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Simulation Model of Divided Wall Distillation Column (DWDC)

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Abstract: Separating three high-purity products from a mixture of three components requires a series of column s for distillation and separation. This process results in significant operational and capital costs, as well as a subst antial footprint within the plant. To address these issues, a type of distillation column referred to as a Divided W all Distillation Column (DWDC) has been recently designed. This design incorporates a wall within the conventi onal distillation column, effectively partitioning the column into four distinct sections: Top, Bottom, Main fracti onation, and Prefractionation. This distillation column effectively separates three components, and in some insta nces, four components, within a single unit. This design minimizes total costs, reduces operating expenses, and o ccupies less space within the facility. However, this type of distillation column (DWDC) is not represented in an y of the simulation software utilized for distillation column simulations, including gPROMS ®, ASPEN Pulse ®, and HYSYS ®, among others. In this research, we developed several models that simulate the operation of (DW DC), achieving favorable verification results between the practical values and the simulation values.

Keywords: Divided Wall Distillation Column (DWDC), simulation, high-purity products, HYSYS ®, operation cost, capital cost and validation

1. Introduction

Distillation columns are essential in manufacturing sectors since they separate two chemicals in a mixture into high-purity products. However, if there are more than two compounds, a succession of distillation columns (two, three, or maybe more) will be required, resulting in increased capital and operational costs, as well as the utilization of extensive spaces inside the plant [1].

Distillation columns account for a significant portion of the energy consumption in industrial businesses. Distillation is the predominant separating technique utilized in industrial businesses. The expansion of the industrial sector has resulted in numerous distillation columns, leading to increased energy consumption, elevated overall costs, and extensive factory space utilization, thereby creating an urgent need to address the issues associated with distillation columns [1].

To solve all the problems mentioned above, we resorted to simulated a new type of distillation columns known as the Divided Wall Distillation Column (DWDC). This type of distillation column contains a divided wall inside the column that helps separate the components inside the distillation column and separate more than two compounds in one distillation column. This type of distillation column (DWDC) contains one reboiler and one condenser, thus leading us to reduce the capital and operating cost and at the same time reduce the area occupied by the plant [3].

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By using this type of distillation columns (DWDC), there is a possibility to reduce the cost to approximately (30%) compared to traditional distillation columns, As a result of reducing the number of boilers and condensers to half the number, while reducing the total column area.. Industrially, this percentage is considered excellent, which has motivated many researchers to search for this topic intensively. There are many types of (DWDC), as shown in Figure (1), where four main types of this type of distillation columns appear [7].

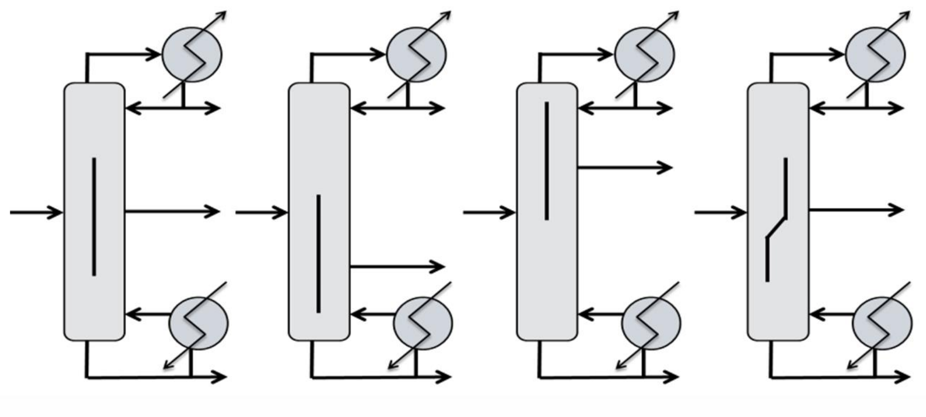

Fig. 1: Different basic types of DWC [7].

Due to the novelty of this type of distillation columns, there is a problem that many researchers have faced in the (DWDC), which is the lack of any model for (DWC) in all simulation programs, which has had a negative impact on research and development processes in (DWC) [1, 2].

In such a type of problem, a specific configuration must be used using a set of columns to be suitable for the operation of distillation columns of type (DWDC) where there is a set of models that are similar in their operation and application to the operation of (DWC) [3].

We used simulation program (HYSYS ®) and we created a group of models. Some of these models were difficult to apply to the programs in terms of operation, and others were easy to operate, but the simulation results were not good. As for the last model, it was excellent in terms of simulation and operation results. These models will be reviewed in detail in the following paragraphs.

2. Backgrounds and chronology

Brugma was the first person to obtain a patent for a thermally coupled distillation column in 1942. Three methodologies exist for the separation of ternary mixtures: fully thermally coupled distillation, side rectifier, and side stripper. The completely thermally integrated distillation column is referred to as a Petlyuk column. The system comprises a main distillation column linked to a prefractionator. Only a single condenser and a single reboiler are necessary. Nonetheless, it is challenging to employ and manage [4, 3, 5].

Wright (1949). proposed the notion of separating a column into two segments by constructing a barrier in the center region, permitting the feed to access the pre-fractionator (feed side) of the partitioned section, while separation occurs in the post-fractionator (side stream side). A side stream can be taken from the center of the column to isolate the third component from the bottom and top products [6].

The main fractionation isolates the intermediate boiling component, whereas the pre-fractionation serves as a boundary between the lowest and highest boiling products. This structure minimizes thermodynamic losses by separating the feed and side product, while also reducing capital costs by requiring just one column to provide a high-purity tertiary separation [7].

The two main techniques for isolating a three-component feed into pure products are the direct and indirect configurations, as depicted in Figs. (2-a) and (2-b) respectively. An alternative is to adopt a three-column arrangement (fig 2-c), in which two columns maintain a clear distinction while one column displays a less apparent or vague division [8].

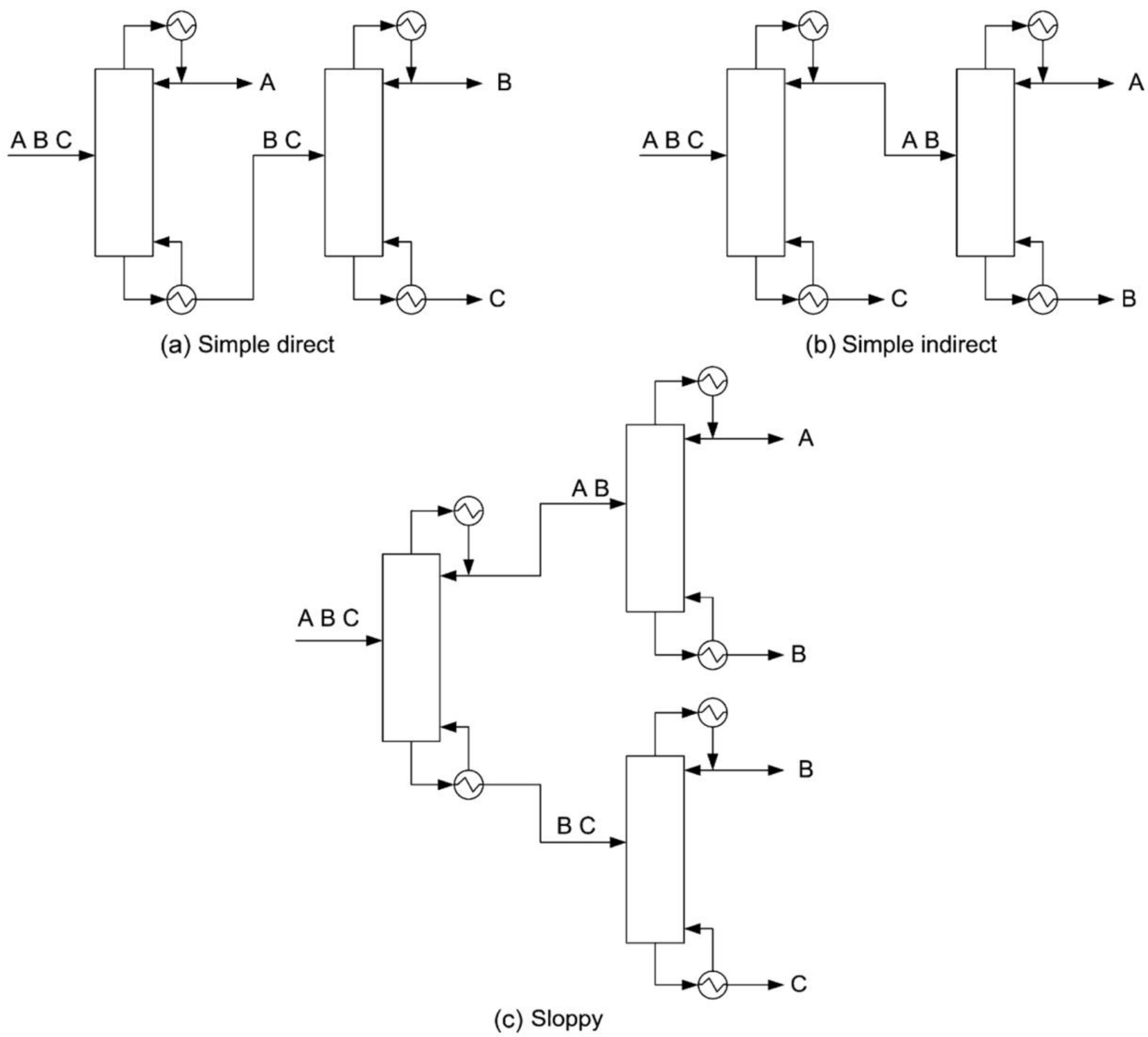

Fig. 2: Common, column-in-series and in-parallel sequences for separating a three-component mixture into pure products [8].

Component B can be extracted as a pure side-stream by linking the bottom of the second column with the top of the third column, as both provide pure component B (see figure 3-a). The overview article and the chapter on distillation sequencing in [Smith]'s book detail various heat coupling configurations for separating three-component mixtures. The prefractionator arrangement illustrated in figure (3-a) requires considerably less energy than traditional column configurations [8].

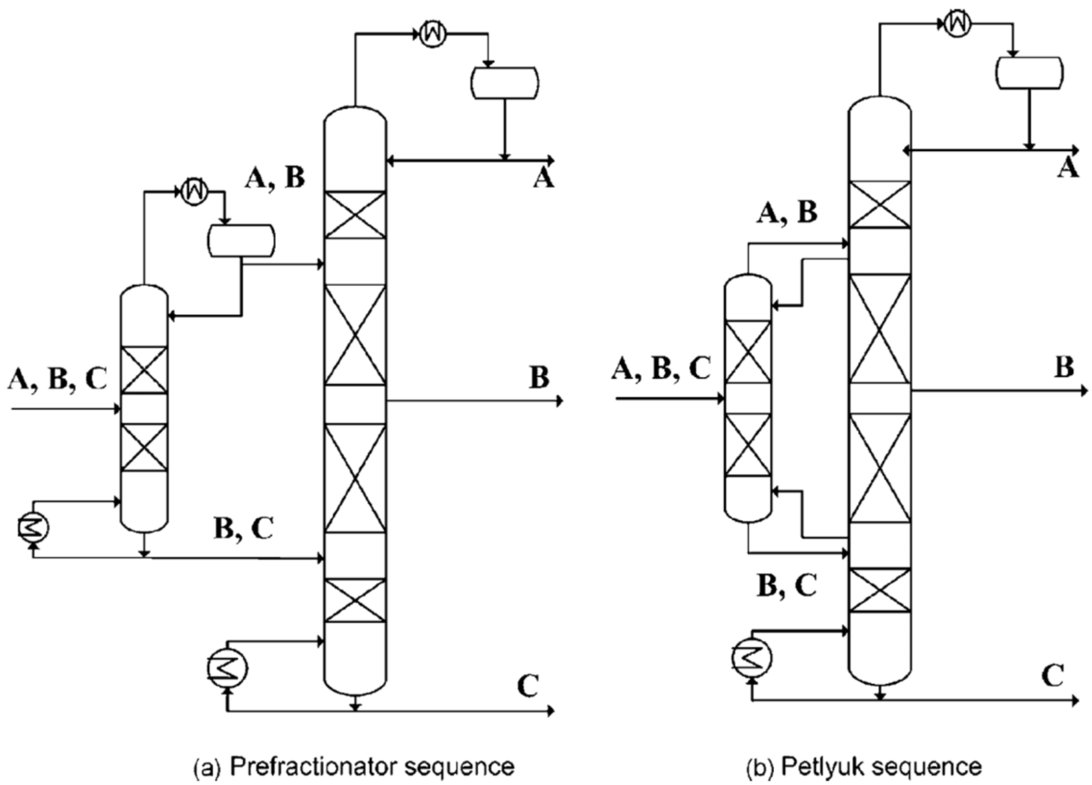

Fig. 3; illustrates three-component separation sequences that are more energy-efficient, which include (a) a conventional prefractionator column and (b) a thermally coupled prefractionator [8].

The elimination of the prefractionator column's condenser and reboiler, when suitable, can result in additional capital savings. This results in the situation depicted in figure (3-b). Three component separation sequences demonstrating improved energy efficiency: (a) a thermally integrated prefractionator; and (b) a standard prefractionator column [8].

Petlyuk et al. (1965). Presented the "Petlyuk column". By thermally integrating the prefractionator column with the main column and attaching the requisite condenser and reboiler to the main column, the missing condenser and reboiler are successfully substituted. This arrangement is commonly referred to as a "fully thermally coupled column" [9].

3. Simulation Software

There are many simulation programs that are used to simulate separation processes such as distillation columns, but all of these programs do not contain a model dedicated to Divided Wall Distillation Column (DWDC) due to the novelty of this type of distillation columns and its limitations in industrial applications. Among the simulation programs that simulate the distillation processes are:

- Aspen HYSYS®
- ASPEN PLUS™

- ChemCAD
- ProSim Plus

In this research, we used HYSYS software because this program has several specifications that make it better than other simulation programs [10]. These features include:

- Equilibrium and Transient Simulation HYSYS® can model steady-state operations, enabling users to comprehend both the short- and long-term behavior of the process [10].
- The software has sophisticated capabilities for simulating complex processes, encompassing heterogeneous chemical reactions and multiphase systems [10].
- The software offers a user-friendly and simple graphical interface that simplifies the visual construction and analysis of processes [10].
- Precise thermodynamic and physical property database for realistic simulation of industrial processes [10].
- HYSYS® provides critical tools for designing divided wall columns that function effectively and produce results similar to real models [10].

Because of these features of the HYSYS software, we will adopt this program in our current research to simulate a Divided Wall Distillation Column (DWDC).

4. DWC Model

We made several models to simulate the operation of DWDC until we arrived at four main models. These four models are:

1) Top Divided Wall Column (T-DWC)
2) Bottom Divided Wall Column (B-DWC)
3) Middle Divided Wall Column (M-DWC)
4) Four columns configuration DWC

Each of these four models has a set of features and uses, and we will discuss these features and uses in detail for each model.

4.1 Top Divided Wall Column (T-DWC)

The setup consists of two columns, labelled "Prefractionator" for the first column and "Main column" for the second, connected by a Recycle tool that serves as a connector between them. This tool operates by balancing the inputs and outputs of the two columns, allowing them to work as a single unit. Figure (4) illustrates the process for connecting the columns.

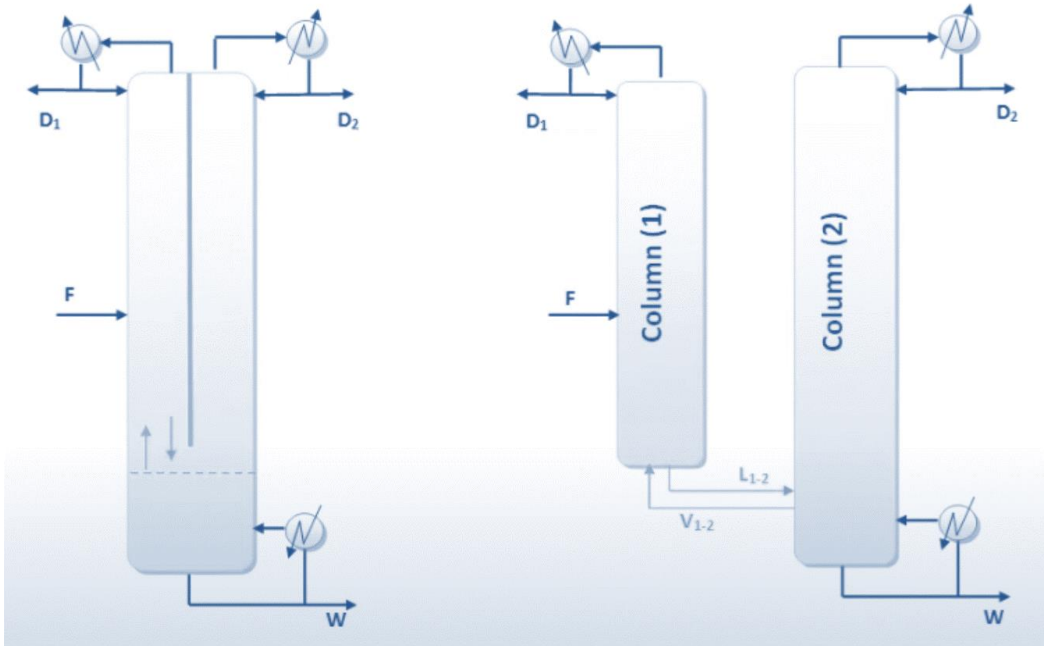

Fig. 4: ‘’Top divided wall column’’ configuration

This variant of DWC features a divide wall positioned at the top of the column, so establishing a connection between the two columns from the bottom, as the higher section is partitioned by the wall. According to this design, a stream will connect from the bottom of the first column, "Prefractionator," to the bottom of the second column, "Main column," for liquid transport. Subsequently, a stream will exit from the bottom of the second column, "Main column," and re-enter the bottom of the first column, "Prefractionator," for vapor transport.

The lightest component (A-top product) is extracted from the top of the first column, "Prefractionator," while the remaining components are extracted from the second column, "Main column." The medium component (B-side stream) exits from the top of the second column, "Main column," while the third component (C-bottom product) is discharged from the bottom of the same column, as illustrated in figure (5).

In this study, we refrained from employing this approach owing to its several drawbacks, which we shall delineate in the subsequent points:

- Challenging to execute in a real DWC simulation.
- Restricted application, as it is utilized solely on columns where the partition is positioned at the top
- It possesses two condensers, distinguishing it significantly from a real DWC.
- The challenge of allocating the number of trays (or packing) for the actual columns into these two columns necessitates the adoption of a specific methodology, either through a shortcut approach or a designated mathematical calculation, with occasional reliance on estimation.
- Three degrees of freedom must be allocated to the second column, complicating the operation of the columns due to the disparity in degrees of freedom.
- Incapable of controlling liquid and vapor distributions.

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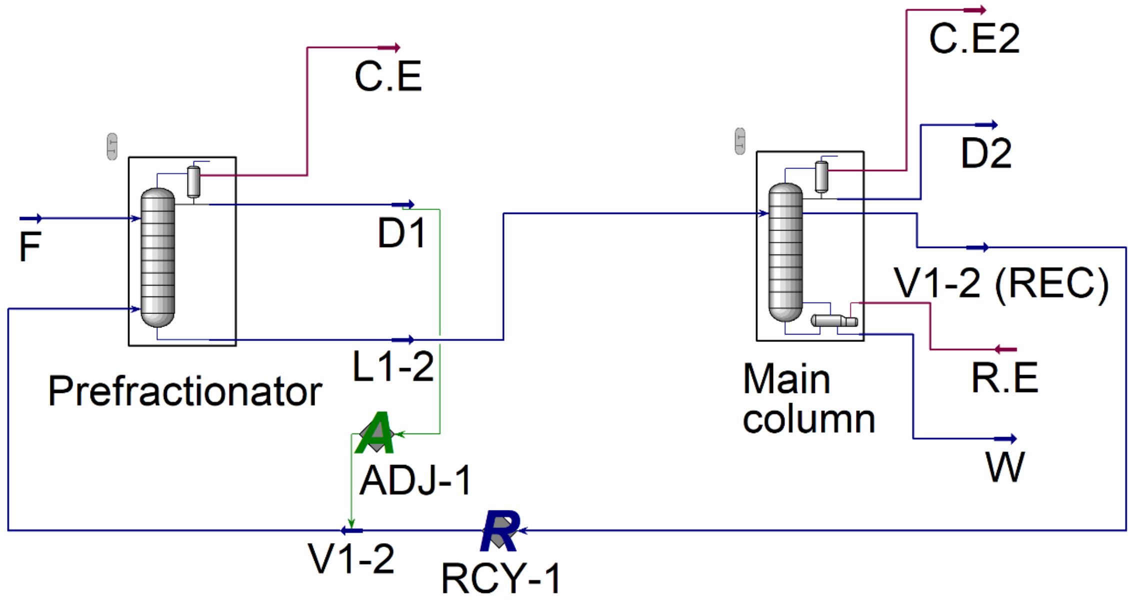

Fig. 5: ‘’Top divided wall column’’ simulation

4.2 Bottom Divided Wall Column (B-DWC)

The setup comprises two columns: the first is labelled "Prefractionator" and the second "Main column." The columns are connected by a Recycle tool that functions as a channel between them. This instrument functions by equilibrating the inputs and outputs of the two columns, enabling them to work as a singular unit. The process for integrating the columns is depicted in the following figure (6).

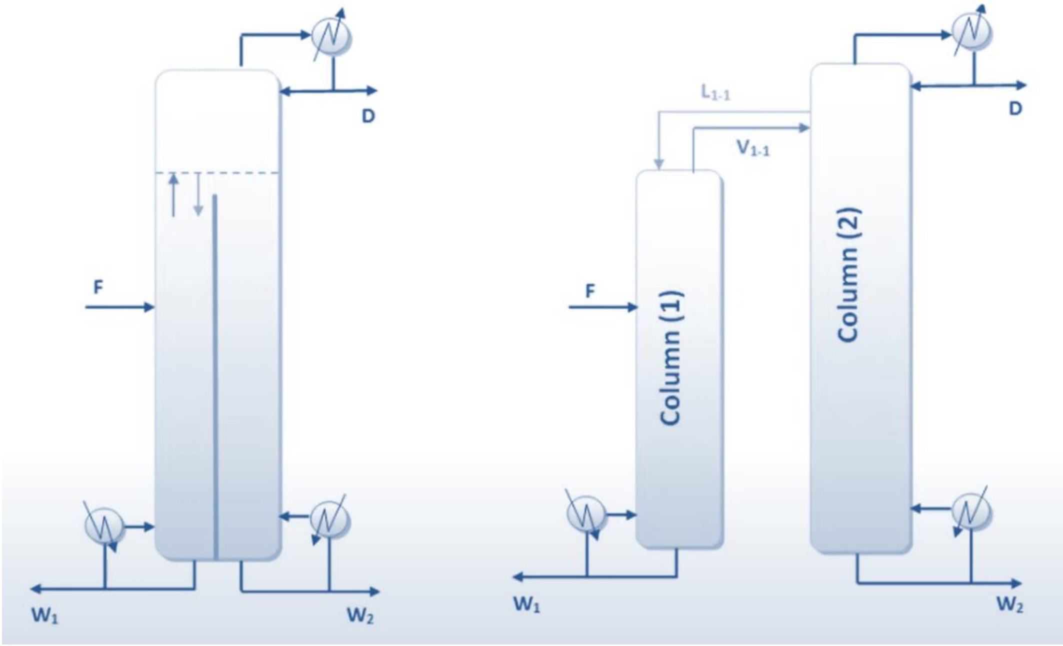

Fig. 6: ‘’Bottom divided wall column’’ configuration

This variant of DWC features a dividing wall at the bottom of the column, establishing that the link between the two columns occurs from the top, as the lower section is divided by the wall. According to this design, a stream will be linked from the top of the first "Prefractionator" column to the top of the second column, "Main column," for liquid transport. Additionally, a stream will exit from the top of the second column, "Main column," and re-enter the top of the first column, "Prefractionator," for vapor transport.

The densest component (C-bottom product) is extracted from the bottom of the first column (Prefractionator), and the remaining components are extracted from the second column. The medium component (B-side product) exits from the bottom of the second column, "Main column," while the lightest component (A-top product) emerges from the top of the second column, as illustrated in figure (7).

Owing to its various disadvantages, we abstained from utilizing this design in the study. The following points will provide a succinct summary:

- Difficult to implement in actual DWC simulation.
- Application is restricted, as it is just utilized on columns with the separating wall positioned at the bottom.
- The difficulty in allocating the number of trays for the actual columns into these two columns lies in the necessity of employing a particular mechanism via a shortcut approach or a specific mathematical formula. Moreover, supposition may be utilized in specific instances.
- It is significantly different from a true DWC because it contains two reboilers.
- Three degrees of freedom must be allocated to the second column, complicating the operation of the columns due to the disparity in degrees of freedom.
- Incapable of controlling liquid and vapor distributions.

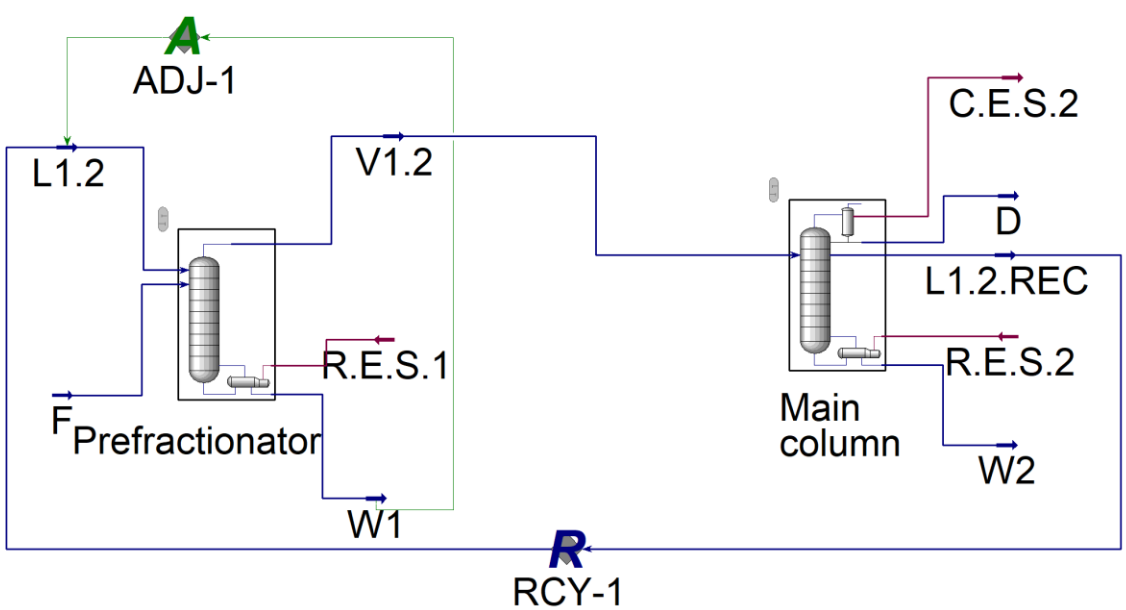

Fig. 7: ‘’Top divided wall column’’ simulation

4.3 Middle Divided Wall Column (M-DWC)

The configuration consists of two columns: the first designated as "Prefractionator" and the second as "Main column." The columns are interconnected by a Recycle tool that serves as a channel between them. This instrument operates by balancing the inputs and outputs of the two columns, allowing them to act as a unified entity. The process for integrating the columns is depicted in the following figure (8).

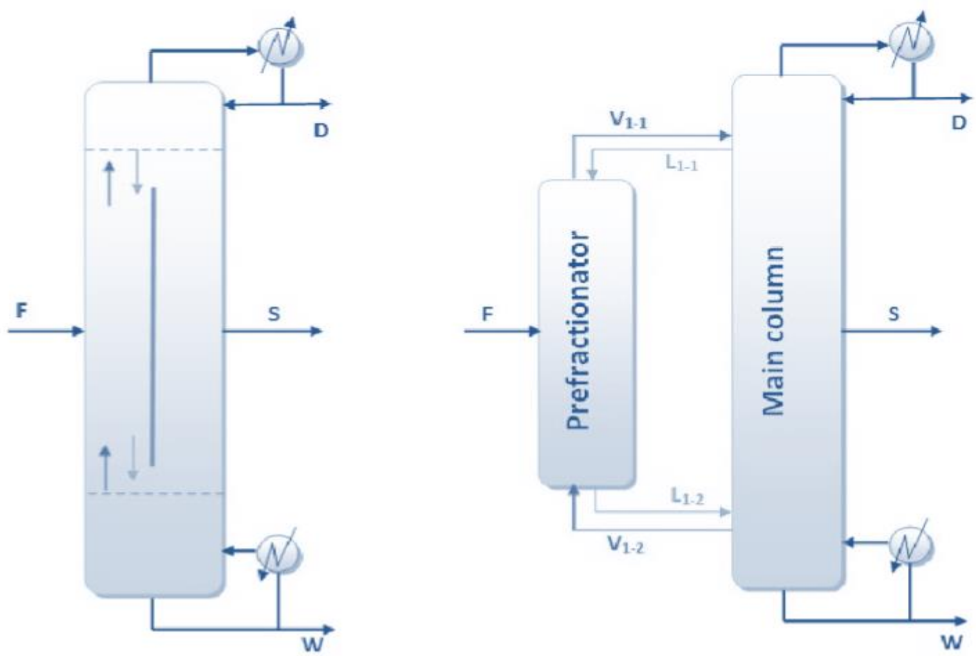

Fig. 8: ‘’Middle divided wall column’’ configuration

This variant of DWC features a central separating wall within the column, facilitating connections between the two columns at both the top and bottom. According to this design, a conduit will extend from the top of the first column to the top of the second column, facilitating the movement of liquids. A stream will be established that exits from the top of the second column and enters the top of the first column, serving to carry vapors. The identical procedure is implemented at the bottom of the two columns until a complete connect is established.

The lightest component (A-top product) is extracted from the top of the second column, the medium component (B-side stream) is extracted from the middle of the second column "Main column," and the third component (C-bottom product) is extracted from the bottom of the second column "Main column," as illustrated in figure (9).

In this study, we refrained from employing this approach due to its several shortcomings, which we will outline in the following points:

- Challenging to execute in a real DWC simulation.
- The challenge in distributing the tray count from the existing columns into these two columns stems from the requirement to utilize a certain technique using a shortcut method or a designated mathematical formula. Moreover, supposition may be employed in some circumstances.

- The allocation of five degrees of freedom to the second column complicates the operation of the columns due to the imbalance in degrees of freedom.
- Incapable of controlling liquid and vapor distributions.

This kind of DWC is deemed superior to the initial two varieties (A and B) notwithstanding these disadvantages. We abstained from using it since the five degrees of freedom significantly complicated the operation of the second column.

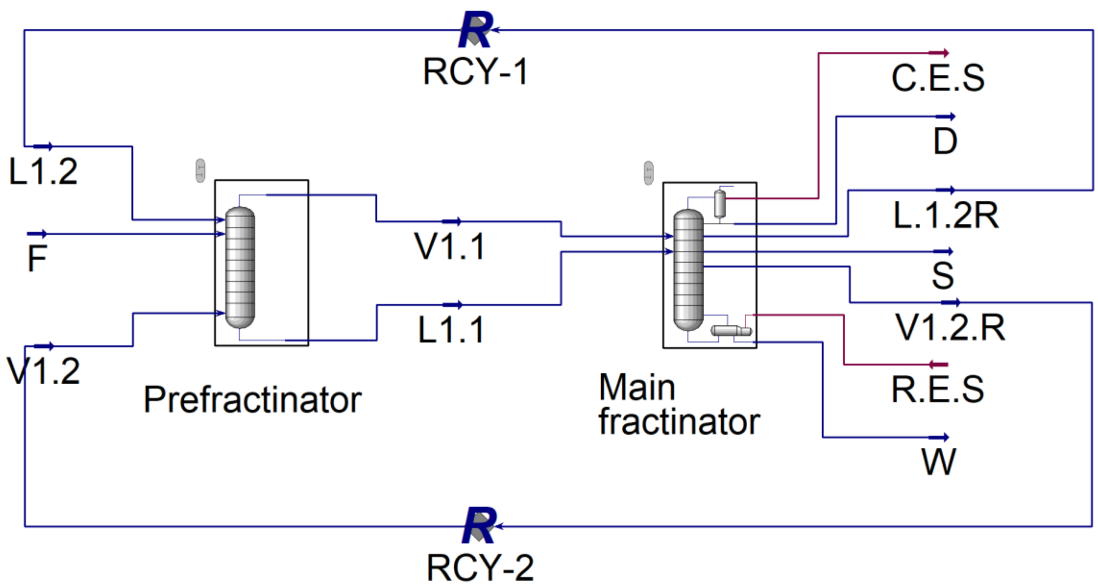

Fig. 9: ‘’Middle divided wall column’’ simulation

4.4 Four columns configuration DWC

The configuration comprises four columns. The first column denotes "Prefractionator" and is positioned on the far left. The second column denotes the "Main column" and is positioned on the far right. The third column denotes the upper section of the DWC and is situated at the top. The fourth and final column denotes the lower section of the DWC and is positioned at the bottom. The columns are interconnected by four Recycle tools, two Mixer tools, and two Tee tools, as illustrated in figure (10).

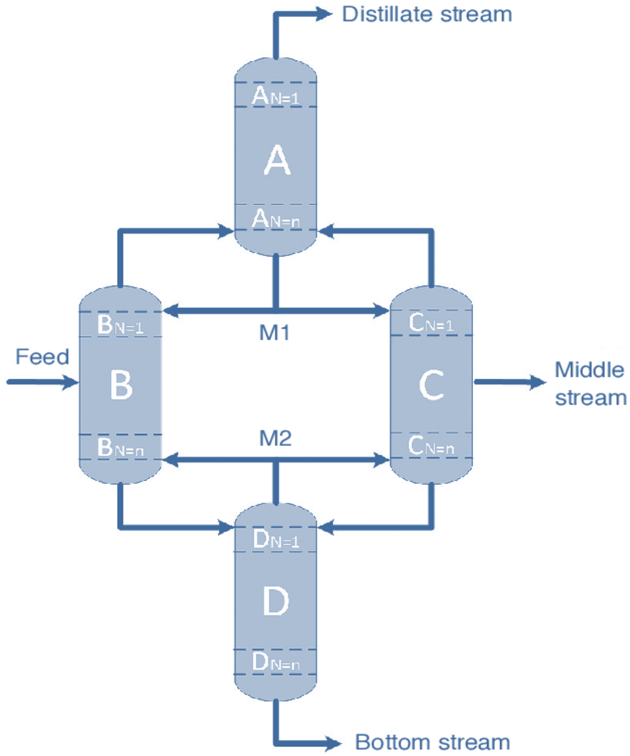

Fig. 10: ‘’Four column DWC’’ configuration

This construction features a somewhat intricate design yet yields efficient effects; the columns are interconnected through multiple stages:

1) The four columns are interconnected by three sorts of tools, specifically:
   - Recycle utilized for the aim of equilibrating between columns.
   - Mixer utilized for the purpose of combining streams.
   - Tee utilized for the split of streams.
2) The four columns are arranged systematically: the first column, "Prefractionator," is positioned on the left; the second column, "Main column," is on the right; the third column is at the top; and the fourth column is at the bottom.
   - "prefractionator" column devoid of both a reboiler and a condenser.
   - "Main column" devoid of a reboiler and a condenser.
   - With a single condenser, the "Top-column" column is presented.
   - Column with a single reboiler located at the bottom.
3) The output from the top of the "Prefractionator" is combined with the output from the top of the "Main column" using the Mixer tool, and the output from the Mixer tool serves as the input to the Top-column.
4) The output from the bottom of the "Prefractionator" is combined with the output from the bottom of the "Main column" using the Mixer tool, and the output from the Mixer tool serves as the input to the Bottom-column.
5) The output from the bottom of the Top-column is directed to the Tee tool, which segregates the incoming material based on the designated ratio. The output from the Tee tool is then routed to two

Recycle tools; the first directs to the top of the "Prefractionator," while the second leads to the top of the "Main column."

6) The output from the upper section of the Bottom-column is directed to the Tee tool, which segregates the incoming material based on the designated ratio. The output from the Tee tool is then routed to two Recycle tools; the first directs to the base of the "Prefractionator," while the second directs to the base of the "Main column."
7) The products are as follows:
   - The output from the upper section of the Top-column functions as the top product (the lightest product).
   - The output from the center of the "Main column" functions as a byproduct (intermediate product).
   - The output from the lowest section of the Bottom-column functions as the bottom product (the heaviest product).

Upon implementing these seven stages in Aspen HYSYS®, the outcome will be shown in Figure (11).

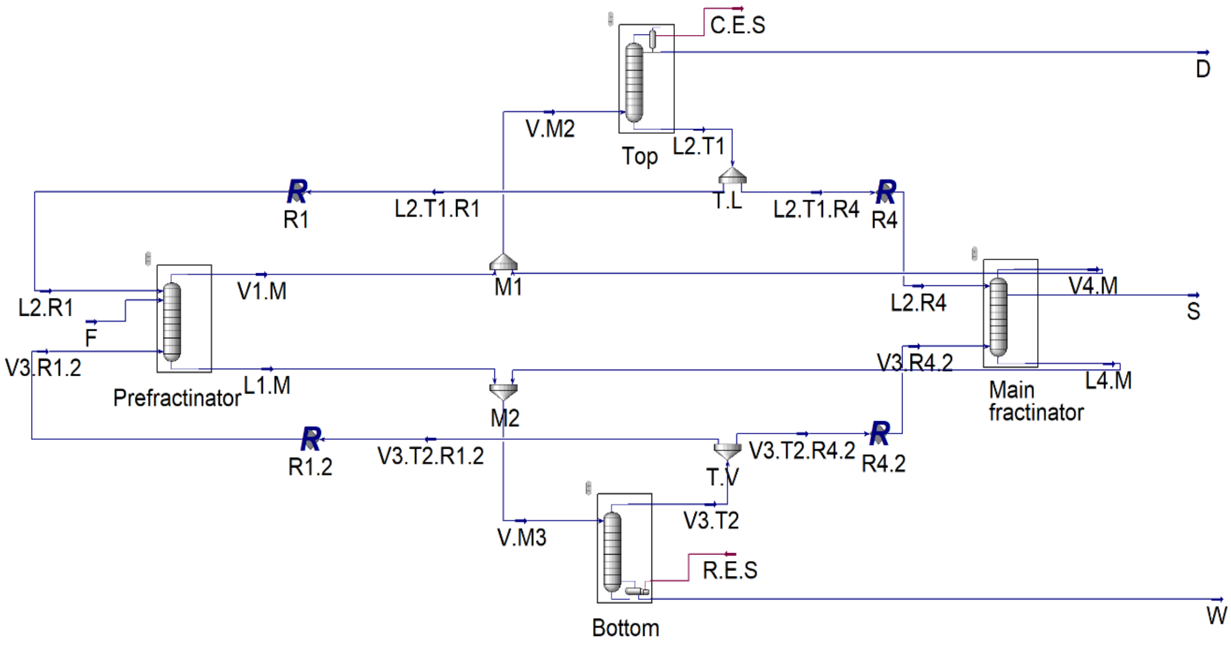

Fig. 11: Four column DWC simulation

This research chose this design due to its advantages, which will be detailed in the subsequent parts;

i. This setup is the most straightforward to install and use compared to other options.
ii. Simple to implement in genuine DWC. The number of trays in the "Prefractionator" corresponds to the right column (1st column), the number of trays in the "Main column" corresponds to the left column (2nd column), the number of trays in the upper section corresponds to the Top column (3rd column), and the number of trays in the lower section corresponds to the Bottom column (4th column).
iii. Controlling the splits of both liquid and vapor is straightforward; the liquid split is regulated by adjusting the Tee Liquid Split (T.L) settings, while the vapor split is managed by modifying the Tee Vapor Split (T.V) parameters.

iv. The application of degrees of freedom is facilitated by their allocation across the three columns: the Top column possesses one degree of freedom attributable to the condenser, the Main column has one degree of freedom due to the side stream product, and the Bottom column includes the final degree of freedom because it contains a reboiler.
v. Upon assessing the outcomes generated by this arrangement and contrasting them with genuine DWC, the results were very precise, justifying our dependence on them.

The combination of these qualities in this design justified its use for simulating a genuine split wall distillation column (DWDC).

5. DWDC-Model Validation

After we have determined the best model for simulating distillation columns (DWDC), we must now verify that the model we designed works efficiently and that the simulation results shown by this model are close to the real results. This will be done by choosing a real model in (Texas) which was studied by the researcher (Michel et al) with Title of his research (Case.1 Separation of ternary mixture).

Four steady-state experiments were performed on the ternary mixture of methanol, 1-propanol, and 1-butanol, using various feed compositions, flow rates, reflux ratios, liquid distributions, and reboiler heat duties. The simulation models executed on the situation were exemplary and yielded minimal error rates, as seen in the table (1).

We used three types of fluid package in this simulation to find out which type is better. These two types were chosen based on the thermodynamic properties of the inputs, as the inputs were hydrocarbon materials with a non-ideal mixture.

The error rate between the actual values and the simulated values was calculated according to the following equation:

$$\text{Err\%} = \frac{simulated - reel}{reel} * 100$$

Table. 1; Validation of separation of ternary mixture case.1

Parameters	exp	Simulation					
		NRTL	Err%	P.R	Err%	Willison	Err%
Feed (kg/h)	5.41	5.41	-	5.41	-	5.41	-
Methanol (wt. %)	0.4	0.4	-	0.4	-	0.4	-
1-Propanol (wt. %)	0.3	0.3	-	0.3	-	0.3	-
1-Butanol (wt. %)	0.3	0.3	-	0.3	-	0.3	-
Distillate (kg/h)	2.66	2.66	-	2.66	-	2.66	-
Methanol (wt. %)	0.814	0.8138	-0.024	0.8122	-0.221	0.8164	0.294
1-Propanol (wt. %)	0.186	0.1862	0.001	0.1878	0.967	0.1836	-1.29
1-Butanol (wt. %)	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Side stream (kg/h)	1.038	1.038	0.0	1.038	0.0	1.038	0.0
Methanol (wt. %)	0.0	0.0002	-	0.001	-	0.0003	-

1-Propanol (wt. %)	0.995	0.99	-0.502	0.9797	-1.537	0.984	-1.1
1-Butanol (wt. %)	0.005	0.0098	0.96	0.0193	96.93	0.0156	59.183
Bottom stream (kg/h)	1.872	1.8724	0.021	1.872	0.0	1.872	0.0
Methanol (wt. %)	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1-Propanol (wt. %)	0.021	0.1394	-	0.1398	-	0.1345	540.47
1-Butanol (wt. %)	0.979	0.8606	-12.09	0.8602	-12.13	0.8655	-11.59
Liquid Split (-)	0.5	0.5	-	0.5	-	0.5	-
Reflux Ratio (-)	3	3.49	16.33	3.571	19	3.881	29.36
Heat Duties (kW)	7.84	7.85	0.1275	7.333	-6.466	7.538	4.006
Press. Drop (mbar)	2.8	2.8	0.0	2.8	0.0	2.8	0.0

We shall analyse the results of Table (1) systematically and in the following order:

1) Distillate (Top product)
   - The NRTL package exhibited the lowest error rate for methanol (wt. %), recorded at -0.024%, indicating superior accuracy relative to alternative packages. The Peng-Robinson package had a greater error rate of -0.221%, whereas the Willson package recorded an error rate of 0.294%. This results in the NRTL package being the most precise in depicting this variable.
   - 1-Propanol (wt.%): The NRTL package demonstrated exceptional accuracy with a 0.001% error margin. The Peng-Robinson and Wilson models had greater errors of 0.967% and -1.29%, respectively. This results in the NRTL package being the most precise in depicting this variable.
   - 1-Butanol (wt. %): All three packages exhibited flawless representation of this component, demonstrating 0% inaccuracy.
2) Side Stream
   - Methanol (wt. %): All packets exhibited little error, with the NRTL packet distinctly surpassing the others, which recorded 0% error.
   - The NRTL package exhibited the minimal error for 1-Propanol (wt.%) at -0.502%, in contrast to Peng-Robinson at -1.537% and Wilson at -1.1%.
   - 1-Butanol (wt. %): The Peng-Robinson (96.93%) and Wilson (59.18%) packages exhibited more errors, but the NRTL package had superior accuracy (0.96%).
3) Bottom Stream
   - The error percentage was omitted in the methanol field because to the presence of a value (0.0) in the (exp) field; nevertheless, upon closer examination, the error is nearly nil (0.0).
   - The NRTL package exhibited the minimal error of 0% for 1-Propanol (wt.%), but the errors of the other two packages were significantly elevated at 540% and 540.47%.
   - The NRTL package had the highest accuracy at -12.09%, followed by Peng-Robinson at -12.13% and Wilson at -11.59%.
4) Performance Metrics
   - The reflux ratio for the package (NRTL) demonstrated exceptional results with an error rate of 3.49, signifying strong performance. The Peng-Robinson and Wilson models exhibited greater accuracy, with respective values of 19% and 29.36%.
   - Heat Duties (kW): The NRTL program demonstrated exceptional accuracy with a mere 0.1275% error, but the other two packages had elevated error rates.

- Pressure Drop (mbar): All packages exhibited perfect accuracy (0% inaccuracy).

The NRTL package has consistently demonstrated superior efficiency compared to alternative packages, with the lowest error rates across most variables. The NRTL package is regarded as the most precise and stable in its representation of findings relative to other packages.

6. Conclusion

Divided Wall Distillation Column (DWDC) are considered a qualitative leap in the separation processes because they have a low capital and operating cost compared to traditional columns, and they also occupy a smaller area compared to traditional columns. For these reasons, there is a great interest in this type of towers, but the problem that researchers faced is that there is no model for this type of columns (DWDC) in the simulation programs, which caused obstacles and many problems for researchers. In this research, we found a group of models that simulate the work of Divided Wall Distillation Column (DWDC). There were four models, the best of which is model (Four columns configuration DWC) because it is easy to operate and smooth to deal with and gives excellent simulation results compared to the other three models. This model helps researchers develop their research by entering a group of inputs and finding the results through simulation, meaning they can know the values of the results before applying them to reality.

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