Comparative study of Heat Pump Assisted Distillation Column and Its Application for Pressure Swing Distillation Process

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Abstract. Two of the well-known heat pumps assisted distillation column scheme are direct vapor recompression and bottom flashing. The comparison between the two schemes was systematically studied for binary mixture of non-azeotropic benzene-toluene system. Simulation was carried out using Aspen Plus software. The best scheme was selected based on economic evaluation (utility cost and TAC reduction). The application of both schemes was also studied for pressure swing distillation process. Pressure swing distillation is one of the most common methods for separating pressure-sensitive azeotropic system. Direct vapor recompression scheme and bottom flashing scheme can be applied to enhance the energy savings. The minimum-boiling homogeneous azeotropic mixture of methyl acetate-methanol was chosen as representative in process simulation.

1. Introduction
Distillation plays an important role in separation process. However, it consumes a huge amount of energy with low efficiency. In order to increase efficiency, several methods have been proposed to enhance the energy efficiency of existing distillation column such as the use of side heating and cooling [1] and pump-around [2]. In the other hand, thermodynamic analysis has been performed to give better understanding in the overall energy balance in distillation system [3-6]. From the design basis point of view, several researchers have been developing new ideas in the recent decade. These ideas mainly based on energy utilization between rectifying section and stripping section. Two of the most common methods to utilize heat in distillation column are heat pump and heat integrated distillation column (HIDiC). Both methods use the same principle of heat integration. The main difference between them is that heat pump only integrate heat in specific section (condenser, reboiler, and some stage in distillation column), but HIDiC integrate heat throughout the column. Although application on industrial scale is still under consideration, the concept of HIDiC is gaining more attention because it gives energy saving up to 30-50% over to the conventional column [7]. However, HIDiC configuration is more complicated compared to the heat pump configuration from the operation and control point of view. Shenvi et al., [8] was conclude that HIDiC configuration does not always superior in heat integration performance when compare to the simpler heat pump configuration in some cases.

Heat Pump Assisted Distillation Column (HPADC) reduce the energy use in distillation column simply by using the heat integration between reboiler and condenser. There are two categories of HPADC: mechanical heat pump and absorption heat pump. Mechanical heat pumps involve compression of the vapor product leaving from the top stage and then using it to heat up the reboiler, or expansion of the liquid product leaving the bottom stage and then using it to cool the condenser. While absorption heat pump involves the circulation of external working fluid and the utilisation of absorption process [9]. Absorption heat pump has been applied in desalination process and give the improvement in the energy efficiency [10-11]. The main issue of absorption heat pump is related to the safety concern toward the toxicity of the working fluid which limit its application. Therefore, mechanical heat pump offers a simpler structure, lower investment and more environmentally friendly [12].
The mechanical heat pumps can be further divided into three configurations: direct vapor recompression, bottom flashing, and external vapor recompression [13]. Direct vapor recompression utilise the latent heat of compressed overhead vapor (hot stream) to reboil the bottom liquid (cold stream) in a combined condenser-reboiler heat exchanger. The hot stream leaving the heat exchanger is expanded to its initial pressure and divided into two streams: reflux and distillate (top product). In the bottom flashing, instead of use the reboiler, the boilup liquid pressure is reduced to a certain value so that the temperature of the stream is decrease and can be used to condensed the overhead vapor. The external vapor recompression using the same idea but the work of heat pump between the reboiler and the condenser employ external working fluid [12]. Only the first two of those configurations is discussed in this paper because external vapor recompression involve the use of working fluid and face identical problem with absorption heat pump.

The application of direct vapor recompression and bottom flashing was investigated by several authors from different point of view. The detailed model on ethanol-water separation with direct vapor recompression was developed by Enweremadu et al. The result showed that the incorporation of several working parameter such as overall heat transfer coefficient and the pressure drop across the compressor gave the greater value on the actual column [14]. Diez et al. performed a simulation on the separation of i-butane/n-butane using four different configurations: conventional column, vapor recompression column, bottom flashing, and absorption heat pump [9]. When compared to conventional distillation column, both vapor recompression column and bottom flashing gave the same degree of energy reduction without significant increase in capital cost. On the other hand, the absorption heat pump was considered to be not applicable for the system. Six different configuration of vapor recompression was chosen by Kazemi et al. to be applied for benzene-toluene separation [15]. The system was simulated using Aspen HYSYS and the best configuration was chosen based on the economic evaluation. The same binary mixture of benzene-toluene is discussed in this paper but the configuration is different. The direct vapor recompression and bottom flashing are applied and comparative study for both configurations is performed. The application of direct vapor recompression and bottom flashing is also studied for pressure swing distillation process.

Azeotropic mixtures are known to be difficult to be separated in conventional column. There are various methods to be chosen, but when the azeotropic composition easily shift with pressure (pressure sensitive), then pressure swing distillation process is the best choice. In the pressure swing distillation process, there are two columns with different pressure. Product with high purity can be obtain from one output stream of the columns and the composition of another stream which close to its azeotrope is recycled to different column. Stream configuration depends on the azeotropic mixture characteristic. Distillate streams are recycled in minimum-boiling azeotropic systems and bottom stream are recycled in maximum-boiling azeotropic system. There are several possibilities of heat integration in pressure swing distillation process due to the inherent opportunity of energy conservation [16]. Simulation on heat integrated pressure swing distillation was investigated on the separation of minimum boiling point azeotropic mixture of ethyl-acetate ethanol [17]. This paper evaluates the possibility of using heat pump in pressure swing distillation of the minimum-boiling homogeneous azeotropic mixture of methyl acetate-methanol. The combination of direct vapor recompression and bottom flashing scheme can be applied to applied enhance the energy savings. All configuration is simulated using Aspen Plus process simulator and Aspen Plus economic analyzer. The objective of this paper is to compare the economic feasibility of direct vapor recompression and bottom flashing in distillation column for the binary system with and without azeotrope.

2. Simulation Process
The simulation covers of two main part i.e. comparative study of heat pump assisted distillation column and its application for pressure swing distillation process. For the first part, benzene-toluene system was used as case study and there are two configurations namely distillation column with direct vapor recompression and distillation column with bottom flashing. For the second configuration there are two categories namely conventional pressure swing distillation columns and heat pump assisted pressure swing distillation columns. Aspen Plus V9.0 and Aspen Plus Economic Analyzer under license from Aspentech [18] are used to simulate all configuration. Peng-Robinson property method was used as based method for comparative study [19] and NRTL property method was used as based method for pressure swing distillation [20].
2.1. Base case for comparative study
The equimolar mixture of 100 kmol/hr benzene and toluene was first heated to reach vapor fraction value of 0.5 and then fed to distillation column. Before execute in rigorous simulation using RADFRAC block, this system was simulated first in shortcut simulation using DSTWU block to obtained main parameters such as distillate to feed ratio, reflux ratio, number of actual stage and feed stage. The column was designed to produce benzene and toluene with minimum purity of 99.5 %wt. From the shortcut method, the total number of actual stages is 40, feed stage is located on the 26th stage, distillate to feed mole ratio is 0.5 and reflux ratio of 2.1 is used. The distillation column operates at atmospheric pressure.

2.2. Distillation column with direct vapor recompression
Column configuration for direct vapor recompression is illustrated in Figure 1a. The vapor stream from the top of the column is compressed to a pressure of 3 atm. The compression process increases the stream temperature from 80 to 124 °C. Therefore, the outlet stream leave from compressor is higher than bottom stream temperature (112 °C). Both streams then exchange heat in a combined condenser and reboiler (HEX1). The hot stream from compressor allow the cold stream to be partially boiled. The boilup ratio is adjusted to meet the column requirement. The vapor-liquid phase from HEX1 is separated in flash drum. The vapor phase is recycled to distillation column and the liquid phase is obtained as bottom product with the purity of toluene is 99.9 wt%. The hot stream outlet temperature of HEX1 is 121 °C with the vapor fraction of 0.29. This can be further utilised to preheat the feed on HEX2 until the stream temperature reach 107 °C and completely condensed before entering the expansion valve. Due to expansion process, some vapor is generated and the vapor fraction of the stream increased to the value of 0.13. Before splitting the stream, cooler is used to condensed the generated vapor. The saturated liquid stream from cooler is then divided into two streams: one stream as a reflux and the other one as distillate with the purity of benzene is 99.9 wt%.

2.3. Distillation column with bottom flashing
Column configuration for bottom flashing is illustrated in Figure 1b. In this configuration, the bottom stream of distillation column is flow through a valve to reduce its pressure up to 0.33 atm. This pressure reducing process allows the stream temperature to decrease and vapor fraction to increase. The outlet stream temperature and the vapor fraction are 73 °C and 0.20, respectively. This stream become the cold fluid in combined reboiler-condenser (HEX1) and receive heat from the vapor stream out of the top of column as the hot fluid. The cold stream outlet temperature is adjusted to be 75 °C to reach the minimum temperature difference within 5 °C with the hot stream inlet temperature. Because of this adjustment, the hot stream outlet vapor fraction is 0.14 and additional cooling is provided by cooler to condense the remaining vapor. This stream is divided into reflux and distillate stream. The cold stream out from HEX1 is then compressed back to 1 atm and consequently the outlet temperature increase to 114 °C. Compressor outlet stream is a superheated vapor, hence it still has high level of energy and this can be utilised to preheat the feed until some vapor is condensed and taken as bottom product. The remaining vapor is recycled back to the column and product purity from both distillate and bottom product is 99.9 wt%.
2.4. Base case for pressure swing distillation columns

The equimolar feed of methyl acetate-methanol is taken as a representative system in this simulation. This system was also investigated by Zhang et al. to study the heat integration possibility and controllability of the system [20]. However, the HP column pressure used in this simulation is lower than the HP column pressure used in their simulation and the detailed column specification is different. The total number of stages of LP column and HP column are 30 and 40, respectively. Fresh feed of methyl acetate and methanol (100 kmol/hr, saturated liquid) enters LP column at the 12th stage and recycle stream from the top of the HP column enters LP column at 26th stage. LP column operates at atmospheric pressure and HP column operates at 9 atm. The bottom product obtained from LP column is methanol 99.9 wt%, while the bottom product obtained from HP column is methyl acetate 99.9 wt%. The top product of LP column is fed to HP column at 24th stage after its pressure is raised to 9 atm and the top product of HP column is recycled to LP column. The process flowsheet is shown in Figure 2.

2.5. Heat pump assisted pressure swing distillation column

The simulation of heat pump assisted pressure swing distillation column consist of three configurations with the combination of direct vapor recompression and bottom flashing for both columns: double direct vapor recompression (DDVR), double bottom flashing (DBF), and combined direct vapor recompression-bottom flashing (CDVRBF). All configuration is setting up to meet the same product requirement with base case configuration for pressure swing distillation and the detailed heat integration scheme is identical with direct vapor recompression and bottom flashing in benzene-toluene separation. DDVR configuration adopt direct vapor recompression in both columns. DBF configuration adopt bottom flashing in both columns. Meanwhile, CDVRBF adopt direct vapor recompression in LP column and bottom flashing in HP column.

DDVR configuration flowsheet can be seen in Figure 3. Compression ratio of 3 and 1.75 are used in LP column and HP column respectively. Li et al. also proposed this configuration in ethanol-acetonitrile separation system and suggested that maximum compression ratio of 4 should be used [21].
3. Simulation Results and Discussion

Heat pump assisted distillation column offer an advantage to reduce the need condenser and reboiler. Consequently, the utility cost is reduced significantly. The reduction in utility cost, therefore, is the important parameter to choose the best configuration. Another important parameter that need to be
incorporated in economic evaluation is total annual cost (TAC). TAC is widely used and well accepted to show the economic feasibility of a process [22] that can be express as follow:

$$\text{TAC} = \frac{\text{total equipment cost}}{\text{payback period}} + \text{total utility cost}$$

(1)

Where the total equipment cost consists of column cost, heat exchanger cost, and compressor cost. The cost of supporting equipment such as pump, expansion valve, and accumulator cost are eliminated because the value is relatively inexpensive and gives the same in all configuration [17]. Payback period of 3 years is chosen for this evaluation and total utility cost consists of cooling water, steam, and electricity cost. All associated costs are given in USD and were obtained from Aspen Plus Economic Analyzer (APEA).

The economic evaluation result from comparative study in benzene-toluene system can be seen in Table 1. Total equipment cost for base case is the lowest, but its total utility cost is the highest, dominantly from steam consumption. In heat pump assisted distillation column, instead of reboiler, the combined condenser-reboiler is used to exchange heat and steam consumption is totally replaced by the electricity consumption. All columns have the same internal specification i.e. total number of stage and molar flow rate, so that the column cost for all configuration is similar. Direct vapor recompression and bottom flashing show different trend in total equipment cost and total utility cost. When compared to bottom flashing, direct vapor recompression has lower total equipment cost but its total utility cost is slightly higher than that of bottom flashing. There are the two main equipment cost in of bottom flashing that contribute to give the higher equipment cost: preheater and compressor. This is mainly due to the stream leaving from compressor is in superheated vapor that gives low heat transfer coefficient. The low value of heat transfer coefficient means additional heat transfer area in the preheater. The calculated exchanger area of preheater in direct vapor recompression configuration is 228 ft$^2$, while in bottom flashing is 338 ft$^2$. Moreover, the compressor in bottom flashing has the larger actual gas flow rate inlet than that in direct vapor recompression, this led to higher compressor cost.

Utility cost reduction for direct vapor recompression and bottom flashing are relatively at the same value. In other words, from utility reduction point of view, direct vapor recompression and bottom flashing give the same benefit. However, From TAC reduction point of view, both heat pump configuration offers an attractive result. The superiority of heat pump assisted distillation column over distillation column also reported by Diez et al in the separation of i-butane/n-butane system [9]. In this simulation, direct vapor recompression gives the higher TAC reduction, almost three times higher than that of bottom flashing configuration. This result is slightly different with the result reported by Diez et al. where bottom flashing showed to be more attractive than direct vapor recompression. This is maybe due to the system characteristic and the difference in detailed configuration.

The economic evaluation for azeotropic system methyl acetate-methanol can be seen in Table 2. Column cost of HP column is more expensive than column cost of LP column because the total number of stages in HP column is higher. The HP column cost in all configuration is at the same value, but the LP column cost in DBF is 10% higher than others. This is due to the fact that column pressure of LP column is adjusted to 3 atm. This adjustment also contributes in the higher value in LP column equipment cost. On the utility cost, the very expensive steam cost in base case configuration is essentially reduced by 68-78 % in heat pump configuration.

| Table 1. Economic evaluation for benzene toluene system |
|--------------------------------------------------------|
| Item | Base case | Direct vapor recompression | Bottom Flashing |
| Distillation column | 269100 | 269100 | 269100 |
| Preheater | 10800 | 12900 | 76900 |
| Reboiler | 16300 | - | - |
| Condenser | 15100 | - | - |
| Heat exchanger | - | 28600 | 14900 |
| Additional cooler | - | 9700 | 8700 |
| Compressor | - | 691900 | 1058700 |
Heat pump assisted distillation column in azeotropic system shows positive effect on the total equipment and total utility cost. Although the total equipment column cost is 4-5 times higher than base case column, the total utility cost is significantly reduced. The TAC for all configuration also gives the same trend heat pump assisted distillation column in non-azeotropic benzene-toluene system. From the utility cost and TAC reduction, among the proposed configuration, DDVR configuration gives the best value. Although the main concern in simulation is different, this result is agreed with simulation result conducted by Li et al [21] that compared the heat pump assisted distillation column with heat integrated distillation column.

Table 2. Economic evaluation for azeotropic methyl acetate-methanol system

| Item | Base case | DDVR | DBF | CDVRBF |
|------|-----------|------|-----|--------|
| **Equipment cost** | | | | |
| **LP Column** | | | | |
| Distillation column | 225300 | 225300 | 247900 | 225300 |
| Reboiler | 18100 | - | - | - |
| Condenser | 40900 | - | - | - |
| Heat exchanger | - | 25800 | 88300 | 25800 |
| Additional cooler | - | 17300 | 19600 | 17300 |
| Compressor | - | 837900 | 1595000 | 837800 |
| **HP Column** | | | | |
| Distillation column | 303300 | 303300 | 303300 | 303300 |
| Reboiler | 37700 | - | - | - |
| Condenser | 14200 | - | - | - |
| Heat exchanger | - | 56300 | 17200 | 17200 |
| Additional cooler | - | 8600 | 10300 | 8300 |
| Compressor | - | 846200 | 877500 | 877500 |
| **Total equipment cost** | 639500 | 2320700 | 3159100 | 2312500 |
| **Utility cost** | | | | |
| Cooling water | 35268 | 11466 | 18266 | 10178 |
| Steam | 2110650 | - | - | - |
| Electricity | - | 453014 | 670541 | 642720 |
| **Total utility cost** | 2145918 | 464480 | 688807 | 652898 |
Simulation on heat pump assisted distillation column on azeotropic and non-azeotropic system was performed. The economic evaluation result shows that the application of direct vapor recompression in the non-azeotropic benzene-toluene system give the higher utility cost and TAC reduction than bottom flashing. When the same system is adopted in pressure swing distillation column on the separation of azeotropic methyl-acetate methanol, the significant reduction in TAC and utility cost is also achieved. The best configuration in azeotropic system was found to DDVR configuration which the total utility cost reduction of 78.36 % and TAC reduction of 47.52 %.

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