Revista de Ciencia y Tecnología
ISSN: 1851-7587

Centro de Investigación y Desarrollo Tecnológico, Facultad de Ciencias Exactas, Química y Naturales, Universidad Nacional de Misiones

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Revista de Ciencia y Tecnología, no. 37, 2022, pp. 11-20

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DOI: https://doi.org/10.7440/res64.2018.03

RECyT
Year 24 / Nº 37 / 2022 / 15–24
DOI: https://doi.org/10.36995/j.recyt.2022.37.002

Simulation of the ethylene oxide production process in ChemCAD® simulator

Simulación del proceso de producción de óxido de etileno en el simulador ChemCAD®

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Received: 01/12/2020; Accepted: 21/08/2021

Abstract

Ethylene oxide is an important industrial chemical compound used as an intermediate in the production of glycols and other plastics. In the present work, the process of ethylene oxide (EO) production from the catalytic oxidation of ethylene was simulated using the ChemCAD® simulator. Heat curves were obtained for each of the shell and tube heat exchangers used, while the flow rate and composition of the most important streams involved in the production process were determined. A sensitivity study was also carried out to establish the influence of a decrease in the feed temperature of the wash water to the absorbers on the amount of EO to be obtained in the distillation column. 22,163.5 kg/h of EO is obtained from the top of the distillation column with a purity of 98.29 %. The wash water should be fed to the absorbers at a temperature of 5 ºC to maximise the amount of EO to be obtained in the distillation column.

Keywords: Sensitivity analysis; ChemCAD®; Heat curve; Ethylene oxide; Simulation.

Resumen

El óxido de etileno es un importante compuesto químico industrial usado como intermediario en la producción de glicoles y otros plásticos. En el presente trabajo se efectuó la simulación del proceso de producción del óxido de etileno (OE) a partir de la oxidación catalítica del etileno, empleando el simulador ChemCAD®. Se obtuvieron las curvas de calor de cada uno de los intercambiadores de calor de tubo y coraza empleados, mientras que se determinó el caudal y composición de las corrientes más importantes involucradas en el proceso productivo. También se llevó a cabo un estudio de sensibilidad para establecer la influencia que presenta una disminución de la temperatura de alimentación del agua de lavado a los absorbedores, sobre la cantidad de OE a obtener en la columna de destilación. Se obtienen 22.163,5 kg/h de OE por la corriente del tope de la columna de destilación con una pureza de 98,29 %. Se deberá alimentar el agua de lavado a los absorbedores a una temperatura de 5 ºC para maximizar la cantidad a obtener de OE en la columna de destilación.

Palabras claves: Análisis de sensibilidad; ChemCAD®; Curva de calor; Óxido de etileno; Simulación.

Introduction

Ethylene oxide (EO) is a colourless gas that liquefies at low temperatures to a mobile liquid. It is miscible in all proportions in water or alcohol, and is very soluble in ether [1].

It is commonly used in the manufacture of ethylene glycol, which is an antifreeze compound, as well as an important raw material for the production of polyethylene terephthalate, used in the manufacture of polyester fibres. It is also used for the preparation of surfactants, the manufacture of ethanolamines, for the production of ethylene glycols used in plasticising agents, solvents and lubricants, and to obtain glycol ethers used as jet fuel additives and solvents [1].

As it is a highly reactive chemical compound, it has several other uses as a reaction agent. However, due to its reactivity, explosion hazard and toxicity, it is rarely shipped out of the manufacturing facility, but instead is pumped directly to the adjacent consumer [2].

Commercial EO production processes involve the direct oxidation of ethylene over a silver catalyst packed in reactor tubes together with promoters, either using air or pure oxygen. The reactions that occur during EO production by partial ethylene oxidation consist of [3]:

Partial oxidation of ethylene to obtain ethylene oxide (epoxidation).

Total oxidation of ethylene to obtain carbon dioxide and water.

The consecutive oxidation of ethylene oxide to obtain carbon dioxide and water.

Since the reactions involved are highly exothermic, the efficiency of heat transfer is critical. In the industrial production of EO, fixed-bed multi-tube reactors are widely used. Heat is removed by means of a cooling agent circulating in the reactor shell. Over time, the silver-based catalysts used for ethylene oxide production exhibit a continuous loss of activity and selectivity, which is accelerated if the reactor is operated at higher than the set temperatures. Undesirable reactions and catalyst burnout can occur if high temperatures are reached. These considerations are particularly important in industrial EO manufacturing, where increasing throughput and reducing risks under varying operating conditions are imperative [4].

Air-based processes operate at low ethylene and oxygen concentrations and higher conversion. In addition to different process technologies, different types of silver catalysts can be used, so catalyst selection is essential to design the best process [3].

Several authors have studied and evaluated the process of ethylene oxidation (epoxidation) to obtain EO, specifically in terms of its kinetics [5] [6] [7] [7] [8], the reaction kinetics in both steady and non-steady state [9], the modelling of a catalytic tubular reactor on an industrial scale [10], the study of the epoxidation reaction in a micro-reaction system [11], the deactivation of the silver catalyst [12], the modelling of the sintering of the catalyst and the evolution of the selectivity of the epoxidation reaction [13], the optimisation of the fixed-bed reactor [14], the modelling and optimisation of the industrial-scale reactor [4], the modelling and dynamic simulation of a catalytic fixed-bed reactor using Artificial Neural Networks [15], the optimisation of the production process and the identification of the best reaction concept [3], and the dynamic optimal design of an industrial-scale reactor using a differential evolution algorithm [16]. The Aspen Plus® simulator has also been used to create a simulation model of the epoxidation reactor, which correlates with reality [17].

In this modern era of powerful computers, the role of process simulation in the chemical industry has grown exponentially. Process simulation is a computer presentation of a real process, plant or system by means of a mathematical model, which is then solved to obtain information about the performance of the process. Simulation allows engineers to model processes in extreme detail without the need to spend time, manpower and money on physical verification of the design in a real industrial environment. Thus, in the competitive world of the chemical industry, process engineering services will not be complete without the presence of process simulators. They are extensively employed as tools to increase, among others, production capacity, company profitability, industrial competitiveness and reduce construction time of new production processes [18].

Among the simulators, most commonly used by engineers today, are Aspen-Hysys®, SuperPro Designer® and ChemCAD®. The ChemCAD® simulator is a sequential modular process simulation programme [19], which allows its users to evaluate the operating conditions of a given process or equipment, to carry out its sizing, and to propose operating alternatives by modifying its variables; while providing, at the same time, a large database of chemical components, thermodynamic models, equipment, accessories, among other options [20].

This simulator has been used to simulate several chemical processes, plants and systems, including the production of dinitrotoluene [18], the reactive distillation of acetic acid and ethanol [21], the thermal-hydraulic analysis of a non-conventional water vapour condenser [22], the fractionation and condensation unit of a waste plastics pyrolysis plant [23], the production of biodiesel from the transesterification of vegetable oils [24], the production of epichlorohydrin from glycerol [25] and the gasification of dried olive pomace [26].

In this article, the simulation of a plant for the ethylene oxide production from the catalytic oxidation of ethylene was carried out using the ChemCAD® simulator, with the aim of determining the mass composition of each of the intermediate and final streams of the production process, as well as their energy content, i.e., to carry out the mass and energy balances. The consumption of the auxiliary services required by all the heat exchangers used in the process was also determined, as well as the heat curves of each of them. Finally, a sensitivity study was carried out to evaluate the influence of the decrease in the inlet temperature of the wash water to the two absorbers on the quantity of EO to be obtained in the distillation column head stream.

Materials and methods

Description of the ethylene oxide production process

The ethylene oxide production process starts with the compression of 500,000 kg/h of dry air at 25 ºC to a pressure of 3 bar by means of a first compressor, which increases the air temperature to 161 ºC, and then cools this compressed stream by means of a shell and tube heat exchanger (Cooler 1) to a temperature of 45 ºC. The air is then compressed again by means of a second compressor to a pressure of 9 bar and a temperature of 206 ºC, and then sent to a second shell and tube heat exchanger (Cooler 2) to reduce its temperature to 45 ºC. The air is then sent to a third compressor to increase its pressure to 27 bar, reaching a temperature of 195 ºC at the outlet of this compressor. In another section of the plant, 20,000 kg/h of ethylene gas is received at a temperature of 25 ºC and a pressure of 50 bar, which is reduced to 27 bar by means of a pressure regulating valve, thus decreasing the pressure of the air at the outlet of the compressor temperature of this stream down to - 6.53 ºC. This ethylene stream is then mixed with a gaseous mixture coming from the top of Absorber 2 (recycle stream), which is at 27 bar and contains ethylene and EO, among other gaseous compounds. The resulting gaseous mixture, which is at 27.3 ºC, is then combined with the previously compressed air stream, and the mixed stream obtained is preheated by means of a shell and tube heat exchanger (Heater 1) to a temperature of 240 ºC, which uses steam at 260 ºC as auxiliary service. Subsequently, this preheated mixture is directed to the first catalytic fixed-bed tubular reactor (Reactor 1), which uses silver catalyst supported on alumina, where three fundamental reactions occur: 1) ethylene epoxidation; 2) total ethylene combustion; and 3) consecutive EO oxidation. The reaction temperature must be controlled at 240 °C by circulating cooling water through the reactor shell, while three reactions are exothermic [4]. The reaction gas mixture at the outlet of Reactor 1, which is at 240 °C and a pressure of 25 bar, is cooled to 45 °C in a shell and tube heat exchanger (Cooler 3) and then compressed to 30 bar by means of a compressor, thereby increasing its temperature to about 64 °C.

This compressed gas stream is sent to a gas-liquid absorption column with perforated trays (Absorber 1), where it is brought into contact with 350,000 kg/h of a liquid water stream at 25 ºC, in order to absorb the EO. The outgoing gas stream at the top of absorber 1 is then preheated to a temperature of 240 ºC using a shell and tube heat exchanger (Heater 2), and its pressure is then regulated to 27 bar by means of a pressure regulating valve. This gaseous reaction mixture is then sent to a second catalytic tubular reactor (Reactor 2), where the three reactions mentioned above take place at 240 ºC temperature and 27 bar pressure, controlling the reaction temperature at 240 ºC by circulating cooling water through the reactor shell. The outlet stream from Reactor 2 is cooled to 45 ºC by a shell and tube heat exchanger (Cooler 4), then compressed by means of a compressor to 30 bar, and then sent to a second gas-liquid absorption column with perforated trays (Absorber 2), where it is mixed with 350 000 kg/h of a liquid water stream. In Absorber 2, an aqueous mixture rich in EO and water is obtained at the bottom, while a gaseous stream rich in ethylene and other gases exits at the top.

This gas stream is split, where 50 % of it is recirculated back into the process (recycle stream), mixing with the pure ethylene feed stream, while the other 50 % is vented to the atmosphere. It should be noted that the recycle stream is pressure reduced to 27 bar by a pressure regulating valve before being mixed with the pure ethylene stream. The aqueous stream from the bottom of Absorber 2 is mixed with the aqueous stream obtained from the bottom of Absorber 1, and the resulting mixture is then sent to a Gas-Liquid Phase Separator where the different gases (carbon dioxide, nitrogen, oxygen, ethylene) that may still exist are vented to the atmosphere through the top, while an aqueous stream containing water and EO is obtained from the bottom. The bottom stream of the Phase Separator is then directed to a shell and tube heat exchanger (Cooler 5) to reduce its temperature to 42 ºC. Finally, the liquid stream cooled at the outlet of Cooler 5 is pumped to the distillation column, where a 98.3% pure EO-rich stream is obtained at the top, water being the main impurity found, while at the bottom an aqueous stream is obtained and sent to the factory's wastewater treatment plant. Figure 1 shows the flow diagram of the process described above.

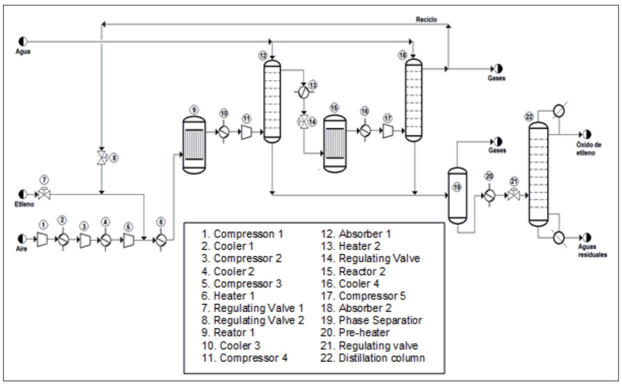


Figure 1: Flow diagram of the ethylene oxide production process by catalytic oxidation of ethylene.

Simulator used

As previously indicated, the ChemCAD® simulator version 7.1.2.9917 [27] from 2017 was used, which is developed by the company Chemstations, Inc. (Wesel, Germany), to carry out the simulation of the EO production process from ethylene.

Catalyst

The catalyst used to carry out the epoxidation reaction is silver supported by an inert support (alumina) [6], which consists of 7.5 mm diameter spheres with a density of 1250 kg/m3 and a void fraction of 0.4 [2].

Table 1: Main chemical reactions taking place in catalytic reactors, their reaction kinetics and fractional conversion.

No.	Chemical reaction	Reaction kinetics	Conv.
1	$C_2H_4 + \frac{1}{2}O_2 \rightarrow C_2H_4O$	$r_1 = \frac{0{,}653 \exp(-2384/RT) p_{etileno}}{1 + 0{,}00098 \exp(11127/RT) p_{etileno}}$	0,72
2	$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$	$r_2 = \frac{454 \exp(-10332/RT) p_{etileno}}{1 + 0{,}00098 \exp(11127/RT) p_{etileno}}$	0,10
3	$C_2H_40 + \frac{5}{2}O_2 \rightarrow 2CO_2 + 2H_2O$	$r_3 = \frac{1{,}4256 \exp(795/RT) p^2_{OE}}{1 + 0{,}000033 \exp(21062/RT) p^2_{OE}}$	0,05

Selection of the thermodynamic model

The Peng-Soave-Redlich-Kwong (PSRK) thermodynamic model with vapour phase association was chosen to carry out the simulation, according to suggestions and indications provided by the ChemCAD® simulator itself through the use of the "Thermodynamics Wizard" option. This is due to the fact that the temperature and pressure limit values used throughout the production process were taken into account, as well as the types of chemical substances being processed.

Chemical reactions involved

Table 1 expresses the main chemical reactions that take place in catalytic reactors, which are, as previously stated, the partial oxidation of ethylene to obtain ethylene oxide (equation 1); the total oxidation of ethylene to obtain carbon dioxide and water (equation 2); and the consecutive oxidation of ethylene oxide to obtain carbon dioxide and water (equation 3). Their reaction kinetics and fractional conversion are also presented [2] [28].

Units of reaction rates are given in kmol/m3.s, pressure is given in bar and activation energies are given in kcal/kmol.

Initial data of the equipment

Tables 2, 3, 4 and 5 show the initial data for the shell and tube heat exchangers, columns, compressors and reactors, respectively, used in the simulation. For the specific equipment name please refer to Figure 1.

Table 2: Initial data for each of the shell and tube heat exchangers used in the simulation.

No.	Name	Heat transfer area (m²)	Type	Material
1	Cooler 1	180	1-2	Carbon Steel
2	Cooler 2	200	1-2	Carbon Steel
3	Heater 1	520	1-2	Carbon Steel
4	Cooler 3	345	1-2	Stainless Steel
5	Heater 2	520	1-2	Carbon Steel
6	Cooler 4	380	1-2	Stainlees Steel
7	Preheater	150	1-2	Carbon Steel

Table 3: Initial data for each of the columns used in the simulation.

N°	Name	Quantity of trays	Reflux Ratio	Material
1	Absorber 1	20	-	Carbon Steel
2	Absorber 2	20	-	Carbon Steel
3	Distillation Column	70	0,89	Carbon Steel

Table 4: Initial data for each of the compressors used in the simulation.

N°	Name	Power (MW)	Adiabatic Efficiency (%)	Material
1	Compressor 1	19,0	80	Carbon Steel
2	Compressor 2	23,0	80	Carbon Steel
3	Compressor 3	21,5	80	Carbon Steel
4	Compressor 4	5,5	80	Carbon Steel
5	Compressor 5	5,5	80	Carbon Steel

Table 5: Initial data for each of the reactors used in the simulation.

N°	Name	N° of pipes	Volumen (m³)	Material
1	Reactor 1	4.722	202	Carbon steel
2	Reactor 2	2.954	95	Carbon Steel

Heat curves

Heat curves were obtained for each of the shell and tube heat exchangers used in the production process, in order to observe the relationship between the temperatures of both fluids with the length of the heat exchanger, thus obtaining a spatial temperature profile that describes the thermal behaviour of the heat exchange process with respect to the length of the equipment. This was done using the "Heat Curves" option contained in the ChemCAD® simulator, thus obtaining 7 heat curves.

Sensitivity study

A sensitivity study was carried out to evaluate the influence of increasing the feed temperature of the wash water to each of the absorbers on the amount of ethylene oxide to be obtained by the current at the top of the distillation column. In this case, the feed temperature of the wash water was varied in the range of 5 - 35 ºC.

Results and discussion

Simulation of the EO production process from the catalytic oxidation of ethylene

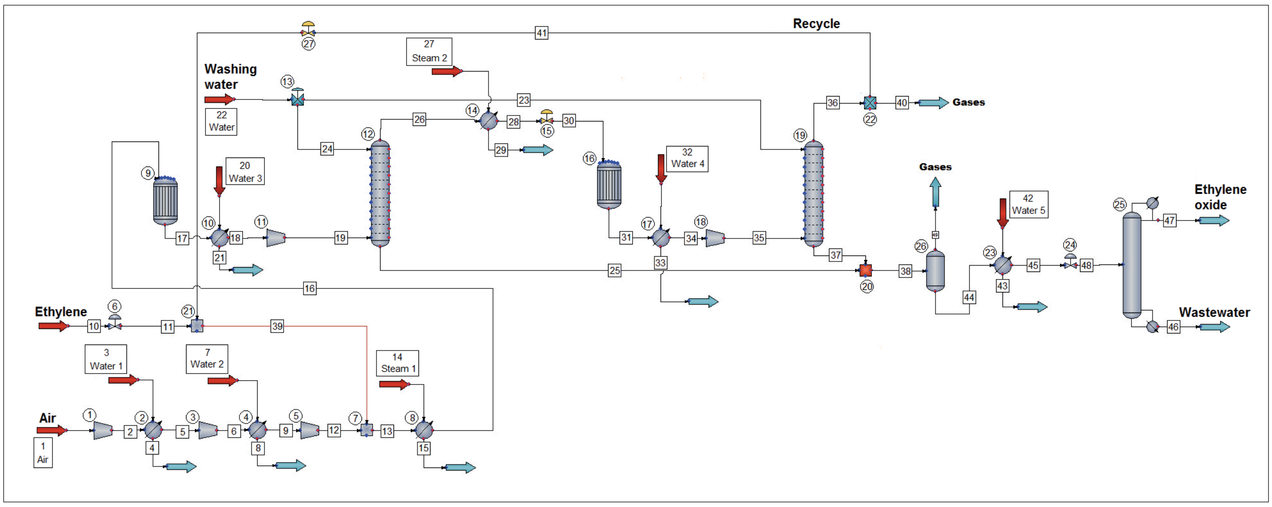


Figure 2: Flow diagram obtained during the simulation of the EO production process using the ChemCAD® simulator.

Figure 2 shows the flow chart obtained during the simulation of the EO production process from the catalytic oxidation of ethylene in the ChemCAD® simulator.

Mass and energy balances of the streams

Table 6 shows the mass flow rates of the main inlet, intermediate and final streams, as well as their enthalpy, temperature, pressure and vapour fraction, which were obtained during the simulation of the production process in the ChemCAD® simulator.

Table 6: Mass and energy balance results obtained for the main inlet, intermediate and final streams.

Variable	Stream number (refer to Figure 2)				
	1	10	11	12	39
Temperature (ºC)	25,00	25,00	- 6,53	195,45	27,30
Pressure (bar)	1,0	50,0	27,0	27,0	27,0
Enthalpy (kcal/h)	- 27,278x10^{3}	8,366x10^{6}	8,366x10^{6}	2,067x10^{7}	- 1,417x10^{7}
Vapour fraction	1	1	1	1	0,99
Compound	Flow rate (kg/h)				
Water	-	-	-	-	706,0
Ethylene oxide	-	-	-	-	3.792,5
Ethylene	-	20.000,0	20.000,0	-	20.363,3
Carbon dioxide	-	-	-	-	9.023,7
Oxygen	105.197,5	-	-	105.197,5	85.543,2
Nitrogen	394.802,5	-	-	394.802,5	394.438,0
Total	500.000,0	20.000,0	20.000,0	500.000,0	513.866,7

Table 6: Continued…

Variable	Stream number (refer to Figure 2)				
	13	16	17	19	25
Temperature (ºC)	108,43	240,00	240,00	63,87	55,21
Pressure (bar)	27,0	26,5	25,75	30,2	30,0
Enthalpy (kcal/h)	6,501x10^{6}	4,072x10^{7}	3,286x10^{6}	- 4,256x10^{7}	- 1,329x10^{9}
Vapour fraction	1	1	1	1	0
Compound	Flow rate (kg/h)				
Water	706,0	706,0	3.479,9	3.479,9	351.850,6
Ethylene oxide	3.792,5	3.792,5	26.625,6	26.625,6	13.804,8
Ethylene	20.363,3	20.363,3	3.665,5	3.665,5	17,0
Carbon dioxide	9.023,7	9.023,7	15.791,4	15.791,4	80,3
Oxygen	190.740,7	190.740,7	175.063,8	175.063,8	57,8
Nitrogen	789.240,5	789.240,5	789.240,5	789.240,5	203,8
Total	1.013.866,7	1.013.866,7	1.013.866,7	1.013.866,7	366.014,3

Table 6: Continued…

Variable	Stream number (refer to Figure 2)				
	26	30	35	36	37
Temperature (ºC)	33,47	240,00	64,34	30,93	54,26
Pressure (bar)	30,0	26,5	30,2	30,0	30,0
Enthalpy (kcal/h)	- 4,035x10^{7}	1,213x10^{7}	- 4,309x10^{7}	- 4,507x10^{7}	- 1,325x10^{9}
Vapour fraction	1	1	1	1	0
Compound	Flow rate (kg/h)				
Water	1.629,3	1.629,3	2.622,2	1.412,0	351.210,2
Ethylene oxide	12.820,8	12.820,8	16.190,1	7.585,1	8.605,0
Ethylene	3.648,5	3.648,5	729,7	726,5	3,2
Carbon dioxide	15.711,1	15.711,1	18.136,7	18.047,4	89,3
Oxygen	175.006,0	175.006,0	171.137,0	171.086,4	50,6
Nitrogen	789.036,7	789.036,7	789.036,7	788.876,0	160,7
Total	997.852,4	997.852,4	997.852,4	987.733,4	360.119,0

Table 6: Continued...

Variable	Stream number (refer to Figure 2)				
	38	**40**	**41**	**48**	**49**
Temperature (°C)	54,74	30,93	30,93	42,42	55,00
Pressure (bar)	30,0	30,0	30,0	10,0	30,0
Enthalpy (kcal/h)	- 2,654x10^{9}	- 2,253x10^{7}	- 2,253x10^{7}	- 1,468x10^{9}	- 1,191x10^{9}
Vapour fraction	0	1	1	0	1
Compound	Flow rate (kg/h)				
Water	703.060,8	706,0	706,0	386.681,0	316.379,8
Ethylene oxide	22.409,8	3.792,6	3.792,5	22.186,1	223,7
Ethylene	20,2	363,2	363,3	-	20,2
Carbon dioxide	169,6	9.023,7	9.023,7	-	169,6
Oxygen	108,4	85.543,2	85.543,2	-	108,4
Nitrogen	364,5	394.438,0	394.438	-	364,5
Total	726.133,3	493.866,7	493.866,7	408.867,1	317.266,2

Table 6: Continued...

Variable	Stream number (refer to Figure 2)	
	46	**47**
Temperature (°C)	180,17	86,58
Pressure (bar)	10,0	10,0
Enthalpy (kcal/h)	- 1,404x10^{9}	- 1,009x10^{7}
Vapour fraction	0	0
Compound	Flow rate (kg/h)	
Water	386.295,0	386,0
Ethylene oxide	22,6	22.163,5
Ethylene	-	-
Carbon dioxide	-	-
Oxygen	-	-
Nitrogen	-	-
Total	386.317,6	22.549,5

Taking into account the results shown in Table 6, it can be established that the recycling stream (number 41 in Figure 2) is composed mostly of nitrogen (79.87 % by mass) and oxygen (17.32 %), contributing 3,792.5 kg/h of EO and 363.3 kg/h of ethylene to the process, which make up 0.77 % and 0.07 % of this stream, respectively. Reactor 1 is fed with 1,013,866.7 kg/h of a gaseous mixture composed mostly of nitrogen (77.84 %) and oxygen (18.81 %), with certain quantities of ethylene (20,363.3 kg/h) and EO (3,792.5 kg/h), which make up 2.00 % and 0.37 % of this stream, respectively.

La corriente de salida del Reactor 1 (No. 17) contiene OE (26.625,6 kg/h) en un 2,63 %; etileno (3.665,5 kg/h) en un 0,36 %; dióxido de carbono (15.791,4 kg/h) en un 1,56 % y agua (3.479,9 kg/h) en un 0,34 %, siendo los principales compuestos químicos encontrados en esta corriente el nitrógeno (789.240,5 kg/h) con un 77,85 %, y el oxígeno (175.063,8 kg/h) con un 17,26 %. Es válido indicar que en el primer reactor se forman 22.833,1 kg/h de OE, y se consumen 16.697,8 kg/h de etileno.

The output stream from Reactor 1 (No. 17) contains EO (26,625.6 kg/h) at 2.63 %; ethylene (3,665.5 kg/h) at 0.36 %; carbon dioxide (15,791.4 kg/h) at 1.56 % and water (3. 479.9 kg/h) by 0.34 %, the main chemical compounds found in this stream being nitrogen (789,240.5 kg/h) with 77.85 % and oxygen (175,063.8 kg/h) with 17.26 %. It is worth noting that 22,833.1 kg/h of EO are formed in the first reactor, and 16,697.8 kg/h of ethylene are consumed.

In Absorber 1, 51.85 % of the EO is absorbed, i.e. of the 26,625.6 kg/h of EO fed to this equipment, 13,804.8 kg/h are absorbed by the wash water, while the rest (12,820.8 kg/h) leave through the gas stream of the buffer (No. 26). Reactor 2 receives 997,852.4 kg/h of a gaseous stream (No. 30) consisting of nitrogen (789,036.7 kg/h) at 79.08 %; oxygen (175. 006.0 kg/h) by 17.53 %; carbon dioxide (15,711.1 kg/h) by 1.57 %; EO (12,820.8 kg/h) by 1.28 %; ethylene (3,648.5 kg/h) by 0.37 % and water (1,629.3 kg/h) by 0.16 %. In the second reactor, 2,918.8 kg/h of ethylene are consumed and 3,369.3 kg/h of EO are produced, resulting in an output gas stream (No. 35) consisting of 79.08 % nitrogen (789. 036.7 kg/h); 17.15 % oxygen (171,137.0 kg/h); 1.82 % carbon dioxide (18,136.7 kg/h); 1.62 % EO (16,190.1 kg/h); 0.26 % water (2,622.2 kg/h) and 0.07 % ethylene (729.7 kg/h).

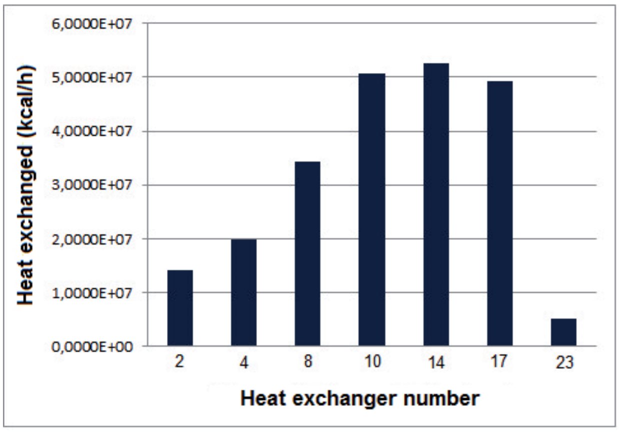
In Absorber No. 2, 53.15 % of the EO is absorbed, i.e. of the 16,190.1 kg/h of EO fed into this unit, 8,605.0 kg/h is absorbed by the wash water, and the rest (7,585.1 kg) leaves through the gas stream at the top of this unit (No. 36). The mixing of the liquid stream from the bottom of Absorber 1 (No. 25), which is mainly made up of 96.13 % water (351,850.6 kg/h) and 3.77 % EO (13,804.8 kg/h), with the liquid stream from the bottom of Absorber 2 (No. 37), which in turn is made up of 96.13 % water (351,850.6 kg/h) and 3.77 % EO (13,804.8 kg/h), with the liquid stream from the bottom of Absorber 2 (No. 37), which in turn is made up of 96.13 % water (351,850.6 kg/h). 37), which in turn is mainly composed of 97.53 % water (351,210.2 kg/h) and 2.39 % EO (8,605.0 kg/h), results in a liquid stream composed of 96.82 % water (703,060.8 kg/h) and 3.09 % EO (22,409.8 kg/h), which is then fed to the Phase Separator. It should be noted that in Absorber 2, a gaseous stream is obtained through the top (No. 36) consisting of nitrogen (788,876.0 kg/h) at 79.87 %, oxygen (171. 086.4 kg/h) 17.32 %, carbon dioxide (18,047.4 kg/h) 1.83 %, EO (7,585.1 kg/h) 0.77 %, water (1,412.0 kg/h) 0.14 % and ethylene (726.5 kg/h) 0.07 %. Half of this gas stream is recirculated back to the production process (Recycle, No. 41), while the other half (Gases, No. 40) is vented to the atmosphere, so it is recommended to design a technological process to recover and purify the 3. 792.6 kg/h of EO leaving this vent stream, in order to increase productivity and profitability, reduce losses of the main product, eliminate the harmful impact on the environment and increase the operational safety of the production process, taking into account that both ethylene and EO are flammable, explosive and reactive chemical compounds in a gaseous state [29].

The buffer stream of the gas separator (No. 49) mainly consists of water (316,379.8 kg/h) at 99.72 %, nitrogen (364.5 kg/h) at 0.11 % and EO (223.7 kg/h) at 0.07 %. In this unit, water is removed by the buffer stream by 45 %, while the other gaseous components are removed by 100 %, with the exception of EO, which has a removal rate of 0.99 %. That is, the EO losses in the phase separator amount to 223.7 kg/h, with a removal rate of 0.99 % compared to the amount of EO fed to this equipment (22,409.8 kg/h).

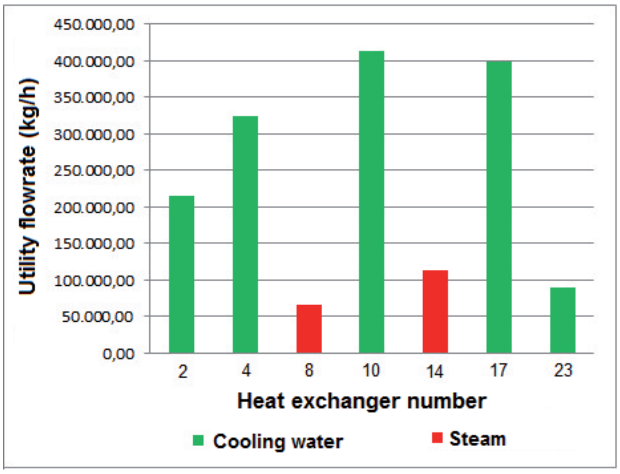
A liquid stream consisting of 94.57 % water (386 681.0 kg/h) and 5.43 % EO (22 186.1 kg/h) is fed to the distillation column. 99.8 % of the EO fed to the distillation column is recovered by the top stream (No. 47), obtaining in this stream 22,163.5 kg/h of EO with a purity of 98.29%, water being the only impurity found. The stream at the bottom of the distillation column (No. 46) produces 386,317.6 kg/h of a stream consisting of 99.99 % water, which is sent to the factory's waste treatment plant to be reused in the production process.

Heat exchanged and auxiliary service consumption of heat exchangers

Figure 3 describes the heat exchanged and the auxiliary service consumption of each of the shell and tube heat exchangers used in the process. For the type of heat exchanger in relation to the number shown in Figure 3, please refer to Figure 2.



a) Heat exchanged



b) Auxiliary service flow rate

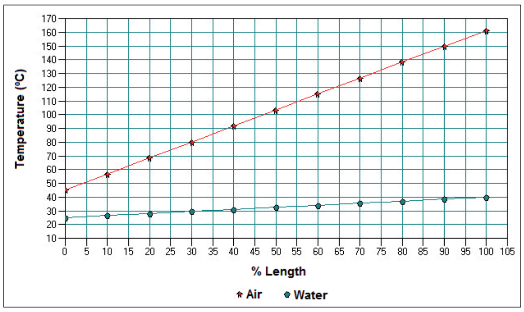
Figure 3: Results obtained for the heat exchangers.

According to Figure 3, the heat exchanger, where most heat is exchanged, is number 14 (refer to Figure 2) with 5.25x107 kcal/h, because it is there where 997,805 kg/h of gas mixture must be heated from 33.47 °C to 240 °C, i.e. it is the largest temperature range found in the production process for a heat exchanger, handling at the same time the second largest working fluid flow. The heat exchanger with the lowest heat load is heat exchanger 23 (5.16x106 kcal/h), where 408,867 kg/h of liquid mixture must be cooled from 55 °C to 42 °C, i.e. it is the smallest temperature range found in the process with the lowest working fluid flow rate.

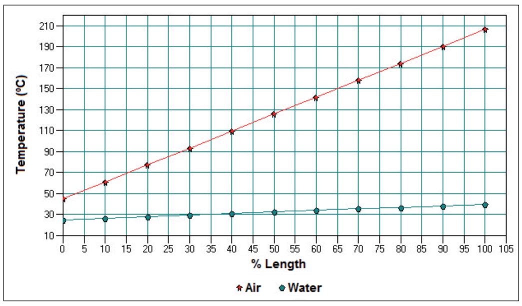
Regarding the auxiliary service flow required, of the heat exchangers that consume cooling water, number 10 is the one that needs the highest flow of this service (412,569.52 kg/h), as it is where the greatest amount of heat is exchanged (5.06x107 kcal/h). The one that needs the least flow of cooling water is number 23, with 89,653.48 kg/h, as it is where the least amount of heat is exchanged in the whole process, as it was previously established. Finally, of the heat exchangers that consume water vapour, number 14 is the one that requires the largest amount of steam (112,857.63 kg/h), as this is where the largest amount of heat is exchanged of all the heat exchangers (5.25x107 kcal/h), as mentioned above.

Heat curves

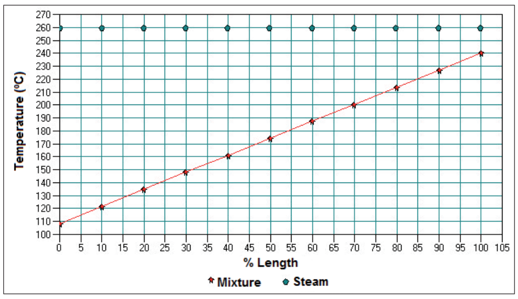
Figure 4 presents the different heat curves obtained using the ChemCAD® simulator for each of the shell and tube heat exchangers used in the production process.



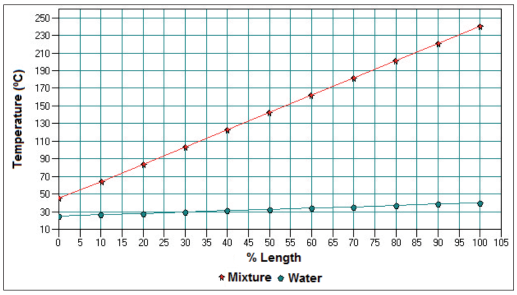
a) Cooler 1



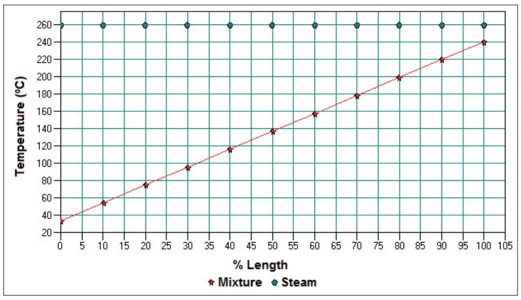
b) Cooler 2



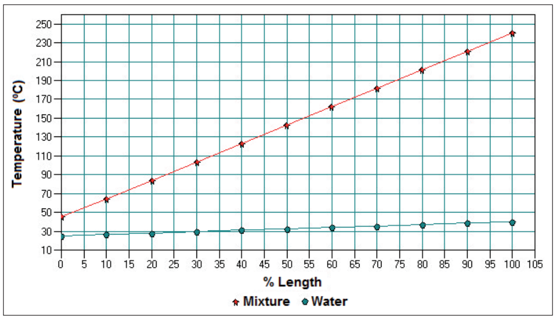
c) Heater 1



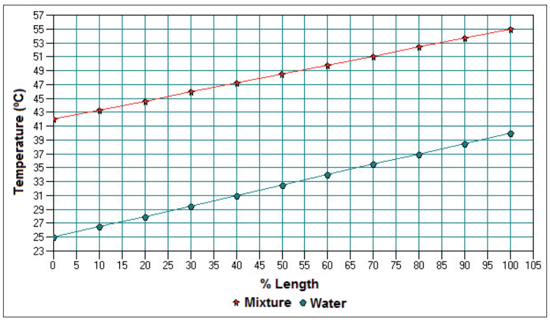
d) Cooler 3



e) Heater 2



f) Cooler 4



g) Cooler 5

Figure 4: Heat curves obtained for the shell and tube heat exchangers used.

Considering the results shown in Figure 4, it can be said that in both Cooler 1 (Figure 4a) and Cooler 2 (Figure 4b) the air experiences a linear decrease in temperature, indicating that sensible heat is transferred without phase change. This behaviour is also observed for both Cooler 3 (Figure 4d) and Cooler 4 (Figure 4f), where the gaseous mixture is cooled without phase change, i.e. sensible heat is transferred. In Cooler 5, linear cooling of the liquid mixture also occurs without phase change.

On the other hand, figures 4c and 4e show that the gaseous mixture is heated up to 240 ºC in both heat exchangers without any phase change, which is demonstrated by the increasing linear behaviour of this stream in the respective heat curves, indicating that sensible heat is transferred in both units. It should be noted that in both curves it is observed that the water vapour changes phase at the same feed temperature (260 ºC), obtaining saturated condensate at the outlet of each unit, which is demonstrated by the rectilinear behaviour of its heat curve.

Finally, in all the coolers, the heat transfer agent (water) does not undergo a phase change (evaporation), which is demonstrated by its linear increasing behaviour in all the heat curves that plot it.

Results of the sensitivity study

Figure 5 shows the results obtained by performing the sensitivity study above, with respect to the determination of the influence of the increase of the wash water feed temperature on the amount of EO to be obtained in the distillation column top stream.

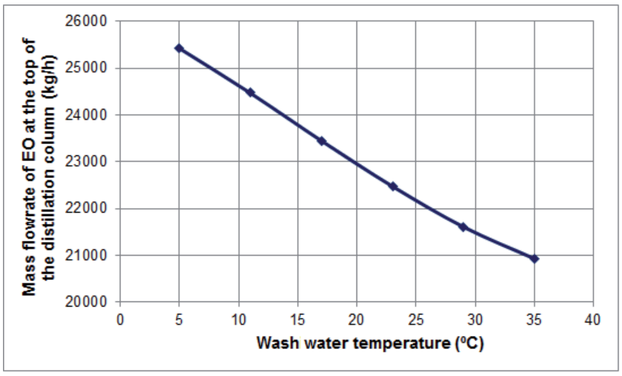


Figure 5: Results of the sensitivity study.

As it can be seen in Figure 5, decreasing the feed temperature of the wash water increases the amount of EO obtained at the top of the distillation column. This is because the amount of EO absorbed by the cold water in the absorbers increases, due to a higher diffusion and mass transfer of the EO into the water as a result of the temperature decrease. Thus, the reduction of the washing water temperature from 35 °C to 5 °C makes it possible to obtain 4,515.2 kg/h of additional EO in the distillation column, which is significant and desirable for the production process, since, considering that EO is priced in the order of USD $ 1,210/t [30], USD $ 5,463.39/h of additional profits will be obtained due to the application and introduction of this change in the production process. Considering the above, it is recommended to carry out technical-economic feasibility studies in order to determine how profitable it can be to install a cooling system for the washing water consumed in the absorbers, with a view to obtaining increased amounts of EO through the top of the distillation column, and thus increase the economic profitability and productivity of the production process. That is, to carry out a cost/benefit study and analysis.

Conclusions

The use of the ChemCAD® simulator made it possible to successfully simulate the EO production process from the catalytic oxidation of ethylene.

EO is obtained from the top stream of the distillation column with a flow rate of 22,163.5 kg/h and a purity of 98.29 %, which can be considered acceptable.

The heat curves obtained for each heat exchanger show the spatial distribution of the temperature inside the unit, depending on its length.

The shell and tube heat exchanger which exchanges the most heat is number 14 with 5.25x107 kcal/h, which in turn requires the most steam flow (112,857.63 kg/h).

The heat exchanger with the highest cooling water flow rate is number 10, with 412,569.52 kg/h.

It is recommended to feed the wash water to the absorbers at a temperature of 5 ºC, in order to increase the amount of EO to be obtained by the flow from the top of the distillation column. In this case, a reduction of the wash water temperature from 35 ºC to 5 ºC allows obtaining an additional 4,515.2 kg/h of EO in the distillation column.

It is recommended to design recovery and purification operations for stream No. 40 (Gases) in order to recover the 3,791.8 kg/h of EO contained in this stream, which is vented to the atmosphere in the current process.

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