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Mechanical design and hydrodynamic analysis of sieve trays in a dividing wall column for a hydrocarbon mixture



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ABSTRACT

Distillation is one of the most widely used separation processes, mainly because it allows obtaining products with high purities. However, it has high energy requirements due to its low thermodynamic efficiency. Among the alternatives to reduce these energy requirements, the dividing wall column (DWC) is one of the most promising technologies, also allowing savings in capital costs compared to conventional distillation sequences. Even so, there is only little information about the physical design of dividing wall columns, and most of the recent developments on this area have been achieved by private industry. Moreover, most of the reported information is for packed columns. Nevertheless, the design of dividing wall columns with trays is important for systems with high vapor loads. Thus, a strategy for the mechanical design of sieve trays for the separation of a hydrocarbon mixture in a dividing wall column is presented in this work. Furthermore, an operational analysis of the trays using Computational Fluid Dynamics (CFD) is reported. Designed trays are tested in terms of weir flooding, active zone flooding and flow regime. Reported strategy allows obtaining operational designs for the trays of the whole column.

1. Introduction

Distillation is the most widely used separation process for liquid mixtures in the chemical and petrochemical industries, mainly because it allows obtaining high purities for the desired products. Nevertheless, due to its inherent low thermodynamic efficiency, it requires high amounts of external energy to perform the separation. Thus, in the last century the structure of distillation columns has been modified in order to reduce their energy requirements and environmental impact.

Although modern distillation equipment, i.e. the thermally coupled distillation columns [1] and dividing wall columns [2], was proposed in the early 20th century, the existing methods of analysis and mathematical models were not robust enough for a comprehensive study on such systems. The development of the Petlyuk column [3] was a breakthrough, because it was the first work that analyzes in detail thermally coupled equipment.

http://dx.doi.org/10.1016/j.cep.2015.09.002 0255-2701/© 2015 Elsevier B.V. All rights reserved. It was not until 1985 that the interest in this technology grew, due to the design and construction of the first industrial DWC by BASF. A year earlier, a patent about a dividing wall column for the separation of a quaternary mixture appeared [4]. However, in that work the complete design methodology of the column is not reported. In recent years, other thermally coupled alternatives have appeared for the separation of quaternary mixtures [5,6].

There are many works dealing with the design of DWC's, in terms of calculating the number of stages and location of the dividing wall. Triantafyllou and Smith [7] proposed the use of short-cut methods, but Amminudin and Smith [8] established that the use of the Kirkbride equation to estimate the coupling stages was inappropriate, and proposed a semi-rigorous method. Halvorsen and Skogestad [9] proposed the method of minimum vapor flow. Other design alternatives include the use of stochastic optimization techniques [10,11] and the response surface methodology [12,13].

Other studies are focused on the calculation of the column size, with particular interest on the diameter of the trays. Shah and Kokossis [14] proposed using the sizing procedures available in the commercial simulator Aspen Plus as a good initial approach. Olujic et al. [15] proposed using the simulator developed at Delft

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Nomenclature	
Symbols used	
$D_{\rm T}$ (m))	trav diameter
$A_{\rm T}$ (m ²)	total area
$A_{\rm D}$ (m ²)	downcomer area
$A_{\rm N}$ (m ²)	net area
$A_{\rm B}$ (m ²)	bubbling area
$A_{\rm h}~({\rm m}^2)$	hole area
Lw (m)	weir length
Wdc (cm)	downcomer width
LFP (m)	flow-path length
<i>S</i> (m)	tray spacing
dH (cm)	hole diameter
A _f	fractional hole area
hw (cm)	outlet weir height
hcl (cm)	clearance under downcomer
<i>t</i> (cm)	tray deck thickness
p (cm)	hole pitch
v _{liq} max (m/s)	maximum liquid velocity
$v_{gas} \max (m/s)$	maximum gas velocity
ΔP (Pa)	pressure drop

University of Technology for packed DWC's. Rix and Olujic [16] proposed a calculation method to predict the pressure drop in the column taking into account the column internals, such as collectors and distributors. Hernandez et al. [17] described the design and pilot-scale implementation of a DWC with non-structured packing. Rangaiah et al. [18] proposed the use of a commercial simulator for the design of a three-product DWC, considering the sections of the DWC as separated columns. Later, Dejanovic et al. [19] established that the better way to design a DWC with trays is considering the column as a combination of various columns and performing the hydraulic design following the method proposed by Stichlmair and Fair [20]. Some other works remark the importance of the DWC at industrial level, and present an overview of the advances on research for such equipment [19,21].

Many design methodologies for DWC's have been published over the last years; however, there is little information about the design of the internal components of such columns. Olujic et al. [22] report that the mechanical design of packing and/or trays can be obtained through a combination of CFD techniques and semiempirical equations, which has been proved as a good approach for already constructed columns.

Different CFD studies have been reported for conventional distillation columns. Krishna et al. [23] and Van Baten and Krishna [24] simulated the hydrodynamics of a sieve tray using a threedimensional mesh. They analyzed circular and rectangular trays, using a two-phase transient flow model. The authors studied the distribution of velocity, the clear liquid height and the volumetric fraction of liquid. Trujillo et al. [25] modelled mass and heat transfer for the evaporation phenomenon. They report the use of different turbulence models, concluding that the $k-\varepsilon$ RNG model represents such systems in a better way. Wang et al. [26] simulated the liquid flow and mass transfer for a system air-water in a column with trays. Wang and Wang [27] studied the mass transfer in bubbling columns using CFD-PBM techniques. Sun et al. [28] analyzed the distillation process using a simplified c2-EC mass transfer model and a $k-\varepsilon$ turbulence model. Noriler et al. [29] developed a CFD model using a eulerian-eulerian approach to predict momentum and heat transfer for a multiphase flow. Rahimi

et al. [30] analyzed, using CFD, the effect of the hole and bubble size in the effectivity of the tray, validating their results with the data reported by Dribika and Bidduph [31]. Finally, Zarei et al. [32] evaluated the weep point for columns with sieve trays, using rectangular and circular geometries.

It can be seen that, over the last decades, there have been many advances in the design and simulation of distillation columns; nevertheless, CFD studies for such systems are few. Furthermore, to the best of the authors' knowledge, there are no works reported on the mechanical design of trays for dividing wall columns. Thus, a methodology for the mechanical design and hydrodynamic analysis for sieve trays in a DWC is presented in this work. Mechanical design is performed through the adaptation of the methodology proposed by Kister [33], which is one of the most used methodologies for design of conventional distillation columns. The hydrodynamic analysis is performed through CFD techniques, by using the commercial software ANSYS Fluent v14.0. The trays are assumed to be at their normal operational conditions, where different parameters have been tested, looking for the proper values of such parameters to avoid flooding and irregular flow patterns.

2. Case of study

A mixture of n-pentane, n-hexane and n-heptane, with molar compositions 0.4/0.2/0.4, separated in a dividing wall column reported by Gómez-Castro et al. [11] has been taken as case of study in this work. 45.35 kmol/h are fed to the column, where recoveries of 99 mol% are desired and purities of 98.7, 98 and 98.6 mol% for each component are expected. The main column has 51 stages, 13 of these stages corresponding to the wall section. The reflux ratio is 6.69, while the heat duty is 3773.6 GJ/h. Pressure at the top of the column. The computed diameter for the main column is 1.07 m. This design has been obtained in a previous work as the one with the lowest heat duty through a multiobjective genetic algorithm coupled to the column because of their low cost and high vapor capacity. Furthermore, for diameters of the column



Fig. 1. Sections of the dividing wall column.

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