

Simulation and Design of a Dividing Wall Column with an Analysis of a Vapour Splitting Device

Andreu Bernad-Serra^a, Kaj Jakobsson^{b,*}, Ville Alopaeus^b

^aDepartment of Chemical Engineering and Analytical Chemistry, University of Barcelona, Barcelona, Spain

^bDepartment of Biotechnology and Chemical Technology, School of Chemical Technology, Aalto University, Espoo, Finland
kaj.jakobsson@aalto.fi

The simulation and control of dividing wall columns are two of the main issues blocking their widespread use. The latter could be mitigated by controlling the vapour split in these columns, but this is rarely considered due to the lack of a device for doing so. The objective of this work is to review the current simulation strategies for dividing wall columns as well as the working principles of a vapour splitting device. To assess its viability, a dividing wall column was simulated, sized and its results were used to study the required pressure drop of the device for a given vapour split. Finally, the vapour splitting device was studied by means of computational fluid dynamics to adjust its geometry in order to fulfill the required pressure drops.

1. Introduction

Recently, new distillation techniques have been developed to decrease the energy consumption of distillation units; however, they usually require a high capital investment. Such is the case for heat pump assisted distillation or internally heat integrated columns (Dejanovic et al. 2010). Instead, a concept of combining distillation columns for a more efficient operation can achieve both energy and capital investment savings. These columns arrangements are typically referred to as Petlyuk columns and consist of an interconnected prefractionator and a main column. The theory behind this type of column has been known for a long time (Petlyuk 2004), but they gained industrial interest when a practical approach for the coupling of the columns, the dividing wall column (DWC), was discovered (Dejanović et al., 2010). Notable recent contributors in this field are e.g. (Kaibel 2014, Kiss and Ignat 2012, Qian et al. 2016).

A DWC is a distillation column with a built-in wall inside. The wall allows for the existence of more than one distillation region within a single shell (Petlyuk 2004). The simulation and design of DWCs is more complex than the simulation of a regular distillation column sequence. The extra complexity arises from the interconnecting streams between column sections; thus, making each of these sections strongly dependent on the others. Therefore, a special simulation strategy is required for their simulation (Dejanović et al., 2011).

DWCs have more degrees of freedom than standard sequences of distillation columns, which make their simulation more complicated but can also be used for control purposes. Two of them deserve special attention: the liquid and the vapour splits. The first can be easily controlled using a mechanical device (Kaibel 2014). The second is rarely controlled but fixed by the position of the partition wall. In the present work, an approach for the control of the vapour split is presented, based on the device designed in Sun et al. 2015.

The objective of this work is to study the operation of a vapour splitting device while taking into account the pressure drops of the different column sections in a DWC. These pressure drops were not considered in the original article (Sun et al. 2015). In this work, a DWC was simulated, sized and its results were used to assess the required pressure drop for the vapour splitting device. The analysis of the device was carried using Computational Fluid Dynamics (CFD).

2. Simulation of Dividing Wall Columns

As the chemical system in the simulations, a crude Benzene mixture from a patent issued by BASF (Kaibel 2007) was used. The objective of the column is to separate its feed into a C₅ cut, a Benzene-Toluene-Xylene

(BTX) cut and a C_{9+} cut. The system was selected because it is well established and allows the work to be focused on the equipment being studied; while still having an industrial interest.

The presented simulation strategy (based on the one reported in Dejanović et al. (2011)) is split in four parts. The first aims to describe a DWC as an equivalent sequence of columns, which can be implemented in available flowsheet simulation programs. The second studies the interconnecting nature of the different sections through a degrees of freedom (DOF) analysis, which values are set in the third part. In the last part, the DWC is simulated using rigorous methods and its convergence discussed.

2.1 Equivalent sequence

A sequence of columns is required to simulate a DWC. Among all available choices, the three-column (see Kaibel (2014)), the two-column Petlyuk arrangement (see Petlyuk 2004) and the four-column sequence (see Dejanović et al. (2011)) are among the most used ones. The latter was chosen for this work because it is the easiest sequence to analyze and size once the flowsheet is converged (Dejanović et al. (2011)). The four-column sequence is formed by two distillation columns with no condenser/reboiler, a stripper and a rectifier. These sequences can be seen in Figure 1.

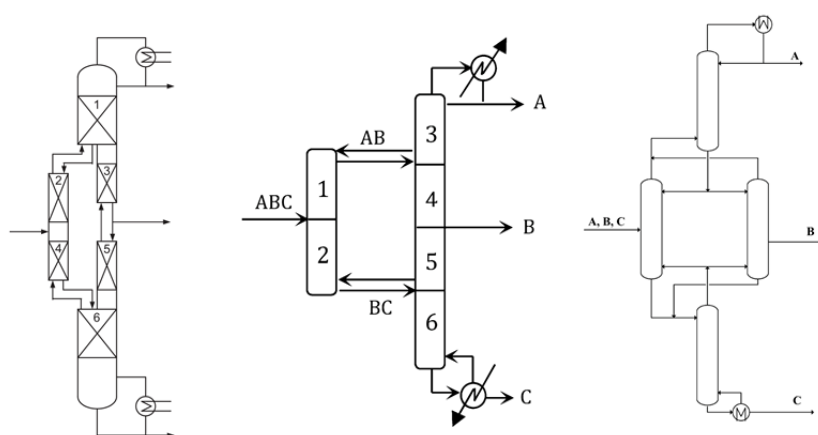


Figure 1: Three column, two column (Petlyuk) and four column sequences (Dejanović), respectively

2.2 Degrees of Freedom Study

The system was first studied through a Degrees of Freedom (DOF) analysis to understand the influence of its interconnecting streams on the overall column. The DOF study was carried out following the methodology described in Seader et al. 2013. This methodology was applied to the four-column sequence (Dejanović et al. (2011)) and the following DOF were obtained:

$$DOF_{DWC} = 2N_T + C + 26 \quad (1)$$

where C stands for the number of components of the working mixture and N_T is the sum of the stages in each of the four columns. Among the found DOF, 11 deserve special attention for their impact in the performance of the overall column and its convergence. They can be seen in Table 1.

Table 1: DOF analysis: Design Parameters

Specification	Number of variables
1.-Number of stages in each column section (see Figure 1)	6
2.-Vapour and liquid splits	2
3.-Side stream rate	1
4.-Boilup ratio or Distillate rate	1
5.-Reflux ratio or Bottom rate	1

2.3 Specification of the Variables

Among the Design Parameters presented in Table 1, the most difficult ones to specify are the vapour and liquid splits. Both splits are defined as the ratio between the vapour/liquid entering the prefractioner and the total being split. Their importance arises from their interconnecting nature. In the present work, the Vapour

Minimum diagram reported in Halvorsen and Skogestad 2003 was used for its simplicity while maintaining a fundamental base. The method is based on the resolution of the Underwood equations for estimating the vapour and liquid splits (Halvorsen and Skogestad 2003). The diagram can also be used for further assessment of the column (Halvorsen 2011). The method was solved in its analytical form for the 23 components mixture described in Kaibel 2007, rather than by using rigorous simulation as in Dejanović et al. 2011. This was found to be important because it provides a more autonomous tool for the initialization of such a column configuration than could be applied in process simulators.

Apart from the liquid/vapour splits, the distillate and side product rates were calculated from the overall material balance. Educated guesses for the number of stages, feed/product stages and reflux ratio were provided and adjusted during the rigorous simulation to achieve the desired separation. The specification for the Design Parameters can be seen in Table 2.

Table 2: Initialized Variables

Specification	Value	Number of variables
1.-Number of stages in each column (see Figure 2)	20 stages	4
2.-Feed stage	10 stages	1
3.-Side stream stage	10 stages	1
4.-Distillate rate	21.6 kmol/h	1
5.-Reflux ratio	12.4 kmol/h	1
6.-Side product rate	63.7 kmol/h	1
7.-Vapour split	0.21 kmol/kmol	1
8.-Liquid split	0.03 kmol/kmol	1

2.4 Rigorous Simulation of a Dividing Wall Column

Once the variables were initialized, the BTX system was simulated using rigorous RadFrac units in Aspen and its equation-oriented method. The Flowsheet used can be seen in Figure 2, together with the internal molar flows of the converged system. The latter representation is reproduced from Dejanović et al. 2011.

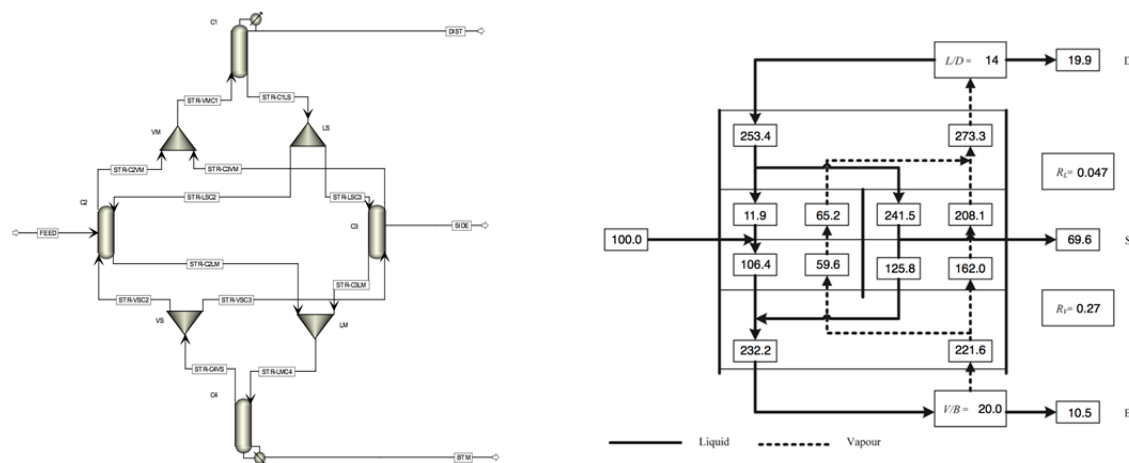


Figure 2: Equivalent Sequence used and internal molar flows, respectively.

The separation of column C1 (see Figure 2) was less effective than expected and the initial values were modified to account for it: the number of stages of C1 and the reflux ratio were both increased while the distillate rate was decreased. The liquid and vapour splits were also adjusted to compensate for the non-constant molar overflow (which is inherently assumed in the Vapour Minimum diagram).

3. Preliminary Design of the Vapour Splitter

The vapour split of a DWC is rarely controlled but fixed because, as reported in Kaibel 2014, there is no reliable mechanical device for this task. Despite its controlling difficulties, the potential of a vapour splitting device to improve operation of DWC justifies its development (Ghadrdan et al. 2013, Sun et al. 2015).

Among the designs available in open literature, this study was carried out based on the vapour splitting device reported in Sun et al. 2015; which can be seen in Figure 3. This device can be divided in two symmetrical parts. Each of these parts includes a vapour channel with a controlling blade and a distribution system. The first adjust the vapour flowing in each of the channels by rotating the channel's blade. The latter is required in order to avoid vapour maldistribution. (Sun et al. 2015)

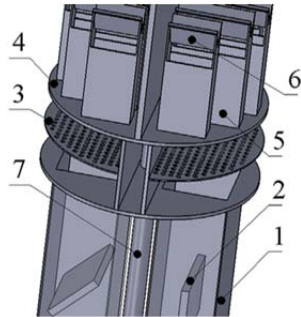


Figure 3: Vapour splitter device from Sun et al. 2015. 1 : vapour channel ; 2 : blade ; 3 : distribution plate ; 4 : chimney tray ; 5 : vapour tube ; 6 : V-type caps and 7 : liquid downcomer.

A DWC with its wall can be seen, from a hydraulic point of view, as a parallel network of pipes. As such, the pressure drop in both sides of the wall must be equal meaning that as the flow resistance increases on one side (decreasing the flow through that side), the flow through the other side will increase to compensate. This is the working principle of the vapour splitting device, where the vapour flow is controlled by modifying the pressure drop of the different channels by changing the blade angle.

In the present work, the operability of this device was studied with pressure drops and volumetric flows corresponding to a real DWC. This is the reason why the system was simulated and sized before analysing the vapour splitting device; in order to set the required pressure drops for a given vapour split.

Experimental validation has been reported in Huaqiang et al. 2016 and Sun et al. 2015, but it did not take into account that if the vapour flow is tried to be controlled by only using one of the blades the overall pressure drop of the column cannot be kept constant. Instead, the approach presented here is based on the control of the vapour split by using both blades at the same time. The advantage of using such an approach is that the pressure drop of the overall column will remain constant at any time. The main disadvantage, inherent to its operation nature, is that at steady state the device will present an additional pressure drop.

3.1 Sizing of the Dividing Wall Column

An approximate sizing of the column is required to obtain the necessary pressure drops in its different sections, which will be the base for the design of the vapour splitting device. Pall Rings were used as column internals because of the amount of available correlations. The diameter was set based on flooding conditions, estimated from the Billet and Schultes correlation. The height was calculated using a rule of thumb for Pall Rings. Finally, the pressure drop of each section was estimated using the Robbins correlation. All the methods used for the sizing can be found in Kister 1992.

3.2 Required Pressure Drops for Operability

The approach works in such a way that the pressure drop of the column remains constant upon flow control. This is achieved by imposing a fixed pressure drop (by using the blades), even when the vapour split is at its set point. If the gas flow of one side needs to be increased, it is done by decreasing the resistance of that side and increasing the resistance of the other one to maintain the same pressure drop on both sides of the wall. Therefore, a compromise arises between the fixed pressure drop and how much the flow is controlled.

The required pressure drops for a vapour splitter that could be used for the column before simulated and sized can be seen in Table 3 (see Figure 2 for the labels), where the gas flow of column C2 (q_{C2}) was changed from a 90% to a 110%. For the construction of Table 3 it was taken into account that modifying the volumetric flows in columns C2 and C3 would modify their pressure drop, which was calculated using the Robbins correlation (Kister 1992).

Table 3: Pressure drops for the column parts (ΔP) where subscripts C2/3 refer to columns in Figure 2, VS stands for Vapour Splitter and Left/Right stand for the Prefractionator and Main column side of the wall.

q_{C2} (m ³ /s)	ΔP_{C2} (Pa)	ΔP_{C3} (Pa)	$\Delta P_{VS,Left}$ (Pa)	$\Delta P_{VS,Right}$ (Pa)	$\Delta P_{\Sigma,Left}$ (Pa)	$\Delta P_{\Sigma,Right}$ (Pa)
0.26	4726	6559	3209	1375	7935	7935
0.29 (set point)	6330	6200	1604	1735	7935	7935
0.32	7935	5841	0	2094	7935	7935

3.3 Design of the Channels

Once the required pressure drops were established, the different channels were designed and analyzed using CFD. Only the left channel was studied, but the methodology presented here could be applied to the other one as well. An example of the geometry studied can be seen in Figure 4.

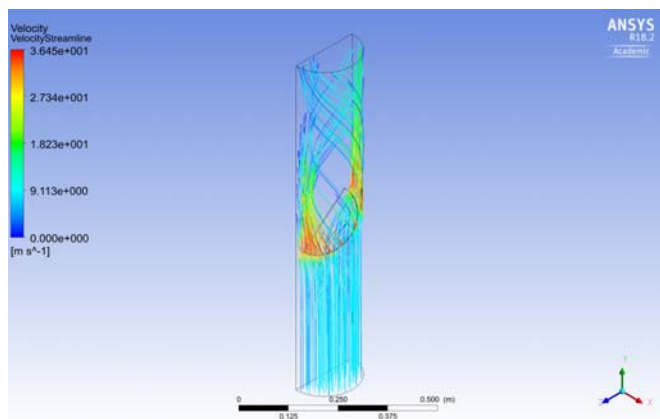


Figure 4: Example of a channel simulation using ANSYS

The diameter of the channel was the only physical design variable studied. The diameter should be small enough to ensure the required pressure drop, but as big as possible to enhance controllability. The initial diameter was set so that the gas superficial velocities were between 5 and 10 m/s. These velocities are higher than the ones reported in Sun et al. (2015), but were found to be required once the pressure drop of the different column sections were taken into account. For each diameter, the influence of both the inlet superficial velocity and the blade angle were studied. This compromise can be seen in Figure 5.

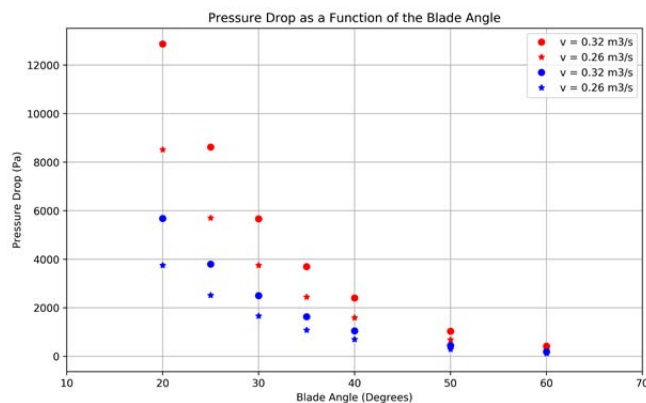


Figure 5: Results for the 200 mm (red) and the 250 mm (blue) diameter channels

Figure 5 shows that the 200 mm diameter channel is able to provide the required pressure drops specified in Table 3, but it is only able to provide it for a narrow range of blade angles (higher than approximately 55 degrees). This could cause controllability problems related to the high sensitivity of the device. Instead, the 250 mm channel is able to provide the required pressure drop in a wider blade angle range. It should be noted that there is still some room for improvement and the diameter could be slightly increased.

4. Conclusions

From the simulation point of view, dividing wall columns can be readily simulated with commercial software (such as Aspen Plus) but they require the use of equivalent sequences. Special attention should be paid to the initialization of their degrees of freedom. In that regard, the Vapour Minimum diagram has proved to be a simple initialization tool for the vapour and liquids splits, which could be easily implemented in process simulators.

From the controllability point of view, it has been proved that a vapour splitter such as the one reported in Sun et al. 2015 could control the gas flow when operating in a DWC. This was proved by simulating and sizing a real case DWC and comparing its pressure drop with that of the vapour splitting device. In addition, the vapour split has been controlled by changing the pressure drop of both channels in the vapour splitter. This allows to control the vapour split while keeping the pressure drop of the overall column constant, at the expense of a fixed pressure drop. These devices can be simulated and designed using CFD tools such as ANSYS Fluent before building any prototype, making the overall design process easier.

References

- Dejanović I., Matijašević L., and Olujić Ž., 2010, Dividing wall column — a breakthrough towards sustainable distilling. *Chem. Eng. Process.*, 49:559–580.
- Dejanović I., Matijašević L., and Olujić Ž., 2011, An effective method for establishing the stage and reflux requirement of three-product dividing wall columns. *Chem. Biochem. Eng. Q.*, 25:147–157.
- Ghadrdan M., Halvorsen I. J., and Skogestad S., 2013, Manipulation of vapour split in kaibel distillation arrangements. *Chem. Eng. Process.*, 72:10–23.
- Halvorsen I. J., S. S. Analytic expressions for minimum energy consumption in multicomponent distillation: A revisit of the underwood equations. In *AIChE Annual Meeting*, Dallas TX, 1999. Paper 221g, presented at Separations Systems Synthesis.
- Halvorsen I. J. and Skogestad S., 2003, Minimum energy consumption in multicomponent distillation. 2. three-product petlyuk arrangements. *Ind. Eng. Chem. Res.*, 42: 605–615.
- Huaqiang G., Xiangwu C., Nan C. and Wenyi C., 2016, Experimental study on vapour splitter in packed divided wall column. *J. Chem. Technol. Biotechnol.*, 91:449-455.
- Kaibel G., Oost C., Stroezel M., Meyer G., Trubenbach P., Sartor K.-H., and Heners J, 2007, Method and device for carrying out the distillative separation of c5+ cuts. US 7,169,267 B2.
- Kaibel B, 2014, *Dividing-Wall Columns. Distillation: Equipment and Processes*, Elsevier Inc., Ludwigshafen, Germany.
- Kiss A. A. and Ignat R. M., 2012, Innovative single step bioethanol dehydration in an extractive dividing-wall column. *Sep. Purif. Technol.*, 98:290–297.
- Kister H. Z., 1992, *Distillation Design*, McGraw-Hill Inc., New York, USA.
- Petlyuk F. B., 2004, *Distillation Theory and Its Application to Optimal Design of Separation Units*, Cambridge University Press, Cambridge, UK
- Qian X., Jia S., Skogestad S., and Yuan X, 2016, Comparison of stabilizing control structures for dividing wall columns. *IFAC-PapersOnLine*, 49:729–734.
- Seader J. D., Henley E. J., and Roper D. K., 2013, *Separation process principles: Chemical and Biochemical Operations*. John Wiley and Sons, Inc., New York, USA.
- Sun J., Ge H., Chen W., Chen N., and Chen X, 2015, CFD simulation and experimental study on vapour splitter in packed divided wall column. *Can. J. Chem. Eng.*, 93: 2261–2265.