coupled distillation column for separation of ternary mixtures is presented and it is more flexible and easy to apply. Also, a study is conducted for theoretical control properties and closed loop dynamic responses for load rejection. The remainder of this manuscript is organized as follows: Section 2 discusses column system design procedure. Section 3 discusses controllability analysis. Section 4 discusses cases studied for validation of the proposed design method, structural design results are presented into Section 5. Section 6 discusses controllability analysis results; finally, conclusions are presented into Section 7.

## 2. Column system design procedure

A brief schematic diagram of FTCDC is shown in Fig. 1a; since there are two interlinking streams between prefractionator and main column, conventional multi-component column design procedure is not directly implemented unless the compositions of the interlinking streams are given. In this work, the design problem is decoupled in two steps: (1) operating conditions and (2) column structure design followed by simulation. At steady state FTCDC has five degrees of freedom; three correspond to design product specifications, the remaining are used to obtain proper values of interconnecting vapor or liquid streams which provide minimum energy consumption.

### 2.1. Model design assumptions and material balance equations for a FTCDC

Suppose  $A$  is lightest component,  $B$  is middle component, and  $C$  is the heaviest component; from Fig. 2, the top product in Section 1 is mostly  $A$  and  $B$  with a little  $C$ , and the bottom product is mostly  $B$  and  $C$  with a little  $A$ . To assume a sharp split in Section 1 would not be a suitable assumption for realistic design, because it requires an infinite number of trays. To start the design of distillation column system, top and bottom products compositions of prefractionator have to be estimated first: what are the recoveries of  $A$ ,  $B$ , and  $C$  in Section 1?

It is assumed that net flow of species  $C$  at the top of Section 1 is equal to the flow of species  $C$  into side draw. Likewise, at the bottom of prefractionator, it is assumed that net flow of species  $A$  at the bottom of Section 1 is equal to flow of species  $A$  into side draw. Chu et al. used these assumptions for the design of divided wall column (DWC) [29]. Composition difference on interlinking trays

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