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Optimization and Retrofit studies for Naphthalene Production Process

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Abstract

In this work process simulations are performed for UNIDAK process for the production of naphthalene. As a part of that to do simulations for the process, UNIDAK process is designed in ASPEN PLUS v9.0 simulation user interface. To assess the environmental impacts of the developed process, potential environmental impacts of constituent chemicals are calculated using Waste reduction algorithm (WAR). Engineering economic evaluation is performed using ASPEN ECONOMIC ANALYZER v9.0 which inherently contains the cost of the consumed energy as an operating cost. For the designed process energy analysis is done using ASPEN ENERGY ANALYZER v9.0. From the retrofit analysis studies 63.27% of the energy savings reported. HEN (Heat Exchanger Network) is developed for the base case process and retrofit studies are performed to improve the process efficiency. One heat exchanger is added to the base case HEN which enhanced the process efficiency by 16% with a payback period of 0.3 years. Energy efficient process reduced total potential environmental index (PEI) to 99.9% compared to the Base case process.

Keywords: Energy Analysis; Heat Exchanger Network (HEN); Potential Environmental Impact (PEI); Retrofit studies; UNIDAK process.

1. Introduction

Process systems engineering is an interdisciplinary research and it deals with the use of process simulators in process design. Process simulators enhance the efficiency of the processes by providing automation techniques to process plants [1-5, 14-17]. Process integration techniques are helpful in increasing the efficiency of the existing plants. Pinch technology is one of the process integration techniques and it is used in designing energy efficient systems [6]. Designing HEN (Heat Exchanger networks) using pinch analysis of processes is the new trend in pinch technology [7-12]. Pinch technology concept saves up to 30% of energy cost in combination with capital cost and payback times in retrofit applications [10]. Heat integration schemes are proposed to improve company's economic performance and to reduce its environmental impacts [13]. Several techno-economic evaluation techniques were reported for the retrofit of chemical processes through waste minimization and process integration [18, 19, 23]. Process alternatives are suggested to reduce the environmental impacts [20, 22]. Optimization techniques incorporated for plant-wide control of industrial processes to design energy efficient and safer processes [21, 24-25]. These studies motivated the present study for the design and optimization of naphthalene production process.

The present study simulates the production of naphthalene process (UNIDAK Process, developed by Union Oil in which 1-hexadecene is the raw material) [26] using ASPEN PLUS v9.0 simulating tool. The designed process was optimized for efficient energy usage using ASPEN ENERGY ANALYZER v9.0. Environmental impacts of modified process and the base case process were evaluated using Waste Reduction Algorithm (WAR). After that, retrofit studies were conducted using ASPEN ENERGY ANALYZER v9.0 for the base case HEN (Heat exchanger network) to improve the efficiency of the process.

2. Methodology

2.1. Process design

Process flow diagram for the production of naphthalene is shown in fig 1. This process contains five pumps, four heat exchangers, one reactor, one separator and three distillation columns. 5 kmol/hr of hydrogen at 25°C and 10 bar pressure is heated to 760°C in heater B14. Mixed stream containing 25 kmol/hr toluene, 15 kmol/hr naphthalene, 55 kmol/hr 1-methylnaphthalene, 5 kmol/hr 1-hexadecene at 25°C are heated using heater (B1) to 760°C. Both hydrogen stream and mixed stream containing toluene, naphthalene, 1-methyl-naphthalene and 1-hexadecene are mixed in a mixer (B2).

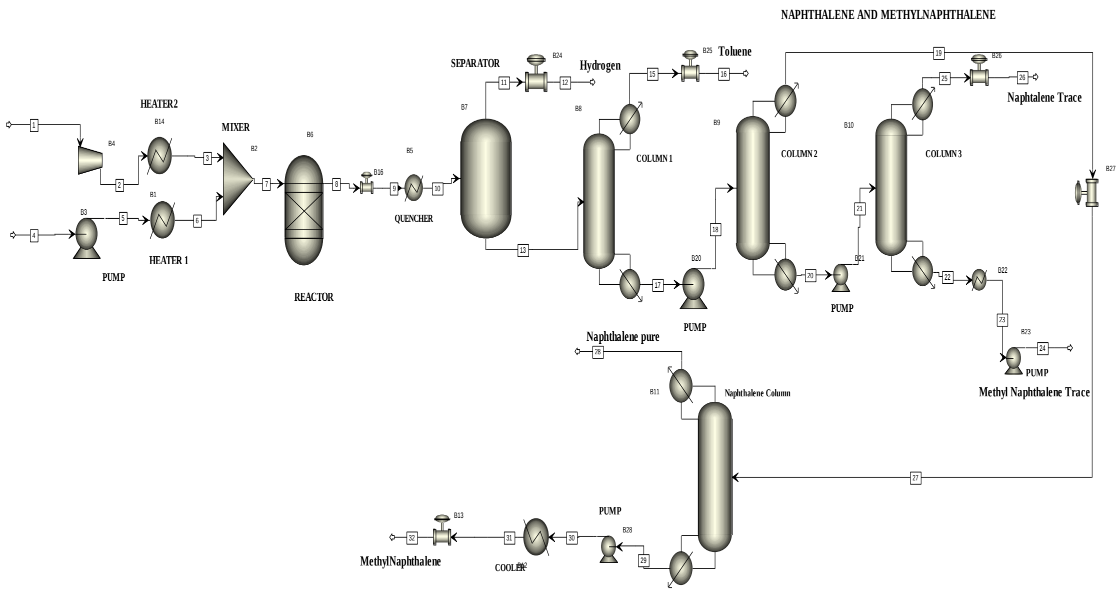

Fig.1. Base case process

The resulting mixture is send to the RGIBBS reactor (B6) in which reaction takes place at 760°C. The resulting reaction products and unreacted reactants containing 15.7872 kmol/hr toluene, 74.2619 kmol/hr naphthale-ne,14.2619 kmol/hr 1-methylnaphthalene, traces of 1-hexadecene, 88.4988 kmol/hr hydrogen are send to the quencher (B5) in which the products are cooled to 25°C. Cooled mixture is send to the separator (B7) having temperature 25°C and pressure 1.5 bar. In separator block all hydrogen is completely recovered. Separator bottoms stream containing toluene, naphthalene, 1-methylnaphthalene in combination with bottoms stream from the naphthalene column (B11) is send to the toluene column i.e column1 (B8). In B8 toluene is separated as tops. Bottom stream from the toluene column containing naphthalene, 1-methylnaphthalene is send to the column2 (B9). Bottoms of the column2 contains naphthalene and 1-methyl-naphthalene is send to the column3 (B10). In column3 the two components naphthalene and 1-methylnaphthalene were get separated. Tops of the column2 are rich of Naphthalene and it is send to the naphthalene column (B11). From B11 99% pure naphthalene is recovered as tops. Bottoms stream containing naphthalene and 1-methylnaphthalene is mixed with the separator (B7) bottoms stream at mixer (B13) and resend for further separation operation to the column1 (B8). It can be seen in fig 2. The purity of the naphthalene produced is 99%.

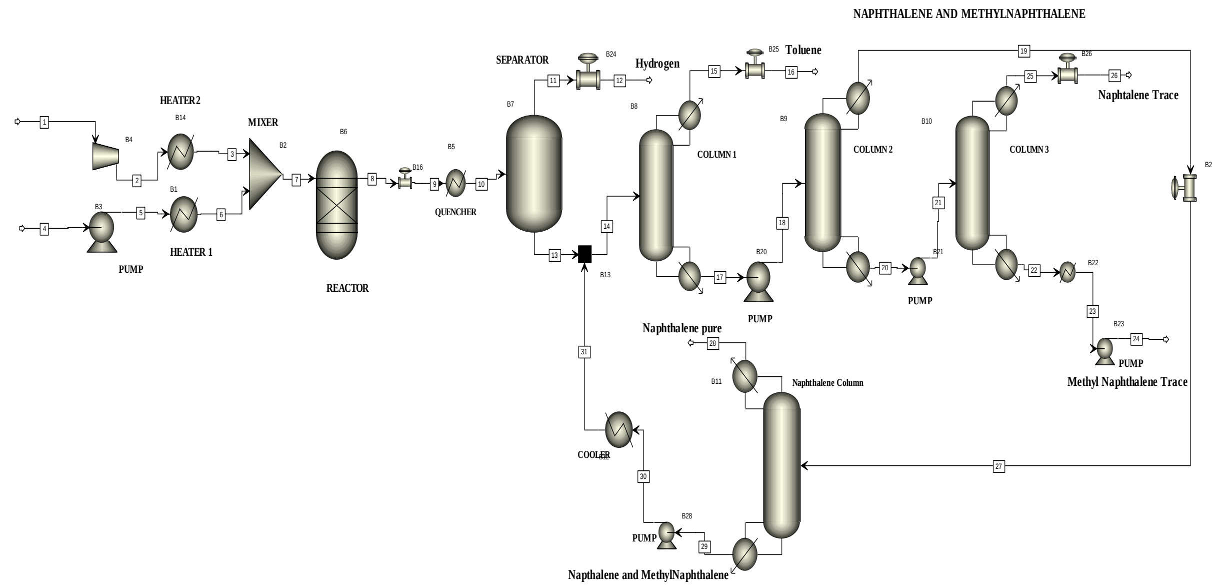

Fig. 2. Modified process

2.2. Energy consumption and total cost estimation

Based on mass and energy balances from the simulations energy consumption and total costs were estimated. In this, the energy used by the reboilers, condensers, exchangers, reactors and the electric power required by the pumps all are included. ASPEN ECONOMIC ANALYZER V9.0 was used to estimate the capital and operating costs of the whole process. In estimating the costs it uses the design information calculated by the ASPEN PLUS v9.0 software.

2.3. Environmental impacts

From ASPEN PLUS simulations, the file with no warnings and no errors, report file was generated with file export option in ASPEN PLUS v9.0. This report file is used as input file for the WAR algorithm. Using the data generated by the ASPEN PLUS, WAR algorithm calculates environmental impacts in terms of PEI (Potential environmental impacts). WAR characterizes the PEI of the streams entering and leaving the process boundaries. WAR includes PEI from eight categories. They are: Human Toxicity Potential by Ingestion(HTPI), Human Toxicity Potential by Exposure(HTPE), Aquatic Toxicity Potential(ATP), Terrestrial Toxicity Potential(TTP), Global Warming Potential(GWP), Ozone Depletion Potential(ODP), Smog Formation Potential(PCOP), Acidification Potential(AP). Based on these eight categories of PEIs the base case process can be modified such a way that the PEIs scores will be minimized.

2.4. Retrofit design

Based on the results from the WAR algorithm, retrofit studies are performed such a way that the reduction in PEIs values. Retrofit studies are helpful in designing the energy efficient processes. Here ASPEN ENERGY ANALYZER v9.0 is used to take design decisions regarding design modifications. ASPEN ENERGY ANALYZER suggests the solutions to minimize the energy losses in the process. Based on these decisions scenario based retrofit designs were conducted and for each retrofit design environmental impact assessment was conducted.

3. Results and discussion

3.1. Process simulation

Simulation results for the naphthalene production process is shown in table 1. Simulation results include the mass and energy balances of all streams in the process flow diagram shown in fig 1. These results are helpful for calculating the PEI (potential environmental impact) values of the process using WAR algorithm.

3.2. Energy integration and economic evaluation

ASPEN ENERGY ANALYZER v9.0 gives the available savings of the process in terms of the absolute utilities savings. These values indicates the total utilities savings opportunity in term of heating and cooling utility usage is 26.91 MW which translates to almost 62.79% potential savings. Recoverable duty at B1 (Heater) is 1.351MW; at B5 (quencher) is 12.1 MW. These values are helpful to increase energy efficiency of the process. Design changes suggested by aspen energy analyser are shown in table 2.

Table 1. Mass and energy balances for naphthalene production process

Substream: Mixed	1	2	3	4	5	6	7	8	12	14
Mole flow kmol/hr	0	0	0	25	25	25	25	15.787	0.356	15.43
toluene	0	0	0	15	15	15	15	74.261	0.0143	77.36
naphthalene	0	0	0	55	55	55	55	14.261	0.00071	17.38
1-methylnaphthalene	0	0	0	5	5	5	5	3.73E-22	0	0
1-hexadecene	5	5	5	0	0	0	5	88.49	88.47	0.027
hydrogen	5	5	5	100	100	100	105	192.8	88.84	110.2
Total flow, kmol/hr	0	0	0	25	25	25	25	15.78	0.356	15.43
Temperature, ^{0}C	25	416.5	760	25	25.876	760	759.82	760	25.01	25.03
Pressure, Bar	1	10.34	10.342	1	10.342	10.3421	10.342	10.34	1	1.5
Enthalpy, cal/mol	0.19	2738.1	5181.3	7793.1	7867.5	70349.8	67246.5	43326.0	54.4	18544.4
Density, mol/cc	4.0E-5	1.79E-4	1.2E-4	6.08E-3	6.09E-3	1.22E-4	1.22E-4	1.2E-4	4.03E-05	6.82E-3
Average MW	2.015	2.015	2.015	131.69	131.69	131.69	125.51	68.35	2.39	125.35

Table 1. Continuation of mass and energy balances

Substream: Mixed	16	18	19	21	24	26	28	29
Mole Flow, kmol/hr	15.4	0.027	0.027	1.09E-08	3.7E-14	1.09E-08	0.027	8.88E-11
toluene	2.47E-05	77.36	70.0	7.36	3.24	4.11	66.8	3.11
naphthalene	5.44E-08	17.38	4.21	13.17	11.28	1.88	1.08	3.12
1-methylnaphthalene	0	0	0	0	0	0	0	0
1-hexadecene	0.02	6.76E-21	0	0	0	0	0	0
hydrogen	15.4	94.7	74.2	20.53	14.53	6	68	6.24
Total flow, kmol/hr	15.4	0.027	0.027	1.090E-08	3.7E-14	1.09E-08	0.027	8.8E-11
Temperature, ^{0}C	109.17	221.34	252.49	266.53	10.201	226.803	218.005	229.001
Pressure, Bar	0.5	2	2	2	2	0.5	1	1
Enthalpy, cal/mol	14345.13	32357.19	45390.69	32090.45	15040.55	42435.02	43881.93	30423.13
Density, mol/cc	1.59797E-05	0.00571076	4.8371E-05	0.0051116	0.00613846	1.22238E-05	2.52906E-05	0.00543504
Average MW	91.97995	130.7366	128.9568	137.1716	139.0657	132.5829	128.3832	135.2004

Table 2. Design modifications suggested by ASPEN ENERGY ANALYZER

	Energy Saving [%]	Payback [year]	New Area [m^2]	Extra Capital Cost [$]	Energy Cost Savings [$/Yr]	Location of new heat exchanger	
						Hot Side Fluid	Cold Side Fluid
Solution 1	16.30	0.033	20.78	19,060	578,027	Upstream to B5	Upstream to Reboiler@B9
Solution 2	9.84	0.04456	11.22	15,535	348,878	Upstream to B5	Upstream to Reboiler@B11
Solution 3	32.91	0.2066	1786	535,324	2,592,710	Upstream to B5	Upstream to B6_heat_Exchanger
Solution 4	5.91	0.2955	54.18	24,339	82,427	Upstream to Condenser@B9	Upstream to B1

Based on solution 1 from table 3, one heat exchanger is added to the process at upstream to B5 and upstream to Reboiler@B9. Energy analysis performed again. From the results the modified process is effective in saving the energy. Remaining three solutions are also tried but the solution 1 is more practical in saving the energy of the process. In Solution 3 ASPEN ENERGY ANALYZER assumed RGIBBS reactor as a heat exchanger and this option can be changed and it is left to the user. The modified energy efficient process flow diagram is shown in fig 3.

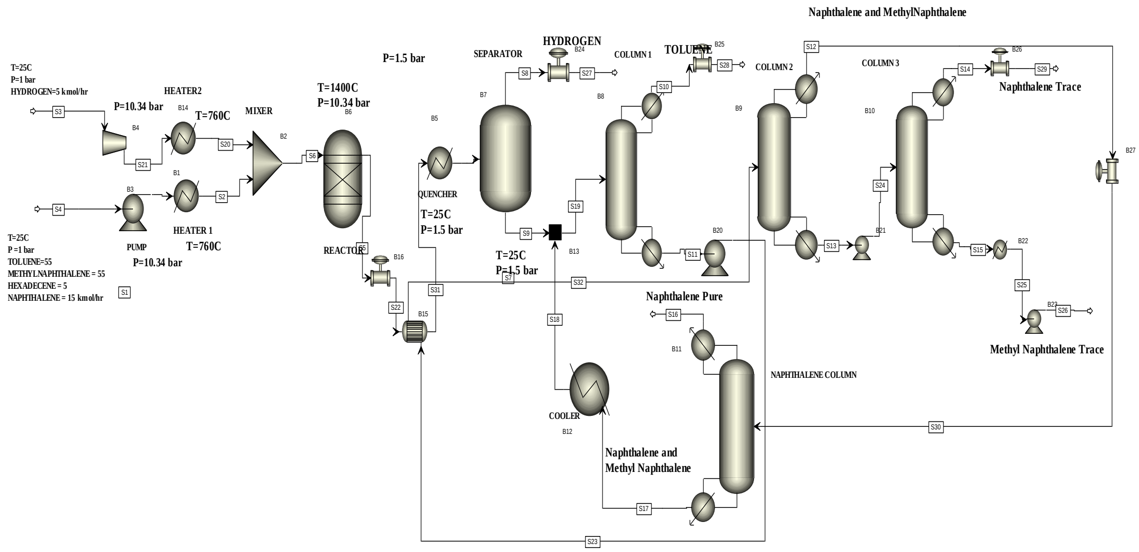

Fig.3. Energy efficient process flow diagram

To check for other feasible process designs retrofit studies were conducted. As a part of that scenario based analysis was done using ASPEN ENERGY ANALYZER. Heat Exchanger Network (HEN) was developed for the base case process and it is shown in fig 4. One heat exchanger was added to the base case HEN. The retrofit design for base case HEN is shown in fig 5. The newly added exchanger reduced the energy and the payback period reported was 0.3829 years which is less than one year.

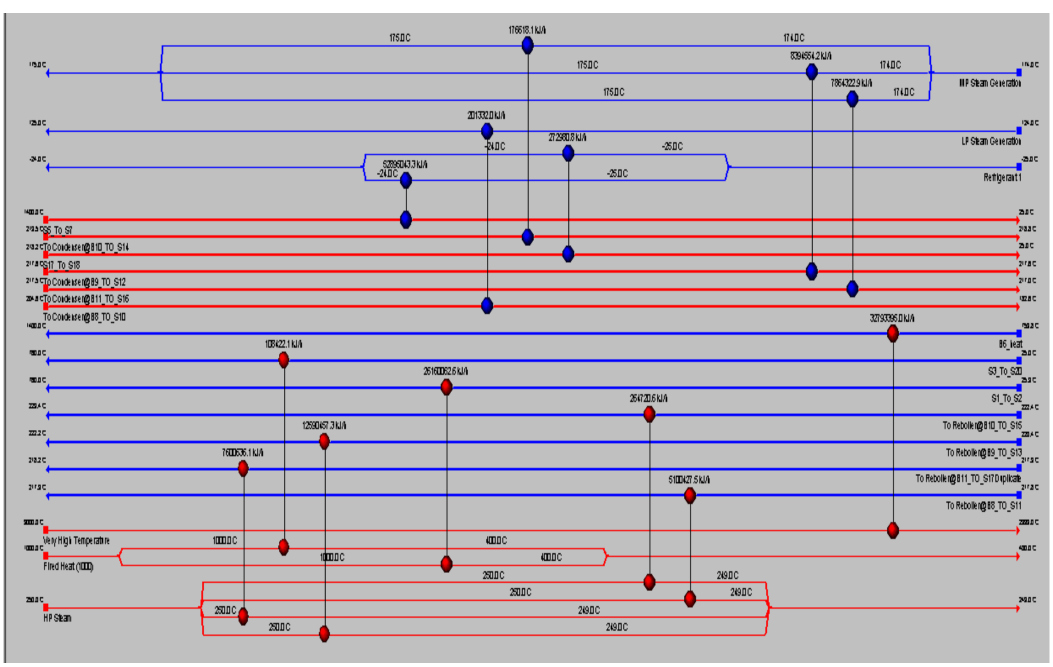

Fig 4. Base Case HEN

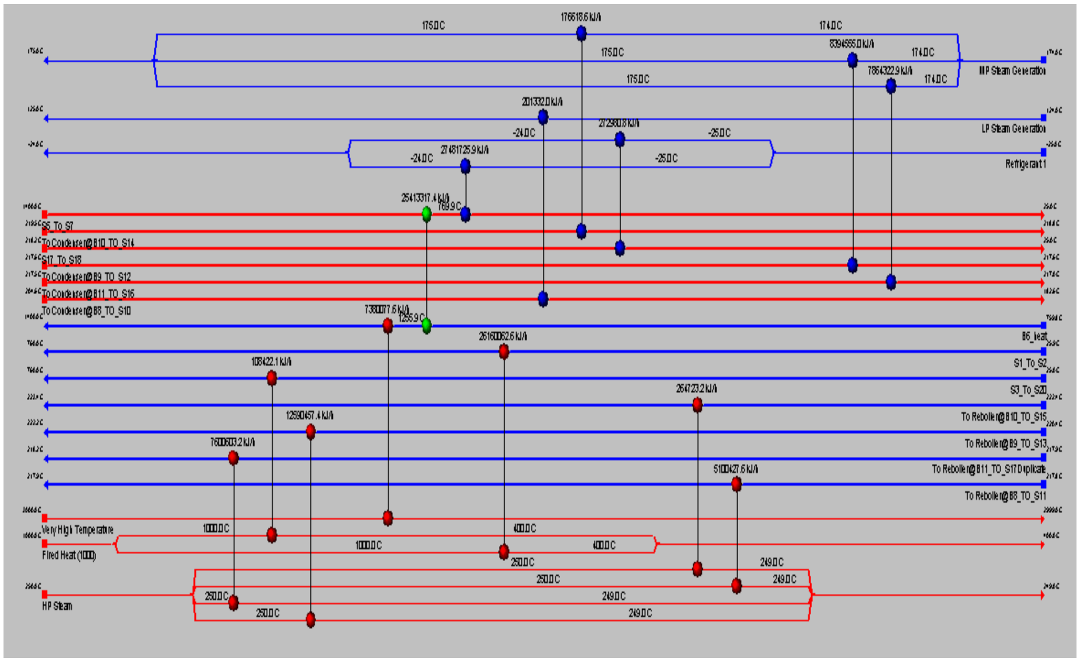

Fig.5. HEN for Retrofit design

In table 3 economic comparisons between the base case process, modified process and the energy efficient process are shown. Modified process capital cost is more but the operating cost and utilities cost are less. The modified process saves 16 % of the energy compared to the original process.

Table 3. Economic comparisons

Cost	Base Case Process	Modified Process	Energy Efficient Process
Total Capital Cost [USD]	10 421 200	9 757 770	9 456 400
Total Operating Cost [USD/Year]	5 259 810	5 292 940	4 267 110
Total Utilities Cost [USD/Year]	3 591 950	3 656 650	2 717 650
Equipment Cost [USD]	1 447 200	974 100	828 100
Total Installed Cost [USD]	3 490 000	3000 800	2 835 500

3.3. Environmental Impact Assessment

The results of the potential environmental impact (PEI) per kilogram of products are tabulated in Table 4. The results show that the energy efficient process reduced total PEI values to 99.9% compared to the base case process. Energy efficient process is the eco-friendly process. It saves both energy and environmental impacts. It emits lower emissions compared to the original process.

Table 4. PEI Values

Case	HTPI	HTPE	TTP	ATP	GWP	OOP	POOP	AP	Total
Base Case Process	9.68E+3	5.96E+1	9.68E+3	8.31E+2	1.66E-2	1.74E-7	1.38E+4	5.13E-1	3.4E+4
Modified Process	2.7	1.67E-2	2.7	2.54E-1	1.66E-2	1.74E-7	3.83	5.13E-1	1E+1
Energy Efficient Process	2.69	1.67E-2	2.69	2.51E-1	1.5E-2	1.58E-7	3.83	4.65E-1	9.97

4. Conclusions

Process simulations for UNIDAK process for producing naphthalene are done using ASPEN PLUS v9.0 chemical process simulator. From the simulations it is evident that formation of naphthalene is favourable at high temperatures and pressures. The simulation results can be used to predict the original process behaviour with varying process conditions. From the energy and economic analysis of the process it is known that energy utilities are reduced by modifying the process. The scope for reducing the energy is 62.75%. Waste Reduction Algorithm results shows that potential environmental impact score can be reduced to 34000 to 9.97. Retrofit analysis results shows that it is possible to improve energy efficiency by 16% by adding one new heat exchanger to the existing heat exchanger network with a payback period of 0.3 years, which is a good investment.

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