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Simulation and Investigation of the Thermodynamics and Energy of Methanol Purification Units

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ABSTRACT

Methanol is an important industrial chemical, and its synthesis and purification units are among the most widely used ones in the field of energy. The two-column separation unit of methanol has been evaluated from the thermodynamic and energy points of view in the present study. The simulation has been done by Aspen Hysys V11 and the SRK equation has been regarded as the most appropriate equation of state (EOS) for this simulation with the mean relative error (MRE) of 2 %. Then, the design of the heat exchanger network (HEN) has been developed using the Aspen Energy Analyzer V11. Both distillation towers have been evaluated using the pinch technology. As a result, the amounts of the used hot and cold utilities have been LP = 1.482 × 10^8, MP = 1.57 × 10^4, and Air = 1.423× 10^8. Besides, the total heating and cooling targets of the process have been 1.482 × 10^8 and 1.423 × 10^8 respectively. Then, the ΔT_{min} (minimum allowable temperature difference between hot and cold currents) and its effect on the annual cost have been investigated. The optimum value of ΔT_{min} is determined to have better-operating conditions and to meet the design of the HEN economically. Reducing ΔT_{min} increases operating costs and reduces energy costs.

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1. Introduction

The chemical processing sector is closely monitoring energy savings due to recent increases in the fuel price. Modern process simulation techniques are one of the most crucial recommendations to lower production costs and boost economic efficiency for the efficient management of energy resources in order to meet energy-saving targets [1]. Powerful technologies are available to

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measure and discover improvement opportunities through a processing unit by developing an accurate model for estimating energy use [2]. The pinch technology and related methods are the main keys for energy savings in the refining industry for a wide range of purposes [3]. Over the past decades, the Pinch Analysis (PA) has provided physical insights into the design of an optimal energy recovery network involving various sources such as heat [4], power [5], and mass [6]. PA has been initially created to help process plants determine their best energy usage and energy-saving tactics. One of the most effective methods for integrating process energy is the pinch technology. For the ultra-ambient process and sub-ambient temperature, a new concept diagram has been developed due to the restrictions and drawbacks of PA in heat exchanger network retrofitting. The rate of the heat transfer as a function of temperature is the basis for this graph. Concepts like increasing the Heat Exchanger Network (HEN) to conserve energy can materialize using this design [7]. The hybrid system's network of heat exchangers connected to heat exchangers with multiple currents is extracted using the pinch approach. The effect of natural gas composition entering the cycle on system parameters is studied and reported [8]. Lei et al. [9] have introduced the pinch technology to the large-scale cryogenic analysis and created temperature enthalpy diagrams for various refrigeration cycles. The pinch technology, lowering CO_2 emissions and enhancing the fuel quality, have been suggested for the energy analysis [10]. Pan et al. [11] have proposed the pinch technology, temperature-heat diagrams and problem tables for adsorption refrigeration systems. Kaveh Petrochemical Methanol Complex has been enhanced based on the energy-oriented pinch technology using Aspen Hysys and Aspen Energy [12]. Deproteinization and a four-stage pyrolysis gas compression cycle are two industrial processes that incorporate carbon emissions into the structure of a heat exchanger network. Li et al. [13] have developed a better heat exchanger network in terms of the total annual cost and energy efficiency in which carbon emission is reduced.

Methanol, which has the potential to be used as an alternative fuel, is made from a variety of carbon-based raw materials, including coal, heavy oil cuts, natural gas, and naphtha. Currently, natural gas is the most common material for the production of methanol. The related industrial chemical pathway involves indirect conversion using synthetic gas, a mixture of H_2, CO, and CO_2. The process of the production of methanol consists of three basic steps, namely the production of synthetic gas through the steam modification, conversion of synthetic gas to methanol, and separation and purification [14]. It should be noted that the most typical method of separation used in manufacturing methanol is distillation. In the low-pressure methanol synthesis with a Cu-based catalyst in the reactor, crude methanol that comprises water and organic impurities has been purified using a standard two-column methanol distillation procedure. To this date, different energy-saving designs have been planned for the methanol distillation process, among which the Lurgi double-impact double-column design is the most important one in the industry [15]. One of these systems involves dividing the filter column of a two-column design into two distinct columns that run at entirely different pressures, allowing the employment of higher-pressure column headers to re-boil the lower-pressure column [16, 17].

The requirement of an accurate simulation is to choose the appropriate equation of state to predict the thermodynamic properties of the system. In the previous studies, the simulation of the methanol purification has been done, however in the present study, the appropriate equation of state has been selected before the simulation to accurately estimate the thermodynamic properties. Also, the network of heat exchangers and the energy integration have been recently investigated in various processes, however there is no outcome about the purification section of the methanol unit with two separation columns. Herein, in addition to examining the amount of the energy consumption in the purification unit of Methanol production, we have investigated the effect of choosing hot and cold utilities as well as ΔT_{min} on the annual cost of the unit.

2. Methodology

Modeling a variety of industrial processes requires the use of equation EOS which benefits precision, compatibility, quick computation, robustness, and prognostication beyond the context of its application [18]. In this study, three EOS's of Peng Robinson, Soave-Redlich-Kwong (SRK), and Lee-Kesler-Plocker are used. The information about the equations of state and the experimental data of a two-phase equilibrium has been obtained from previous studies [19]. After determining the appropriate equation of state, the simulation process has been performed using the Aspen Hysys V11 software, and the process energy analysis has been performed using the Aspen Energy Analyzer V11 software. In the methanol purification section, the raw methanol output from the synthesis unit, which contains some dissolved gases, especially CO_2, is due to the reduction of two-phase pressure and enters the two-phase separator D-5001 in order for the liquid and vapor phases to be separated. The effluent from the bottom of this separator is sent to the T-5001 distillation tower with the temperature of 40 °C and the pressure of 3 bar. In this tower, the gases dissolved in crude methanol are excreted. The upper and lower operating pressures of the tower are 2.1 bar and 2.4 bar respectively. The exhaust steam from the top of the tower is sent to the AE-5001 air conditioner at a temperature of 84 °C and condenses with air flow. The air conditioner reduces the vapor temperature from the top of the tower by 64 °C, and as a result of this temperature reduction, the vapor is condensed and is sent to the two-phase separation vessel D-5002 for the liquid and vapor phases to be separated. The output steam from the top of this two-phase separator with a temperature of 64 °C and a pressure of 1.9 bar, after passing through the heat exchangers E-5003 and E-5004, reaches the temperature of 120 °C and is sent as fuel to the reforming unit. The output stream from the bottom of the two-phase separating vessel returns to the T-5001 distillation tower as a recycle flow with a temperature of 64 °C and a pressure of 3 bar. The output stream from the reboiler is sent to the T-5002 distillation tower for the final purification. The exhaust vapor from the top of the tower with the temperature of 66 °C is sent to the air conditioner AE-5002, for the initial condensation to the temperature of 65 °C, and in the heat exchanger E-5007, it is completely condensed by the heat exchanger with the flow of cooling water. The condensed stream with the temperature of 40 °C and the pressure of 1.1 bar enters the two-phase separating vessel D-5003. Part of the effluent from the bottom of the flash drum, after passing through the P-5003 pump, is discharged from the unit as a methanol product with the temperature of

40 °C and the pressure of 4 bar, and the rest returns to the tower as a recycle flow (Figure 1).

The process pinch analysis has been carried out to assess the energy usage. It is possible to think about the pinch technology as a means to improve the heat transfer in a processing unit. There are a lot of strategies to reduce the energy consumption in chemical plants, such as refineries, however, mathematical programming approache is one of the most effective ways to conserve the regenerated energy. PA provides trustworthy, practical, and simple thermodynamic information that permits and optimizes the energy use, significantly lowers the resource usage, and lowers manufacturing costs. [20]. In late 1978, Budo Linhoff developed an alternative way to explain energy flows in the heat exchanger networks of the process. Then the principles of thermodynamics are now known as the process synthesis and heat exchanger network design, and are known as the pinch technology and have a long industrial history. Figure 2 shows the network diagram of the existing heat exchanger design.

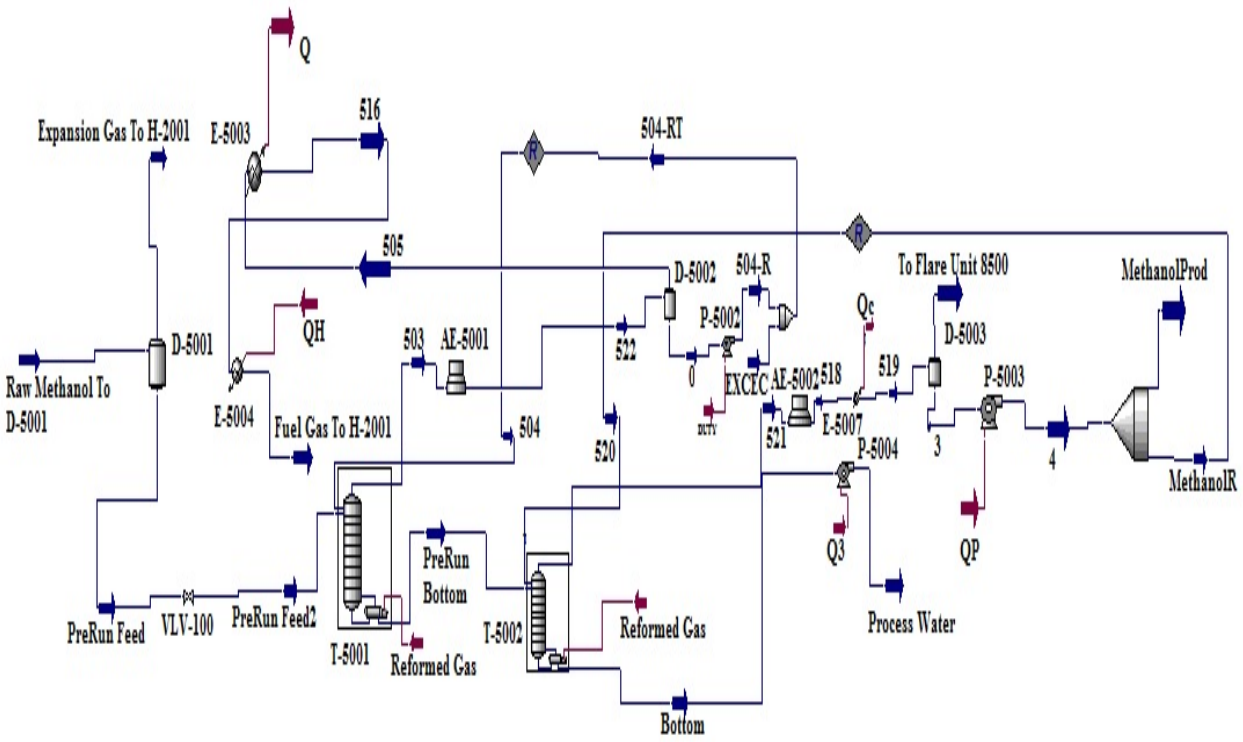

Figure 1. Methanol purification unit.

Table 1
Process and utility streams.

Name	T_{in} (°C)	T_{out} (°C)
505-516	64	40
516-Fuel Gas	40	120
521-519	71.7	40
503-522	85.9	64
PreRun Feed2-PreRun Bottom	93.4	94

PreRun Bottom-Bottom	82.2	85
LP Steam	125	124
MP Steam	175	174
Air	30	35
Cooling Water	20	25

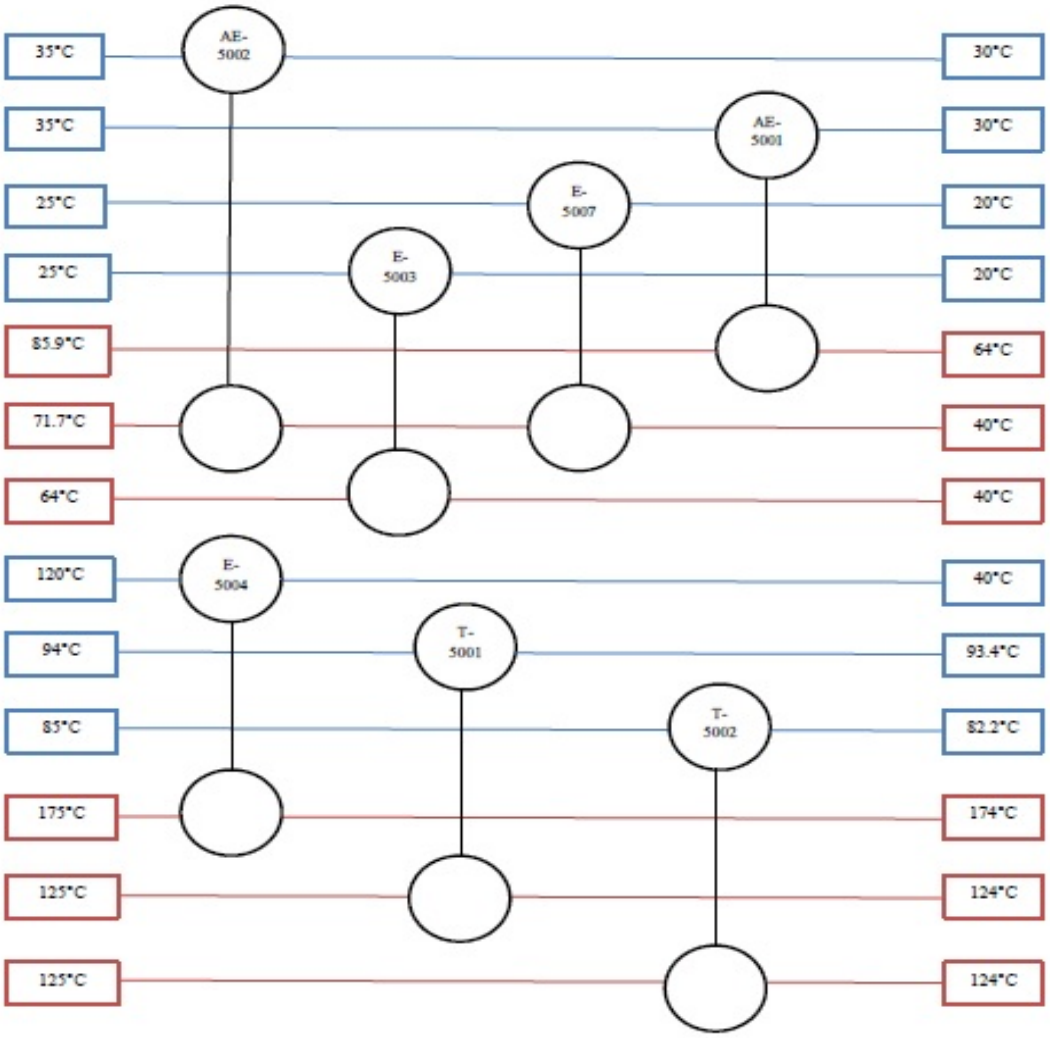

Figure 2. HEN diagram of the methanol synthesis unit design.

3. Results and discussion

For an accurate simulation it is needed to predict the thermodynamic properties of the fluid by selecting the appropriate state equation. It has been shown that the results obtained from the SRK and Peng-Robinson equations of state are not much different from each other [21]. Peng-Robinson and SRK EOS have been successful for vapor-liquid equilibrium computations [22]. Lee-Kesler-Plocker equation has shown significant deviations from the experimental results for highly polar fluids [23]. Interestingly, the SRK equation of state is consistent with the experimental results [24]. As a result, we have employed the SRK equation of state as the most suitable option for simulation. Figures 3, 4 and 5 show a comparison between the

prediction results of the two-phase equilibrium data using thermodynamic models, Peng-Robinson, Lee-Kesler-Plocker and SRK with experimental data respectively.

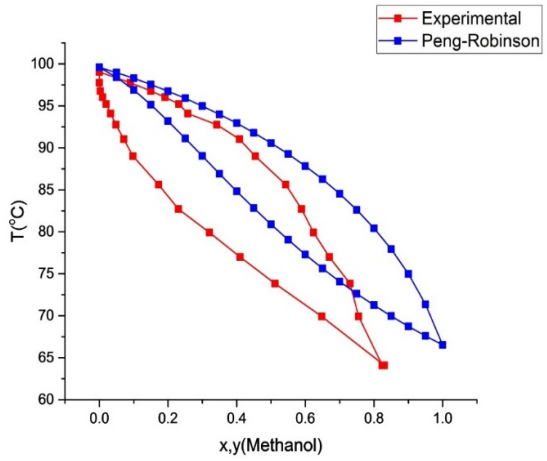

Figure 3. Comparison of the prediction of two-phase equilibrium data using Peng-Robinson thermodynamic model with experimental data.

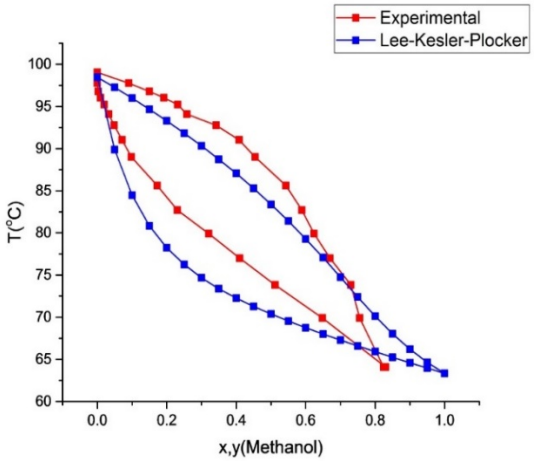

Figure 4. Comparison of the prediction of biphasic equilibrium data using Lee-Kesler-Plocker thermodynamic model with experimental data.

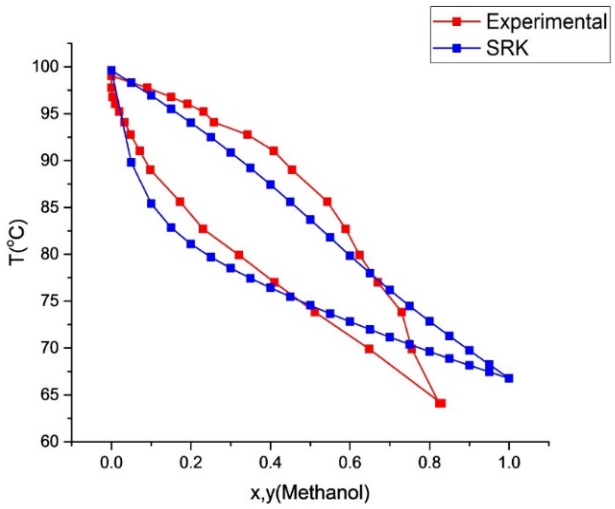

Figure 5. Comparison of the prediction of two-phase equilibrium data using SRK thermodynamic model with experimental data.

Table 2 shows the validation results of the simulation data. By comparing the simulation data with the industrial data, a good agreement has been observed (Mean relative error of 2 %).

Table 2
Simulation data validation results.

Data	Simulation data	Industrial data	RE (%)
PRERun Feed2 (Input feed to the tower 5001)			
Temperature (°C)	40.08	40	0.2
Pressure (bar)	3	3	0

Flow ($\frac{kmol}{hr}$)	3370	3426.2	1.6
503 (top exit of tower 5001)			
Temperature (°C)	85.92	84	2.3
Pressure (bar)	2.1	2.1	0
Flow ($\frac{kmol}{hr}$)	760.2	816.5	6.9
PRERun Bottom (Bottom outlet of Tower 5001)			
Temperature (°C)	93.97	92	2.1
Pressure (bar)	2.4	2.4	0
Flow ($\frac{kmol}{hr}$)	3416	3416	0
504 (Backflow of Tower 5001)			
Temperature (°C)	64.02	64	0.03
Pressure (bar)	3	3	0
Flow ($\frac{kmol}{hr}$)	806.3	806.3	0
Methanol Prod (The final methanol product)			
Temperature (°C)	40.04	40	0.1
Pressure (bar)	4	4	0
Flow ($\frac{kmol}{hr}$)	2162	2600.7	16.9

The heat exchanger network has been then designed, which is the first step in energy integrating of a process. The simulation has been performed with the Aspen Hysys V11 software, and the process energy analysis has been developed using the Aspen Energy Analyzer V11 software. Horizontal blue and red lines represent hot and cold currents respectively. The heat exchangers are shown as circles attached to vertical lines. The input and output currents, power supply, target temperature for the hot and cold currents, and heat duty of each heat exchanger are all displayed in Tables 3 and 4 (data extraction table). Figure 6 displays the composite curve (CC) diagram of hot and cold flows, which shows the enthalpy-temperature relationship. The pinch technology enables reinforcement schemes to review hot and cold energy targets in the net or higher thermal zone, below or above the Grand Composite Curve (or GCC) (Figure 7) to achieve the minimum energy targets of QH_{min} and QC_{min} [25].

Table 3
Enthalpy streams.

Stream	Enthalpy (kJ/h)
505-516	2.138×10^5
516-Fuel Gas	2.512×10^5
521-519	1.13×10^8
503-522	2.913×10^7
PreRun Feed2-PreRun Bottom	5.05×10^7
PreRun Bottom-Bottom	9.755×10^7

Table 4
Heat loads of heat exchangers.

Exchanger name	Q (kJ/h)
E-5003	213800
E-5004	251200
AE-5002	24246183
E-5007	88783817
AE-5001	29130000
T-5001	50500000
T-5002	97550000

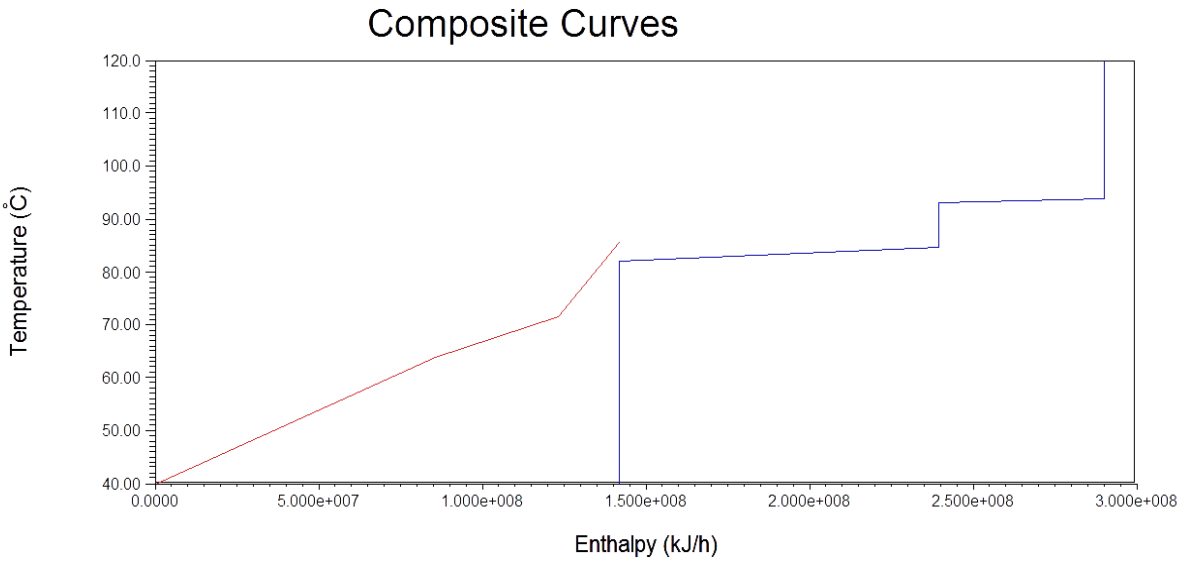

Figure 6. Combined diagram of the enthalpy temperature for the methanol purification unit.

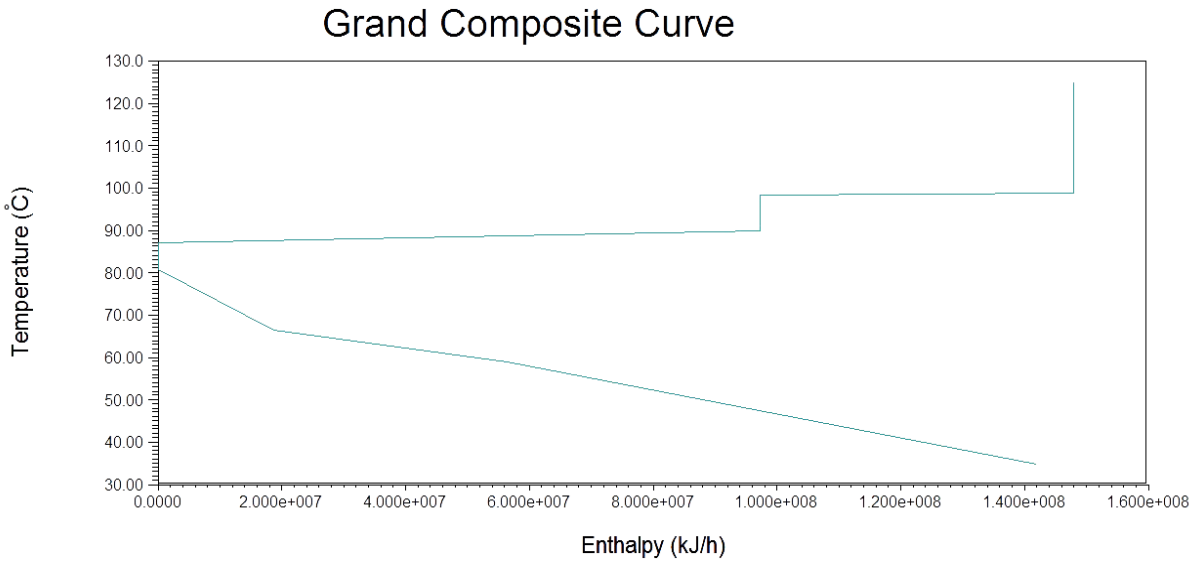

Figure 7. Grand Composite Curve.

The Grand Composite Curve (GCC) is an innovative diagram created from CC. First, the hot composite curve with $\frac{1}{2}\Delta T_{min}$ and the cold composite curve with $\frac{1}{2}\Delta T_{min}$ are moved downwards. This causes the CCs to be felt in the pinch. Process currents are not shown on converted composites at their actual temperature and are shown in temperature ranges. Therefore, hot currents are $\frac{1}{2}\Delta T_{min}$ warmer and cold currents are $\frac{1}{2}\Delta T_{min}$ colder. In order to create goals for the minimum energy goals, the value of ΔT_{min} has been set to solve this problem. ΔT_{min} is the smallest temperature difference between hot and cold currents in a heat exchanger in which the current is assumed to be reciprocal. In the design of HEN, an important parameter that should be considered is ΔT_{min} which is used to balance the energy and cost of capital. The energy-capital balance is achieved with this design. According to several academics, one should aim for and create the ideal HEN cost in order to optimize the HEN design. The goal of designing and

optimizing the optimal HEN cost should be achieved using ΔT_{min}. To provide the minimum of a lower and more accurate heat transfer design, the common idea is to select the value of ΔT_{min} to balance operating costs and capital [26]. Baker et al. [27] have used a variety of facilities and various kinds of heat exchangers to examine the various impacts of ΔT_{min} on the initial and ongoing costs of HEN. A lower value of ΔT_{min} maximizes capital expenses while minimizing running costs. Higher values of ΔT_{min}, however, enhance operational expenses while minimizing capital costs. The energy recovery will be lowered if a lower value of ΔT_{min} is used, however, a larger heat exchanger area will be needed. The energy recovery will be lowered, but the size of the heat exchanger will be smaller if a higher value of ΔT_{min} is chosen. To prevent the rigidity and inefficiency of HENs, it is crucial to select the ideal value of ΔT_{min} during the early stages of the design. The method of confirming the intended value of ΔT_{min}, which may have superior performance conditions and be economically advantageous, is the question that needs to be addressed in this situation.

There are two types of hot utility streams in the methanol unit, which include LP vapor and MP vapor. Table 5 shows the amount of each of these streams separately.

Table 5
Hot Utility Data.

Utility	Load (kJ/h)	Cost index (Cost/s)	Total targets (kJ/h)
LP steam	1.482×10^8	0.078	Heating target
MP steam	1.57×10^4	9.6×10^{-6}	1.482×10^8
Cooling water	0	0	Cooling target
Air	1.423×10^8	3.952×10^{-5}	1.423×10^8

Figure 8 shows the total cost index versus the minimum temperature method for the methanol distillation unit. This diagram shows that the best total cost index is achieved at $\Delta T_{min} = 20$ °C.

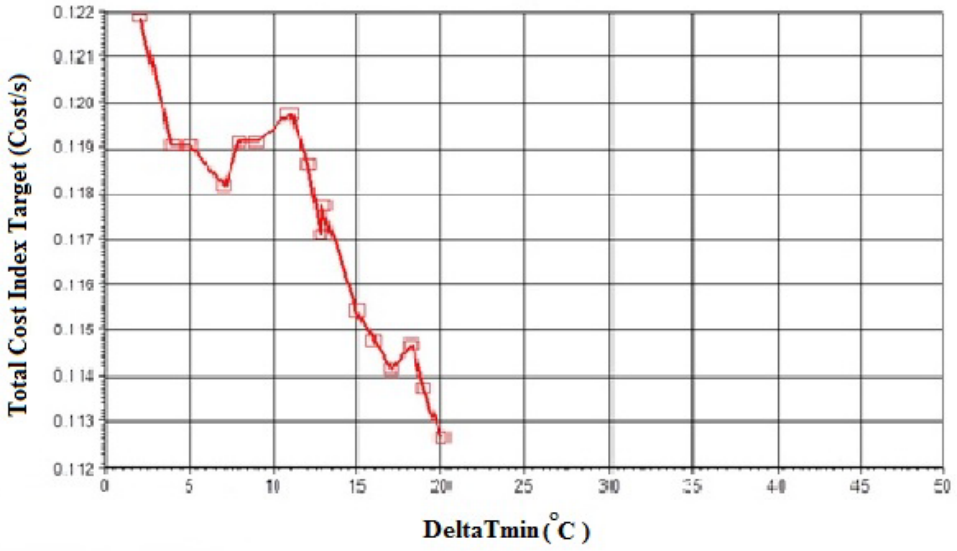

Figure 8. Total cost versus ΔT_{min}.

The ΔT_{min} parameter represents the exchange between the investment cost (which increases as the value of ΔT_{min} decreases) and the energy cost (which decreases as the value of ΔT_{min} decreases). Herein, the ranges of typical values of ΔT_{min} are used, which represent the compensation for each category of processes. Figures 9 and 10 show the ΔT_{min} for hot and cold utilities respectively.

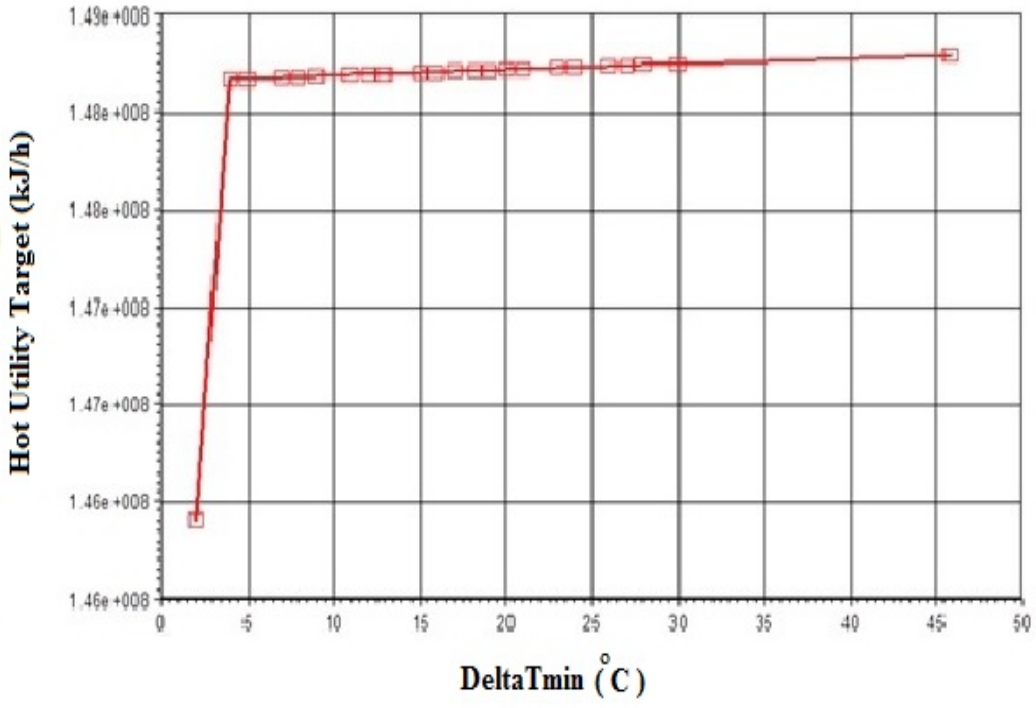

Figure 9. Range of ΔT_{min} for the hot utility flow.

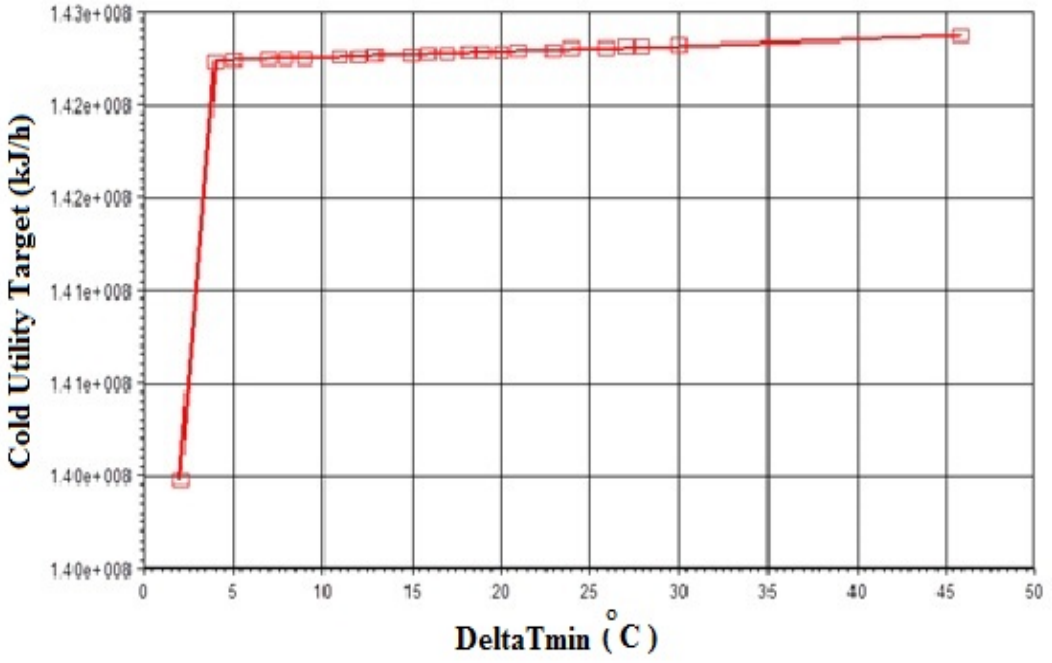

Figure 10. Range of ΔT_{min} for the cold utility flow.

4. Conclusions

In this study, the separation part of the methanol unit has been evaluated. The two-column separation section of the methanol production unit has been thermodynamically simulated using the SRK, as the best equation of state for this design, and the Aspen Hysys V11 software.

- The MRE has been obtained as 2 % for this simulation.
- The design of the heat exchanger network has been done by the Aspen Energy Analyzer V11 software. CC and GCC diagrams have been drawn, demonstrating the combination of the instantaneous temperatures and minimum energy QH_{min} and QC_{min} of hot and cold flows respectively. Furthermore, two distillation towers have been analyzed using the pinch technology.
  - The amount of hot and cold utilities have been obtained as the LP steam = 1.482×10^8 kJ, MP steam = 1.57×10^4 kJ and Air = 1.423×10^8 kJ.
  - The total heating target and cooling target of the process have been 1.482×10^8 kJ and 1.423×10^8 kJ respectively.
  - The MP steam and other high-temperature hot utilities cost more than the LP steam and other low-temperature hot utilities. Despite the fact that the MP steam is more expensive than the LP steam, the consumption of the MP steam has been less than that of the LP steam, which has led to a lower net cost for the consumption of MP steam.
  - The analysis of the minimum temperature difference between hot and cold currents with ΔT_{min} has been performed and its effect on the annual cost has been investigated. Through decreasing the amount of ΔT_{min}, operating costs increase and energy costs decrease.

As a consequence, we suggest using a heat pump in the distillation column in future works to reduce the energy consumption and to investigate its effect on reducing the energy consumption and subsequently reducing annual costs.

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