

Simulation Study of Propylene Glycol Formation from Propylene Oxide and Water: Effect of Reactor Type, Reactant Ratio, Temperature, and Reactor Configuration

Eko Ariyanto^{1,2}, Eka Sri Yusmartini^{1,2*}, Robiah Robiah¹, Feby Ardianto³

¹ Department of Chemical Engineering, Engineering Faculty, University of Muhammadiyah Palembang, Jalan Jendral Achmad Yani 13 Ulu Palembang, Indonesia, 30263

² Master Program of Chemical Engineering, University of Muhammadiyah Palembang, Jalan Jendral Achmad Yani 13 Ulu Palembang, Indonesia, 30263

³ Department of Electrical Engineering, Engineering Faculty, University of Muhammadiyah Palembang, Jalan Jendral Achmad Yani 13 Ulu Palembang, Indonesia, 30263

*Corresponding Author: eka.yusmartini@gmail.com

Abstract

This study investigates the influence of reactor type, reactor configuration, reactor temperature, and reactant ratio on the formation of propylene glycol from propylene oxide and water using HYSYS simulation software. The examined reactor types include Continuous Stirred Tank Reactors (CSTR) and Plug Flow Reactors (PFR). The impact of reactant ratio is explored by varying the mole ratio of propylene oxide to water. The effect of temperature is studied by altering the reaction temperature from 24 to 40 °C. HYSYS simulation results reveal that PFR yields the highest conversion compared to CSTR. Furthermore, consecutive CSTR configuration produces higher conversion than parallel CSTR configuration. Additionally, an increase in reaction temperature from 24 to 40 °C enhances the conversion of propylene oxide to propylene glycol. The reactant ratio 1:1 (propylene oxide to water) yielding the highest conversion compared to other reactant ratios. The implications of these findings are to provide insights into more efficient and economical propylene glycol processes. The study suggests that PFR configuration, consecutive CSTR configuration, elevated reactor temperatures, and optimal reactant ratios can significantly improve the efficiency of propylene glycol formation.

Keywords: Propylene Glycol, CSTR, PFR, Conversion, HYSYS Simulation

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Abstrak

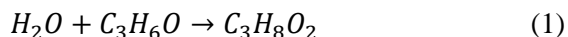
Studi ini menginvestigasi pengaruh beberapa parameter pada pembentukan propylene glycol dari propylene oxide dan air menggunakan Perangkat Lunak Simulasi HYSYS. Jenis reaktor yang dievaluasi adalah Continuous Stirred Tank Reactors (CSTR) dan Plug Flow Reactors (PFR), sementara konfigurasi CSTR berturut-turut dan CSTR paralel juga diperbandingkan. Pengaruh suhu reaktor terhadap reaksi dijelajahi dalam rentang 24 hingga 40 °C, sementara rasio reaktan, yang diwakili oleh perubahan rasio mol propylene oxide terhadap air, juga menjadi fokus penelitian. Hasil simulasi menggunakan HYSYS menunjukkan bahwa PFR memberikan konversi tertinggi dibandingkan dengan CSTR. CSTR konsekutif memberikan konversi yang lebih tinggi daripada CSTR paralel, menunjukkan bahwa urutan reaktor dapat memengaruhi efisiensi konversi. Peningkatan suhu reaksi dari 24 hingga 40 °C meningkatkan konversi propylene oxide menjadi propylene glycol. Rasio 1:1 (propylene oxide ke air) memberikan konversi tertinggi dibandingkan dengan rasio reaktan lainnya. Implikasi dari temuan ini adalah bahwa konfigurasi PFR, konfigurasi CSTR berturut-turut, peningkatan suhu reaktor, dan pemilihan rasio reaktan yang optimal dapat secara signifikan meningkatkan efisiensi dan ekonomi proses pembentukan propylene glycol. Studi ini memberikan wawasan yang berharga untuk desain dan optimalisasi proses industri propylene glycol, memungkinkan pengembangan solusi yang lebih efisien dalam produksi bahan kimia tersebut.

Kata Kunci: Propylene Glycol, CSTR, PFR, Konversi, Simulasi HYSYS

INTRODUCTION

Propylene glycol is a non-toxic chemical. Propylene glycol is a versatile chemical found in liquid detergents, paints, cosmetics, moisturizers, solvents, surfactants, and preservatives [1]. It is commercially produced by hydrolyzing propylene oxide [2, 3]. Glycerol hydrogenolysis is a method for producing propylene glycol by using a catalyst and hydrogen [4].

The reaction for the formation of propylene glycol is as follows [5]:



This reaction can occur with or without a catalyst. Without a catalyst, the reaction can occur at high temperatures and require excess water [6]. This method is very inefficient and produces a lower-quality product. A catalyst can be added to a chemical reaction to increase the reaction rate or produce a particular product [7]. In the case of propylene oxide hydration, an acid or base catalyst can be utilized to increase the conversion process. Various catalysts, including homogeneous and heterogeneous catalysts, can be used to hydrate propylene oxide. Homogeneous catalysts include sulfuric acid [6] and salts of several other acids [8], whereas heterogeneous catalysts include ion exchange resins [9], solid bases [10], and solid acid catalysts [11]. Heterogeneous catalysts are preferred because they are non-corrosive, can help reduce side reactions, and provide a higher product purity [12].

The reaction of water with propylene oxide to generate propylene glycol has become an exciting research topic in the chemical industry. This reaction may occur in several reactors, including the Continuous Stirred Tank Reactor (CSTR) [9, 13] and the Plug Flow Reactor (PFR) [14].

Several studies have investigated the effect of various factors on the propylene glycol formation reaction, such as the reactant ratio and reaction temperature [9, 15, 16]. Meanwhile, the reaction temperature can affect the selectivity of the resulting propylene glycol.

In addition, the influence of the type of reactor used also needs to be considered in this study. The most popular types of reactors used in chemical processes are CSTR and PFR. CSTR is frequently utilized on an industrial scale because of its ease of operation and modification, but PFR offers advantages in terms of reaction efficiency and response time reductions.

Aspen HYSYS is an example of a commercially available computer program used for simulation processes that can observe the influence of operating parameters and provide a good analysis of chemical

and physical phenomena in chemical industrial processes, allowing the optimization process to take place efficiently [17]. Many studies have been conducted using the Aspen HYSYS software to observe the optimization process in reactors, namely the tubular reactor [18], membrane reactor [19], and CSTR [20]. Several studies have been conducted to optimize the propylene glycol production process using the HYSYS software. Jiménez R. et al. [21] used HYSYS to calculate manufacturing costs and analyze raw material and utility usage in the propylene glycol plant. Janoovsk J et al. [22] utilized HYSYS to identify hazards in the propylene glycol plant induced by changes in process parameters. Bauer P and Filho R [23] utilized HYSYS to estimate the environmental impact of the propylene glycol plant.

From these studies, there are still few HYSYS studies simulating the propylene glycol process, mainly studying the effects of reactor-type and reactions such as reactant ratio and temperature. Therefore, research on the reaction of water and propylene oxide to produce propylene glycol needs to pay attention to these factors, such as the ratio of reactants H₂O: propylene oxide, reaction temperature, type of reactor used, and the configuration of the reactor using Aspen HYSYS. The aim of this study is to predict the conversion reaction with various variables that affect the propylene glycol reaction process in the CSTR and PFR. The results of this research can help increase the efficiency of propylene glycol production and provide new insights into the development of better propylene glycol production processes.

MATERIALS AND METHODS

Propylene glycol reactor simulation model

Simulation programs can be used to develop and optimize the physical and chemical systems of a chemical industry process, particularly chemical reactions in reactors. Aspen HYSYS is a process simulator that optimizes process parameters while reducing operational time and costs [24]. The reaction for the formation of propylene glycol in the CSTR and PFR reactors occurs in a steady state simulated using Aspen HYSYS V11. Calculation of physical properties using the Soave-Redlich-Kwong (SRK) equation. The simulation is made based on several assumptions as follows:

- The reaction process that occurs in the reactor takes place in a steady state.
- The total volume of the reactor is 5 liters for a single reactor and 2.5 liters for double reactors.

- The reactors are configured in series, each with the same residence time.
- The reactor is configured in parallel, so the flow entering the reactor is combined into one stream before being split into two streams with the same flow rate.

Reaction kinetic data

It can be seen in Eq. (1) that propylene oxide reacts with water to produce propylene glycol. The reaction is first-order and exothermic with $\Delta H = -8.955$ kJ/kg mol. The Arrhenius equation is used to calculate the reaction rate of propylene glycol, and the frequency factor value is 16.96×10^{12} as follows [5].

$$k = 16.96 \times 10^{12} e^{-\frac{76000}{RT}} \quad (2)$$

where R is the ideal gas constant, and T is the temperature.

Kinetic data and chemical reactions in the HYSYS simulation can be seen in **Figure 1**.

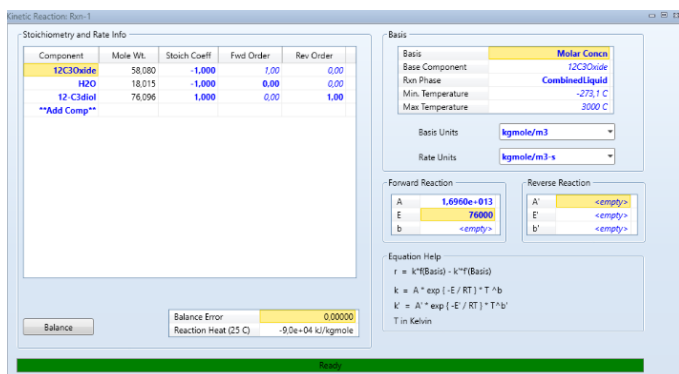


Figure 1 Kinetic Data and Chemical Reactions of Propylene Glycol in HYSYS Simulations

Input reactor data

The mass flow rates of propylene oxide and water used in the HYSYS simulation can be seen in **Table 1**.

Table 1. HYSYS Reactants Stream Simulation Data

Parameter	Propylene Oxide	Air
Temperature (°C)	23.89	23,89
Pressure (atm)	1.1	1,1
Mass Flowrate (kg/hr)	5000	5000

Mathematical modeling

CSTR mathematical modeling

The CSTR mathematical model equation is as follows:

$$\tau = \frac{V}{v_o} = \frac{C_{A0} \cdot V}{F_{A0}} = \frac{C_{A0} \cdot X_A}{-r_A} \quad (3)$$

where τ is the residence time (hour), V is reactor volume (l), v_o is the flow rate (l/hour), C_{A0} is the initial concentration (mol/l), F_{A0} is the mass flow rate of fluid (kg/hour), X_A is the reaction conversion, and r_A is the reaction rate.

The reaction rate can be calculated using the following Eq. (4).

$$-r_A = -\frac{dC_A}{dt} = kC_A \quad (4)$$

where dC_A/dt is the change in concentration over a change in reaction time, C_A is the reactant remaining from the reaction products (mol/l), and t is the reaction time.

The following equation may be used to calculate the remaining reactants as a function of time t during the reaction process.

$$C_A = C_{A0} - C_{A0} \cdot X_A \quad (5)$$

or

$$X_A = \frac{C_{A0} - C_A}{C_{A0}} \quad (6)$$

Eq. (5) may be rewritten as reaction conversion (X_A) by substituting Eq. (6).

$$-r_A = -\frac{dX_A}{dt} = k(1 - X_A) \quad \dots \quad (7)$$

Eq. (7) is substituted into Eq. (3), so:

$$\tau = \frac{V}{v_o} = \frac{C_{A0} \cdot V}{F_{A0}} = \frac{C_{A0} \cdot X_A}{-k(1 - X_A)} \quad (8)$$

For CSTR reactors arranged in series, as shown in **Figure 2**

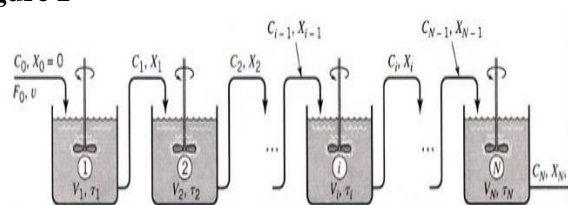


Figure 2. CSTR Series Configuration [25].

The mathematical model for the series CSTR is as follows:

$$\frac{C_0}{C_N} = \frac{1}{1 - X_N} = \frac{C_0}{C_1} \frac{C_1}{C_2} \dots \frac{C_{N-1}}{C_N} = (1 + k \cdot \tau_i)^N \quad (9)$$

where N is the number of reactors arranged in series, X_N is the conversion reaction in the N reactor, C_0 is the initial concentration (mol/l), C_1 and C_2 are the concentrations leaving the first and second reactors (mol/l), C_{N-1} is the concentration leaving reactor $N-1$ (mol/l), C_N is the concentration leaving the N -th reactor (mol/l), and τ_i is the residence time (hours). Eq (8) can be rewritten to become Eq. (10).

$$\tau = \frac{C_{A0} \cdot V}{F_{A0}} = \frac{C_{A0} \cdot (X_{AF} - X_{Ai})}{-r_A} \quad (10)$$

or

$$\tau = \frac{C_0 \cdot V_i}{F_0} = \frac{C_0 \cdot (X_i - X_{i-1})}{-r_{Ai}} \quad (11)$$

where X_{AF} is the final conversion, X_{Ai} is the conversion in the i -th reactor and r_{Ai} is the reaction rate. Assuming that τ_i has the same value for each reactor, the conversion of the reactors up to N can be calculated as follows:

$$X_N = 1 - \frac{C_{AN}}{C_{A0}} = 1 - \frac{1}{(1+k \cdot \tau_i)^N} \quad (1)$$

PFR mathematical modeling

The mathematical model equation for the PFR reactor is as follows:

$$\tau = \frac{V}{v_0} = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} \quad (13)$$

Substitute Eq. (6) into Eq. (10) to become:

$$\tau = \frac{V}{v_0} = C_{A0} \int_0^{X_A} \frac{dX_A}{-k(1-X_A)} \quad (2)$$

RESULTS AND DISCUSSION

Effect of reactor type

The type of reactor greatly influences the conversion of propylene oxide to propylene glycol products. In this study, the reactors used were CSTR and PFR as seen in **Figure 3**.

Figure 3 shows the reactor type used in the HYSYS Simulation to produce propylene glycol utilizing propylene oxide and water as reactants. **Figure 3** shows the CSTR (**Figure 3(a)**) and PFR (**Figure 3(b)**) process flows. The reactant stream is combined into the mix point (MIX-100) before entering the reactor.

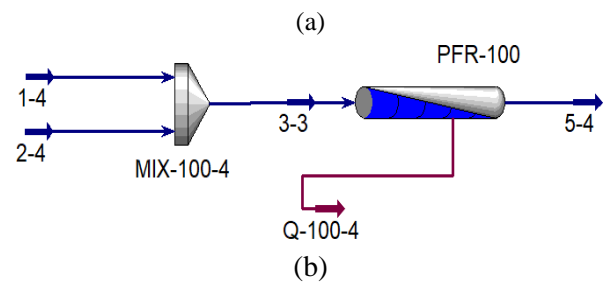
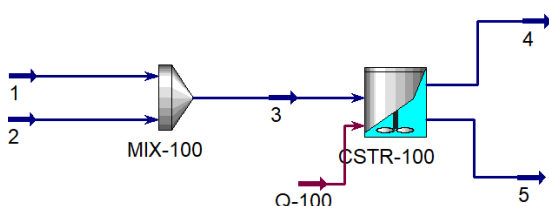


Figure 3. Flow Diagram HYSYS Simulation (a) CSTR; (b) PFR.

Table 2 shows the results of HYSYS simulation from the two reactors.

Table 2. HYSYS Simulation Results of 2 Reactor Types

Reactor Type	Conversion (%)
CSTR	60.53
PFR	82.30

Table 2 indicates that the PFR outperforms the CSTR regarding conversion. The conversion HYSYS estimating values for the CSTR is 65% and 82.30% for the PFR. CSTR conversion simulation results are lower due to back-mixing, which occurs when reactants interact with unreacted reactants [26]. However, CSTR has the advantage of producing a more homogeneous product, easier to control and more suitable for large-scale production [27, 28].

Geometry	
Orientation: <input checked="" type="radio"/> Vertical <input type="radio"/> Horizontal	
<input checked="" type="radio"/> Cylinder	
<input type="radio"/> Sphere	
Volume [m3]	5,000e-003
Diameter [m]	0,1619
Height [m]	0,2429

(a)

Tube Dimensions	
Total Volume	5,000e-003 m3
Length	10,00 m
Diameter	2,523e-002 m
Number of Tubes	1
Wall Thickness	5,000e-003 m

(b)

Tube Packing	
Void Fraction	1,000
Void Volume	5,000e-003 m3

Figure 4. Reactor Volume in HYSYS Simulation (a) CSTR; (b) PFR

PFR supply reactants continuously flow through a pipe, causing reactions at various rates along the pipe. Because the PFR lacks back-mixing, the reactants have more time to react than the CSTR [26]. The output of the HYSYS simulation for CSTR and PFR volumes can be seen in **Figure 4**.

Effect of reactor arrangement

The conversion of propylene oxide to propylene glycol can be carried out using CSTR operated in series or parallel (**Figure 5**).

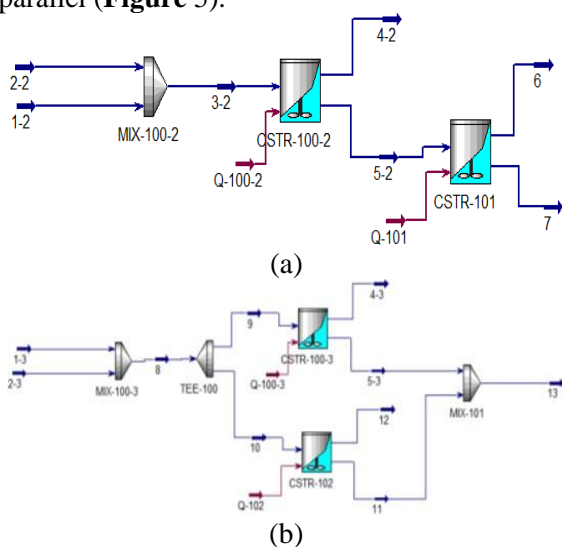


Figure 5. Reactor configuration in the HYSYS simulation (a) Series; (b) Parallel.

The configuration of the reactors significantly affects the conversion. The HYSYS simulation was conducted, as shown in **Figure 5**, with the reactor capacity of both reactors set to 2.5 L. A series reactor configuration is shown in **Figure 5(a)**. **Figure 5(b)** shows a parallel reactor configuration with feed divided into two streams (streams 9 and 10) with the same flow rate. The temperature and pressure in both reactors were set at 23.9 °C and 111.5 kPa, respectively. Figure 6 shows the HYSYS simulation's CSTR dimensions.

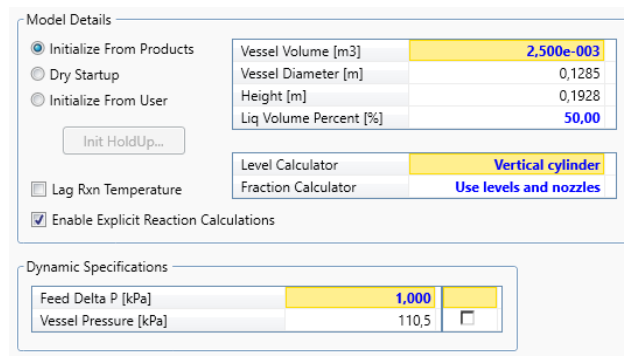


Figure 6. Reactor Volume in HYSYS Simulation (a) CSTR Series Configuration; (b) CSTR Parallel Configuration.

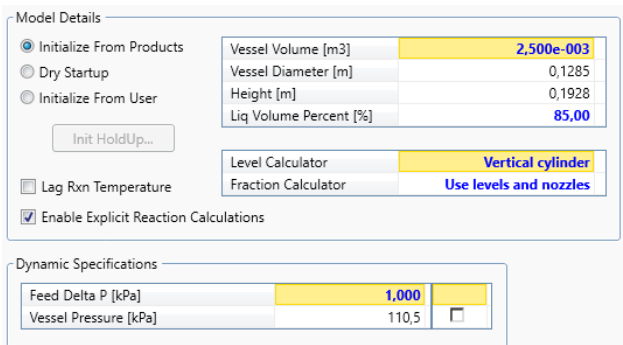
Table 3 shows the HYSYS simulation results for the differences in series and parallel reactor configurations. The series configuration in the first reactor shows higher conversion than the second reactor. It is due to the feed concentration that enters the first reactor having a higher initial concentration. So that it can help increase the rate of reaction and conversion in the first reactor. However, the concentration decreases when the feed enters the second reactor so the resulting conversion will be lower.

Table 3. HYSYS Simulation Results on the CSTR Configuration

Reactor Configuration	Conversion (%)	
	Reactor I	Reactor II
Series	43.38	31.09
Parallel	60.53	60.35

The CSTR parallel configuration simulation results in the first and second reactors indicated that the propylene oxide conversion was higher (60.53%) than in the series configuration. However, the average conversion of parallel reactors is 60.53%, whereas the conversion result for reactors arranged in series with two reactors is calculated by adding all conversions that occur for the two reactors. The overall conversion of the two reactors in series was 74.44%. The series configuration on the CSTR showed an increase in the conversion value, and the results were close to that of the PFR [29].

Motegh et al. [30] investigated the performance of slurry bubble column reactors connected in series. The study concluded that increasing reactors increases conversion; however, gradually increasing the number does not substantially increase conversion. As a result, increasing the number of reactors will be ineffective, costly, and significantly complicate reactor system



(a)

control [29].

In the case of the propylene glycol production reaction, the reaction is a step reaction, so higher conversion in the first reactor can improve overall reaction efficiency. As a result, a parallel reactor configuration can achieve higher conversion in the first reactor than a series reactor configuration.

Furthermore, in a parallel reactor configuration, each CSTR can be operated with optimal operational conditions to achieve maximum conversion. In contrast, in a series reactor configuration, the operational conditions in each reactor must be adjusted to the previous reactor's reaction conditions, so limiting the reaction in subsequent reactors is possible.

In practice, production needs and available resources determine the ideal reactor configuration. Parallel reactor configuration may necessitate a significant investment in reactor number and flow controller, whereas series reactor configuration may necessitate longer residence times and higher operating costs. Therefore, the reactor configuration must be carefully selected to achieve optimum conversion with economical operating costs.

Effect of reactor temperature

The reaction temperature is a significant parameter to increase in conversion of reactions because it affects the rate and equilibrium of chemical reactions. In general, an increase in the reaction temperature will increase the rate of the chemical reaction, thereby increasing the conversion of the reaction. **Table 3** shows the HYSYS simulation results at various temperatures for both reactor types (CSTR and PFR).

Table 4. HYSYS simulation results with various reactor temperature

Temperature (°C)	Conversion (%)	
	CSTR	PFR
23.89	60.53	82.30
30	73.84	90.73
35	83.04	95.52
40	87.91	98.26

Table 4 indicates that increasing the temperature may increase propylene oxide conversion in both reactors. An increase in temperature can increase the kinetic energy of molecules, thereby increasing the frequency of collisions between molecules and breaking chemical bonds so that chemical reactions increase [31]. Therefore, the reaction temperature can increase the reaction rate and conversion.

In addition, an increase in temperature may impact the equilibrium of chemical reactions, thereby influencing the conversion reaction. Some chemical reactions can only occur at certain temperatures, while others are more likely to produce products at higher temperatures. In this case, increasing the reaction temperature could shift the reaction equilibrium toward the formation of products, thereby increasing the conversion of the reaction.

However, it should be noted that a temperature limit can be used in chemical reactions because the highest temperature can produce unwanted reactions or even damage the reaction equipment. As a result, the reaction temperature must be carefully monitored to ensure optimal reaction conversion while maintaining product safety and quality.

Effect of reactant ratio

Ratio reactant is the ratio between the amounts in moles of any two compounds involved in a balanced chemical reaction. Changes in the ratio of reactants can affect the rate and conversion of chemical reactions. The results of the HYSYS simulation on both reactors for different reactant ratios are shown in **Table 5**.

Table 5. HYSYS simulation results on various in reactant ratios

Reactant Ratios (H ₂ O : C ₃ H ₆ O)	Conversion (%)	
	CSTR	PFR
1:1	71.84	94.02
2:1	67.07	89.61
1:2	70.91	54.31

Table 5 indicates that the ratio of reactants significantly influences propylene oxide conversion, with increasing the ratio of reactants H₂O: C₃H₆O decreasing propylene oxide conversion in both types of reactors. The ratio of the reactants can influence their capacity to react with each other and generate products. Chemical reactions may not proceed efficiently if the ratios of the reactants are not optimal. For instance, if the reactants are less than stoichiometric and insufficient reactants are required to generate products, the reaction conversion will decrease. If the reactants are overly concentrated, the reaction rate may be inhibited due to competition among the reactant molecules, which is referred to as diffusion barriers.

At increasing the concentration of C₃H₆O where the reactant ratio was 1:2, the yield of propylene oxide conversion in the PFR was lower (54.31%) compared to the CSTR of 70.91%. The high CSTR conversion results from the stirring process. Stirring can ensure that the concentration of the reactants is constantly uniform throughout the reactor. Thus, the reaction can

continue until the reaction equilibrium is reached. In the case of the propylene glycol production reaction, excess propylene oxide will react with H₂O until equilibrium is reached so that high conversion can be achieved [16]. In contrast, the reactants in a PFR only proceed through the reactor once and are not continually mixed during the reaction. Under these conditions, the excess reactant (propylene oxide) will only react with H₂O for a short time before passing through the reactor as an unreacted product mixed with ethylene glycol. Because the reactions do not reach equilibrium, the conversions in the PFR are lower.

On the other hand, increasing the concentration of H₂O may increase the conversion of propylene oxide in the PFR. From **Table 5**, an increase in the H₂O ratio can significantly increase the conversion from 54.31% to 89.61%. However, the conversion decreased when using the CSTR. This significant difference is influenced by the residence time of the reactants in the PFR, which can be reduced so that the reaction can occur efficiently, and higher conversions can be achieved.

CONCLUSION

Based on the results of a HYSYS simulation study of the reaction for the formation of propylene glycol from the reactants propylene oxide and water, it is possible to conclude that the type of reactor, the ratio of reactants, the temperature of the reaction, and the configuration of the reactors all have a significant effect on the conversion of the reaction.

The type of PFR produces the most significant conversion compared to the CSTR. According to the HYSYS simulation, CSTR is 65%, and PFR is 82.30%. The reaction temperature significantly impacts reaction conversion; the higher the reaction temperature, the higher the conversion reached.

The reactant ratio of 1:1 resulted in the most significant conversion compared to other reactant ratios, namely 71.84% and 94.02% for CSTR and PFR, respectively. Furthermore, there is a decrease in conversion as the ratio of reactants increases. In addition, the CSTR configuration in series produces the highest conversion compared to the CSTR configuration in parallel. The overall conversion of the two reactors in series was 74.44%.

In practice, the findings of this study may be applied to maximize propylene glycol production by selecting the appropriate reactor type, reactor configuration, reaction temperature, and reactant ratio. Furthermore, this research can be a foundation for future research into developing a more efficient and

environmentally friendly propylene glycol production process.

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