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# Process modeling and simulation of ethylene oxide production by implementing pinch and cost analysis

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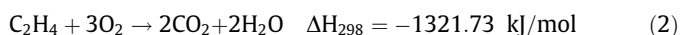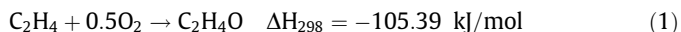
ABSTRACT

This study focused on the modeling and simulation of the Ethylene Oxide (EO) production process in Aspen plus software and energy optimization of the whole process using the Pinch analysis. This work focused on ethylene oxide production by the air-based system and modeled and simulated the whole process in Aspen plus® using the S.R.K. and PSRK thermodynamic models. By process design, modeling and simulation, the behavior of the actual process has been predicted. After process simulation, it has been concluded that control the oxygen concentration by controlling the airflow and controlling the reactor's temperatures causes an impact on our desired product. When the oxygen concentration increases, ethylene is oxidized completely and generated useless products such as carbon dioxide and water to enhance production. Energy optimization of ethylene oxide production is completed through Pinch analysis and saves 18.27 million $ per year, which is consumed in heating or cooling streams.

## 1. Introduction

Most petrochemical processes require ethylene oxide as an initiator. It serves as a necessary ingredient in manufacturing several petroleum products like ethylene, glycol (primary element in antifreeze's), Poly oxirane, Monoethyl ether ethylene glycol, Amino derivatives, Surface active agents, Lubricants and Plasticizers [1,2]. Commercially ethylene oxide is produced by direct catalytic ethylene oxidation with air or oxygen supported over to catalyst silver and additional selectivity. All this process and activity is done in packed bed reactors [3–5]. Reactions occurring during the ethylene oxidation process are [6,7]:

$$C_2H_4 + 0.5O_2 \rightarrow C_2H_4O \quad \Delta H_{298} = -105.39 \ kJ/mol \quad (1)$$

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \quad \Delta H_{298} = -1321.73 \ kJ/mol \quad (2)$$

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Ethylene oxidation reaction (1) is the primary step of this oxidation process, with (2) co-occurring. The reaction mechanism has been reported in the literature [8]. The structure of these oxidation reactions has been described, further inspecting the catalytic deactivation system (catalyst silver supported) through accelerated appearance to ethylene oxide process. In chemical industries, process retrofitting is mainly an ordinary and challenging movement. The retrofit process aims to overcome project barriers. However, several of them, such as mass distribution, heat distribution, and equilibrium reaction restrictions, could not cope with the old chemical engineering methods. Therefore, we need process reinforcement technology (process intensification) to significantly develop the chemical manufacturing process and defeat complex development issues.

On the other hand, the quantity of effective process intensification used the industries partially. A reason for hesitation is not having appropriate retrofitting methods that offer both to identify the mainly hopeful process intensification choice of bottlenecks to assess the potential improvements with the execution of the P.I. technique. That option is recognized with technical and practical issues using different shortcuts headed for a rapidly measuring development method. Ethylene oxide is important inventions among rising requirement along with its manufacturing consume a significant quantity of energy. With an effective ethylene oxide production method, re-reaction regeneration is deliberate when it influences the respondent. Process benefits along with the design

of heat exchanger network and can be quickly and efficiently adjusted. The EO manufacturing procedure's reusability depends on a combination of heat exchanger networks and reactors. Resting on the source of thermodynamic and kinetics equilibrium, the relationship between reusable rate, retail temperature and dissipation temperature is reduced. Considering both the HEN and reactor, an integration model was developed. A cost-effective investigation illustration was produced to show the conflict in returns and costs associated with the reuse rate; the recurrence rate is identified 1.7 and the highest yearly earnings is about 8.39 % [9]. Ethylene epoxidation might serve as an ideal process for studying nonlinear behavior and modeling the reaction system. As the processes involved in ethylene oxide production are complex, it justifies computer-based simulation methods. These advanced digital methods also have an advantage over time-consuming and costly experiments. Analysis has shown that under real's operating conditions during modeling and simulation of fixed bed catalytic reactor, the steady-state (conventional) simulation and transient state (dynamic) simulation are available [10]. Some significant areas for transient simulation of oxidized ethylene reactor mainly consist of investigations during start and shut down, studies for safety and control, dynamic behavior and optimization, and system identification. To get the desired temperature and concentration outline for the catalyst utilizing process during transient conditions must combine both the transient properties of catalyst and reactors at the micro and macro level, respectively [11,12]. While studying operations, the researcher prefers dynamic simulation over conventional simulation because it realistically describes the reactor's transient states. Nowadays, in advanced EO production methods, $C_2H_4$ with catalyst $Ag/Al_2O_3$ is oxidized using air or oxygen ($O_2$), which packs in a fixed bed reactor. Due to the following four advantages [10].

(i) Enhanced selectivity and productivity
(ii) It decreased initial capital cost.
(iii) Low price catalyst is required.
(iv) From purge gas reduced air pollutant amount, it is very desirable to use the oxygen-based reaction process.

An oxirane producing plant is divided into two segments, i.e., reactions and recoveries sectors, the structure of the reactions segment is very important compared with the recovery segment. The primary focus in this study would be the ethylene oxide reaction section because most reactions occur. A diagram of a typical oxygen-based oxygen plantation process is shown in Fig. 1. Ethylene ($C_2H_4$) feed greater than 99.9 % pure is mixed with liquefied gas in the mixer1 and $O_2$ feed with nitrogen gas in mixer 2. The discharge solution is heated at a constant temperature/temperature before being fed to the oxidation agent. Next, the flow of cool water cools. Warm feed from the responder flows to the tube's side when Ag-filled connectors support $Al_2O_3$ [13]. Ethylene is oxidized in the catalytic environment, and ethylene oxide produces other water and carbon dioxide $CO_2$ products. This oxidation reaction is very disruptive, so cooling required the reactor's shell side to restore the heat. This cooling waste sent the ethylene oxide scrubbers. Rich ethylene oxide, also called the rich rotating water, collects at the bottom and moves further to the ethylene oxide building below the section. $C_2H_4$, $O_2$, $CO_2$, and less ethylene oxide, argon vapors spread over a coil back mainly to compressors and increase pressure at 330psi. Compress gas is divided into different streams. One was used also integrated with the new $C_2H_4$ stream. The S19 element transmits the carbon dioxide screw to reduce the amount of $CO_2$ it contains. S18 combines with debris dropped in Mixer 3. Dust (S10) and then into ethylene oxide scrubbers. For regular operation, the zero flow at S18.

All compressed electricity is still distributed forth and back in response feed with minimal $CO_2$ removal. However, at the beginning of the EO plant, the S18 flow rate is not zero and is a vital variant. Starting a new batch is often a complicated process involving inefficient operating processes and radical changes in several points established by regulatory bodies [14]. Also, one of the most critical times when the risk of uncertainty is higher [13]. Several accidents were reported during the launch of the petrochemicals plant [15]. Therefore, the initial safety of the work is a significant problem for chemical plants. In implementing EO plant operations, safety requirements are paramount. They can lead to significant changes in high temperatures and stress, failure due to failure, high air pollution and significant economic losses. Especially in the early stages, the catalyst is subjected to the so-called "fragmentation phase," which has very high O2 conversion and low selectivity and is very difficult to control the oxidation process. In the meantime, the responsive traffic congestion of ethylene ($C_2H_4$) and oxygen ($O_2$) should control well under 8% and 25% safety limits, correspondingly. If not, blow up the reactants directly. The primary product, ethylene oxide, is tasteless gas. Therefore, the detonation caused damage/ casualty, mechanical brake, also released a significant amount of poisonous ethylene oxide and extremely active V. O.C.'s. It leads to severe environmental pollution and the loss of raw materials. Therefore, starting with the ethylene oxide plant's safety as critical financial and ecological capabilities [16].

An innovative technique for finding the best reaction concept from a whole process perspective is proposed in the literature. In this approach, the optimal reaction path is determined impartial of current systems and the recycling influencing the reactor is fully considered. The reaction model and the design factors of the process are all optimized together [17]. An Alternative methodology develops on process analysis, bottleneck identification and choice of the perfect process intensification (P.I.) options from a large databank of P.I. technologies. These options are recognized by studying the technical and process limits and employing different shortcut approaches to measure possible process advancements rapidly. Lastly, the most appropriate equipment for adjusting a given bottleneck is incorporated with the process flowsheet. This approach is illustrated utilizing ethylene oxide production as a case study [18]. For a workable ethylene oxide production process, the reaction block's recycling is studied as it influences the reactor, the Heat Exchanger Network (HEN), and the process's profit and could be adjusted quickly and efficiently. The recycle optimization of a practical EO production process is studied established on the integration of HEN and reactor. Based on the kinetic and thermodynamic equilibrium, relations between the recycle ratio, outlet temperature and the removed heat of the reactor are determined. With both HEN and the reactor considered, the integration model is built. An economic analysis diagram is developed to demonstrate the range of income and expenditure and the recycling ratio [19].

A review of the literature found a demand for a cost-effective and reliable technique to simulate and economically evaluate the EO production process. This work simulates the Ethylene Oxide (EO) production process in Aspen plus and energy optimization of the whole process is performed using the Pinch analysis based on the simulation results. The research aims to develop a model of the ethylene oxide process in Aspen Plus® software to improve the energy optimization of the chemical process industry. Research target on simulation, energy optimization and cost analysis of whole ethylene oxide process. Another aim of this study is to develop process modeling and simulation in Aspen Plus® software, generate the pinch analysis of the ethylene oxide process, and do the cost analysis of the ethylene oxide process. Initially, the cost analysis is done before the energy optimization and the second cost analysis is done after the energy optimization and shown the cost comparison. The use of pinch analysis in this study is novel
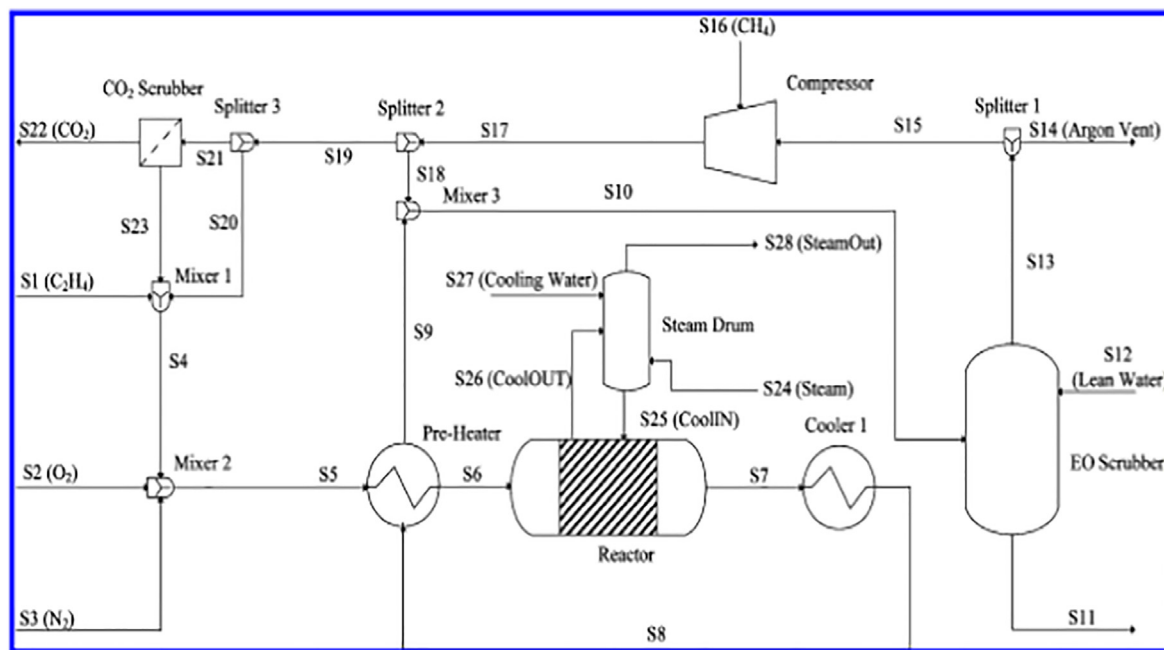
**Fig. 1.** Flowsheet of EO Plant [15].

since it has not been used previously for the economic analysis of an EO process.

## 2. Process design

The first developed ethylene oxide process was developed in 1859 to remove hydrochloric acid from ethylene chlorohydrin using potassium hydroxide. This lead is the industrial development of oxirane (EO), which started in 1914. Direct oxidative of ethylene ($C_2H_4$) exposed by Leffort in 1931 was replaced gradually with the chlorohydrin method. Nowadays, ethylene oxide is commercially generated by ethylene directly oxidation with oxygen or air [20].

### 2.1. Direct oxidation process

The first EO marketing programs to use direct oxidation were Carbide and Carbon Chemicals Corp., which started their first plants based on air in 1937. In 1953 a process for the development of air-cooled scientific (S.D.) projects was introduced, and in the late 1950 s, a natural binding process began to substitute the chlorohydrins process. Shell improvement in 1958 introduces the initial process base on direct oxygenation. The following year, the process oxygen-based was marketed by Halcon in 1969 and 1976 Union Carbide [21].

The primary cause that the chlorohydrins process works are no longer costly. The oxirane production by chlorohydrins method costs 3–4 times more than the direct oxidation method. An additional drawback of chlorohydrins is the quandary of handling vast quantities of desecrate products containing hydrocarbon and calcium chloride levels in chlorine and glycols. The direct oxidation method's significant disruption and ineffectiveness are the low yields of oxirane. Each component of the ethylene supply is used for carbon dioxide and water at a 20–25% ethylene loss. All oxirane directly oxidized industries are based on the first chemical method reported in the literature [22]. At 220–300 °C and a pressure bar of 10–30, a small product is produced without direct $CO_2$ and $H_2O$, $C_2H_4$ and $C_2H_4O$ vapors in silver catalysts. The most important

actions are: In addition to the silver alumina filtration, ethylene is mixed with oxygen to make oxirane.
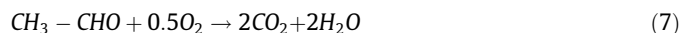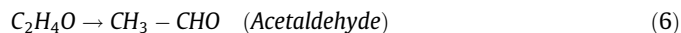
$$C_2H_4 + 0.5O_2 \rightarrow C_2H_4O \quad \Delta H_{298} = -1067 \ kj/mol \quad (3)$$
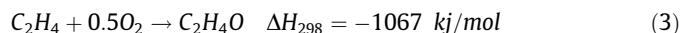
Ethylene is completely oxidized to form carbon dioxide and water.

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \quad \Delta H_{298} = -1323 \ kj/mol \quad (4)$$
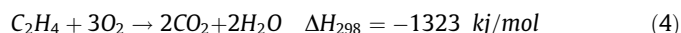
Ethylene oxide is also oxidized to form $CO_2$ and $H_2O$.

$$C_2H_4O + 2.5O_2 \rightarrow 2CO_2 + 2H_2O \quad \Delta H_{298} = -1323 \ kj/mol \quad (5)$$

To prevent excess liquid $C_2H_4O$, the exchange of ethylene to business processes is usually 10 to 20%, leading to gas redistribution, explained in more detail in the literature [22]. With a direct oxidizing process, a minor ppm of ethyl-chloride (2.5 to 3.0 ppm)/ vinyl-chloride (4 to 6 ppm) can be added to the gas supply to prevent oxidization entirely and raise the oxirane selectivity [23]. Both products are available in small quantities, but generally, an amount less than 0.1% acetaldehyde with small amounts of formaldehyde formed:

$$C_2H_4O \rightarrow CH_3 - CHO \quad (Acetaldehyde) \quad (6)$$

$$CH_3 - CHO + 0.5O_2 \rightarrow 2CO_2 + 2H_2O \quad (7)$$

$$C_2H_4 + O_2 \rightarrow 2CH_2O \quad (Formaldehyde) \quad (8)$$

Directly oxidized processes (EO) can separate addiction to the atmosphere and air process. Description of Air-to-Air Flow Process The Halcon SD air system's overflow and filling process is considered a representation of the bulk oxirane process.

### 2.2. Airbase direct oxidation method

The compressed air purifies by removing impurities mixed with renewable gases and new ethylene in an initial step [21]. Ethylene dichloride, vinyl chloride, and halogenated compound are placed in the gas phase of oxidation inhibitors in reaction space to slow carbon dioxide production [22]. The gas is fed into a powerful multi-tube facility where the converter's temperature is controlled by the

distribution of boiling water or crude oil on the side of the shell. It cools in a smoke generator with oil and has a very high power to be used in this process. The garbage from a large reactor contains oxirane, cools in a hot tub with a cold generator. Then cooling is applied to the main component. Ethylene oxide is added to the water, resulting in a robust solution. The electricity released from the absorber is suppressed. A large portion of the gas is reused in a large reactor. Fraction of gas stream is sent to second (vacuum) reaction arrangement to purify the $N_2$ deposited in atmosphere source and $CO_2$ formed in reactors.

### 2.3. Oxygen-base direct oxidation method

Extremely purified $O_2$ is mixed with used gas, and new and $C_2H_4$ the resulting gas mixture is injected into a multi-bulb reactor like air. A heat transfer gas heats waste gas containing ethylene oxide before entering the absorber. In absorption, ethylene oxide is dissolved in water-absorbing water, creating a strong reduction solution. The gas is purified, pressed, and used in the reactor. The fraction of recycled gases is initially transferred to the carbon dioxide connector, where $CO_2$ is formed chemically in the reactor treated in re-allocated hot $K_2CO_3$ solution. Carbon dioxide cooling gas is returned to used fuel and returned to reactors. Rich carbonated $CO_2$ solution reconstituted in carbon dioxide shale use carbon dioxide also steam emanating from the top of the column [21]. A small amount of circulating gas is released into the atmosphere or at room temperature to prevent the accumulation of non-artificial substances such as argon, oxygen pollutants. If not released argon, it accumulates 30–40% in gas cycles. Due to the low-temperature content of argon, circulating gases can enter the combustible environment. As an outcome, the concentration of oxygen in gas circulation should be reduced [22]. Fig. 2 is the block flow diagram of the ethylene oxide production process, which spreads the scenario of the whole process.

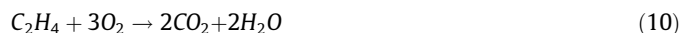## 3. Modeling and simulation of ethylene oxide production process

For ethylene oxide (Oxirane) production, the significant reactants are Ethylene and Oxygen; either the oxygen comes from air or used oxygen cylinders. The modeling and simulation of ethylene oxide are done in ASPEN PLUS ®. Process flow diagram of the process is:

Fig. 3 is the process flow diagram of ethylene oxide in Aspen plus; as from the process flow diagram, first, the air passes through multistage compressors (B11, B12, B13). The heat exchangers (B14, B15) are present between the multistage compressors for temper-

ature control. After passing through multistage compressors (stream 6), the temperature is 196.7 °C and the pressure is at 27 bar the other raw material (stream 7), ethylene gas, whose temperature is 25 °C and the pressure is at 50 bar, is first mixed with recycle stream in the mixer (B19) then moves forward. Both streams air and ethylene gas are mixed in a mixer and the temperature and pressure of the mixed stream are 106.7 °C, 26.8 bar (stream 7A). After that, the mixture is passed through the heat exchanger(B16) to get it to the desired temperature. When the mixed stream entered the reactor, the temperature and pressure of the mixed stream at the outlet of the heat exchanger is 240 °C and 26.5 bar pressure (stream 8). The mixed stream is then entered into the first reactor (B1). The reactions occur between the reactants in the presence of catalyst and ethylene oxide desired product is formed with unconverted ethylene and other byproducts carbon dioxide and water. It passes the separation column (Absorber) to separate the desired product from the mixture (stream 11), it passes the separation column (Absorber). The ethylene oxide is mixed with water and separated from the column (stream 14). The unconverted raw material (stream 13) is moved up in a column and further moves to the heat exchanger(B5) to attain the desired temperature and pressure again at 240 °C and 26.5 bar. Then enter the second reactor(B6), where unconverted raw material is converted into ethylene oxide (stream 18). The separation of ethylene oxide from the mixture again passes through the next separation unit (Absorber). Ethylene oxide is mixed with water and remove from the bottom (stream 24). The little unconverted ethylene is recycled back (stream 22). Next to purifying the ethylene oxide and improving its purity, the mixture of ethylene oxide and water carbon dioxide moves further to the separation column (B17). The purified ethylene oxide (stream 25) is separated from the distillation column at 98 °Cand pressure at 10 bar.

### 3.1. Reaction kinetics

The following reactions occur in the proposed model.

$$C_2H_4 + 0.5O_2 \rightarrow C_2H_4O \tag{9}$$

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \tag{10}$$

$$C_2H_4O + 2.5O_2 \rightarrow 2CO_2 + 2H_2O \tag{11}$$

Kinetic expressions and the reaction rate units are mol/m³ s. PSRK and UNIFAC thermodynamic packages are used for the simulation of reactors and absorbers, respectively.

$$r_1 = \frac{1.96 \exp\left(-\frac{2400}{RT}\right) P_{ethylene}}{1 + 0.00098 \exp\left(\frac{11,200}{RT}\right) P_{ethylene}} \tag{12}$$
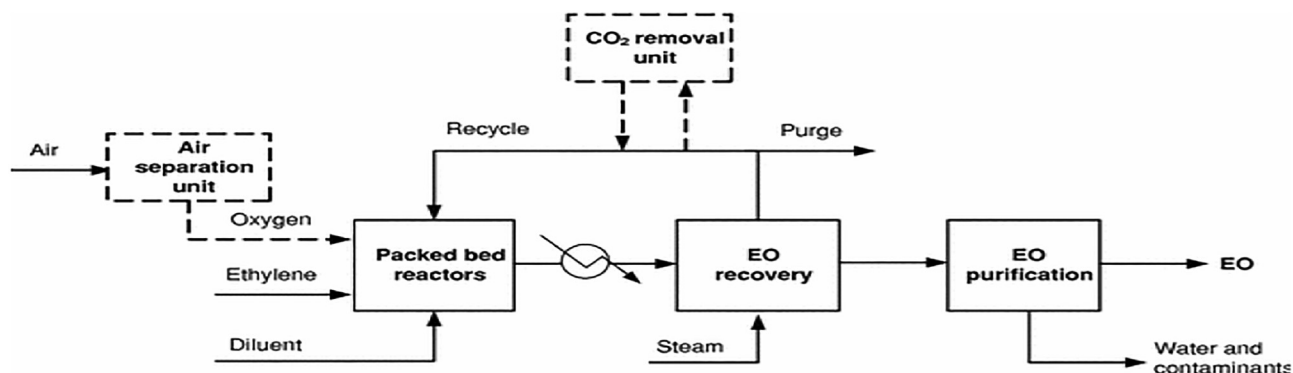


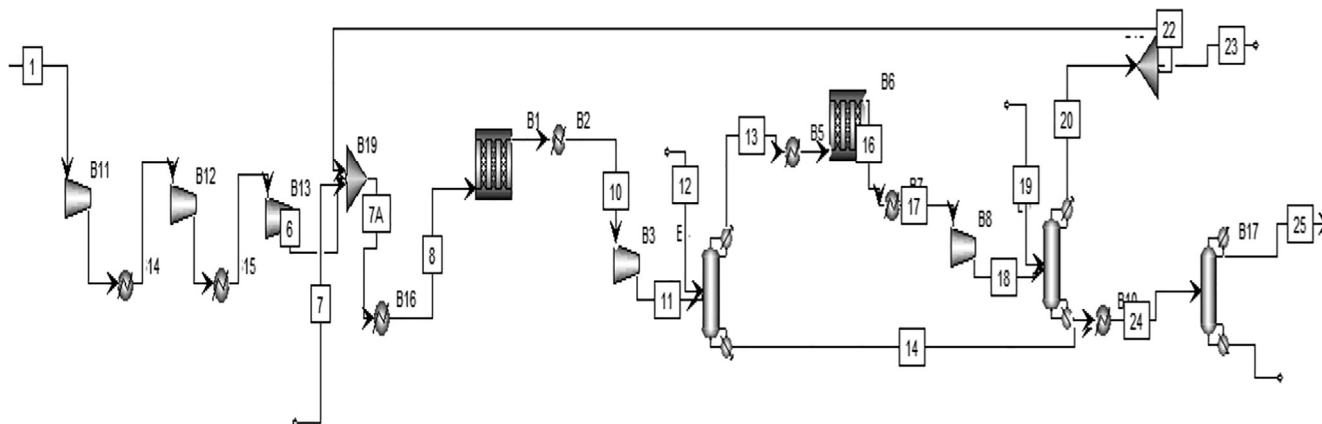**Fig. 2.** Block flow diagram of EO production process [8].

**Fig. 3.** Process Flow Diagram of Ethylene oxide production process in Aspen plus.

$$r_2 = \frac{0.0936 \exp\left(-\frac{6400}{RT}\right) P_{ethylene}}{1 + 0.00098 \exp\left(\frac{11,200}{RT}\right) P_{ethylene}} \tag{13}$$

$$r_3 = \frac{0.42768 \exp\left(-\frac{6200}{RT}\right) P_{ethyleneoxide}^2}{1 + 0.000033 \exp\left(\frac{21,200}{RT}\right) P_{ethyleneoxide}^2} \tag{14}$$

### 3.2. Simulation of EO process

Table 1 shows the results of various streams in the whole process; stream 6 shows the result after passing through the multistage compressor, and the feed enters the first reactor. Stream 9 shows the result after passing through the absorber, a mixture of unconverted ethylene and the air is entered into the second reactor. Stream 16, after passing through the second absorber, the mixture of ethylene oxide, water, and carbon dioxide is entered into the heat exchanger. Stream 24 after achieving the desired temperature, the mixture of ethylene oxide, water, carbon dioxide, and little unconverted ethylene gas is fed in a distillation column.

## 4. Pinch analysis of EO process

The study of an algebraic approach is as followed. Thermal data of the process stream are collected. The temperature interval diagram was made on the suitable temperature difference. The utility target is determined, and stream splitting technology was employed to create a network. Fig. 4 shows the grid diagram of the Ethylene oxide production process. Table 2 shows the area and cost estimated at different temperature intervals $\Delta T = 10$ and 20. It seems clear that when the $\Delta T = 10$, the area target is

increased because for more heat recovery greater the overall area of the heat exchanger network, which also increases the capital cost target. This study used $\Delta T = 20$ where the lesser area is required, which causes a lower capital cost target and causes an impact of $1.32 \times 10^6$ \$/yr. Table 3 represented the temperature intervals of the Ethylene oxide production process. Table 4 presents the grid diagram explaining that the minimum temperature difference between the interaction of hot and cold streams is 20 K.

### 4.1. Composite and grand composite curves

The composite curve containing a hot stream and cold stream in a process plant and a curve gives the overall profile of both available heat and required demand in a specific process. The curve represents the minimum cold and hot utilities required. Moreover, the minimum driving force is required for the process. The next stage to the grid diagram used to identify the location and number of heat exchangers is required in the process industry. It is noted that a change in process parameters due to optimization and modification will change the pinch point and change the hot and cold utilities. The composite curve diagram is shown whether nor or not the heat exchanger is correctly arranged. Fig. 5 presented the composite curve of the ethylene oxide production process, which represents how a cold stream collects much energy from the hot stream. Fig. 6 shows the grand composite curve of the ethylene oxide production process.

### 4.2. Area and cost targets

Fig. 7 represents the network design after the pinch analysis. Most of the waste heat recovery in the process and use of external

**Table 1**
Summary of results from various streams of a process flow diagram.

| | Stream 6 | Stream 9 | Stream 16 | Stream 24 | Stream 25 |
|---|---|---|---|---|---|
| Temperature (℃) | 196.7 | 240 | 240 | 45 | 98.2 |
| Pressure (bar) | 27.19 | 26.5 | 25.8 | 10 | 10 |
| Vapor Fraction | 1 | 1 | 1 | 0 | 1 |
| Mole Flow (kmol/hr) | 17381.7 | 42424.8 | 41542.8 | 41625.9 | 1798.24 |
| Volume Flow (cum/hr) | 24968.6 | 68303.9 | 68698.9 | 68066.9 | 5551.96 |
| Mass Flow (kg/hr) | 500,000 | $1.22 \times 10^6$ | $1.94 \times 10^6$ | $7.74 \times 10^5$ | $5.63 \times 10^4$ |
| Enthalpy | 20.94 | 66.18 | 58.91 | −2722.03 | −13.25 |
| Mole Flow (kmol/hr) | | | | | |
| Ethylene | | 974.635 | 781.663 | 21.52 | 21.52 |
| EO | | 217.89 | 218.78 | 350.70 | 350.70 |
| $CO_2$ | | 51.99 | 63 | 7.25 | 7.25 |
| $H_2O$ | | 73.20 | 111.96 | 39992.5 | 164.8 |
| $O_2$ | 3281.4 | 7048.55 | 6706.21 | 459.12 | 459.12 |
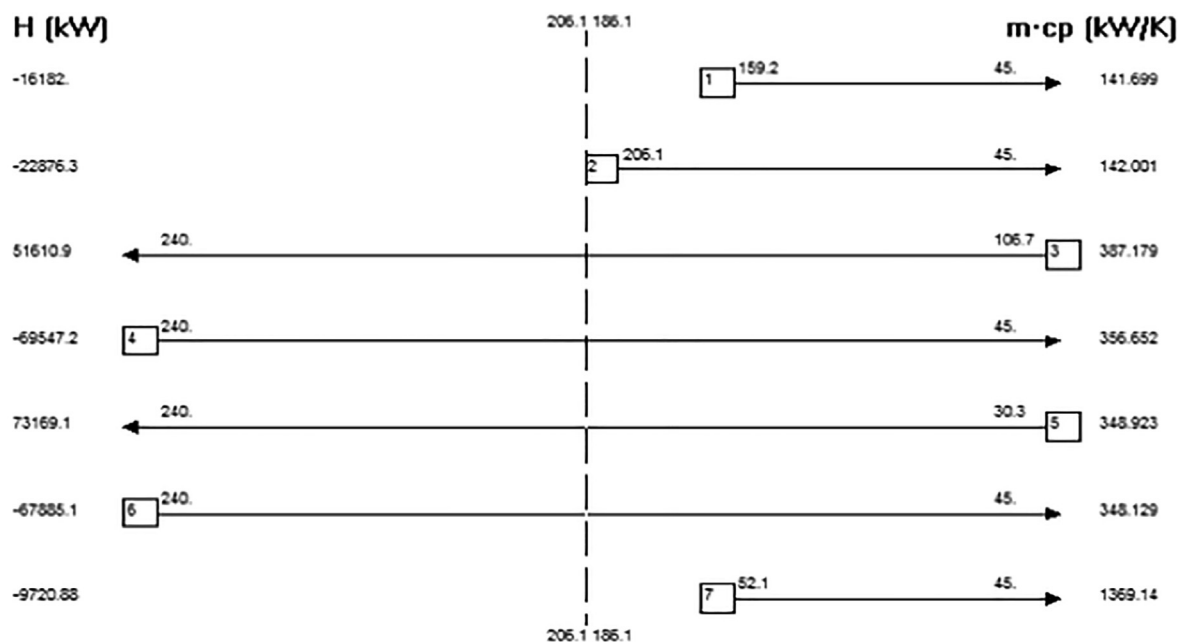
**Fig. 4.** Grid diagram of EO production process.

**Table 2**
Area and Capital cost target at different minimum temperature difference intervals.

| Minimum Temperature Difference | Area Target (m$^2$) | Capital Cost Target ($/yr) |
|---|---|---|
| At $\Delta T$ = 10 | 9,268 | $5.049 \times 10^6$ |
| $\Delta T$ = 20 | 5,824 | $3.707 \times 10^6$ |
| Difference | 3,444 | $1.342 \times 10^6$ |

**Table 3**
Temperature Intervals of EO production process.

| Temperature (K) | Enthalpy (kW) |
|---|---|
| 250 | 15783.8 |
| 230 | 1061.76 |
| 196.1 | 0 |
| 149.2 | 5190.91 |
| 116.7 | 13393.2 |
| 42.1 | 61104.2 |
| 40.3 | 64719.9 |
| 35 | 77215.3 |

**Table 4**
Information of grid diagram shown in Fig. 4.

| Minimum temperature difference: | 20 K |
|---|---|
| *Calculating the energy cascade, the following results are obtained:* | |
| Pinch Temperature: | 196.1 K. |
| Energy Target (Heating): | 15783.8 kW. |
| Energy Target (Cooling): | 77215.3 kW. |



**Fig. 5.** Composite curves of EO production process.

targets of the EO production process at a minimum temperature difference of 20 K.

## 5. Results and discussion

The ethylene oxide process's modeling and simulation mainly control the reactor's temperature. When the temperature is not controlled, there is complete oxidation of ethylene and produces byproducts such as Carbon dioxide and water. Ethylene oxide, the desired product, is produced by partial oxidation of ethylene. Results available when the mixture of ethylene and air is entered in the first Reactor in ASPEN PLUS®. The unconverted ethylene is again entered into the second reactor. The unconverted ethylene is again partially oxidized in air and the results are generated in ASPEN PLUS®.

### 5.1. Optimization results

For the energy optimization of the ethylene oxide process, pinch analysis is applied to the process. After the pinch analysis, recover most heat energy waste when there is no interaction between the

utilities reduces by utilizing heat. Before pinch analysis, need 15783.8 kW of heat to achieve the desired temperature, but after pinch analysis, recover 6962.7 kW of heat from hot streams and only provided 8821.1 kW of heat. Before pinch analysis, we need 77215.3 kW of cold heat utility to achieve the desired temperature. However, after pinch analysis, the proposed model recovers 6963.1 kW of heat from cold streams and only provided 70252.2 kW of cold heat utility. Table 5 shows the area and cost
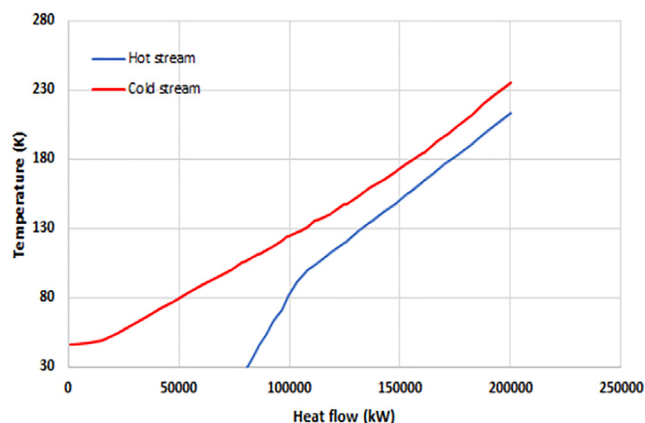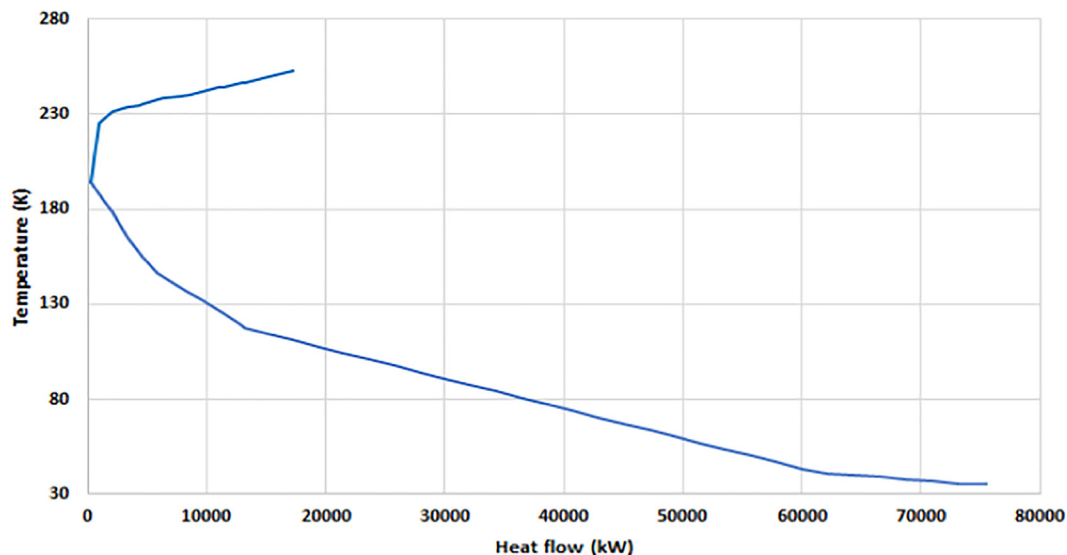
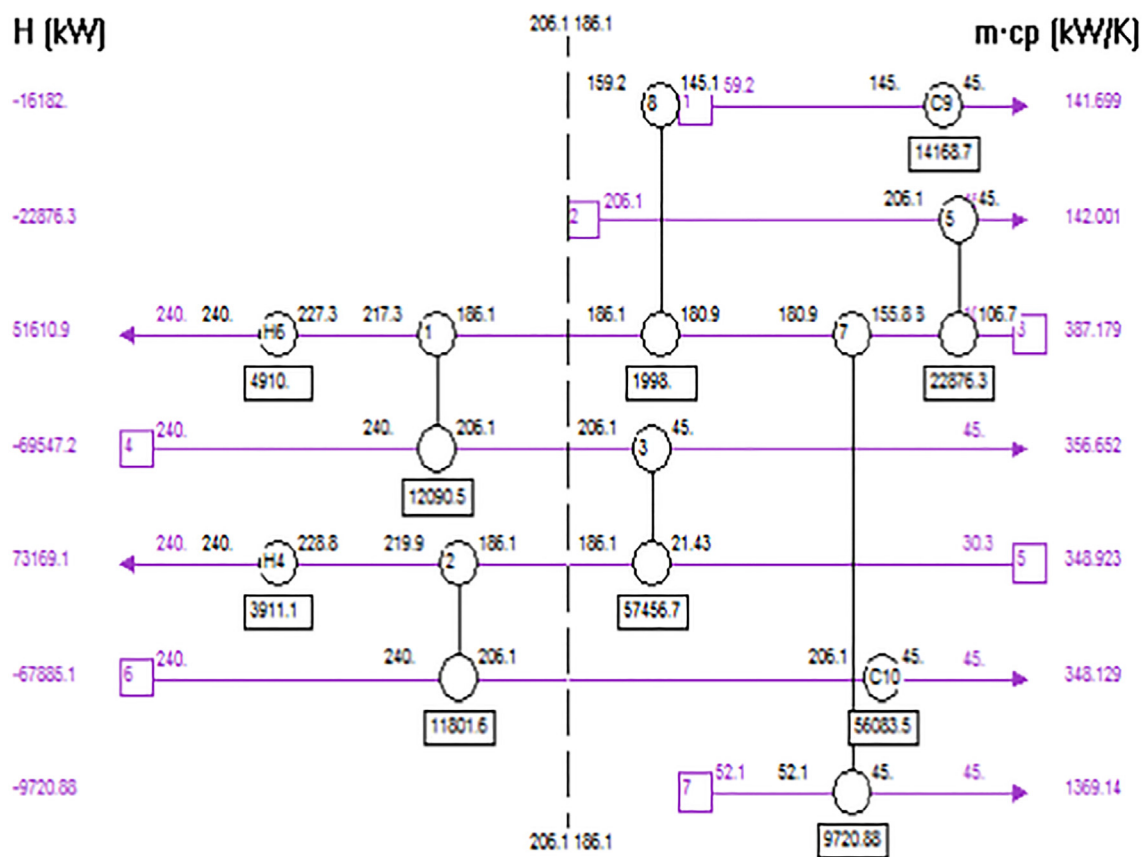**Fig. 6.** Grand composite curves of EO production process.



**Fig. 7.** Heat exchanger network design of EO production process.

heat exchangers. After the pinch analysis, most of the waste heat recovery in the process and use of external utilities reduces by utilizing heat. Before pinch analysis, need 15783.8 kW of heat to achieve the desired temperature, but after pinch analysis, recover 6962.7 kW of heat from hot streams and only provided 8821.1 kW of heat.

Before pinch analysis, the process needed 77215.3 kW of cold utility to achieve the desired temperature. However, after pinch

analysis, recover 6963.1 kW of heat from cold streams and only provided 70252.2 kW of cold utility. Therefore, the operating cost (Utility cost) of the whole process is also reduced by Pinch analysis after recovering most of the heat from the process. Table 6 shows the annual utility cost of the ethylene oxide production process before the pinch analysis.

Before utilizing the pinch technology, 21 M.\$ in cost is consumed per year to achieve the whole process's desired tempera-

**Table 5**
Area and cost targets of EO production process.

| | |
|---|---|
| Minimum Number of Heat Exchangers: | 11 |
| Area Target: | 5824.13 m$^2$ |
| Minimum Temperature Difference | 20 K |
| *Cost Targets:* | |
| Operating: | 4.65 × 10$^6$ $/yr. |
| Capital (Total): | 3.71 × 10$^6$ $. |
| Capital (Annualized): | 370,742 $. |
| Annualized total: | 5.02 × 10$^6$ $. |
| *To calculate cost targets and annualize them, the following data have been used:* | |
| Heating cost: | 50 $/kJ. |
| Cooling cost: | 50 $/kJ. |
| Pay-back time: | 10 years. |
| Interest Rate: | 5 %. |
| Lang Factor: | 3.4 |

ture. When the pinch technology is used, it recovers the waste heat from the process, but no heat exchangers are increased and decreased in external utilities. Total utility cost after the pinch technology is shown in Table 7. After the Pinch technology, only 2.7 M.$ costs are consumed per year to achieve the desired temperature in the whole process and save 18.266 M.$ per year.

Table 8 shows the economic analysis of the whole Ethylene oxide production process. All equipment costs, the land cost in terms of gross root and total module cost, the raw material cost, utility cost is calculated, and the overall profit is found. After the economic analysis, the results clearly show that after the energy optimization and cost analysis of the ethylene oxide production process, profits increased by 22.39 M$/year.

Table 9 compares Aspen Plus results with the literature results at the second reactor outlet in the production of the ethylene oxide process. Unconverted oxygen and ethylene are separated and recycled again to the reactor.

**Table 8**
Economic analysis of the EO production process.

| Before energy optimization results | | After energy optimization results | |
|---|---|---|---|
| Total module Cost | 185.9 M$ | Total module Cost | 187.67 M$ |
| CRW (Cost of raw material) | 110.18 M$ | CRW (Cost of raw material) | 110.2 M$ |
| Annual Cost of Utility | 20.97 M$ | Annual Cost of Utility | 2.71 M$ |
| Gross root cost | 233 M$ | Gross root cost | 236.2 M$ |
| **Profit** | **51.73 M$** | **Profit** | **74.12 M$** |

**Table 9**
Literature result comparison with Aspen plus result [24].

| | Literature Result | ASPEN PLUS Result |
|---|---|---|
| Temperature (°C) | 45 | 45 |
| Pressure (Bar) | 10 | 10 |
| Mole flow (kmol/hr) | 40,355 | 41,626 |
| *Components flow rate (kmol/hr)* | | |
| Ethylene | 1.27 | 21.52 |
| $O_2$ | 2.89 | 459.2 |
| EO | 354.22 | 350.7 |
| Water | 40,000.7 | 39992.5 |
| $CO_2$ | 0.02 | 7.245 |
| $N_2$ | 5.35 | 795 |

## 6. Conclusions

This study focused on ethylene oxide production by the air-based system and modeled and simulated the whole process in ASPEN PLUS®. By virtual experiments, predict the actual process's behavior. Finally, it is concluded that we control the oxygen concentration by controlling the airflow and controlling the reactors'

**Table 6**
Utility summary of EO production process before pinch analysis.

| Name | Total module cost ($) | Grass root cost ($) | Utility used | Actual usage (MJ/h) | Annual utility cost ($) |
|---|---|---|---|---|---|
| E-101 | 365,012 | 520,000 | Cooling water | 58,500 | 184,000 |
| E-102 | 369,000 | 525,000 | Cooling water | 83,200 | 262,000 |
| E-103 | 761,000 | 1,080,000 | High pressure steam | 148,000 | 6,950,000 |
| E-104 | 740,000 | 1,050,000 | Cooling water | 210,000 | 660,000 |
| E-105 | 750,000 | 1,070,000 | High pressure steam | 230,000 | 10,830,000 |
| E-106 | 730,000 | 1,030,000 | Cooling water | 21,500 | 68,000 |
| E-107 | 190,000 | 265,000 | Cooling water | 207,000 | 650,000 |
| R-101 | 8,000,000 | 8,900,000 | Medium pressure steam | 33,100 | 766,000 |
| R-102 | 8,000,000 | 8,900,000 | Medium pressure steam | 26,200 | 606,000 |
| P-101 | 26,700 | 34,000 | Electricity | 4.65 kW | 2,610 |
| **Total** | **19,931,712** | **23,374,000** | | | **20,978,610** |

**Table 7**
Utility summary of EO production process after pinch analysis.

| Name | Total module cost ($) | Grass root cost ($) | Utility used | Actual usage (MJ/h) | Annual utility cost ($) |
|---|---|---|---|---|---|
| E-101 | 466,481 | 664,000 | N/A | – | – |
| E-102 | 485,000 | 690,000 | N/A | – | – |
| E-103 | 2,178,000 | 3,090,000 | N/A | – | – |
| E-104 | 160,000 | 222,000 | Low pressure steam | 14,100 | 238,000 |
| E-105 | 1,537,000 | 2,180,000 | N/A | – | – |
| E-106 | 174,000 | 246,000 | Low pressure steam | 17,700 | 299,000 |
| E-107 | 141,000 | 199,000 | N/A | – | – |
| E-108 | 126,000 | 179,000 | N/A | – | – |
| E-109 | 218,000 | 310,000 | Cooling water | 51,000 | 161,000 |
| E-110 | 535,000 | 760,000 | Cooling water | 202,000 | 640,000 |
| R-101 | 8,000,000 | 8,900,000 | Medium pressure steam | 33,100 | 766,000 |
| R-102 | 8,000,000 | 8,900,000 | Medium pressure steam | 26,200 | 606,000 |
| P-101 | 26,700 | 34,000 | Electricity | 4.65 kW | 2,610 |
| **Total** | **20,810,712** | **24,623,000** | | | **2,712,610** |

temperature throughout virtual experiments. When the oxygen concentration increases, ethylene is oxidized completely and generates useless carbon dioxide and water products. Enhancing ethylene production must partially oxidize that generates our desired product ethylene oxide. The energy optimization of the whole ethylene oxide process is also completed through Pinch analysis and recovers most of the valuable energy that is causing external utilities to be low and saves money in heating or cooling of streams. The critical contribution of this work is the solution it provides for process simulation and cost analysis of ethylene oxide production by applying pinch analysis. An overall summary of the economic analysis results is given in Table 7. The results clearly show that after the energy optimization and cost analysis of the ethylene oxide production process, profits increased by 22.39 M $/year. The results were directly compared with the previously reported findings on process simulation of ethylene oxide (Table 8). These findings are in line with results reported by other publications in the literature.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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