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SIMULATION OF ETHYLENE GLYCOL PRODUCTION FROM USED ETHYLENE OXIDE IN STERILIZATION OF SYRINGES

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ABSTRACT

The production of ethylene glycol from used ethylene oxide was simulated by Aspen HYSYS® V9.0 based on actual data got from Ava-med for syringes in Khartoum. The effect of temperature and EO-water ratio on the EG mass flow was studied. Results showed that the amount of EG produced is 38.7 kg/h. As the temperature increased the mass flow of EG oscillated. The best temperature that gave the best amount of EG was 190°C. As the EO-water ratio is increased the EG mass flow is increased and the DEG byproduct is decreased. The ratio of EO-water in the Case Under Study (CUS) was 1:108 while the ratio that the literature recommended was 1:20, and it is found that the results were slightly improved in the CUS.

KEYWORDS: Simulation, Ethylene Glycol production, Sterilization, Aspen HYSYS®.

1. INTRODUCTION

Ethylene Glycol (EG) is an important organic compound and chemical intermediate used in a large number of industrial processes. Ethylene glycol is a colorless and odorless, high boiling point, hygroscopic liquid completely miscible with water and many organic liquids (Matar and Hatch, 2001; Speight, 2002). Mono-ethylene glycol (MEG) is the most important type of ethylene glycol. Di-ethylene glycol (DEG) and tri-ethylene glycol (TEG) glycol are obtained as a co-product during the manufacturing process of MEG (Seider et al., 2003).

Currently, the predominant method used worldwide for the production of ethylene glycol is the hydrolysis of ethylene oxide. EO is obtained by the direct oxidation of ethylene with air and oxygen in the presence of silver catalyst (Seider et al., 2003).

The hydrolysis reaction occurs at a temperature range of 50-100°C. The Contact time is approximately 30 minutes. Di and triethylene glycol are coproducts with the monoglycol. Increasing the water/ethylene oxide ratio and decreasing the contact time decreases the formation of higher glycols. A water/ethylene oxide ratio of 10 is normally used to get approximately 90% yield of the monoglycol. However, the di and the triglycols are not an economic burden, because of their commercial uses (Matar and Hatch, 2001; Turto et al., 2008). Figure 1 below shows this process.

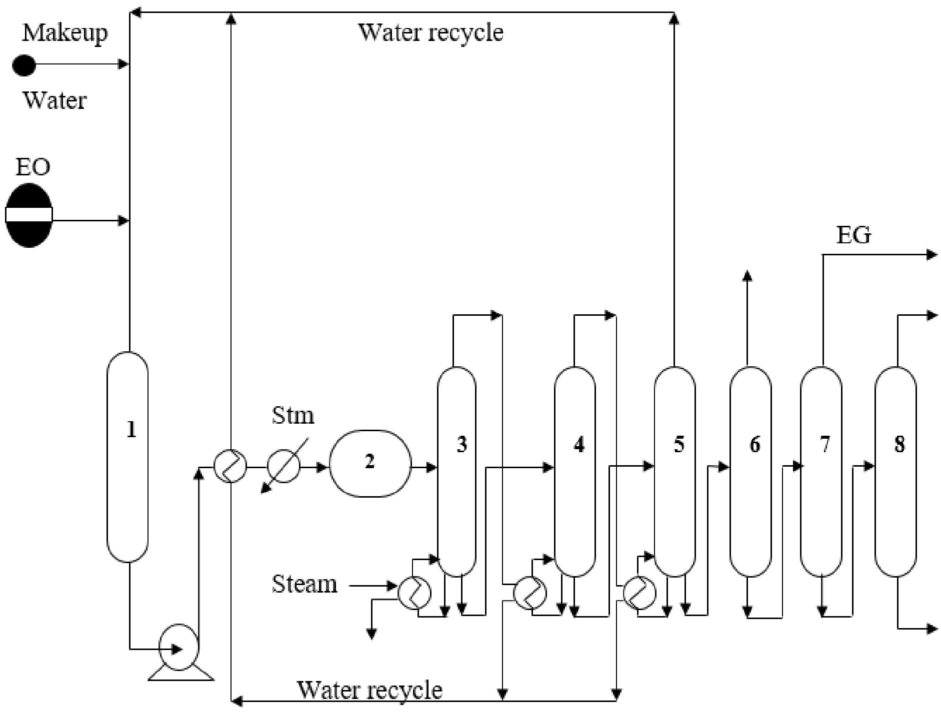

Figure 1: The Scientific Design Co. process for producing ethylene glycols from ethylene oxide: (1) feed tank, (2) reactor, (3,4,5) multiple stage evaporators, #4 operates at lower pressure than #3, while # 5 operates under vacuum, evaporated water is recycled to feed tank, (6) light ends striper, (7,8) vacuum distillation columns (Matar and Hatch, 2001).

In many plants and facilities where the sterilization process is needed, ethylene oxide is used as sterilant gas. In *Ava-med* plant for Syringes, ethylene oxide is used for sterilization of produced syringes. When the process is completed the EO is evacuated from the chamber with a pump and purged with water, then the mixture is discharged to a storage tank without any other further treatments, and finally, the effluents disposed by sewage authority.

There is a chance to use the produced solution for the production of the ethylene glycol in a commercial quantity after further treatments.

The main objective of this paper is the simulation of the production of Ethylene Glycol from the used EO in the sterilization process.

2. Methods

To carry out this research a process modeling method is chosen, and a simulation program that is Aspen HYSYS®V9.0 is used.

2.1 Kinetic Model and Reaction Mechanisms

The non-catalytic hydrolysis process of ethylene oxide to ethylene glycol follows these elementary steps: reaction of EO with water to give MEG and subsequent reaction with EO to form di and tri ethylene glycol (Gunorubon and Paschal, 2018):

$$C_2H_4O + H_2O \xrightarrow{k_1} C_2H_6O_2 \qquad (1)$$

$$C_2H_4O + C_2H_6O_4 \xrightarrow{k_2} C_4H_{10}O_3 \qquad (2)$$

The rate expression for any component j from equation (6,7,8) are showed below:

For j= A, B, C, and D: let A represent C_2H_4O; B ≡ Water; C ≡ $C_2H_6O_4$; D ≡ $C_4H_{10}O_3$; Then,

$$(-r_A) = -K_1C_AC_B - K_2C_AC_C \qquad (3)$$

$$(-r_B) = -K_1C_AC_B \qquad (4)$$

$$(r_c) = K_1C_AC_B - K_2C_AC_C \qquad (5)$$

$$(r_D) = K_2C_AC_C \qquad (6)$$

The reaction rate constant (K_i) for any reaction path (i) given by Arhenius law as follows (Batiha, 2004):

$$K_i = Ae - \frac{Ei}{RT} \qquad (7)$$

The reaction rate constant (K_i) for reaction 1 as a fuction of temperature is given as follows:

$$K_1 = 7.123E{+}08e \frac{(-21193)}{RT} \qquad (8)$$

The ratio of the rate constant for the reaction paths are (Batiha, 2004):

$$\frac{K_2}{K_1} = 2.946, \quad (9)$$

2.2 The flowsheet of the process

The feed is pumped out of the storage tank and the pressure is raised during the pumping from 1 atm to 13 atm. The stream leaving the pump is called Stream 1 (S1), then S1 is heated up from 35°C to 190°C to meet the desired conditions that the process of the producing of ethylene glycol required and the heated stream is called S2. S2 is fed to the reactor, where the reactions took place. After the reactions are completed, liquid products and vapors are produced. The vapors contain a minor amount of EG, DEG, and steam. The liquid products comprise the bulk of EG, a minor amount of DEG, and a huge amount of water. Since the vapors and the liquid products contain the same constituents a mixer is used to ensure that the whole amount of the products are present in the produced stream. The produced stream was labeled as (product), and before this stream is directed to a separation unit a control valve is used to reduce the pressure of the stream to send to the distillation which is an atmospheric distillation where it is separated to EG, DEG, and water. Below is Figure (2) that shows the flow sheet of the process created by Aspen HYSYS®V9.0.

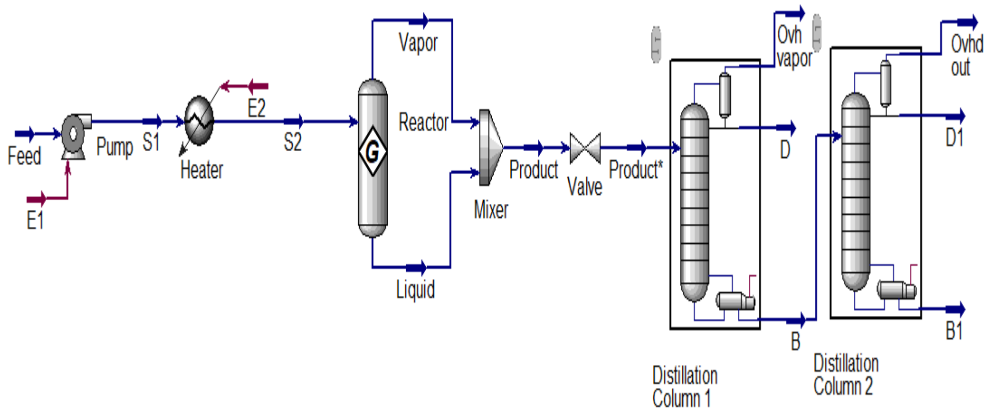

Figure 2: The flow sheet of the process created by Aspen.

3. Solution Method

In Ava-med there are two cycles of sterilization process carried out per day every eight hours. The period time of each cycle is six hours. In every cycle, the amount of gases used in sterilization is 10-12 kg/cycle, 70% of that gas is CO_2 where 30% of it is EO.

3.1 Calculated Variables

To evaluate the values needed in Aspen HYSYS® some calculations are made as follows:

To evaluate the amount of gases used per day, the mean of the values mentioned above-which are 10-12- is taken and the mean is 11 kg/cycle. - Since there are two cycles per day, the amount of gases from the chamber equals 22 kg. and the composition of EO is 30%, therefore, 30% of EO of that amount = 0.3×22

Amount of EO per day = 6.6 kg

Amount of EO in 25 days = 165 kg

Amount of water based on the ratio 1:20 = 3300

The total amounts of effluents in 25 days = 3465 kg.

- Assuming that there will be one cycle/day to produce EG and it takes 6 hours,

That means:

Feed = 577.5 kg/h

- Composition of the Feed:

EO = 27.5 kg/h

Water = 550 kg/h

The fluid package chosen is UNIQUAC Ideal.

Table 1: The amount and the composition of the feed.

Ratio	Amount of water (kg)	Total amount of effluents (kg)	Feed (kg/h)	Composition (kg)	
				EO	Water
1:20	3300	3465	577.5	27.5	550
1:108.4	17886	18051	3008.5	27.5	2981

Table 2: Conditions of the Feed.

Stream Name	Feed
Vapor/Phase Fraction	0.0000
Temperature [C]	35
Pressure [kPa]	101.3
Molar Flow [kgmole/h]	31.15
Mass Flow [kg/h]	577.5

Table 3: Conditions of the stream fed to the reactor (S2).

Stream Name	S2	Vapor Phase	Aqueous Phase
Vapor/Phase Fraction	0.3959	0.3959	0.6041
Temperature [C]	190	190	190.0
Pressure [kPa]	1317	1317	1317
Molar Flow [kgmole/h]	31.15	12.33	18.82
Mass Flow [kg/h]	577.5	237.8	339.7

3.2 Parameters effect

A case studies of the effect of water-EO ratio used in the process from 1:1- 1:120, and the effect of the temperature on EG mass flow are carried out. The table 1 below shows that.

Table 4: Case study of effect of water amount on EG mass flow.

Ratio	Amount of water (kg)	Total amount of effluents (kg)	Feed (kg/h)	Composition(kg)	
				EO	Water
1:1	165	330	55	27.5	27.5
1:5	825	990	165	27.5	137.5
1:10	1650	1815	302.5	27.5	275
1:15	2475	2640	440	27.5	412.5
1:20	3300	3465	577.5	27.5	550
1:40	6600	6765	1127.5	27.5	1100
1:60	9900	10065	1677.5	27.5	1650
1:80	13200	13365	2227.5	27.5	2200
1:100	16500	16665	2777.5	27.5	2750
1:108.4	17886	18051	3008.5	27.5	2981
1:120	19800	19965	3327.5	27.5	3300

4. RESULTS

Table 5: Composition of liquid product.

Component	Mass Flows [kg/h]
EO	0.0000
H_2O	297.6617
EG	36.2407
DEG	0.1154

Table 6: Composition of Vapor product.

Component	Mass Flows [kg/h]
EO	0.0000
H2O	311/228
EG	0.0000
DEG	0.0000

Table 7: Composition of Bottoms (B) 8: Composition Ovhd & Dist (D).

Component	Mass Flows [kg/h]
EO	0.0000
H2O	0.0000
EG	38.5869
DEG	0.1357

Table 9: Composition of Bottoms (B1).

Component	Mass Flows [kg/h]
EO	0.0000
H2O	0.0000
EG	0.0015
DEG	0.1341

Table 10: Composition of Distillates (D1).

Component	Mass Flows [kg/h]
EO	0.0000
H2O	0.0000
EG	38.5854
DEG	0.0015

Table 11: Condition of the Product entering the Distillation (Product*) in CUS.

Stream Name	Product*	Vapor Phase	Aqueous Phase
Vapor/Phase Fraction	0.2227	0.2227	0.7773
T [C]	101.1	101.1	101.1
P [kPa]	105.0	105.0	105.0
Molar Flow [kgmole/h]	165.5	36.85	128.6
Mass Flow [kg/h]	3008	664.1	2344

Table 12: Composition of Bottoms (B).

Component	Mass Flows [kg/h]
EO	0.0000
H_2O	0.0000
EG	0.1460
DEG	0.0109

Table 13: Composition of Bottoms (B1).

Component	Mass Flows [kg/h]
EO	0.0000
H_2O	0.0000
EG	38.7326
DEG	0.0109

Table 14: Composition of Distillates (D1).

Component	Mass Flows [kg/h]
EO	0.0000
Water	0.0000
EG	38.5867
DG	0.0000

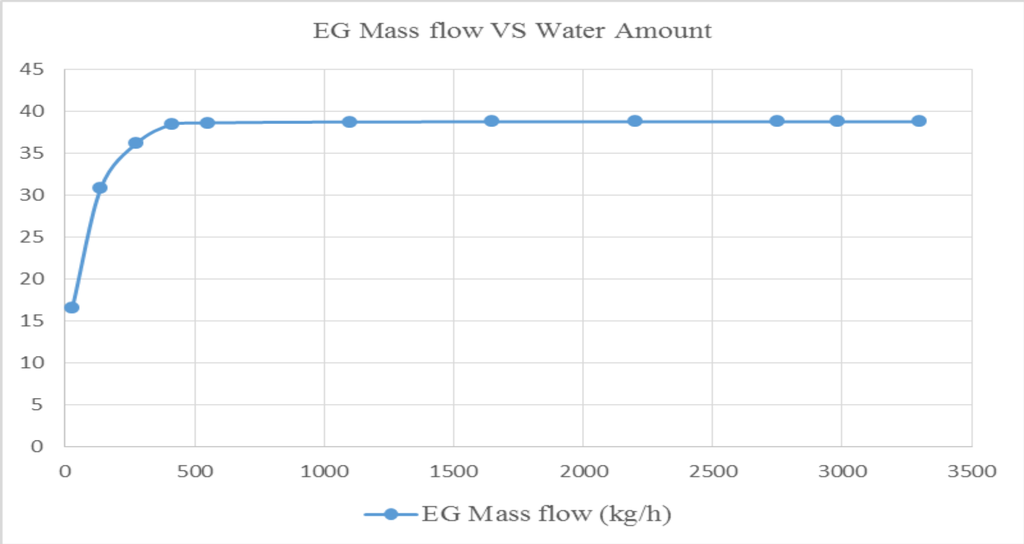

Figure 3: ***Water amount vs EG mass flow.***

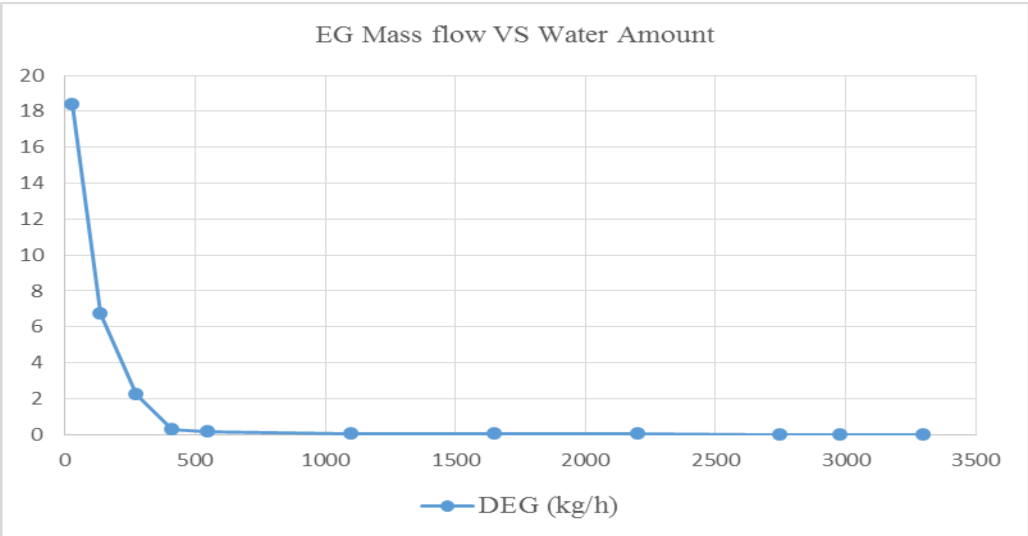

Figure 4: ***Water amount vs DEG mass flow.***

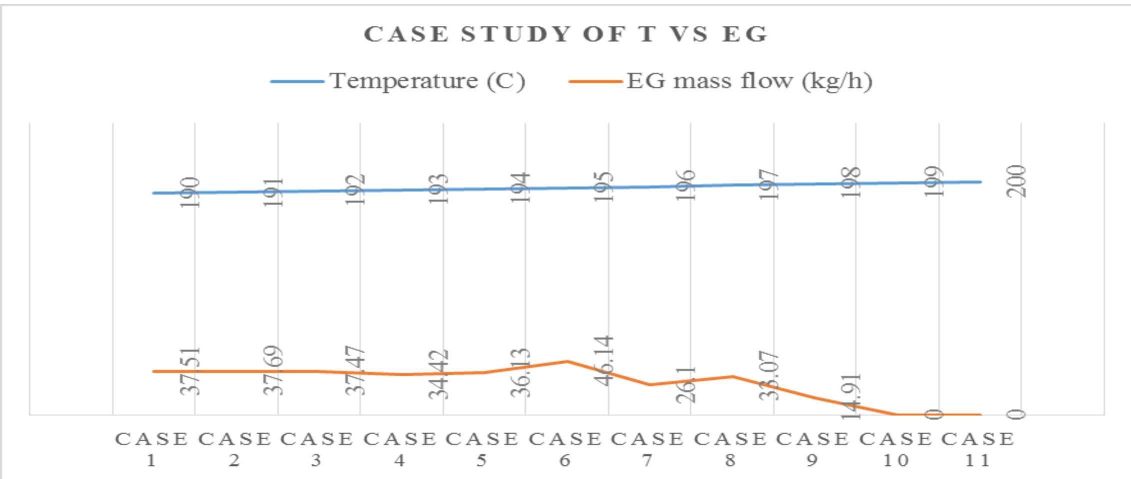

Figure 5: ***Case study of T vs EG in SDC.***

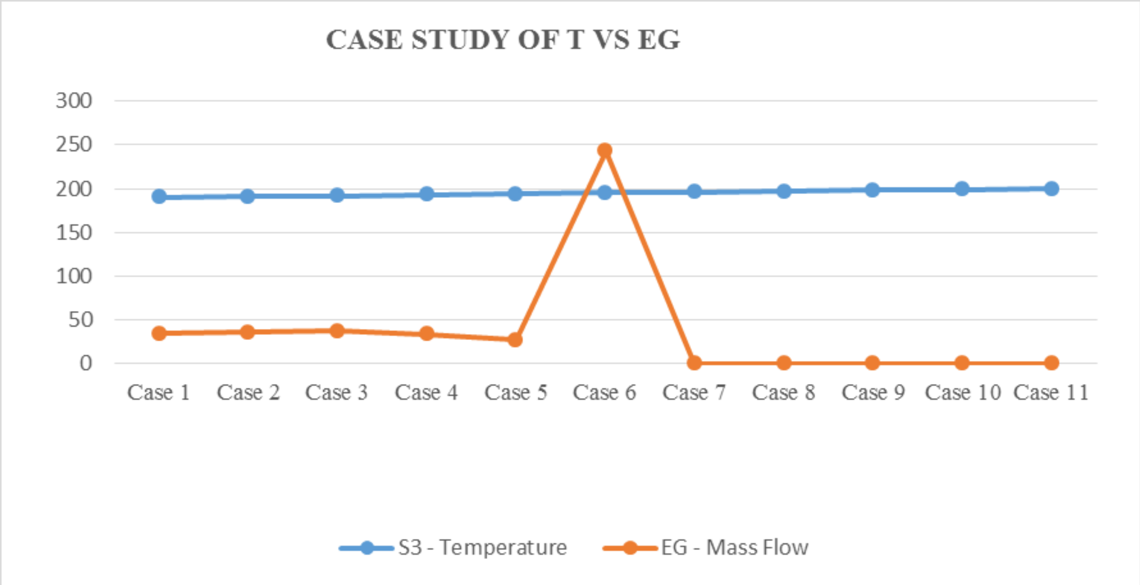

Figure 6: *Case study of T vs EG in CUS.*

From the results, it has been found that a considerable amount of ethylene glycol was produced in one cycle which is 38.7 kg/h. Also, it has been found that DEG has resulted as a byproduct. It has been found that 100% of ethylene oxide that was present in the feed is removed successfully and converted into useful and less harming environmentally products which is EG mainly. From the case studies carried out, it has been found that the amount of water in the case under study (CUS) had a positive effect and improved the mass flow of EG despite it was more than the suggested amount by literature, and the results found are quite better than that results found in the suggested standard amount of water. Furthermore, it is found that amount of water has a directly proportional to the mass flow of EG, and inverse proportional to the DEG mass flow. The temperature has a random influence on the mass flow of EG, but the best temperature was found to be 190^{o}C.

5. CONCLUSION

In this paper two cases were studied, standard case (SDC) and the case under study (CUS). After analyzing all the results, it can be seen that there is much similarity in the two cases, and they followed the same pattern in the most stages. In CUS the amount increased slightly and it is found that around 38.5 kg/h is produced rather than 36 kg/h in SDC, which is a very good indication and shows that this process is promising.

These results are in great agreement with what the literature suggested. The amount of water used in the case under study (CUS) has a positive effect on the amount of EG produced in the process, where remarkable improvement has been seen in the mass flow of EG.

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