Assessment of heat pumping technology in oleochemical fatty acid fractionation

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Assessment of heat pumping technology in oleochemical fatty acid fractionation

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Abstract. Similar to petroleum industry, major energy consumption in oleochemical plants is also dominated by separation process in order to obtain purified oleochemical cuts. Combination of the distillation column with heat pumping system has emerged as one of the most popular techniques in heat integration. Although heat pumping technology has been proven to be effective in petroleum separation, the research on this technology in oleochemical separation has not yet been discovered. Hence, it would be appealing to investigate the feasibility of integrating heat pump technology with distillation units in hopes of reducing energy usage in the separation of oleochemical products. In this study, two configurations of heat pumping system, namely direct vapor recompression (VRC) and bottom flashing heat pump (BFHP) are simulated in Aspen Plus particularly for fractionation of palm kernel oil (PKO) fatty acid. Proper selection of thermodynamic package is discussed in detail. Only three major components of PKO-based fatty acid are involved in the simulation in order to arrive at simple simulation and easy convergence. Simulation results indicates that both configurations of heat pump can be feasibly integrated with the distillation column. However, to satisfy the heating and cooling requirement, supply of make-up utility is necessary.

1. Introduction

Over the past decades, most research in separation processes has emphasized the use of heat integration approach which not only provides economic benefits but also reduces the greenhouse gas emissions [1]. Principally, the effective separation process involves the supply of heat at an elevated temperature in the reboiler and reject the heat at a low temperature in the condenser [2]. Due to the significant temperature difference between the reboiler and condenser, the overall thermodynamic efficiency of a distillation column is considerably low, which is typically ranging from 5% to 20% [1]. In light of this, distillation has become an utmost priority for general improvement in energy efficiency in most chemical plants.

In the history of energy-efficient distillation development, heat integration has been thought of as a key factor in reducing the energy consumption in the column. The most promising external heat integration approach is the association of heat pumping with distillation unit. The idea of heat-pump assisted distillation (HPAD) lies in the fact that available heat sources and heat sinks within the distillation process may be used for heat recovery. A heat pump is purposely used in an effort to fully utilize the waste heat released from the condenser to assist the evaporation in the reboiler [3]. Of all the available systems, vapor recompression (VRC) is the most popularly known HPAD amongst the researchers. Application of HPAD system would be beneficial to reduce the associated utility costs, by making use of waste heat either from excess vapor at any stages in the stripping section or directly from overhead vapor to aid the evaporation process in the reboiler. There are various possible VRC flowcharts can be employed depending on the influencing factors of the process system. Typical VRC configurations in distillation process are direct VRC and bottom flashing heat pump (BFHP).

The research on heat-integrated distillation using HPAD method to date has tended to focus on petroleum processes and very few writers have been able to draw on any systematic research into energy-efficient distillation process in oleochemical plants, let alone the integration of the column with heat pumping and other intensified technologies. The main challenges are coming from the limitations in familiarity and flexibility of oleochemicals which will lead to a complexity in operation; high degree of freedom [4]. Nonetheless, one published literature has successfully developed a model of fatty acid fractionation in a dividing wall column (DWC), closely represented by a four-column configuration [5]. Though the study requires more works on its design controllability, it offers some important insights into integrating the heat integration system to the existing column design.

This present work attempts to demonstrate that the fractionation of palm-based fatty acid in conventional distillation column can be feasibly integrated with the VRC technology. The models are developed using Aspen Plus V10 simulator and the thermodynamic package that is well-suited the process is selected based on the validation process as explained in the methodology section.

2. General process description of fatty acid fractionation

Fractional distillation of oleochemical fatty acid is commonly carried out by means of sequential separation, employing two units of conventional distillation column (CDC) to purify and separate heavy cut (C16-C18), medium cut (C12-C14) and light cut (C8-C10) [5]. The process is operated under vacuum, most of which ranges from 5 to 80 mbar [6]. Due to its heat sensitive characteristic, the chemical decomposition of fatty acids can be avoided if the operating temperature is kept between 180-250°C [7]. The pressure drop within the column should be retained as low as possible, in such a way that the difference between top column pressure and bottom column pressure is 40-60 mbar [7].

3. Principle of distillation column with vapor recompression system

3.1. Direct vapor recompression (VRC)

As illustrated in figure 1, this configuration eliminates the employment of a condenser, as the vapor leaving the top of the column is straight out sent to a compressor. For the purpose of introducing the latent heat of condensation into the reboiler, the overhead stream must be compressed to a point where the temperature is sufficiently high for an efficient heat exchange [8]. In the compression stage, saturated vapor might condense in the compressor. The consequence from this unfavorable situation is that the available latent heat cannot be fully utilized to vaporize the liquid stream in the reboiler [9]. Nonetheless, condensation of the fluid can be avoided by superheating the stream in a superheater prior to compression [8-9]. Large temperature difference indicates high compression ratio, which requires more mechanical works [9-10]. For that reason, the VRC is only considered as cost-effective if the temperature difference is small [10]. The heat transfers from compressed vapor to bottom product occurs through a heat exchanger which operates as a combination of a reboiler and a condenser [11]. In practice, partial condensation might take place during heat transfer process. In view of this, the stream must be further cooled in a trim condenser to a temperature that will not make it vaporized when its pressure is reduced to a column pressure through a throttling valve [9, 12]. The saturated liquid will be then returned to the column, whilst the remaining liquid is discharged as distillate [12]. On the other hand, the saturated vapor in bottom stream is separated from its liquid in the flash drum and recycle to the column whereas the liquid outlet is discharged as bottom product [9, 12].

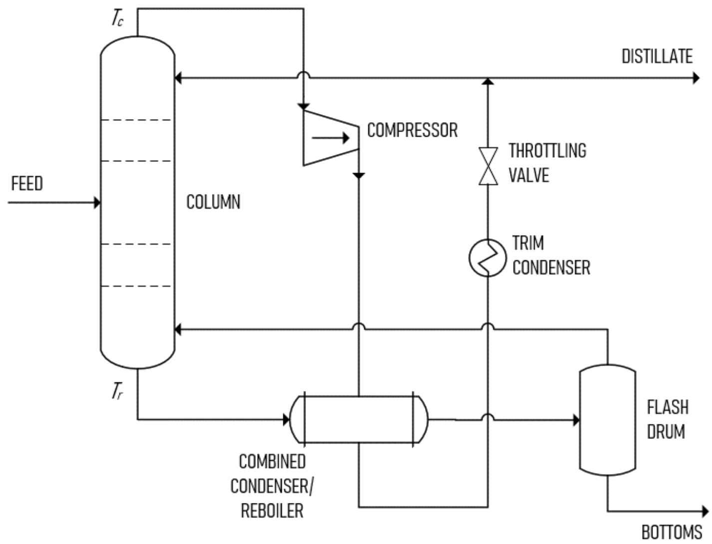

Figure 1. Typical configuration of distillation column with direct VRC system.

3.2. Bottom flashing heat pump (BFHP)

In this heat pump system, the bottom liquid is expanded in a valve to decrease its temperature, bubble point and pressure so that it can be heat exchanged with top vapor stream in a heat exchanger [13]. The bottom stream is flashed until its dew point temperature is much lower that the top vapor temperature [14]. After passing through the heat exchanger, the bottom outlet stream is recompressed in a compressor to the column pressure, increasing the temperature as well. Due to that, the stream needs to be air-cooled so that it can be recycled to the column. Similar to direct VRC system, the vapor is separated from liquid in a flash drum and sent to the column as boil-up, whilst the liquid is discharged as final bottom outlet. In the event that the boil-up is not sufficiently produced, a trim reboiler might be needed to supply the remaining boil-up. For comparison purposes, the condensed top outlet with similar distillate flow rate in the CDC is discharged as a final top product, and the rest is recycled to the column as reflux. Figure 2 shows the standard configuration of BFHP.

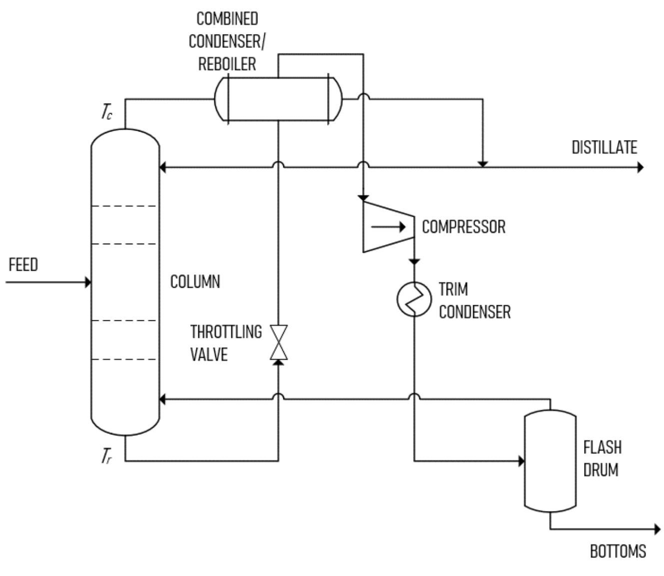

Figure 2. Typical configuration of distillation column with BFHP system.

4. Simulation Methodology

4.1. Feed data selection

In this study, the feed was adopted from Othman and Illner [5] which utilizes industrial palm kernel oil (PKO) based fatty acid. To ease the simulation process, three major compositions of the fatty acid as tabulated in table 1 were used for feed stream input.

Table 1. Major components in PKO based fatty acid.

Component	ID (Aspen Plus)	Formula	Mass fraction	Dipole moments (MUP)
Lauric acid	1-DOD-01	$C_{12}H_{24}O_2$	0.663	2.761
Myristic acid	N-TET-01	$C_{14}H_{28}O_2$	0.227	1.679
Palmitic acid	N-HEX-01	$C_{16}H_{32}O_2$	0.110	1.739

4.2. Selection of thermodynamic model

Many researchers and engineers overlook the importance of choosing an appropriate thermodynamic model prior to carrying out the process simulation in the process simulator. Improper selection will result in a poor performance of the developed process model, or worse, inaccurate result will be generated for the overall simulation. Apparently, there are many thermodynamic models available to choose from and the selection method can be facilitated by using a decision tree [15] which provides appropriate heuristic for better screening options.

As can be seen in Table 1, all three major components of PKO based fatty acid possess dipole moments (MUP) value larger than zero, so as to indicate that the feed to the distillation column is polar fluid. Given that the fatty acid is non-electrolyte system with pressure under 10 bar, it is suggested by the decision tree that the suitable models for this study are NRTL, Wilson, UNIQUAC and UNIFAC. This is inconsistence with previous studies where the thermodynamic model used in fatty acid fractionation were Soave-Redlich-Kwong [5] and Lee-Kesler-Plocker [16]. To determine whether the suggestion from the decision tree is the best choice, further validations for the suggested models as well as the ones used in the published literatures were thoroughly carried out. The validation process using average absolute deviations (AAD) calculations using equation (1) is summarized in table 2.

$$AAD = \frac{\sum_i^n \left| T_i^{exp} - T_i^{pred} \right|}{n} \tag{1}$$

The model predictions results were validated against experimental data from National Institute of Standards and Technology (NIST) available in the Aspen Plus databank. The binary experimental data that could be retrieved from NIST Thermodata Engine (TDE) is only myristic acid/palmitic acid binary system. Under these circumstances, analysis for all listed models was also done for myristic and palmitic acid system to generate more reliable comparison data. The AAD value for each model indicates how much it deviates from the base data. For comparison purposes, the temperature for model predictions was extracted at similar liquid mole fraction of experimental data.

From table 2, it was clearly observed that NRTL, Wilson, UNIQUAC and UNIFAC models acquired considerably small differences which is in agreement with the decision tree. UNIQUAC model has the lowest AAD value which suggests that it is the most suitable model to be used when involving fatty acid components. LK-Plock model, on the other hand, proved the invalidity of previous researches that have employed the particular model for fatty acid process simulations. While SRK model deviations was very much smaller than that in LK-Plock, it is still not the best one to be used.

Table 2. AAD of thermodynamic model predictions from experimental data in Aspen Plus.

Liquid	TDE	Model prediction, T_{pred} (K)					
fraction	T_{exp} (K)	NRTL	Wilson	UNIQUAC	UNIFAC	LK-Plock	SRK
0.000	465.150	463.908	463.908	463.908	463.908	457.611	461.960
0.044	563.149	462.752	462.760	462.751	462.659	455.850	460.728
0.160	461.148	459.904	459.921	459.917	459.664	452.124	457.772
0.303	458.147	456.751	456.765	456.790	456.461	448.746	454.605
0.502	454.145	452.926	452.931	452.983	452.689	445.327	450.866
0.629	452.145	450.770	450.779	450.829	450.603	443.606	448.795
0.840	449.644	447.630	447.630	447.654	447.565	441.208	445.769
1.000	447.143	445.546	445.546	445.546	445.546	439.631	443.751
AAD		**1.3095**	**1.3038**	**1.2865**	**1.4469**	**8.3209**	**3.3030**

4.3. Base case: Conventional distillation column (CDC)
The shortcut model in Aspen Plus, DSTWU is usually used to estimate the column performance such as number of stages and reflux ratio, which will later be used for rigorous distillation known as RADFRAC. The column capacity for PKO based fatty acid fractionation in this simulation study was 9000 kg/hr and feed mass compositions were set as tabulated in Table 1. The feed vacuum pressure and temperature throughout this work were taken to be 20 mbar and 180°C, respectively. The estimation of reflux ratio value was determined using DSTWU results and with reflux ratio value of 0.88, 19 stages were required to reach the desired separation. Due to its very low-pressure operation condition, it was assumed that there was no pressure drop across the column. A simulative investigation into the performance of two VRC configurations was carried with comparison to this base case. In all simulations, the feed was introduced to the column at the same condition, and both distillate and bottom product were required as saturated liquid at 20 mbar.

4.4. Distillation column with direct VRC system
For the purpose of arriving at simple process simulation in the simulator, the degree of freedom must be reduced to avoid convergence issues. In this study, the assumption made was that no condensation occurs during compression. The overhead outlet of CDC was directly fed to the compressor with an outlet pressure of 40 mbar, where the temperature was hot enough to supply required heat for bottom liquid heating. The temperature difference was kept within 5-7°C for economical reason. In the heat exchanger, compressed vapor exchanged heat with the bottom liquid stream, where the pressure drops of shell and tube side were neglected. However, the recovered heat was insufficient to satisfy the heating requirement in the reboiler. Thus, a trim reboiler was employed to provide the remaining heat. The throttle valve brought back the stream to its column operating pressure and was then subcooled in the cooler or trim condenser prior to stream splitting. It is very important to make sure that the stream does not vaporize because the reflux stream must return to the column as liquid as well as for comparison purposes, the product streams must be discharged as saturated liquid. In the splitter, mass flowrate of distillate stream was set to be the same as in base case. A portion of liquid is recycled to the top column as reflux. Meanwhile, the heated stream was introduced into the flash drum. The vapor stream was returned to the bottom of the column as boilup. The final product of bottom liquid with similar flowrate as in the CDC was obtained by manipulating the operating temperature of the flash drum. Figure 3 shows the simulated process flow diagram of the system in Aspen Plus. In this simulation, the typical RADFRAC column was substituted with a simple RADFRAC absorber without both condenser and reboiler.

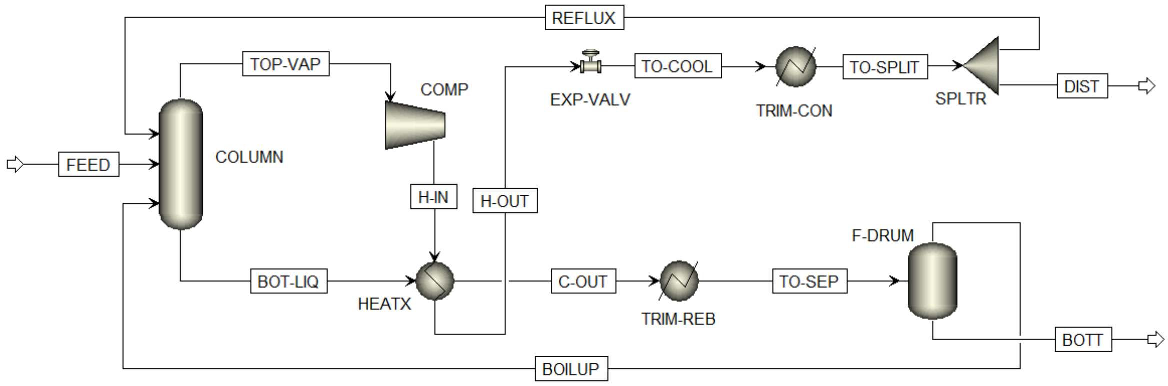

Figure 3: Flowsheet of the direct VRC-assisted distillation column.

4.5. Distillation column with BFHP system

In this configuration, the pressure of the bottom liquid was reduced to 8.5 mbar and the temperature was decreased to 172.38°C to enable heat exchange with the column top vapor stream. Similarly, make-up heat was also required in this system due to insufficient heating duty provided by top column vapor. Hence, additional of a trim reboiler in the flowsheet as can be seen in figure 4. The bottom column outlet entered the compressor to be recompressed to the column operating pressure before being separated in the flash drum. However, a superheater was needed to ensure the stream entering the compressor contained maximum amount of vapor for compression, otherwise the system would not be converged. The recompressed bottom column outlet stream was cooled and sent to the flash drum. Vapor outlet was recycled as boil up and liquid product was discharged as final bottom product. The hot outlet stream of the heat exchanger was straight away divided in the splitter as no cooling needed. Liquid reflux returned to the column while the other portion of liquid was withdrawn as final distillate product.

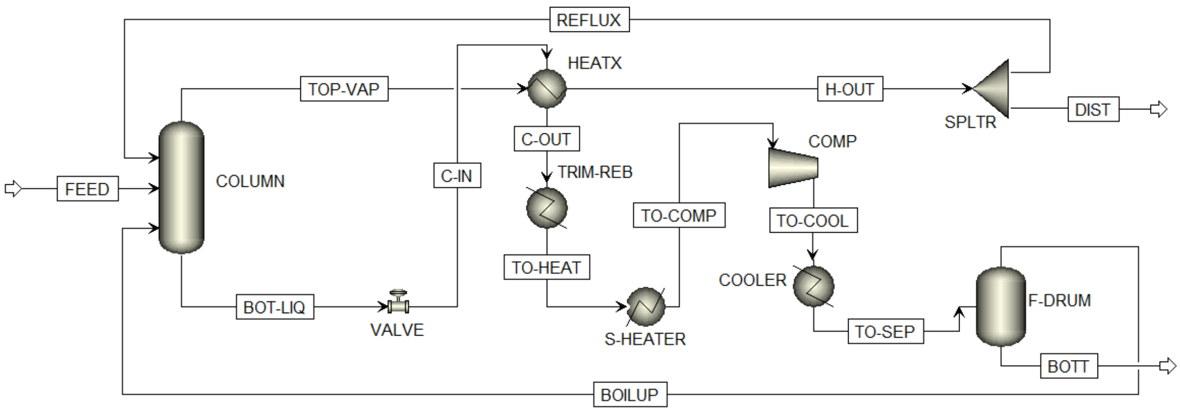

Figure 4. Flowsheet of the BFHP system.

5. Results and discussions

In reviewing the literature, no study was found on the simulation of oleochemical separation using heat pumping scheme. In the current study, comparing the conventional column with two HPAD configurations generates significant differences in energy requirement. The simulation process was straightforward for the VRC model, however for the BFHP, some manipulations of the variables were needed to get the system converged. The process conditions of product streams for all simulations are presented in table 3.

Table 3. Process conditions of product streams.

	CDC	VRC	BFHP
Purity of $C_{12}H_{24}O_2$ in distillate (%)	99.89	99.89	99.78
Distillate temperature (°C)	181.11	180.40	181.50
Bottoms temperature (°C)	195.18	195.17	195.17
Condenser load (kW)	882.27	-	-
Reboiler load (kW)	943.15	-	-
Recovered top vapor heat (kW)	-	822.31	882.26

*(-) Not applicable

As can be seen from the table, both HPAD configurations recorded high purity of the desired product, $C_{12}H_{24}O_2$ in the distillate stream. Product temperatures of integrated columns also showed very minimal differences than in the CDC. Meanwhile, the systems proved an excellent performance in recovering heat from column overhead vapor to aid in heating process of the liquid in the column bottom stream.
It is no doubt that an immense amount of energy could be conserved with both HPAD systems. Heat pumping technology, though not completely, but reduced more that 80% of reboiler duty and more than 70% of condenser duty. Table 4 summarises the external heating and cooling duty for direct VRC and BFHP arrangements after the elimination of the condenser and reboiler units as compared to conventional column. The mechanical work in the compressor is also compared in the table for both integrated systems.

Table 4. Summary of relative performance of all simulations.

System	CDC	Direct VRC	BFHP
Cold utility requirements (kW)	882.27	97.56	285.74
Hot utility requirements (kW)	943.15	127.21	425.14
Mechanical work requirements (kW)	-	38.95	76.53

*(-) Not applicable

In direct VRC case, approximately only 11% of cold utility is required than in the CDC. Further cooling was necessary to decrease the vapor fraction of the reflux stream. The hot utility input in this system is coming from the trim reboiler which was purposely used to supply auxiliary heat for bottom liquid reboiling. Even so, 87% of column top vapor heat could be recovered to provide heat for the bottom liquid, which is quite a promising option.

For BFHP case, if we look closely at the utility requirement values, it is apparent that this system requires substantially high external utilities to satisfy the process requirement in comparison to direct VRC. The high heating duty was contributed by two equipment as depicted in figure 4. Even though the recovered heat using this method was 94%, higher than that in the VRC, the superheating of the bottom column outlet has directly escalated the number of hot utility requirements. This situation could not be avoided because the vapor content in the stream after exchanging heat was insufficient to undergo compression, therefore the need to superheat it until vapor fraction has reached 1.00. Due to this, 364.36 kW of energy was demanded only for superheating. On the other hand, the cooling duty for the BFHP as shown in the table is also considerably high due to an increased temperature after the compression.

The elimination of overhead condenser and bottom reboiler implies that the amount of external cooling utility is significantly decreased thus will be reducing more operation costs. However, it is compulsory in heat pumping method to employ a compressor unit. Unlike the conventional operation, the HPAD economic feasibility highly depends on the compression ratio value, because as a matter of fact, higher compression ratio means more mechanical work. Principally, the operation and capital costs for the implementation of the compressor that is driven by electricity is outrageously expensive. Table 4 reported that the compression work in the BFHP is obviously higher than that in the direct VRC. Not only the BFHP system demanded more external utility supply, but it also consumed more electricity. Taken together, the VRC configuration is in favour in this assessment over the BFHP.

6. Conclusions

This study set out to conduct an assessment of heat pumping method in oleochemical fatty acid separation. The results of this study indicate that it is technically feasible to integrate the system with the process. The performance of the direct VRC configuration is apparently better than the BFHP. Although the consumption of external heat source is decreased in the reboiler, along with the reduction of condenser and its utility usage, the HPAD additionally employs a compressor that is operated by electricity, which is far more expensive than the thermal utility. It is a proof that a systematic analysis of the HPAD is necessary from the energetic and economic aspects. There will be certainly a trade-off between operational and capital costs to operate the system. Also, it will be more promising if the simulation process is thermodynamically correct and one of the ways is to properly select the thermodynamic package prior to run the simulation. Further studies, which take the effects of thermodynamic measures to the HPAD system into account, involving all components in the feed stream, will need to be undertaken. This research will serve as a base for future studies in energy efficient oleochemical separation.

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