THE MIXING OF NITRATION GLYCEROL USING MICROCHANNEL HYDRODYNAMIC FOCUSING UNDER DIFFERENT FOCUSING RATIO

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ABSTRACT

The paper aims to examine the effect focus ratio on the focus width of the microchannel and mixture efficiency on the glycerol nitration. In this study is using two microchannels. First, by measuring the flow mixing. Second, by measuring the temperature, using a K-type thermocouple connected to Analog Converter Data. The independent variable is the focus ratio of the inlet channel. Focus ratio of 1:2 (DSheath=300 μm), focus ratio of 1:1 (DSheath=150 μm), the focus ratio of 2:1 (DSheath=75 μm). The result of the study is focused ratio affects the efficiency mixture and wide focus. The focus ratio relates to several reactants and the mixing time. The smaller the focus ratio, the higher the mixture efficiency, and the smaller the width of focus. Diffusion-related to the speed of reaction, the flow shear stress influenced by differences in the volume of the inlet channel, the greater of shear stress will accelerate the diffusion of molecules—the smaller the focus ratio, the more increase the reaction temperature.

KEYWORDS: Nitration Glycerol, Focus Ratio, Mixing Efficiency, Microchannel

Received: Jun 06, 2020; **Accepted:** Jun 26, 2020; **Published:** Aug 07, 2020; **Paper Id.:** IJMPERDJUN2020680

INTRODUCTION

The Nitroglycerin ($\text{C}_3\text{H}_5(\text{ONO}_2)_3$) is a compound formed from the glycerol nitration process. Equation nitroglycerine formation as follows: (1)

The glycerol nitration process is essential, but it is hazardous. It is due to the process that is very quick and exothermically. Furthermore, a rapid temperature rise, if unchecked, leads to an explosion [1]–[5][6]. The risk of the explosion shows the importance of controlling this process. Several studies have focused on the design of Microfluid for control of the liquid mixture [6]–[15].

One of the processes to control of glycerol nitration is using microchannel [7], [16]–[22]. Microchannel widely uses in the fields of biology, chemistry, physics, medicine, and its application [23]–[26]. Microchannel, as a mixer, provides full contact between molecules, increasing the speed of chemical reactions [27], [28]. The micromixer mechanism affects the speed of chemical reactions. It caused reactants to react only through micromixer[29]. Mixing reactive fluids associated with the diffusion process [22]. Mixing in a microchannel depends on the diffusion of molecules, but it is slow and takes a long microchannel [11]. One of the microchannel as the micromixer is hydrodynamic focusing. This type used to improve the efficiency of mixing the fluids [30]. [31], [32] Examining the ratio focused on hydrodynamic inlet channel on selective seeding technique (SES-PIV). The results showed that two aspects affect the flow deformation [33]. First, it is a wide distribution of non-uniform flow.

Second, determining the angle of the inlet channel flow is symmetrical or not. [34]–[35] found that the level of efficiency and a wide mix of focused flow depends on the flow shear stress. [36] States that the ratio of the flow velocity, Reynolds number, and concentration of the solution affects the flow of the mixture. Focus ratio ($Q_1/(Q_2+Q_3)$) is the ratio between the flow rate focused on focusing flow rates. The study's purpose is to investigate the effect of the focus ratio of the focus width microchannel and efficiency of mixing.

The microchannel is one of the new technologies in the pharmaceutical field. In the pharmaceutical field, the microchannel assumed to be a blood vessel of a living thing [37], [38]. The flow in the microchannel can change dynamically under certain conditions, such as the blood flow of people with diabetes mellitus. Diabetes mellitus is a disease related to blood plasma. Increased blood plasma viscosity causes diabetes [39][40]. The viscosity of human blood that is higher than the normal limit will have a negative effect. One negative effect is the heart's performance to pump blood heavier and can damage the walls of blood vessels. The two channels on the microchannel that insulated with a membrane represent external and internal fluids in human cells. Diffusion that occurs through aporous membrane describes the process of absorption of nutrients or drugs that enter the body through the blood [8], [29].

EXPERIMENTAL METHODS

The purpose of the study is to know the characteristics of the hydrodynamic microchannel ratio focus. The research used to Investigate the behavior of the mixture flow in the microchannel. The microchannel schema shown in figure 1, and the specification of microchannel shown in Table 1. The dimensions of hydrodynamic focusing microchannel comprise three inlet channels. The glycerol supplied to the core channels and nitric acid in the sheath channel. The volume of reactants shown in Table 2.

Figure 1: Schematic of Microchannel [9].

Table 1: Table Specification Microchannel

Focusing Ratio Type	1:2	1:1	2:1
The width of the inlet channel core D1 (μm)	300	300	300
The width of the inlet channel sheath D2, D3 (μm)	300	150	75
The width of the outlet channel D4 (μm)	300	300	300
Channel height w (μm)	200	200	200
The angle of junction α(o)	45	45	45
Long inlet channel L1,L2,L3 (μm)	2000	2000	2000
Long outlet channel L4 (μm)	4000	4000	4000

Table 2: Table Specification of the Fluid

No	Reactan	Molar Massa (gr/mol)	Density (gr/cm3)	Reactan Volume (ml)
1	Glycerol	92,09	1,26	73
2	Nitric Acid	63,01	1,51	120
3	Sulfuric Acid	98,08	1,84	5

The microchannel made of acrylic with a thickness (T1 and T2) 5 mm, as shown in figure 1. Two microchannels made each treatment. First, It uses the mixture flow measurement, using a different color additive between glycerol and nitric acid. The yellow color is for glycerol and red for nitric acid. Second, measure the reaction temperature and place a K type thermocouple every 500 μm in the microchannel outlet channel, starting from the inlet channel's junction point.

EXPERIMENTAL SETUP

The experiment used a variation of focus ratio (1:2, 1:1, 2:1) with a flow rate of 5 mm/min. The setup consists of four main components: lighting system, an optical system, a Dino capture camera, and a control system. Lighting system using Fluorescent Bulb type lamp, Daylight MA305-05. It is to clarify the color of the resulting image. The optical system uses the Olympus BH2 BH-P microscope. This system is equipped with two-way movement control. The AM7023B dino-lite camera used to record reactant mixing. Data stored in the form of images on a computer. The control system uses a syringe pump type TS-1B / W0109-1B. This pump has four flow drive units. The four driving units operate independently. Image data is processed using color-based segmentation using the color space of the MATLAB program. The result is color data of the reactants and products, as well as a focus width (d) and mixing efficiency.

To test the reaction temperature using a K type thermocouple with a diameter of 50 μm . It placed starting from the intersection point up to 4000 μm at intervals of 500 μm . It connected with the data converter analog-type RAY-SF1-M13100-1M CB3. Temperature data plotted into a graph. The scheme experiment setup shown in figure 2.

Figure 2: Scheme of Experiment Setup.

RESULT

Figure 3 shows the difference in the flow of the mixture variations focus ratio. It is known to mix a color change. Nitroglycerine products at most of a ratio of 1:2. It is due to the discharge shroud channel this ratio is higher than other ratios discharge. It increases the shear stress at the boundary layer between the surface of nitric acid and glycerol. Thus facilitating the process of molecular diffusion and improve the efficiency mixture of the reactant.

Figure 3: The Behavior of the Flow of Glycerol Nitration a Ratio of Focus (1:2, 1:1 and 2:1).

VARIATION FOCUS RATIO VERSUS WIDTH OF FOCUS

Figure 4: Variation Focus Ratio to Focus Width.

Figure 4 shows a graph which tends to be equal between the research and the theoretical, but smaller than the theoretical research. It is due to surface roughness increase turbulence and therefore contributes to the mixing of the reactants. Focus ratio increases, so the smaller the width of the focus of the core flow. It is due to several reactants and the mixing time and the shear stress effect on molecular diffusion. The effect causes more loose-fitting molecular bonds to facilitate the mixing of flow. In 2500 m, indicate that the width of the focus on a 1:2 ratio reached 0.01 being a ratio of 1:1 and 2:1, respectively 0.06 and 0.19. It means the number of glycerol almost entirely mingled with nitric acid.

VARIATION RATIO FOCUSES ON THE EFFICIENCY OF THE MIXTURE

Figure 5 The Effect of Focusing Ratio on the Efficiency of the Mixture.

Figure 5 shows the effect of focusing ratio on the efficiency of the mixture. The smaller the focus ratio, the higher the efficiency of mixing. It is due to the smaller focus ratio, the greater the amount of nitric acid. One mole of nitroglycerin requires three moles of nitric acid and one mole of glycerol. It means that it takes three times the amount of nitric acid glycerol. At a focus ratio of 1: 3, the more reaction products, the higher the mixture's efficiency. The results of measurements at a distance of 4000 μm demonstrate the efficiency of the mixture ratio of 1:2 is 0,89, a ratio of 1:1 and 2:1 respectively 0,68 and 0,52.

VARIATION OF THE FOCUS RATIO ON THE REACTION TEMPERATURE

Figure 6: Variation of the Focus Ratio on the Reaction Temperature.

Figure 6 shows that the smaller the focus ratio, the higher the temperature of the reaction. Due to the smaller focus ratio, the amount of nitric acid increased, thereby increasing the reaction product. By the reaction equation, increasing the reaction product, the higher the heat generated. It causes the reaction temperature to rise. The 1: 2 focus ratio is the highest compared to other focus ratios. At a ratio of 1:2 in the average temperature 30,4°C, being a ratio of 1:1 and 2:1 are 29,3°C and 28,95°C respectively temperature.

DISCUSSION

The glycerol nitration reaction is a reaction in the solution system so that the nature of the solvent will determine the reaction rate. Solvents are media that will control the attraction between molecules, determine the mixture's viscosity, and determine the polarity of the molecules. Water is a universal polar solvent. The ability of water to dissolve in compounds is influenced by the degree of ionization or hydration of the compound to produce electrostatic forces (hydrogen bonds).

The mechanism of $\text{HNO}_3\text{-H}_2\text{SO}_4$ reaction in the sheath channel and $\text{C}_3\text{H}_5(\text{OH})_3$ in the core channel takes place through several stages, given separately, as shown in Figure 7 and 8.

Figure 7: Mechanisms for the Formation of Nitronium Ions in the Sheath Channel.

Figure 8: The Mechanism of the Electrophile Glycerol Substitution Reaction and Nitronium Ion.

In the first stage, in the sheath channel, a strong acid, H_2SO_4 , as a catalyst, will collide with nitric acid causing protonation of HNO_3 , forming a product between activated complexes. The activated complex in the second stage dehydrates and forms nitronium ion, NO_2^+ , as a reactive species that are electrophilic. Both stages of the reaction occur quickly and reversibly, with the equilibrium constant (K) = 22. Furthermore, in the third stage, nitronium ions will diffuse towards the interface phase in the core channel and collide with glycerol through the electrophilic substitution mechanism.

The third stage mechanism runs slow so that it is a determining step in the overall reaction rate. It is influenced by, among others, the formation of water by-products in the mechanism of stage 2 and the steric effect on the products formed. In stage two, the reaction is reversible, so water will tend to shift the equilibrium towards the reactants. The steric effect due to the size of the nitronium ion on NO_2 is a barrier to further nitration reactions. However, the presence of excess nitric acid reactants, according to Le Chatelier's principle, causes the reaction's equilibrium to lead to product formation and increase the reaction rate. Therefore, the two conflicting influences cause an irregular front reaction.

VARIATION OF FOCUS RATIO

Figure 9 show that there are differences in image data between solutions with different focus ratios. Therefore the difference in reactant flow discharge causes a difference in the reactant flow volume ratio so that it affects the ratio of the number of moles of the two reactants. The number of moles of reactants affects the reactant volume in the initial and transition states. The initial hydration process causes this. If the activated complex volume is smaller than the total reactant molecule volume, hydrostatic pressure will occur.

In this study, the difference in the flow volume ratio causes one reactant to act as a limiting reagent so that the other reactants will be excessive. Therefore some molecules will be unpaired. It shown in Figure 9.

Figure 9: Schema A. Electrostatic Force (Ion-Dipole Interaction) B. Load Transfer, Adhesion, and Friction Forces Occur. C Diffusion Process Occurs, and Ion-Dipole Bonds Formed.

The existence of the remaining reactant molecules causes the amount of reactant volume to be greater than the activated complex volume. It will result in increased hydrostatic pressure and increase the concentration of activated complexes, thereby increasing the rate of reaction.

CONCLUSIONS

From the results of the study, it can summarize as follows:

- The focus ratio affects the surface shear stress of the reactants. The smaller the focus ratio, the higher the shear stress. It causes a more tenuous bond of molecules. So the process of molecular diffusion is faster. It increases mixing efficiency and reduces the width of focus.
- The smaller the focus ratio leads to greater mixing efficiency, and increase the reaction temperature.

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