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MODELING AND SIMULATION OF A DIVIDING WALL COLUMN FOR FRACTIONATION OF FATTY ACID IN OLEOCHEMICAL INDUSTRIES

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ABSTRACT

The dividing wall column (DWC) is particularly useful for separating multi-component mixtures into their pure fractions within one column shell and has attracted many researchers and companies for various applications. In the oleochemical industries, it is observed, that the fractionation of fatty acid commonly uses conventional two stage distillation columns. In this research, DWC was studied for a more efficient fractionation of fatty acid mixtures. A unique four column configuration model was used to represent the four sections in DWC. Using Aspen Plus as computer aided process engineering tool, a rigorous steady state simulation was performed. The results show that a more logical and realistic model for describing the process operation was obtained, compared to a common more two or three-column approach. In addition, some technical aspects were also highlighted to comprehend the design and operational configuration of DWC.

Keywords: *Dividing wall column; fatty acid; oleochemical; modeling; simulation*

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1.0 INTRODUCTION

Distillation is one of the most common separation methods, as it is widely understood and used to a great extent in mixture separation techniques. Although the thermodynamic efficiency of distillation processes is low, the ease and confidence in operation makes it one of the most preferred separation methods [1]. However, Sangal et al. [1] argue that distillation columns consume a substantial part of the entire energy requirement for chemical industry. This motivates researchers to focus on developing and improving the efficiency of distillation processes. The separation of multicomponent mixture has typically been done by sequential distillation columns [2]. This configuration has basic drawbacks related to operation and capital cost. Over the years, researchers proposed several designs to improve the efficiency of distillation processes such as the Petlyuk column and divided wall column (DWC).

DWC are especially advantageous for separating ternary mixtures [3] into pure fractions, especially for medium boiling components. The column configuration is thermodynamically equivalent to the Petyluk column configuration, consisting of a pre-fractionator and a main distillation column. Instead of an external pre-fractionator in the Petyluk design, a vertical wall is introduced in the middle part of the main distillation column of the DWC. This creates a feed pre-heater and draw off section in the middle section. When multicomponent mixtures are introduced into the column, the low boiling component goes overhead as distillate and the high boiling components goes out as bottom product, while the intermediate boiling component draws off in the side stream. The reflux is split between the two wall of the divided sections in the column and the vapour flow is split according to the pressure drop in both section [4]. Such configurations save a second column, where compartments like the column shell, internals, evaporator, condenser, control and maintenance are significantly reduced. Julius Montz GmbH claimed that by using DWC, the investment costs can be cut by 20% - 30% and operating costs by around 25%. In detail, the energy consumption can be reduced up to 50% [5]. This leads to lower carbon dioxide emission and smaller column diameter due to reduction in internal flows [5]. Because of these advantages, DWC’s have attracted many researchers and companies for various applications.

It is observed that the most common approach to fractionate fatty acid mixtures in oleochemical industry is through sequential separation using two distillation columns to separate the light cut (C8-C10), middle cut (C12-C14) and heavy cut (C16-C18) components. Because of distinctive boiling point differences, it is interesting to analyse the possibility of fractionating the three cuts using DWC. In doing this, we proposed a four column configuration model, representative of the DWC in which Aspen Plus is used as computer aided process engineering tools for rigorous steady state simulation of the model. In addition to that, a review of some technical aspects will also be highlighted to comprehend the design and operation configuration of DWC for fatty acid fractionation and significantly open the possibility for industrial implementation.

2.0 MODELING AND SIMULATION APPROACH

Modelling and simulation of DWC has been studied in the open literature using commercial simulators such as Aspen HYSYS and Aspen Plus. However, most often two [4, 6] or three columns [7] configurations were investigated. Due to simulation convergence issues and resulting simplified models most researchers avoid using four column configurations. As illustrated in Fig. 1a, typical DWC configuration can be divided into four sections. Therefore, attempting to represent the real process it is logical to use a four column configuration as represented in Fig. 1b. Such an arrangement could describe the DWC operation in a more realistic and logical approach for the modeling work. Moreover, all main streams and straws could be taken into account even under rising the degree of freedoms, as to be found for a real plant [8].

In this representation (see Figure 1b), the feed stream is introduced to a pre-heat section (section B) which is equivalent to the pre-fractionator of the Petyluk distillation column. It has two output streams. The vapor output stream is introduced to the rectifying column (section A), while the liquid output stream is introduced to the stripping column (section D). The rectifying section (section A) has two input and output streams. The input streams are the vapor streams from the pre-heat (section B) and middle column (section C). While the output streams are the vapor distillate stream and liquid bottom stream. The bottom stream is then split into reflux streams for section B and section C. A split factor could be applied here to control the reflux and rectification behavior of the regarded sections. Section C has two input and three output streams. The input streams are the liquid reflux from section A and vapor boil up from section D. The output streams are the distillate vapor stream, middle product stream and bottom liquid stream. Section D has two input stream and output stream. Input to this column are the liquid refluxes from section B and C. Whereas the output stream is the bottom liquid stream and the vapor boil up, which then split to section B and C according to the fluid dynamic conditions in the sections, mainly pressure drop.

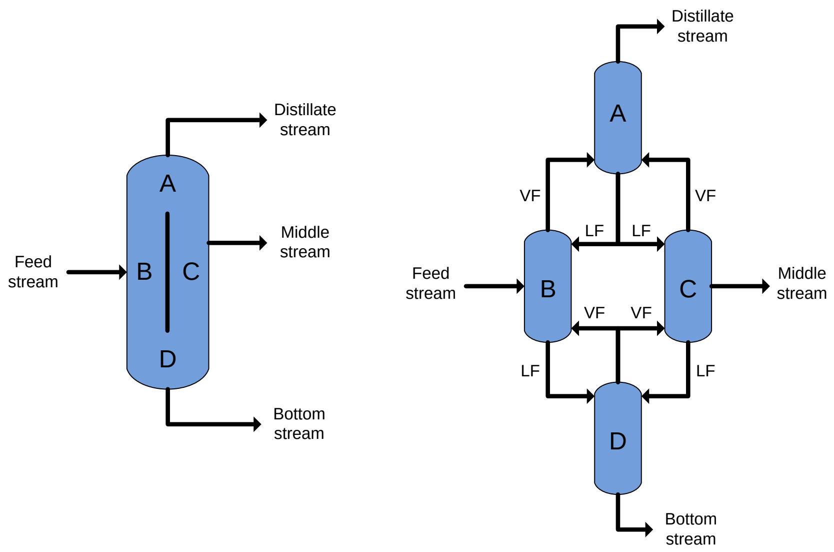

Figure 1: (a) Typical DWC column configuration (b) Equivalent 4 column DWC configuration used for the modelling work

2.1 Modeling Set-Up

Basic steps to process modeling and simulations, using process simulators, include defining chemical components, selecting thermodynamic models and methods, designing the process flowsheet by choosing proper operating units, determining plant capacity and setting up input parameters. Based on the information from our industrial partner, the feed information for fatty acid fractionation based on palm kernel oil (PKO) is shown in Table 1. Note that there are residues of triglyceride and unsaponifiables in the feed, which are represented by pseudo-components methyl oleate and n-hentriacontane respectively. For the determination of the thermodynamic and hydrodynamic properties, different property packages can be used to estimate the required parameters, according to the case under study. With PKO based fatty acids being non-polar components and few experimental data, as well as a variety of properties to be estimated, equations of state have the priority. Therefore, the thermodynamic model SRK (Soave-Redlich-Kwong) is used for the modelling work [9].

The simulated capacity of the column to handle is 9000 kg/hr of PKO-based fatty acids. The DWC column configuration uses four rigorous RADFRAC units with splitters to manage the vapour and liquid load from and towards the two areas of the dividing wall section as shown in Fig. 2. Section A (rectifying column) and section D (stripping column) are set to only have a condenser and reboiler respectively. Whereas, both section B (pre-heat column) and section C (middle column) have no condenser or reboiler. By using this set-up, the DOF is reduced compared to a typical column compartment, which usually has a degree of freedom (DOF) of 2. Section A has only 1 DOF, where the distillate rate is then selected

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and specified. Section B and C have no DOF and so no specification to be given. Section D has 1 DOF, where the reboiler duty is selected and specified. In addition to that, the DWC has two additional DOF which are the liquid (RECT-SPL) and vapour (STR-SPL) load split [10]. Since vapour split is difficult to control, an equal split ratio is specified, whereas liquid split can be manipulated.

Table 1: PKO-based fatty acid compounds and its mole fraction defined in Aspen Plus.

Component name	Alias	Mole fraction
Water	H_2O	0.00035
Caproic acid	$C_6H_{12}O_2$	0.0012
Caprylic acid	$C_8H_{16}O_2$	0.033
Capric acid	$C_{10}H_{20}O_2$	0.034
Lauric acid	$C_{12}H_{24}O_2$	0.474
Myristic acid	$C_{14}H_{28}O_2$	0.162
Palmitic acid	$C_{16}H_{32}O_2$	0.079
Oleic acid	$C_{18}H_{34}O_2$	0.1562
Linoleic acid	$C_{18}H_{32}O_2$	0.026
Stearic acid	$C_{18}H_{36}O_2$	0.0188
Triglyceride (methyl-oleate)	$C_{19}H_{36}O_2$	0.0099
Unsaponifiables (n-hentriacontane)	$C_{31}H_{64}$	0.00555

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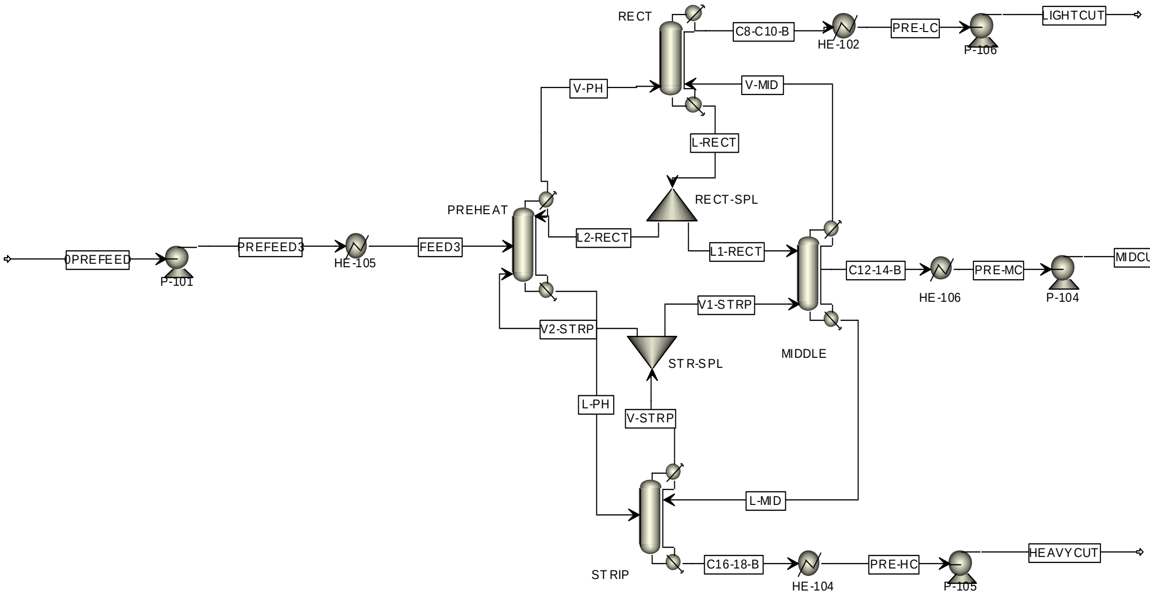
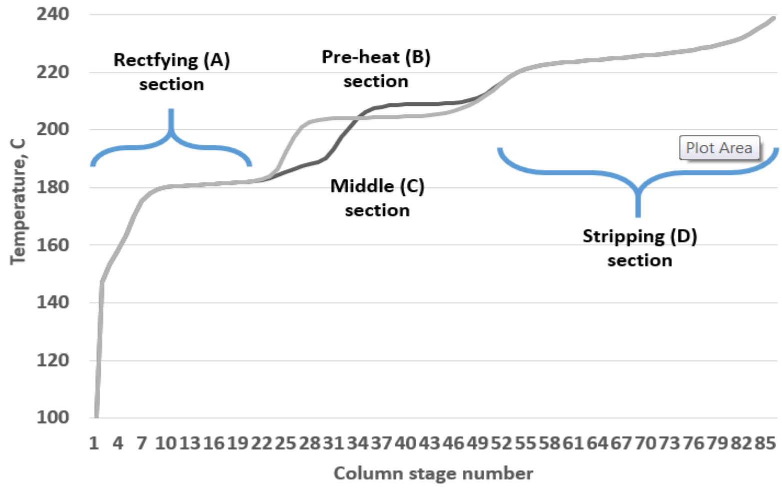
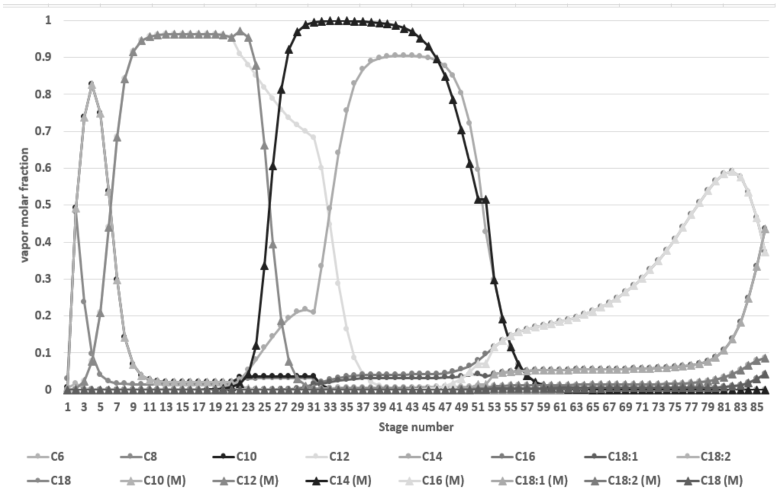


Figure 2: DWC four column configuration in Aspen Plus

The approach for rigorous simulation is based on equilibrium-stage models, taking into account the packing rating. Using packing rating we were able to specify the column section diameter and packing details. Accordingly, the model calculates performance and hydraulic information such as flooding, downcomer backup, and pressure drop. In addition, using packing rating the dimension of the DWC column diameter can be specified and thus gives a more accurate behaviour of the column. Section A has 21 stages with a diameter of 2 meter. Both section B and C have 30 stages with 2 meter in diameter each. Section D has 35 stages with a diameter of 2 meter. The column is design for a packed column with packing factor of 72 m-1. For all stages a HETP of 0.3 meter is assumed. The feed stream is introduced at stage 10 of the pre-heat column, whereas the middle product stream draws off at stage 3 of the middle column. To prevent product degradation, the column the reboiler temperature must be below 240 ˚C. Therefore, the top column pressure is set to 20 mbar with total column pressure drop of 12.25 mbar. The column is design to have >99.0 mole% product purity for each cut.



(a)



(b)

Figure 3: Column (a) temperature and (b) composition profile

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3.0 Simulation Results

The simulation is done in Aspen Plus Ver. 8.3. We do encounter convergence problems. These issues result out of the lack of proper initial values and mainly the multiple internal streams, which need to be initiated, calculated for one section and concurrently serve as feed for another section i.e. simulated unit. However, convergence issues can be minimized by changing the convergence method in the RADFRAC specification tab to other than standard such as strongly non ideal liquid. Other than that the minimum convergence iteration can be increase appropriately, besides the choice of an appropriate solver method (Newton instead of Wegstein e.g.). Note that the model is not in optimal condition. Further sensitivity analysis need to be done and will be the scope of our future work. Fig. 3 shows the temperature and composition profile of the column. The temperature difference between the two sides is around 20 ˚C. Such conditions seem to be easily achievable in the practical application, as little heat transfer and negligible effect on the column performance is expected [4]. Table 2 shows summary of the simulation results.

Table 2: Result summary of the simulated DWC.

Parameters	Value	Unit
Flow rate of feed stream	9000	kg/hr
Flow rate of distillate stream	430.3	kg/hr
Flow rate of middle stream	5276.3	kg/hr
Flow rate of bottom stream	3293.5	kg/hr
Liquid split ratio	0.756	-
Vapour split ratio	0.5	-
Light cut purity (C6-C10)	99.02 / 99.34	%mol / %wt
Middle cut purity (C12-C14)	99.94 / 99.95	%mol / %wt
Heavy cut purity (C16-C18, TG, wax)	99.99 / 99.99	%mol / %wt
Reboiler duty	2300	kW
Condenser duty	-2130	kW

4.0 Technical Insights

The successful implementation of unfixed wall technology by Julius Montz GmbH has increased the acceptance and implementation of DWC in industries. The application ranges from chemical to petrochemical industries. However, in the literature, Schultz et al. [11] and

Kaibel et al. [12] indicate that, while theoretical researches have shown the economic advantages of DWC's, industry has been avoiding investments in these columns. One reason to avoid this type of application is a lack of understanding of its design and control.

Unlike DWC, common distillation columns are well investigated and, for moderate separation tasks, could be designed and planned via models and simulations only. For dividing wall columns however, the design process and technical aspects are more tedious. Detailed simulations and mini-plant scale experiments are necessary for model validation and general investigation of controllability [13].

The general structure and necessary utilities are similar to common distillation columns. Therefore, the set-up of general units, like reboilers, the column shell and sensors underlies a large variety of available products and expertise in establishing. But the aspect of the dividing wall leads the focus on optimal fixation of the wall, mostly within structured packages, to avoid short cut flows to gain an optimal surface area over the column diameter [8]. Therefore, it is important to understand the hydrodynamics behaviour of the column i.e. pressure drops, vapour and liquid flows, which depends on column internals such as packing selection.

Start-Up and controllability are far more complex for DWC's, due to more complex fluid dynamic relations. One issue is the above mentioned vapour split, which cannot be controlled properly. Design and simulations refer to a fixed value, which must be maintained while operation and under the influence of disturbances [10]. Here, it is possible to maintain steady state in the desired operation point via plant control or a rigorous modelling of the fluid dynamic behaviour, to determine the dependant vapour split and resulting product purifications. This behaviour could be shown via simulations, as the product specifications are sensitive regarding the vapour split. The different rectifying zones inside the DWC result in a higher necessary amount of sensors to observe vital measurements to enable sufficient plant control, as well as well-trained plant operators.

Thus the higher effort in simulation, control and construction of a DWC limits applications to more complex separation processes, like close boiling multi-component system, where no simple side straw column could be used. One asset is the higher degree of freedom of DWC's, as it enables multi-purpose plants for a variety of separation tasks for a fixed design of column and utilities [14]. For suitable applications in multi component systems DWC could be a unit of choice, as it reduces installation costs and offers the vital advantage of an internal heat integration concept compared to common applications.

5.0 Conclusion and Outlook

This work outlines the modelling and simulation work of a DWC using four column configuration model for fatty acid separation. In addition, an insight to the technical aspects is also highlighted. Our steady state rigorous simulations show the feasibility of the DWC under satisfying purification specifications. However, the overall technical process is more complex in terms of controllability and set up. Especially the fluid dynamic behaviour has to be understood to carry out proper rigorous modelling and simulation and thus be able to set up

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an appropriate plant control. In conclusion, it is feasible to fractionate fatty acid using DWC instead of the conventional two column separation. It is interesting however to compare both option and will be our future works. Other than that, our future work will also focus on the installation of a mini-plant, based on first simulations and design. Hence, existing models could be validated, extended or parameterized. Furthermore, start-up and dynamic behaviour will be investigated, as well as control and optimization strategies.

6.0 Acknowledgement

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