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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.

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_T (m))	tray diameter
A_T (m^2)	total area
A_D (m^2)	downcomer area
A_N (m^2)	net area
A_B (m^2)	bubbling area
A_h (m^2)	hole area
Lw (m)	weir length
Wdc (cm)	downcomer width
LFP (m)	flow-path length
S (m)	tray spacing
dH (cm)	hole diameter
A_f	fractional hole area
hw (cm)	outlet weir height
hcl (cm)	clearance under downcomer
t (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 semi-empirical 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 three-dimensional 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–ε 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-εc mass transfer model and a k–ε 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 is 1.45 atm, with a pressure drop of 0.68 atm along 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 commercial simulator Aspen Plus v. 7.2 [11]. Sieve trays are used in the column because of their low cost and high vapor capacity. Furthermore, for diameters of the column

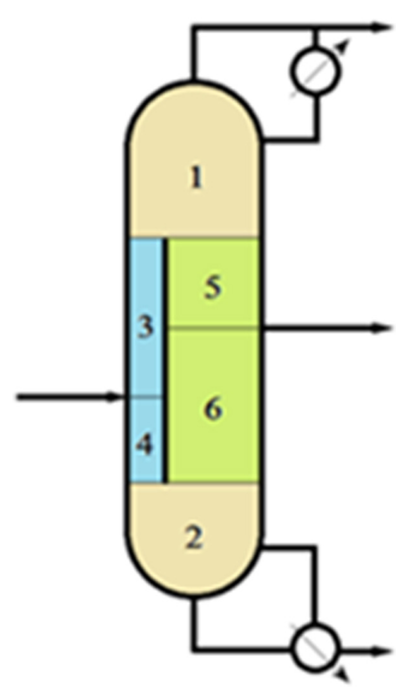

Fig. 1. Sections of the dividing wall column.

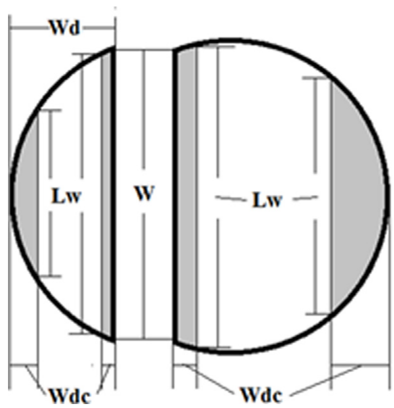

Fig. 2. Geometric variables obtained from the mechanical design step.

higher than 0.6 m, columns with trays are preferred over packed columns [34].

3. Methodology

In this section, the methodology for the mechanical design of the trays is presented first. Then, the methodology used for the hydrodynamic analysis of the trays is described.

3.1. Mechanical design

The proposed methodology for the mechanical design of the trays is based on that reported by Kister [33]. It must be taken into account that, due to the existence of the dividing wall, simulated trays have semicircular shape, which will cause changes on the flow patterns, and the distribution of liquid will be quite different of the distribution for conventional trays. In a first step, the column is divided into sections, whose boundaries are selected where strong changes in the volumetric vapor flowrate occur. A representation of the sections for the dividing wall column is shown in Fig. 1. It is observed that a new section is defined where an external stream is fed, a side stream is withdrawn, or where a split occurs. For each section, the trays with the highest and the lowest vapor flowrates were selected for analysis. Mechanical design is then obtained for the tray with the highest flowrate for each section, and that design is tested for the tray with the lowest flowrate. This strategy is selected because it is more likely to have operational issues on the tray with the highest flowrate. Since the matching trays in sections 5 and 3 are actually parts of a single tray, they are designed simultaneously, following an iterative approach until both designs are consistent. The same occurs for trays in sections 6 and 4.

For the design of the trays, the physical properties of the components on the mixture are required. Since the column works at low pressure and the mixture is close to ideality, the ideal gas equation has been used to calculate the density of the gas phase. The Hankinson–Brobst–Thomson method [35] has been employed for the density of liquid phase, the method of Grunberg and Nissan [36] has been used for the viscosity of liquid mixtures, and the method of Macleod–Sugden [37,38] has been used to compute the surface tension.

Once the physical properties have been computed, an initial design of the tray is proposed. According to Kister [39], the following values for the initial hydraulic design were proposed: hole diameter of 1.27 cm, separation between trays of 45.72 cm, clarity height of 3.81 cm, outlet weir height of 5.08 cm, flooding percent of 80%. Taking into account these values, a foaming factor of 0.9 and a maximum flowrate of 8.15 $(m^3/min)/m^2$ were selected,

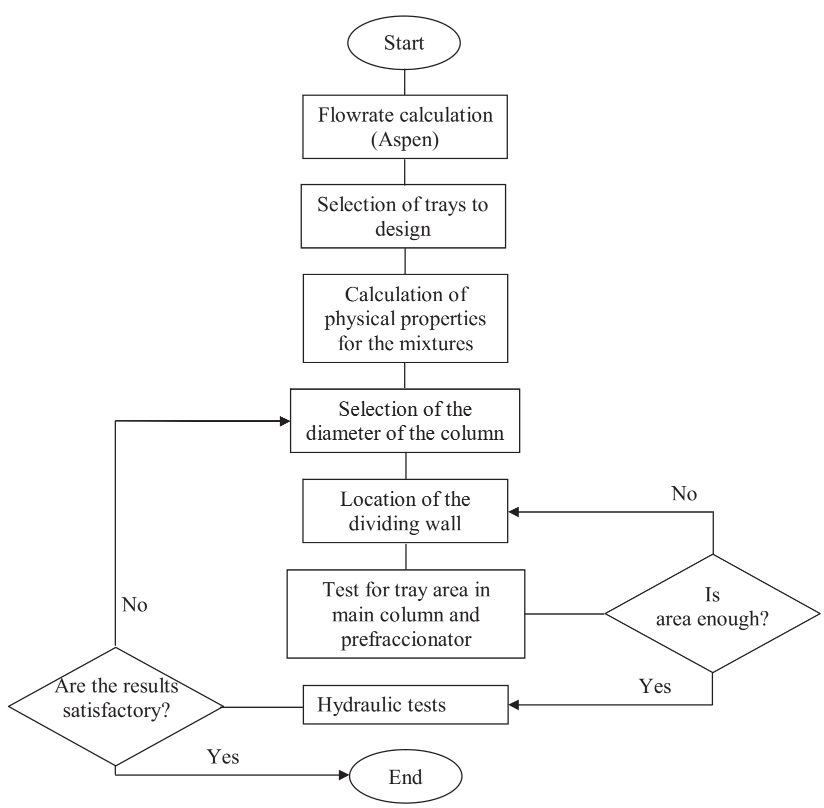

Fig. 3. Flowchart for the methodology of the mechanical design.

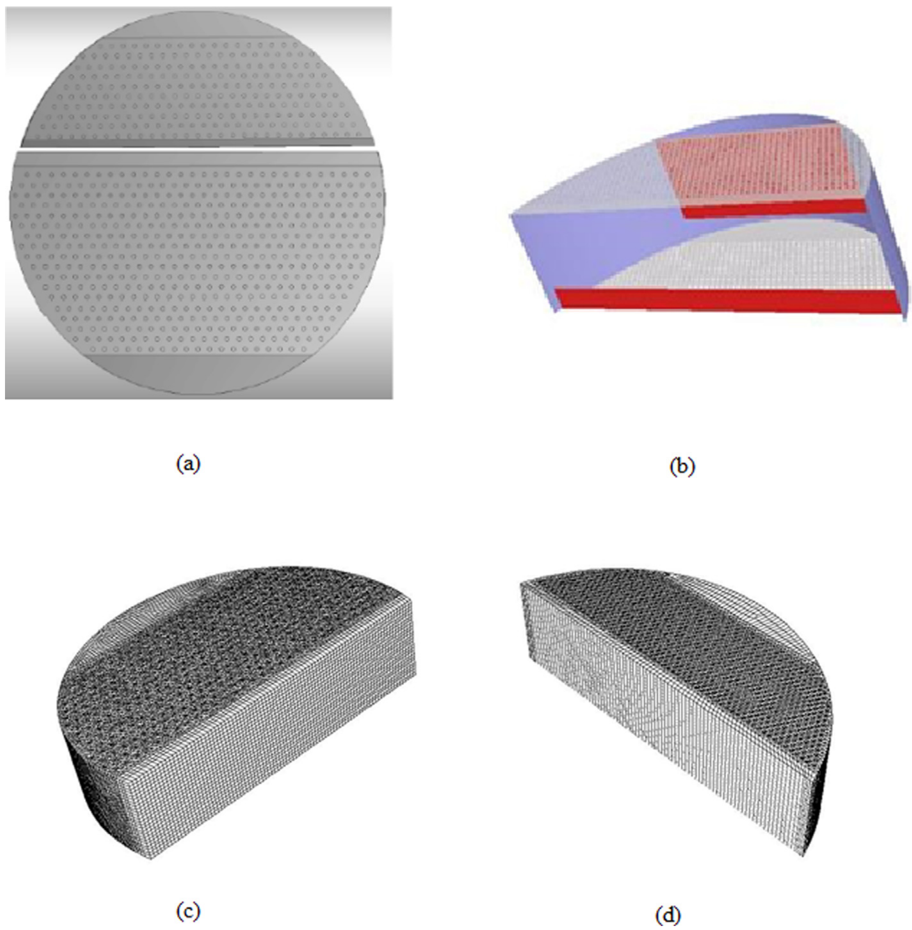

Fig. 4. Geometry and meshing of a tray on the dividing wall section, (a) two-sections geometry, (b) three-dimensional geometry of the tray, (c) meshing for the tray in main column, (d) meshing for the tray in prefractionator.

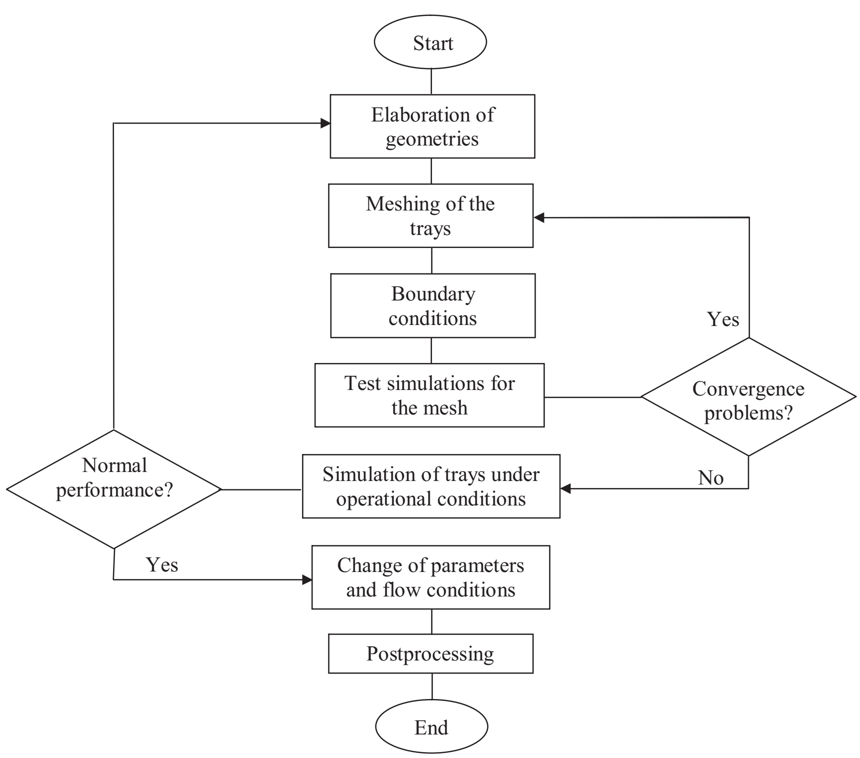

Fig. 5. Flowchart for the methodology of the CFD analysis.

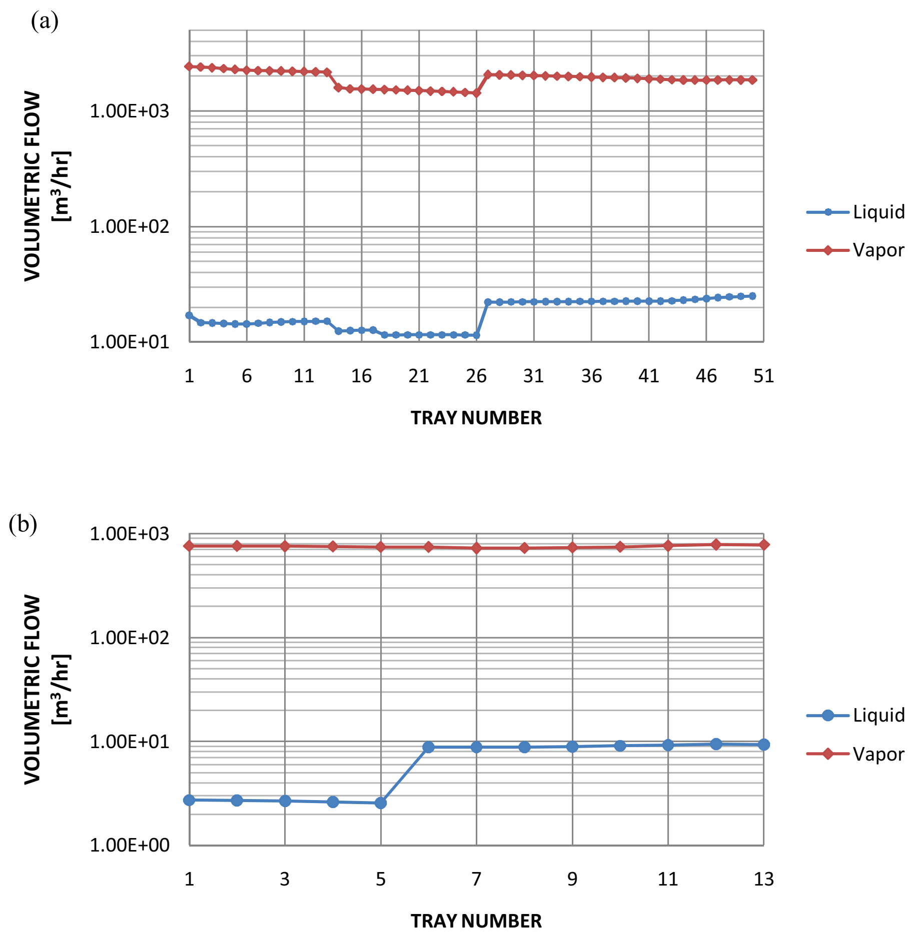

Fig. 6. Volumetric flow rates across the column, (a) main column, (b) prefractionator.

which are values recommended for hydrocarbons at low pressure. Then, the following calculations are performed:

1. Gas velocity, net area and flooding percent for a given diameter.
2. The fraction of the total area covered by the net area.
3. The actual downcomer length and the weir width.

Once the calculations have been performed, the tray is tested for flooding percent, following the procedures of Kister and Haas and Fair and Smith, as reported by Kister [33]. The tray is considered as operable is flooding percent is below 100%. Then, the tray is tested for liquid entrainment, which must be lower than 1% to avoid flooding. If liquid entrainment is higher than 1%, the efficiency of the tray is reduced [40]. Flooding percent is then recalculated by considering the height occupied by the liquid and the froth.

Weeping point tests have also been performed, assuming a reduction of 60% on the flow rates from their original value, to calculate the weeping point. The value of weeping point must be slightly higher that 100%. The calculation of the liquid seals height is also performed.

For the regions 3 and 5, next to the dividing wall, the trays are designed separately for each region, requiring that the total area of the matching trays corresponds to the area of a single tray in regions 1 and 2. It is important to notice that a matching pair of trays in regions 3 and 5 is the same as a single tray in regions 1 and 2, but separated by the dividing wall. The same occurs for a tray in regions 4 and 6. The wall is located such that its distance from the wall of the shell is proportional to the fraction of the area occupied

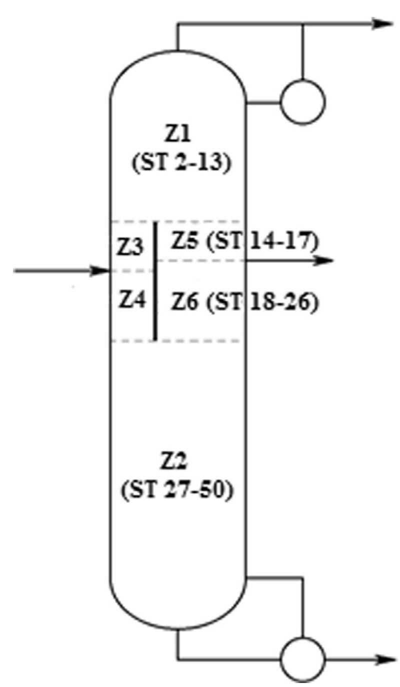

Fig. 7. Distribution of sections in the dividing wall column.

Table 1
Maximum and minimum vapor flowrate for selected trays on each section.

Section	Type	Number of stage	Mass flowrate (Kg/h)	Volumetric flowrate (m^3/h)
1	Maximum	2	10,110	2400
	Minimum	13	10,520	2163
2	Maximum	27	11,463	2065
	Minimum	44	11,828	1850
3	Maximum	14	7739	1591
	Minimum	17	7897	1540
4	Maximum	18	7911	1530
	Minimum	26	7859	1428
5	Maximum	14	2806	758
	Minimum	17	2703	741
6	Maximum	18	3050	781
	Minimum	26	2651	723

by the section equivalent to the prefractionator. Nevertheless, the location of the dividing wall with respect to the shell wall was treated as a degree of freedom, thus, it must be modified if the tray fails the flooding test. The selection of the best location of the dividing wall requires an optimization procedure, having as objective the minimization of the total diameter. The procedure also involves a systematic adjustment of the parameters which depend of the total area, such as the weir area, the active area, and even the diameter and distribution of the holes in the tray. To reduce the total diameter, those parameters should be reduced. Nevertheless, care must be taken with the lower boundaries, which are those values for which the column shows operational problems. Different tray diameters were tested until the minimum value for which the column can be operated is obtained.

From the design stage, the main parameters computed were: the diameter of the tray, the location (Wd) and width (W) of the dividing wall, and the width (Wdc) and length (Lw) of the downcomers, which are shown in Fig. 2. The width of the dividing wall column has a value of 1.18 m, and it is not modified through the simulations. A flowchart of the methodology used for the mechanical design is presented in Fig. 3.

3.2. CFD analysis

CFD analysis has been performed using the software ANSYS Fluent v. 14.0. The three-dimensional geometry of the trays (designed by following the method presented in the previous section) was first created. The geometries for the trays with a dividing wall were created first as separated sections, taking special care on ensuring the continuity required for a single tray. A top view of the tray is shown in Fig. 4a. The holes in the tray were located in a triangular pitch to minimize the required space. Once the geometry of the trays was created, it is processed and the trays are discretized. For the meshing, the trays were divided in three regions: two of them corresponding to the downcomers, and another region for the active zone. It has been decided to mesh such regions because of the following reasons:

1. The mixing of the phases and the mass and heat transfer take place only in the active zone of the tray, therefore, in this zone the mesh should be refined. In the other two zones, there is only liquid flow.
2. The mesh on the active zone should take into account the existence of the holes. Thus, different geometries of the elements may be required.

For the case of the trays in the dividing wall section, the active zone was further divided into two sub-regions: one equivalent to the main column of a Petlyuk column, from where the side stream is withdrawn (Fig. 4b); and another corresponding to the prefractionator of a Petlyuk column, where feed stream enters (Fig. 4c). Weir regions were discretized using a mesh with hexahedral elements of 0.5 in; for the active zone, tetrahedral elements have been used because hexahedral elements cannot be adjusted, due to the presence of holes. For a better adjustment of the cells on the active zones, the holes were first meshed using triangular cells. The contour of the active zone is then meshed so the space between nodes is the same than that of the holes mesh. Then, the other zones of the tray are meshed using triangular cells, mapping it to order the cells. Additional modifications to the size of the cells are performed to reduce its number, and, as a consequence, the computational effort. This modification has been done systematically, always taking care on the values of the cell aspect ratio and the skewness, which must take numerical values close to 1 to avoid convergence problems.

For the CFD simulations, the pressure-based solver was used, taking as reference the atmospheric pressure at the gas outlet. For the multiphase flow, the eulerian–eulerian model was used, because the bubbles are too small in comparison with the whole system. Turbulence was represented through the k–ε RNG model. All the simulations were performed until the errors in the residuals reached a specified convergence value, checking periodically the

Table 2
Design parameters for selected trays on each section.

	Section 1	Section 2	Section 3	Section 4	Section 5	Section 6
D_T (m)	1.37	1.37	1.22	1.22	1.22	1.22
A_T (m^2)	1.48	1.48	0.48	0.48	0.79	0.79
A_D (m^2)	0.16	0.19	0.13	0.12	0.06	0.04
A_N (m^2)	1.32	1.28	0.35	0.35	0.73	0.75
A_B (m^2)	1.16	1.09	0.22	0.23	0.66	0.71
Lw (m) W–S	1.02	1.07	0.97	0.95	0.80	0.81
Lw (m) S–W	–	–	1.15	1.15	1.19	1.19
Wdc (cm) W–S	22.61	25.91	20.31	19.06	14.99	15.49
Wdc (cm) S–W	–	–	3.08	2.80	4.67	4.83
LFP (m)	0.92	0.85	0.96	0.99	0.59	0.58
S (m)	0.46	0.46	0.46	0.46	0.46	0.46
dH (cm)	1.27	1.27	1.27	1.27	1.27	1.27
A_f	0.1	0.1	0.1	0.1	0.1	0.1
hw (cm) W–S	5.08	5.08	5.08	5.08	5.08	5.08
hw (cm) S–W	–	–	5.08	5.08	5.08	5.08
hcl (cm) W–S	3.81	3.81	3.81	3.81	3.81	3.81
hcl (cm) S–W	–	–	3.81	3.81	3.81	3.81
t (cm)	0.34	0.34	0.34	0.34	0.34	0.34
p (cm)	3.81	3.81	3.81	3.81	3.81	3.81

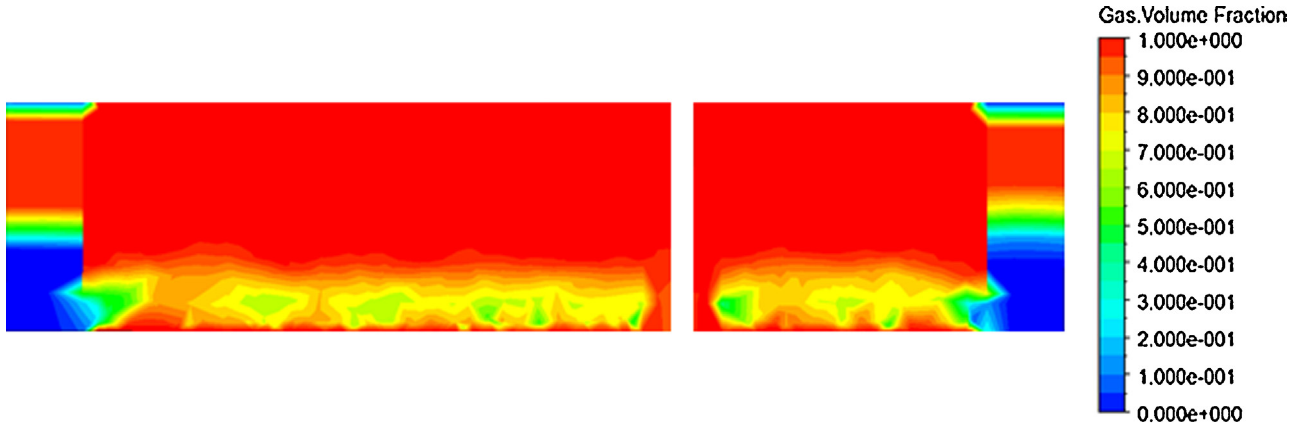

Fig. 8. Volumetric fraction contours for vapor phase in the trays with dividing wall under operational conditions (side view in a plane cutting through the downcomers).

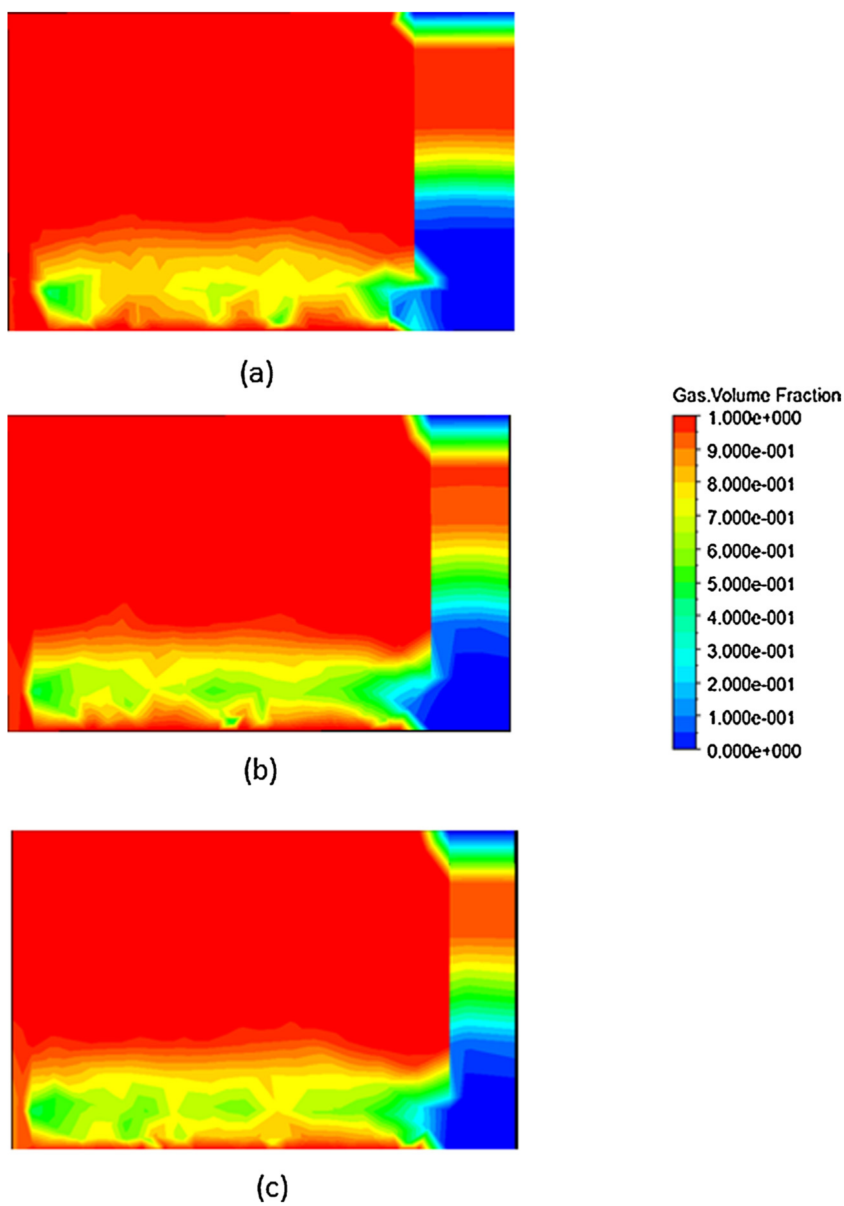

Fig. 9. Volumetric fraction contours for vapor phase in the trays under operational conditions with modifications on weir area: (a) no modification, (b) reduction of 20%, (c) reduction of 40% (side view of the prefractionator section in a plane cutting through the downcomer).

Table 3
Final design for the trays under maximum charge.

	Prefractionator		Main column	
A_T (m^2)	0.48		1.00	
A_D (m^2)	0.02		0.05	
A_h (m^2)	0.04		0.08	
Wdc (cm)	6.35 (S)	1.91 (W)	10.16 (S)	3.81 (W)
hw (cm)	5.08		5.08	
hcl (cm)	3.81		3.81	
S (cm)	30.48		30.48	
dH (cm)	0.978		0.978	
p (cm)	2.95		2.95	
v_{liq} max (m/s)	0.09		0.06	
V_{gas} max (m/s)	6.62		7.68	
ΔP (Pa)	381		480	

flow rates, temperatures and volumetric fraction for both phases. When these criteria are achieved, it is considered that the column works in steady-state, which is taken as the normal operation state of the column. Once the simulations were completed, the results were analyzed. If operational issues were observed, the trays were re-designed and tested again. A flowchart of the methodology used for the CFD analysis is presented in Fig. 5.

4. Results

In this section, the results for both parts, mechanical design and CFD analysis, are presented and discussed.

4.1. Mechanical design

To initialize the mechanical design of the trays, it is important to know the volumetric flow rate for both phases across the stages. Volumetric flow rates for the main column and the prefractionator sections are presented in Fig. 6. These data were obtained from steady-state, rate-based simulations in Aspen Plus v.7.2. As aforementioned, the column was divided into sections, the trays contained in each section are shown in Fig. 7, where Z1, Z2, etc., are the zones or regions of the column; the numbers following the abbreviation ST indicate the number of stages (corresponding to the main column on the Petlyuk-like structure) included in each section. The trays selected for analysis are presented in Table 1; these trays are the ones with the highest and lowest volumetric vapor flowrate in each section. Data shown in Table 1 has been obtained from the steady-state simulations. It is also important to notice that the trays in sections 3 and 5 are the same in the DWC, but they have different flowrates due to the vapor split. The same occurs for sections 4 and 6. As aforementioned, the mechanical design of the trays was carried out by proposing an initial design and then testing it until it is operable. This was done using a Visual Basic routine and Microsoft Excel worksheets. Final designs of the trays are shown in Table 2, where W–S implies that the flow goes from the dividing wall to the shell, while S–W is the opposite. It is important to recall that sections 3 and 5 (and sections 4 and 6) are complementary, thus the diameter of 1.22 m in sections 3 and 5 implies that the whole tray has a diameter of 1.22. Trays reported in Table 2 have successfully overcome all the tests mentioned in Section 3.1.

4.2. CFD analysis

In order to test the mesh for convergence, transient simulations were performed using the water-air system, running the system until the values of residuals are small enough and it has been proved that no convergence issues occur. Once those simulations have been successfully finished, the hydrocarbons mixture is loaded to the geometry, re-initializing the system to continue with the analysis. The tray in section 3 presented some problems when it was charged, because the vapor stream caused the liquid to leave the tray almost completely. Thus, the tray was redesigned, taking into account the following considerations:

1. Since there was an excessive liquid entrainment, the area for vapor flow must be increased;
2. the liquid column in the weir was smaller than expected, thus the distance between trays must be reduced; and
3. the vapor velocity in the holes was high, thus the hole area must be increased by reducing the diameter of the holes, thus reducing the pitch and increasing the number of holes.

Taking into account the previous ideas, distance between trays was reduced to 30.48 cm (12 in), and the hole diameter was modified to 0.9525 cm. The trays were redesigned and a diameter of 1.37 m was obtained as the minimum diameter for which no operational issues were observed. After these modifications, no excessive liquid entrainment was further observed for this new

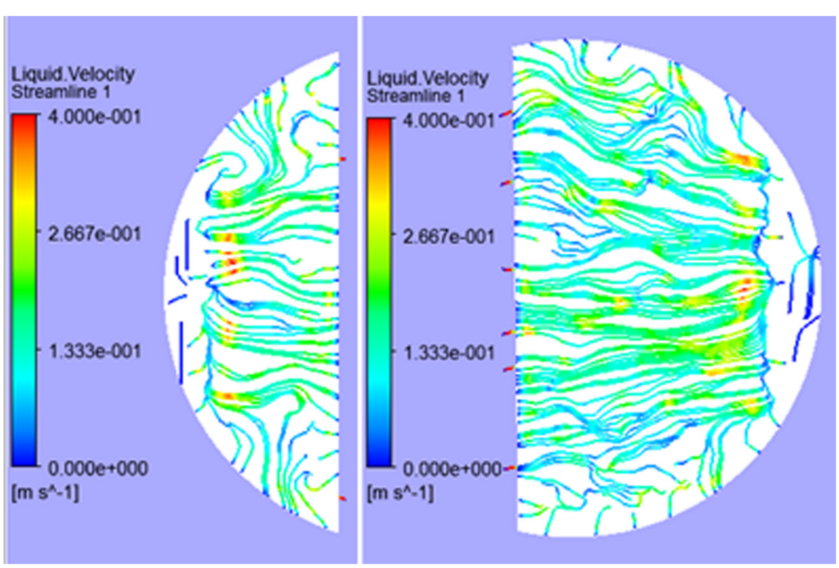

Fig. 10. Streamlines of the liquid mixture in a top view at the gas-liquid interface.

design. The complete tray for sections 3 and 5 under operational conditions is shown in Fig. 8, where a lengthwise projection of the tray can be observed. Patterns in Fig. 8 shows the volumetric fraction of the gas, where the darkest zones indicates a higher volumetric fraction.

The tray in section 3 operates under a bubbling regimen, while the tray in section 5 operates under a spray regimen. Since it is desired that the trays operate under bubbling regimen, additional modifications were performed on the weir area, looking for an increase on the active area. Two cases were examined: the first by reducing the weir area 20% and the second by reducing it 40%. Results of the simulations with those modifications are shown in Fig. 9, where the volumetric fraction of the gas phase is observed. As the weir area is reduced, the liquid fraction increases. Mean liquid fraction for the basis case is 0.416. Once the reduction of 20% is applied, liquid fraction increases to 0.4639. When the reduction of 40% occurs, liquid fraction is 0.4844. Nevertheless, it is not possible to reduce further the weir area because it would cause an excessive pressure drop and capillarity phenomenon may occur. Thus, the reduction of 40% has been taken as the maximum reduction for the weir area. The final design for the trays under maximum charge is shown in Table 3.

Stream lines for the liquid phase are shown in Fig. 10. A high-turbulence region can be observed, due to the crossflow between the liquid from the weir and the vapor entering to the tray. The liquid emerges following a wave-like movement, causing a constant contact between the particles along the tray. The temperature profiles for the liquid and the vapor phases are shown in Fig. 11. Liquid temperature profiles show a random temperature distribution on the tray in section 3, while a slow variation on temperature is observed as the liquid pass by the tray in section 5. This is because in section 5 there is a higher contact time between the phases. It can be observed that the temperature distribution is almost symmetric for the gas phase. Finally, the designed trays under operational conditions are presented in Fig. 12, where the volumetric fraction of liquid is observed. The mixing between both phases is almost homogeneous, thus a proper operation of the distillation column is expected.

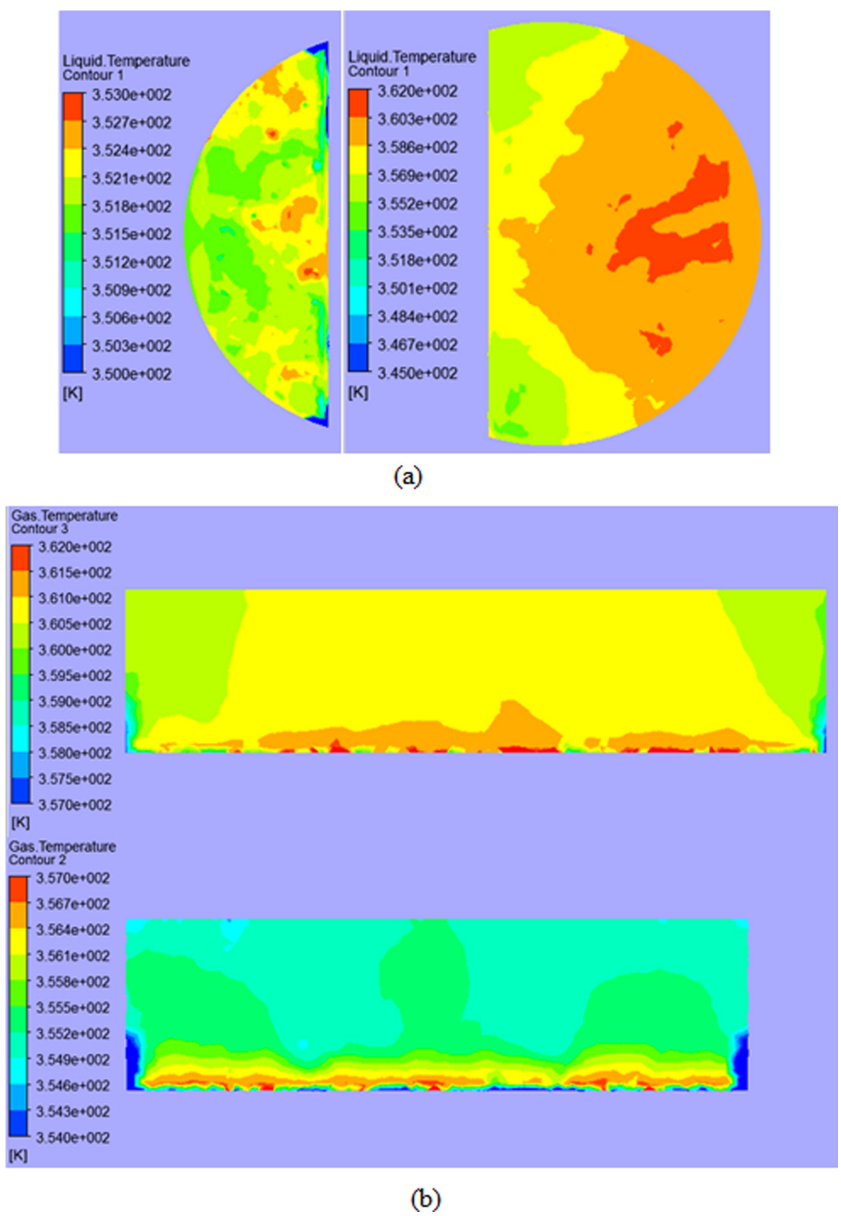

Fig. 11. Temperature profiles (a) liquid phase, (b) gas phase.

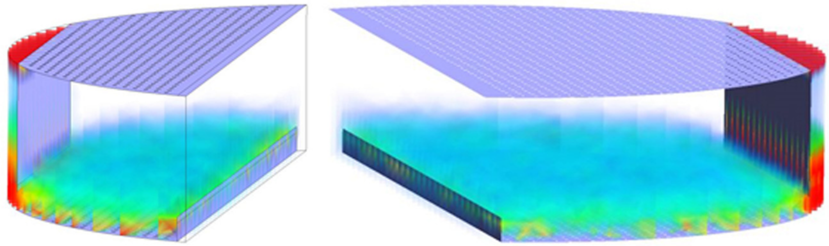

Fig. 12. Volumetric fraction of the liquid mixture in the trays under operational conditions (3D view of the trays).

5. Conclusions

A methodology for the mechanical design and analysis of the trays in a dividing wall column has been presented. The methodology is divided in two steps: an initial design; and a hydraulic analysis of the trays using CFD. The proposed method is based on a traditional design methodology for conventional trays, modified in this work to take into account the geometry of the trays. The parameters have been adjusted for the dividing wall section, taking into account the area of the main column and the prefractionator.

During the hydraulic tests, some flooding problems were observed; therefore the trays were systematically re-designed to make them operable under the flow conditions reported. It has been shown that, for a given diameter of the column, it is possible to change the operational regimen by increasing the total area of holes. This implies an increase on the pressure drop and the liquid high on the weir. Nevertheless, simulations show that, for a mixture of low viscosity, the increase on such parameters is minimal.

The final trays were subjected to different hydraulic tests, showing a good performance in their operational point. No flooding was observed, neither in the weir nor in the trays, and a good mixing resulted in an increase in the contact between phases. The temperature profiles showed a gradual increase along the tray, and an appropriate pressure drop. Thus, the designed trays are functional, and may operate properly in the dividing wall distillation column. Finally, it is important to notice that the operational regimen of the trays has been supposed to be a quadratic function of the bubbling area. Nevertheless, additional data could be necessary to ensure the quadratic approach is good enough for the studied system. Furthermore, the method should be tested for pilot-scale systems, so that experimental validation could be achieved; and for non-ideal mixtures.

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