Tubular Reactor Performance for Hydrolysis Reaction Of Propylene Oxide

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Abstract

This study aims to investigate the performance of the tubular reactor for the hydrolysis reaction of propylene oxide to produce propylene glycol with sulfuric acid as a catalyst. The performance of the reactor studying using mathematical modelling and computer simulation. The reactor model base on a homogeneous model with an emphasis on the dispersion model and assumption steady-state condition, nonadiabatic, and the gas phase follows the ideal gas rule. The kinetic reaction follows the previous study by Gordon (2003).
The performance of a tubular reactor for the hydrolysis reaction of propylene oxide affected by operating conditions. Rising temperature and C_3H_6O/H_2O ratio increase the yield, and on the other hand, increasing superficial velocity and reactant concentration will decrease the reaction conversion.

Keywords
tubular reactor, propylene oxide, hydrolysis, propylene glycol

1. Introduction
Recent technological advances are developing rapidly. Everything has used the ability of computers, ranging from household needs, offices, factories to lectures also have used it. In the discipline of chemical engineering, its use has been so widespread, ranging from simple things to more complex situations, for example, in the process of modelling and simulation of a system or a process tool such as a reactor.

Tubular reactor or plug flow reactor (PFR) is a device used to react a reactant into a product by flowing the fluid in a pipe continuously. One reaction that uses a tubular reactor is the hydrolysis of propylene oxide to propylene glycol. Glycol is used in the manufacture of unsaturated polyester resins, solvents, antifreeze, and softeners. Propylene glycols are a valuable commodity with a wide range of applications, from food, pharmacy to the automotive industry. Propylene glycols are suitable solvents for many polar organic substances, a preservative in food and pet food products, and anti-freeze systems in automotive.(Gu et al., 2020; Hirano et al., 2015; Prabhakaran et al., 2016; Sullivan et al., 2018; Sun et al., 2015; Wang et al., 2019)

The selection of reactors to be used based on chemical reactions and various hydrodynamic factors that exist determine the size of the reactor and how to determine the best-operating conditions are the problems faced in planning to increase production from laboratory scale to industrial scale. The scale-up process has traditionally been carried out in stages from a laboratory scale to a pilot-scale to finally a larger scale. However, this experiment requires a considerable cost, time, and energy to obtain the results of excellent or optimum operating conditions. Using models and simulations can reduce the risk of danger, save time and money in analysing reactor performance.(Fogler, 2016; Froment et al., 2011)

The research that will be carried out is modelling and simulating a tubular reactor for the hydrolysis of propylene oxide, which refers to Gordon (2003) to determine the reactor's performance. The tubular reactor model developed is

a two-dimensional homogeneous model with a dispersion model, steady-state, nonadiabatic, and gas-phase operating conditions following the ideal gas law.

2. Methodology

The research carried out begins by collecting data and parameters needed in compiling the model, including supporting theories about propylene oxide hydrolysis reactions, experimental data for model validation.

Develop a mathematical model of the tubular reactor system, a mass balance that considers hydrodynamic factors in a reactor consisting of convection and dispersion. Complete mathematical models with numerical methods with the help of computers and conduct validations and simulations to determine the effect of operating conditions on reactor performance.

The model described in the tubular reactor is as follows

$$\frac{\partial C_i}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}\left[\left(-D_e\frac{\partial C_i}{\partial r}r\right) + U_rC_ir\right] - \frac{\partial}{\partial z}\left[-D_e\frac{\partial C_i}{\partial z} + U_zC_i\right] + r_i \qquad (1)$$

where: C_i = concentration (mol/m³)
D_e = diffusivity factor (m²/s)
U_z & U_r = superficial velocity (m/s)
r_i = reaction kinetics (mol/m³.s)

The reaction is studied under steady state conditions, so the equation can be simplified by ignoring accumulation.

$$0 = -\frac{1}{r}\frac{\partial}{\partial r}\left[\left(-D_e\frac{\partial C_i}{\partial r}r\right) + U_rC_ir\right] - \frac{\partial}{\partial z}\left[-D_e\frac{\partial C_i}{\partial z} + U_zC_i\right] + r_i \qquad (2)$$

Convective flux in the radial direction (U_r) is smaller than diffusive flux, so it can be ignored.

$$0 = -\frac{1}{r}\frac{\partial}{\partial r}\left[\left(-D_e\frac{\partial C_i}{\partial r}r\right)\right] - \frac{\partial}{\partial z}\left[-D_e\frac{\partial C_i}{\partial z} + U_zC_i\right] + r_i \qquad (3)$$

Furthermore, Uz is assumed to be constant throughout the reactor then:

$$0 = -\frac{1}{r}\frac{\partial}{\partial r}\left[\left(-D_e\frac{\partial C_i}{\partial r}r\right)\right] + D_e\frac{\partial^2 C_i}{\partial z} - U_z\frac{\partial C_i}{\partial z} + r_i \qquad (4)$$

So, the final equation for the tubular reactor mass balance model is as follows:

$$0 = D_e\frac{\partial^2 C_i}{\partial z} + \frac{D_e}{r}\frac{\partial C_i}{\partial r} + D_e\frac{\partial^2 C_i}{\partial z^2} - U_z\frac{\partial C_i}{\partial z} + r_i \qquad (5)$$

3. Result and Discussion

The model can be used to estimate reactor performance, and it is necessary to validate the model with experimental data. In this validation, the model compares with data based on experiments conducted by Gordon et al. (2003). Calculations with the model in various conditions in accordance with the experiments conducted by Gordon et al. With a small deviation (4.78%), the model is appropriate for estimating reactor performance. (Jatmiko et al., 2018; Yan et al., 2014)

3.1 Effect of Temperature on Reaction Conversion

The effect of temperature on the reaction conversion observes with varies the operating conditions in temperature from 298 K (25 C) to 335 K (62 C).
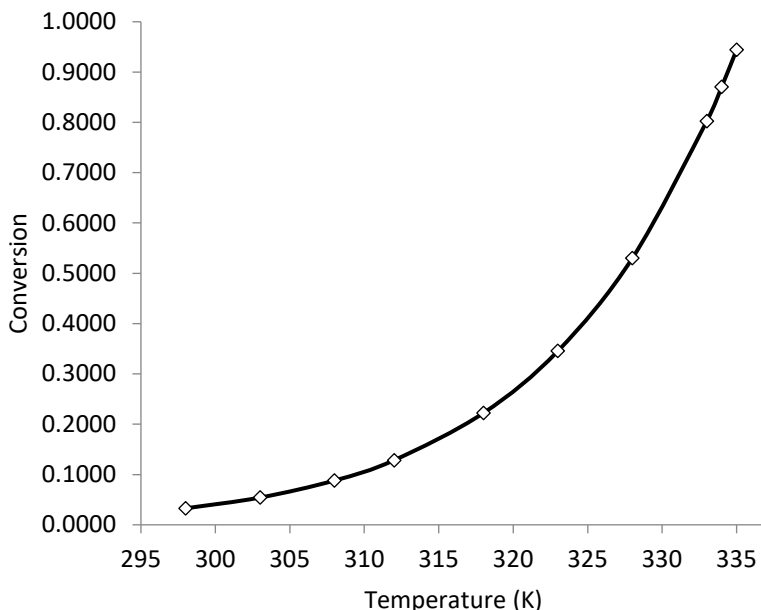

Figure 1. Effect of temperature on reaction conversion

Figure 1 shows the effect of temperature directly proportional to the conversion of the reaction where the higher the temperature, the greater the reaction conversion. It is related to the reaction rate directly proportional to the temperature (Arrhenius equation) (Fogler, 2016), whereas the temperature increases, the reaction rate will increase. An increase in temperature from 298 K to 335 K rose the reaction conversion from 0.0328 to 0.9443.

The simulation results carried out showed that the permissible temperature threshold is 335 K (62C), with a reaction conversion of 0.9443. If the temperature varies above 335K or exceeds the maximum temperature threshold, the reaction conversion results obtained also exceed the equilibrium conversion value.

3.2 Effect of C_3H_6O concentration on reaction conversion

To study the effect of initial C_3H_6O concentration on reaction conversion, variations were made from 3109.7528 mol/m^3 to 5884.9078 mol/m^3 with a temperature of 312 K, superficial velocity of 0,0008 m/s and a C_3H_6O/H_2O ratio = 1/2.5.

Figure 2 shows the effect of the C3H6O concentration is inversely proportional to the conversion of the reaction where the higher the C3H6O concentration that occurs, the reaction conversion will be smaller. The initial variation made at a concentration of 3109.7528 mol/m^3, obtained a reaction conversion of 0.168643 (16.8643%). At a concentration of 3895.6202 mol/m^3 to 4398.66582 mol/m^3, the optimum concentration with the conversion reaction is from 0.134623 to 0.119227. Meanwhile, according to Gordon et al. (2003), the optimum concentration was carried out at 4081.9839,

with a reaction conversion of 0.128476. Until the final concentration of 5884.9078 mol/m^3, the reaction conversion decreases to 0.089116 or 8.9116%.
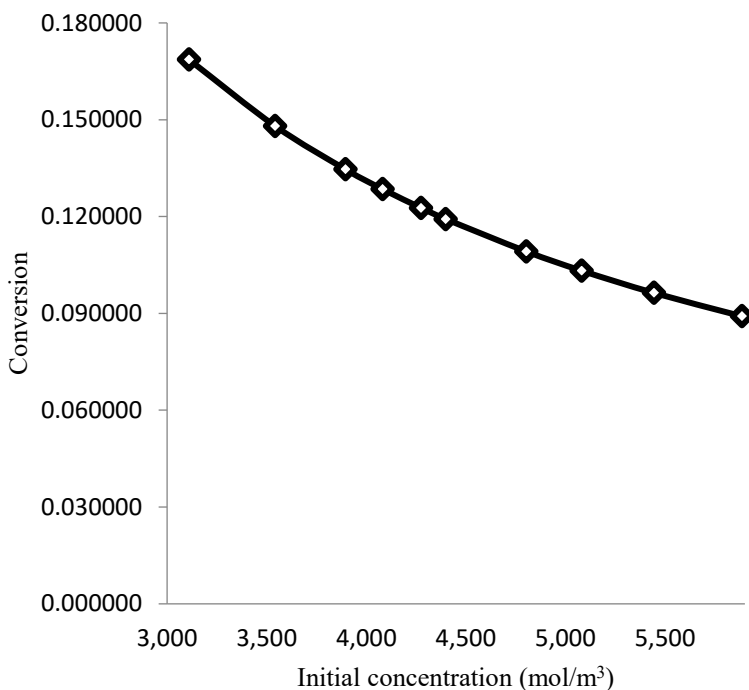

Figure 2. Graph of Effect of C_3H_6O Concentration on Reaction Conversion

3.3 Effect of Superficial Velocity on Reaction Conversion

The effect of superficial velocity on reaction conversion studied with variations was made from 0,0008 m/s to 0.0026 m/s with a temperature of 335 K, a concentration of 4081.9839 mol/m3, and a C_2H_6O/H_2O ratio = 1/2.5.

Figure 3 shows that superficial velocity is inversely proportional to the conversion of reactions where the higher the superficial speed that occurs, the smaller the conversion of reactions. The increase in superficial velocity from 0.0008 m/s to 0.0026 m / s results in the conversion of the reaction decreasing from 0.920896 to 0.283353. As the superficial velocity increases, the residence time that occurs will decrease, and the contact between the reactants and the catalyst lasts briefly, resulting in the resulting conversion also decreases. (Froment et al., 2011; Jatmiko et al., 2018; Patel et al., 2013)

Figure 3 shows the relationship of superficial velocity to Peclet numbers. Peclet number is a parameter that can be used to predict the ratio of convection to dispersion or can also show the flow patterns that occur. The higher the Peclet value, the flow pattern approaches plug flow pattern, and the smaller the Peclet number, the flow pattern approaches the perfectly mixed flow pattern.

The change in superficial velocity from 0,0008 m/s to 0.0026 m/s increased the Peclet number from 49,632.26 to 161,304.80. With increasing Peclet numbers, the convection rate is greater than the dispersion, and the flow pattern in the reactor approaches the stopper flow pattern so that it can reduce the conversion. (Froment et al., 2011)
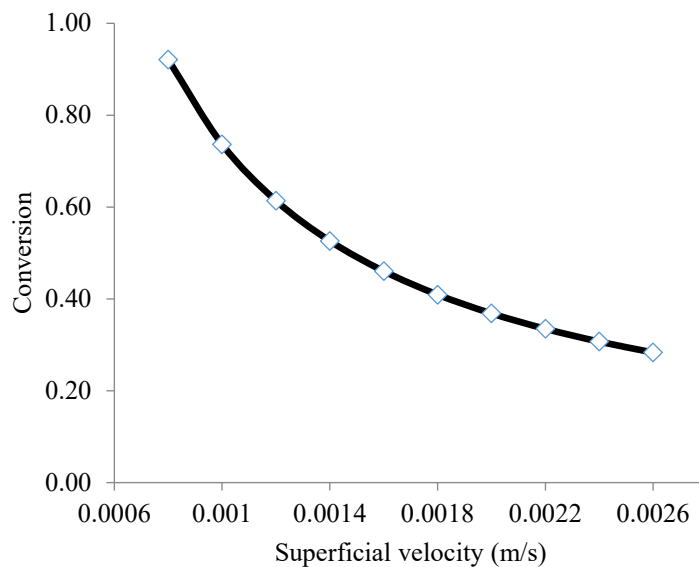
Figure 3. Effect of Superficial Speed (m/s) on Reaction Conversion

3.4 Effect of C_3H_6O/H_2O ratio on reaction conversion

To determine the effect of the C_3H_6O/H_2O ratio on reaction conversion, variations of $1:0.5$ to $1:2.8$ with a temperature of 335 K, superficial velocity of 0,0008 m/s, and a concentration of 4081.9839 mol/m³ are carried out. Figure 4. shows the effect of the C_3H_6O/H_2O ratio is directly proportional to the reaction conversion, where the higher the C_3H_6O/H_2O ratio is given, the greater the conversion of the reaction.
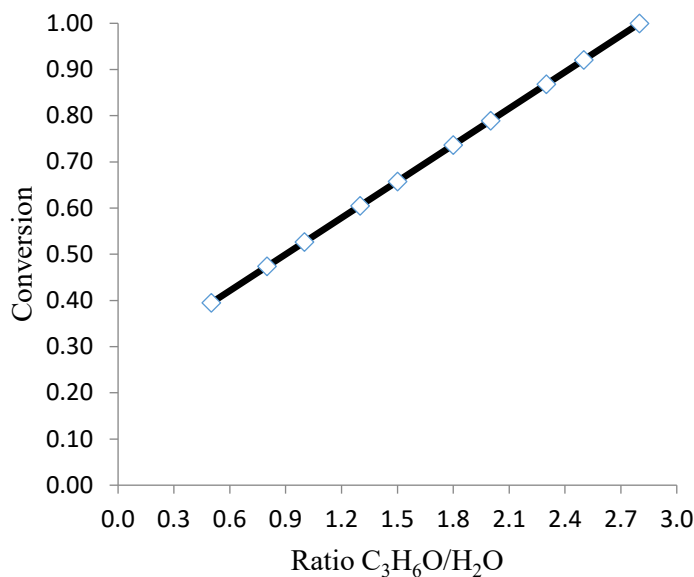

Figure 4. Graph of Effects of C_3H_6O/H_2O Ratio on Reaction Conversion

An increase in the C_3H_6O/H_2O ratio from 0.5 to 2.8 indicates a significant increase in reaction conversion, from 0.301 to 0.959. Based on the reaction stoichiometry, it appears that C_3H_6O becomes a limiting reactant. The higher the ratio,

then C3H6O can react with abundant H2O so that the converted C_3H_6O becomes large. As the conversion increases, the reaction also increases due to the rise in the amount of C3H8O2 produced by propylene's oxidation reaction. It is consistent with experimental results; when the C_3H_6O/H_2O ratio is enlarged, the reaction conversion also increases. (Gordon et al., 2007)

4. Conclusion

A mathematical model of the tubular reactor for the propylene oxide hydrolysis reaction can be used to predict the reactor's performance well. From the results of simulations carried out, it can be seen several factors that influence the significant hydrolysis of propylene oxide, including temperature, initial concentration of propylene oxide, superficial speed, and reactant ratio. The temperature and reactant ratio are directly proportional to the conversion of the reaction. On the other hand, the initial concentration of propylene oxide and superficial velocity is inversely proportional to the conversion of the reaction

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Biography

Tri Hadi Jatmiko is a researcher at Research Division for Natural Product Technology, Indonesian Institute of Sciences, Indonesia. He obtained his Bachelor of Chemical Engineering from Sepuluh Nopember Institute of Technology (ITS) and his master's in chemical engineering from University of Indonesia (UI), Indonesia. He has been involved in various studies at Research Division for Natural Product Technology, Indonesian Institute of Sciences, Indonesia and has published the results of his research in conference papers and in journals. He also has a number of patents that have been registered. His research interests are in chemical engineering, biomass utilization, including modeling and simulation.