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Design and Pinch Analysis of Methyl Acetate Production Process using Aspen Plus and Aspen Energy Analyzer

K. Nagamalleswara Rao[1*], *G. Koteswara Reddy*[1], *P.Rajendra Prasad*[2], *V. Sujatha*[2]
[1]Department of Chemical Engineering, Bapatla Engineering College, Andhra Pradesh, India.
[2]Department of Chemical Engineering, AU College of Engineering, Andhra University, Andhra Pradesh, India.

Abstract

This study deals with the design and heat integration of Methyl Acetate production process. Initially, Methyl Acetate production process plant is designed using Aspen Plus. Methyl acetate obtained is 99.99% pure and the designed plant is safe to environment with less emissions. For the developed process plant, pinch analysis is applied using Aspen Energy Analyzer. Improved Heat exchanger networks (HEN) is obtained with retrofit analysis of the process plant. The retrofit design saves the energy of the process by minimizing the operating costs. In retrofit analysis, four new heat exchangers are added to the base case HEN which reduced the operating cost with the payback period of 0.9 years.

Keywords: *Pinch analysis, Aspen plus, heat exchanger networks (HEN), Aspen energy analyzer, retrofit analysis*

***Author for correspondence:** *Email ID: kanidarapunag2001@gmail.com*

INTRODUCTION

Designing of automated process plants having good control and safe to environment is the present trend in chemical engineering practice[1,5,6]. To improve the process efficiencies process engineers and technical service engineers are continuously searching for design alternatives[7]. For that it is desirable to develop rigorous models for realistic and large-scale processes with recycle streams, energy integration and non-ideal systems, and use them for evaluating plant-wide control schemes[2,3,7].

The concept of pinch technology was introduced by Linnhoff *et al.* and Umeda based on Hohmann's work[8]. Energy efficient systems can be designed by pinch technology[9]. Designing heat exchanger networks (HEN) using pinch analysis of processes is the new trend in pinch technology[10–12]. It is proved in the case of new plant designs that industrial energy cost can be saved up to 30% in combination with capital cost[13,14] and payback times in retrofit applications were reported to be less than one year[13,15]. Pinch analysis was derived from combined first and second law analysis, as a technique ensuring a better thermal integration, aiming the minimization of entropy production or equivalently energy destruction by heat exchangers networks[16].

Heat integration schemes are proposed to improve companies economic performance and to reduce its environmental impacts[4,14]. To reduce the drawbacks in pinch analysis different techniques are proposed for example total entropy generation minimization techniques etc.,[17–19]. To improve process efficiencies heat integrated distillation columns and process equipment alternatives are designed[20–21].

Pinch analysis concept can be understood in terms of composite curves, grand composite curves, grid diagram, grid diagram for retrofit analysis etc.

The principles already applied in the process industries are first one is heat flow across the pinch should be zero, second principle is utilities consumption both hot and cold can be minimized by integrating streams above and below the pinch separately and the third one is excess energy flows tend to incur high capital costs due to the extra heat transfer capacity needed for both utility heating and cooling. Improved energy recovery may lead to capital savings[22]. The above established principles allow us to set energy targets prior to design, to design minimum energy networks by keeping the portion of the process above and below the pinch separate and to avoid black box i.e. giving decision power to engineers[22].

The present study aims at designing a process plant for the production of methyl acetate using Aspen Plus v8.0 and applies the established pinch principles in designing an alternative energy efficient HEN by applying retrofit analysis by using Aspen Energy Analyzer.

METHODOLOGY

Optimization of operating conditions and retrofit of HEN are the two methods frequently used energy saving methods in designing the process plants[10]. In optimization of operating conditions set points of the process are determined. In retrofit method the pinch techniques had to be applied to improve the project performance. Retrofit had its advantages compared to optimization *i.e.,* in optimization approach HEN is fixed but in the case of retrofit it is possible to incorporate real plant information in the design step. Based on this reason only, retrofit is preferred for most of the industrial plants to improve the process efficiency by saving the energy. The fundamental steps followed in the retrofit analysis are:

1. Extracting the process data from the process plant.
2. HEN design for the base case process and retrofit analysis.
3. Design improvement.
4. Economic analysis is performed for the base case and retrofit design.
5. If the economic analysis of retrofit is satisfied compared to base case then the modified design is implemented.

The extracted data from the step one contains hot and cold stream temperatures heat duties of all streams are calculated by using heat capacity data of each stream. Generally hot streams contains more energy this energy is recovered by matching the cold streams with hot streams and this matching can be achieved by several combination of hot and cold streams. Once the quantity of the energy is known heat exchange area calculation is very easy. Segmentation streams are useful in the case of large temperature range of the process streams to calculate accurately the heat capacity of a phase changing stream. From stream data HEN grid diagram is designed. Next step is to improve the HEN it can be done by knowing the gap between ideal energy consumption and current energy consumption of the HEN. If there is no gap between ideal and retrofit then retrofit project ends there. This is the situation where energy savings were poor. Ideal energy consumption can be achieved by recovering heat in the process by several ways.
Composite curves were used to analyze the gap between the ideal and current HEN. If it is not possible to get ideal energy consumption by current HEN then the HEN was subjected to redesign by the pinch design method.

After the designing the HEN the next step is the economic analysis. In economic analysis capital investment and hot and cold utility load energy consumption costs were evaluated. The same economic procedure was applied to retrofit of the HEN. Retrofit was a trade-off problem between the energy saving and the capital investment[22]. If the new HEN developed by retrofit satisfies the desired economy of the process then the next step to be followed is detail engineering step. If the proposed HEN does not satisfy the economic criteria search for a new HEN design step was necessary for the design improvement.

The present study explains the production of methyl acetate by Aspen plus v8.0 and the pinch analysis of the process is done by using Aspen energy analyzer.

PROCESS DESCRIPTION

The present process contains two heat exchangers, two compressors, plug flow reactor, flash column and two distillation columns. Process is designed by using Aspen Plus user interface v8.0. Process flow diagram is shown in Figure 1. Raw materials for the process are di-methyl ether; carbon monoxide and hydrogen (synthesis gas) are preheated before sending to the plug flow reactor.

In the reactor reaction occurs and the product mixture contains methyl acetate, methanol, and unconverted reactants of carbon monoxide, hydrogen and di-methyl ether. The products are separated from the unconverted reactants in flash column and two distillation columns. In flash column di-methyl ether and carbon monoxide are separated. In the first distillation column di-methyl ether obtained at the top of the column is compressed and recycled. In the second distillation column product methyl acetate of purity 99% is obtained. Steady state process data is shown in Tables 1 and 2.

DATA EXTRACTION FROM THE PROCESS

Process stream data is extracted from the steady state process using Aspen energy analyzer. The data extracted contains temperatures, heat duty, heat capacity of each stream, utility data and the cost data which is helpful in determining the energy cost and capital investment. Calculation of heat duty for each stream is done by Aspen Energy analyzer. The extracted data of process is shown in Tables 3–6. The process contains three hot streams and four cold streams. Two hot streams, three cold streams are segmented to satisfy the condition of phase change followed by large temperature change in a single phase. Utilities present in the process are two heating utilities and two cooling utilities. Heating utilities are LP (Low pressure) steam and HP steam. Cooling utility is Air, Refrigerant 1.

After process data extraction pinch analysis is applied to get HEN for the process. In the next step retrofit analysis is performed. Retrofit is a trade-off problem between energy saving and capital investment[22]. Results are evaluated by the relative amount of the cost saved and investment needed. Utility cost index for the present process is 0.03 and base operating time 8765.76 hours are needed to calculate the energy cost saving and the heat exchanger cost is needed to estimate the investment cost[10].

Costs of the heat exchangers are calculated by the following equations *i.e.* Eqs. (1–5)[23]. Each type of heat exchange equipment had its own equation for calculating the capital cost:

For shell and tube

$$CC = a + b(Area/N_{shell})^{c} \times N_{shell} \qquad \text{Eq. (1)}$$

Fired heater

$$CC = a + b(Duty)^{c} \qquad \text{Eq. (2)}$$

CC is installed capital cost of a heat exchanger, a is installation cost of the heat exchanger, b, c are the duty or area related cost set coefficients of the exchanger, Area is the heat transfer area of the exchanger, N_{shell} is the number of heat exchanger shells in the heat exchanger, Duty is the amount of energy being transferred in the heat exchanger. Operating cost is a time dependent cost that represents the energy cost to run the equipment. For Aspen Energy Analyzer, the operating cost is dependent on the calculated energy targets in the HEN:

$$OC = \Sigma(C_{hu} \times Q_{hu,min}) + \Sigma(C_{cu} \times Q_{cu,min}) \quad \text{Eq. (3)}$$

OC is the operating cost, C_{hu} is utility cost for the hot utility, $Q_{hu,min}$ is energy target of hot utility(kW), C_{cu} is utility cost for the cold utility(\$/kW yr) $Q_{cu,min}$ is energy target of hot utility (kW). Total annualized cost (TAC) accounts for both the capital cost and operating cost associated with the heat exchangers in the HEN. The equation used to calculate the TAC is

$$TAC = \Lambda \times \Sigma CC + OC \quad \text{Eq. (4)}$$

CC is the installed capital cost of a heat exchanger (\$), OC is the operating cost(\$/yr), Λ is the annualization factor (1/yr).

The annualization factor accounts for the depreciation of capital cost in the plant. It must be considered since the capital cost and operating cost of a heat exchanger network do not have the same units. The following equation is used to calculate the annualization factor:

$$\Lambda = (1 + ROR/100)PL/PL \quad \text{Eq. (5)}$$

ROR is the rate of return (percent of capital), PL is the plant life (yr).

BASE CASE HEN ANALYSIS FOR RETROFIT

Heat integration studies are performed for the process flow diagram shown in Figure 1. In the first step of the analysis data is extracted from the steady state process and the grid diagram is developed and is shown in Figure 2. In the next step an alternative design for the base case design was developed and it is shown in Figure 3. Results are explained with composite curve as shown in Figure 4, Grand composite curve shown in Figure 5. HEN for the current process is represented as grid diagram and is shown in Figure 2. Hot streams are represented by thick red color lines in the upper portion of the grid diagram and the cold streams are represented by blue thick lines in the lower portion. The base case has seven exchangers between process streams. Hot and cold composite curves are combined and are shown as composite curve in Figure 6. Composite curve represents heating and cooling demand of the process corresponding to the temperature range. Quantity of maximum energy recovery can be calculated from the composite curve. The close gap in the diagram shows the ΔT min, it means the minimum driving force for heat exchange. Pinch point is the point where the two curves approach closest and the temperature difference of two composite curves is ΔT_{min}. Economic efficiency and is decided by ΔT_{min} and it affects heat exchange area. For the present study ΔT_{min} is identified as 4.5 °C.

HEN IMPROVEMENT

From the process flow diagram as shown in Figure 1, heat is exchanged in heaters and coolers respectively. Names for the heat exchangers are Condenser@B14, Reboiler@B7, Condenser@B7, Reboiler@B14, B16_heat_Exchanger, B5, B1.

All the heating and cooling requirements of the process were combined together, the result is the Grid diagram and it is shown in Figure 2. Simply the Grid diagram is an overview of all the heating/cooling requirements of the process. The local heat transfer coefficient associated with the individual stream is the default values calculated by Aspen energy analyzer. Flow rate, effective C_P and ΔT, the minimum approach temperature are the parameters used in Aspen energy analyser.

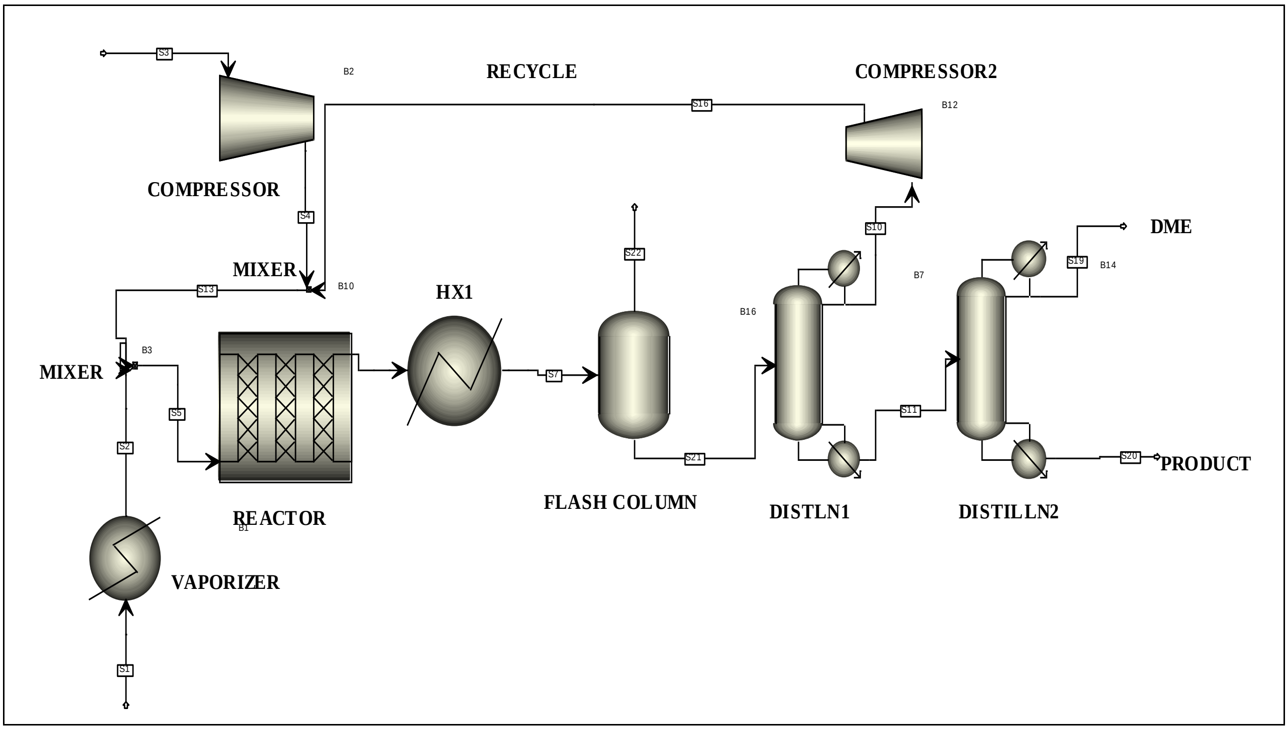

Fig. 1: *Process Flow Diagram for Methyl Acetate Production.*

Table 1: *Process Data of Methyl Acetate Process.*

Name	S1	S2	S3	S4	S5	S6	S7
Mole Flow (kmol/hr)							
CO	0	0	262	262	276.4071	212.5313	212.5313
DME	249.75	249.75	0	0	858.4985	794.6228	794.6228
MEACH	0	0	0	0	0.0603921	63.93615	63.93615
H2	0	0	5.24	5.24	5.268909	5.268909	5.268909
MEOH	0.25	0.25	0	0	0.2506142	0.2506142	0.2506142
Total Flow (kmol/hr)	250	250	267.24	267.24	1140.486	1076.61	1076.61
Temperature (K)	273	372	273	535.1483	361.9754	458.9449	459.1468
Pressure (atm)	32	32	5	32	32	32	32.424
Enthalpy (cal/mol)	–49151.49	–45555.5	–26056.92	–24214.96	–38601.82	–40892.08	–40888.34
Entropy (cal/mol-K)	–77.88362	–67.8140	17.28959	18.32503	–40.79331	–40.55921	–40.57719
Density (mol/cc)	0.0150493	0.01085	0.000223201	0.000728728	0.00107736	0.000849726	0.000860606
Average (MW)	46.05501	46.05501	27.5007	27.5007	41.48724	43.9487	43.9487

Table 2: *Process Data.*

Name	S10	S11	S13	S16	S19	S20	S21	S22
Mole Flow (kmol/hr)								
CO	14.40658	0	276.407	14.40658	0	0	14.40658	198.1248
DME	608.7369	92.2441	608.748	608.7369	92.24416	1.27422E –8	700.9811	93.64169
MEACH	0.0603871	63.3184	0.06039	0.060387 1	1.000191	62.3182	63.37878	0.557365
H2	0.0289175	0	5.26890	0.028917 5	0	0	0.0289175	5.239992
MEOH	0.0006141	0.24581	0.00061	0.000614 14	0.240661	0.005152 4	0.2464276	0.004186
Total Flow (kmol/hr)	623.2334	155.8084	890.485	623.2334	93.48501	62.32334	779.0418	297.568
Temperature (K)	292.1177	311.1776	411.837	391.887	293.2409	386.8518	320	320
Pressure (atm)	5	5.16	32	32	5	5.16	30	30
Enthalpy (cal/mol)	–43661.77	–71438.66	–36649	– 41981.36	–49189.6	–102700	–51985.78	–31384.5
Entropy (cal/mol-K)	–58.59382	–80.15105	–33.459	– 57.35354	–75.9519	– 84.00506	–72.56628	–8.54084
Density (mol/cc)	0.0002085	0.013222	0.00094	0.000995 12	0.014379	0.010774 5	0.0133495	0.001142
Average (MW)	45.65226	57.42995	40.2048	45.65226	46.33261	74.07596	48.0078	33.32187

Table 3: *Process Hot Stream Data.*

Hot stream name	Hot T_{in} °C	Hot T_{out} °C
To Condenser@B14_TO_S19	20.59	20.09
LP Steam	125.0	124.2
To Condenser@B7_TO_S10	19.46	18.96
LP Steam	124.2	124.1
B16_heat	185.9	46.85
HP Steam	250.0	249.0
LP Steam	124.1	124.0

Table 4: *Process Cold Stream Data.*

Cold stream name	Cold T_{in} °C	Cold T_{out} °C
Refrigerant 1	–25.00	–24.78
To Reboiler@B7_TO_S11	37.527	38.027
Refrigerant 1	–24.78	–24.00
To Reboiler@B14_TO_S20	113.20	113.70
Air	30.000	35.000
S6_To_S7	185.79	186.29
S1_To_S2	–0.149	98.850

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Table 5: *Process Heat Exchanger Load and Area Data.*

Heat exchanger name	Load (MW)	Area(m^2)	ΔT_{min} Hot	ΔT_{min} Cold	Overall heat transfer coefficient ($kJ/hr\text{-}m^2\text{-}^{\circ}C$)
Condenser@B14	1.170	120.8	45.37	45.09	771.09
Reboiler@B7	6.869	408.6	86.97	86.72	696.77
Condenser@B7	4.360	576.8	43.46	43.75	624.00
Reboiler@B14	1.323	637.4	10.55	10.91	696.77
B16_heat_Exchanger	6.765	1591	150.9	16.85	256.97
B5	4.69e-3	0.38	63.70	63.20	697.31
B1	1.045	11.0	25.26	124.1	5778.6

Table 6: *Process Utility Stream Data.*

Utility Name	Load (MW)
Refrigerant 1	5.531
Air	6.765
LP steam	9.238
HP Steam	4.69e-3

Table 7: *Performance Summary.*

	HEN	% of Target
Heating(MW)	8.202	352.2
Cooling(MW)	11.256	209.1
Number of Units	11	137.5
Number of shells	16	57.14
Total Area(m^2)	3327.8	152.4

Grid diagram contains process streams, utility streams, heat exchangers, and split mixers. Streams are named as:
Refrigerant 1, To Reboiler@B7_TO_S11
Refrigerant 1, To Reboiler@B14_TO_S20
Air, S6_To_S7, S1_To_S2 are cold streams. To Condenser@B14_TO_S19, LP Steam, To Condenser@B7_TO_S10, LP Steam, B16_heat, HP Steam, LP Steam are hot streams. In the grid diagram blue color represents cooler, red represents heater, and green shows that the heat exchanger has been added or modified by a retrofit action.

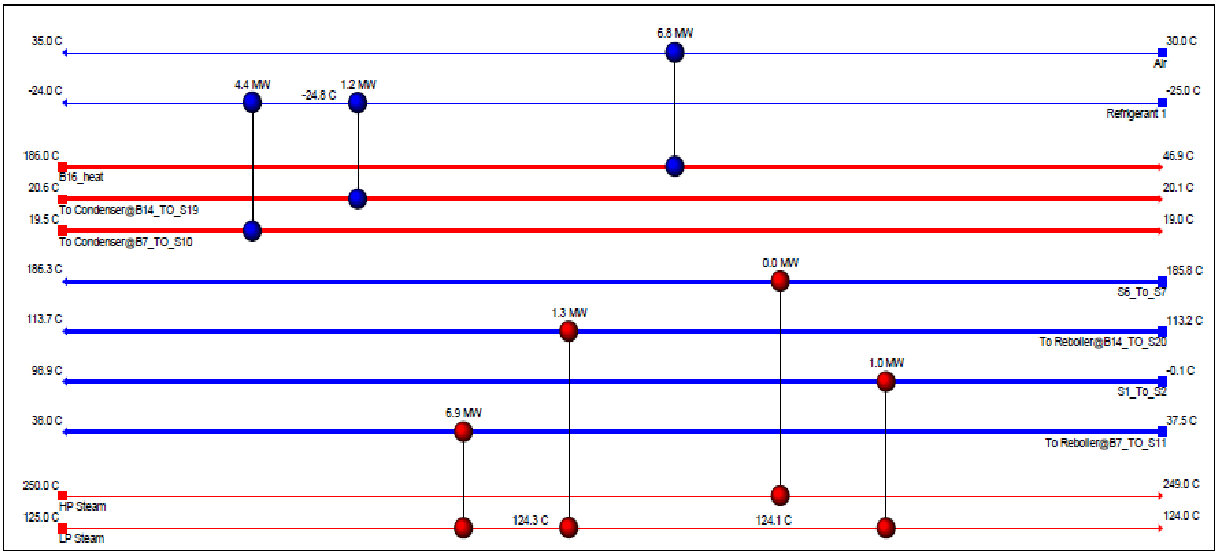

Fig. 2: *Base Case HEN Design of the Methyl Acetate Process.*

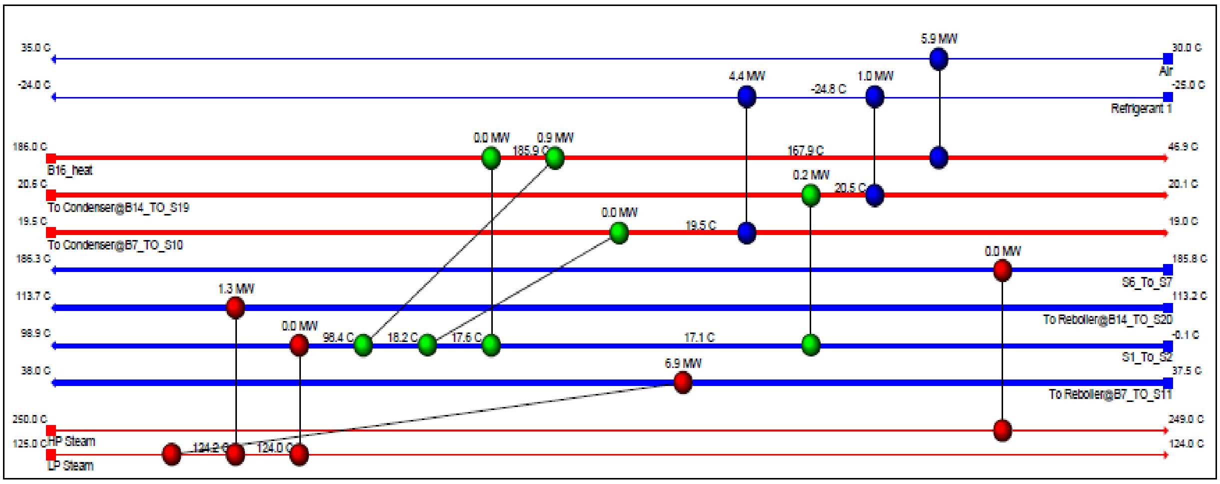

Fig. 3: *Retrofitted HEN for the Base Case Design.*

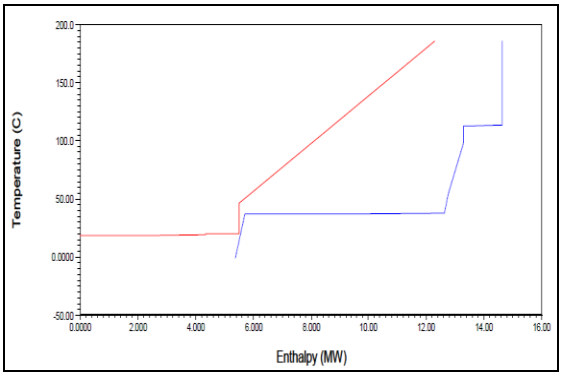

Fig. 4: *Composite Curve.*

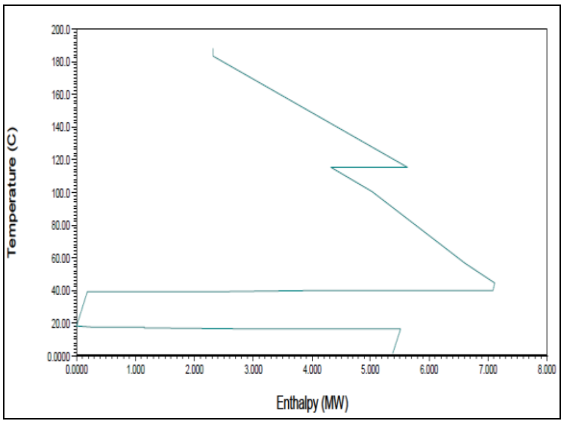

Fig. 5: *Grand Composite Curve.*

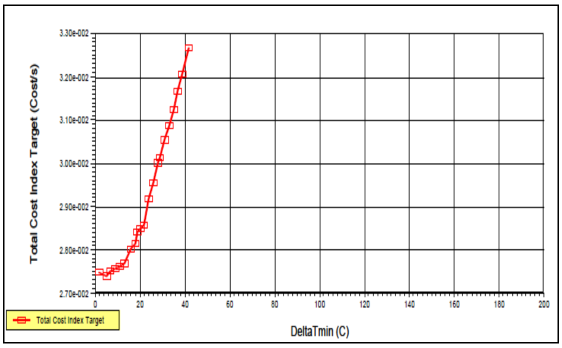

Fig. 6: *Range Targets Plot.*

Figure 4 shows the temperature versus enthalpy plot or composite curve. Composite curves set the energy targets prior to design. Energy targets from the composite curve are heating 2.329 MW and cooling load 5.383 MW. Figure 5 shows the Grand composite curve (GCC). GCC is a plot of shifted temperatures versus the cascaded heat between each temperature interval.

Figure 6 shows the range targets plot. Range target gives the information corresponding to the optimization of the minimum approach temperature. It is calculated by minimizing the total annual cost. It means finding the best compromise between utility requirements, heat exchange area and unit shell number. As the minimum approach temperature is varied the total annual cost of the network is calculated. There will be a ΔT_{min} which will yield a minimum total cost. Here the ΔT_{min} calculated is 4.5°C.

It shows the heat available in various temperature intervals and the net heat flow in the process (which is zero at the pinch). ΔT_{min} is noted as 4.5 $^{\circ}$C. Total number of unit targets is 9. It explains the minimum number of heat exchangers required, minimum number of exchangers required (MER) to achieve maximum energy recovery, and the sum of the minimum

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number of shells from all the exchangers. The number of shells required is 28.

PERFORMANCE EVALUATION

Retrofitted HEN is compared with the base case HEN to know the improvement in energy savings and capital cost investment. The parameters include the heating, cooling, operating, capital, total cost values relative to the target values, the amount of energy being transferred for heating and cooling purpose in the design, number of exchangers, number of shells, the total heat transfer area values relative to the target values, the individual utility cost and load for all the utilities in the design, and the percentage values of the utility load relative to the target values.

Here, the number of shells added is 16 and added heat transfer area is 3328 m^2. The individual utility cost and load for all the utilities in the design. The percentage values of the utility load relative to the target values.

Grid diagram are shown in Figure 2. The process has three hot streams and four cold streams. The current HEN has seven heat exchangers between process streams. Utility use is represented by thin lines and the utility streams are HP steam, LP steam, Air, Refrigerant 1. The grid diagram efficiency can be improved by recovering the heat energy from hotstreams.

By using Aspen energy analyzer retrofit analysis is performed for the base case design. Capital and payback period data were recorded. In retrofit analysis four new heat exchangers are added. For each addition of the exchanger payback period and capital cost were noted. Table 7 explains the performance summary of the new retrofit design compared to the base case design. Figure 3 shows the alternative design obtained from retrofit analysis with payback period less than one year (0.9 years).

CONCLUSIONS

Process for production of methyl acetate is designed and the product purity obtained is 99.9%. The plant designed is safe to operate and environmentally friendly with less emissions. By using Aspen Energy Analyzer the entire plant energy data is extracted. From the extracted data HEN is designed for the base case. Retrofit analysis is done for the base case using Aspen Energy Analyzer. The base case HEN capital index is 8.159×10^5 and the improved HEN cost index is 9.534×10^5 with a payback period of 0.9 years which is acceptable retrofit design for the process.

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