



Mass transfer phenomena of partially miscible liquids under liquid-liquid slug flow in a circular microchannel

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ABSTRACT

Micoreactors have been demonstrated to become an effective tool for increasing mass and heat transfer in heterogeneous chemical processes that are unachievable in batch or continuous stirred tank reactors. The key to superior performance is the availability of a large specific surface area (A/V) in the microsystem for mass and heat transfer between phases. Among the flow patterns generated in the two-phase liquid-liquid flow, slug is an ideal flow with a high stability characteristic, regular velocity, and uniform dimension throughout a micro-channel system. The flow behavior gives slugs great potential to increase mass and heat transfer between phases, so optimizing the utilization of micoreactors in many chemical process applications needs an in-depth understanding of the liquid-liquid hydrodynamic. Therefore, the current work aims to determine *the mass transfer coefficient under liquid-liquid slug flow and the influence of slug dimensions, channel material, volumetric flow rate, and the flow rate ratio of the organic-aqueous phase on the mass transfer coefficient*. The experiments were performed in 1 mm (ID) circular PTFE and silicone tubes, with a 30–40 ml/hour flow rate, and sodium hydroxide concentrations of 0.1, 0.13, and 0.15 M were used. The results exhibit that the most prominent overall mass transfer coefficient was 0.121/s, attained at 0.15 M sodium hydroxide concentration, with 40 ml/hour total discharge within the silicone channel. *Microchannels generated smaller slug sizes at a higher aqueous phase flow rate than the organic phase. The smaller size provided a large specific surface area (A/V) for enhancing the mass transfer coefficient.*

1. Introduction

Microdevice technology plays an increasingly important role nowadays and has many positive impacts on the development of science and industrial applications. One of the rapidly developing fields in micro-technology is microstructure reactors (micoreactors). Micoreactors consist of several channels with an inner diameter of less than 1 mm (Prakash and Ghosh, 2021; Zhang et al., 2019). Because of the small dimension, the surface area (A) to volume (V) ratio that can be provided on a micro-scale under a hydraulic diameter range of ten to hundreds of micrometers is very high, attaining 10,000 – 50,000 m^2/m^3 (Dessimoz et al., 2008), a much greater value than conventional reactors which are only able to provide 100 – 400 m^2/m^3 (Jähnisch et al., 2004). The high surface area to volume ratio is a crucial aspect required for enhancing mass and heat transfer performance between phases in a unit process. The huge specific surface found in a microfluidic system is able to encourage the provision of a high mass and heat transfer coefficients up

to 1.1/s (Ratchananusorn et al., 2011) and 25,000 $\text{W}/\text{m}^2\cdot\text{K}$, respectively, which allows intensification of highly exothermic and or endothermic takes place effectively (Dessimoz et al., 2008; Wang et al., 2020; Ghaini et al., 2010).

The hydrodynamic of two-phase microfluidic systems has three different aspects to be considered: the first, the surface area to volume ratio; the second, the flow is characterized by a small Capillary number (C_a), which expresses that the influence of surface tension force is more predominant than viscous force in the system; and the third, micro-roughness and wettability channel wall exert significant influence to the formation of flow pattern. In a laminar multiphase flow system, the domination of interfacial tension and inertial force leads to various interfaces in regular shapes (Plutschack et al., 2017). There are many types of liquid-liquid flow patterns on a micro-scale. The main flow patterns observed in silicone and Teflon microchannels are annular, slug, and droplet flow (Tsaoulidis et al., 2013), but among the flow patterns, slug flow is ideal for enhancing mass and heat transfer due to the high stability characteristics shown by this flow pattern, and its ability to

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Nomenclature		Greek Letters	
a	specific surface, m^2/m^3	τ	reaction time, s
A_i	interfacial area, m^2	ρ	fluid density, kg/m^3
C	concentration, mol/liter	μ	fluid viscosity, Pa s or $\text{kg}/\text{m s}$
C_a	Capillary number	σ	surface tension, kg/s^2
D	diameter, m	Subscripts	
$D_{i,j}$	molecular diffusivity, m^2/s	A	species of CCl_3COOH
Ei	enhancement factor for instantaneous reaction	B	species of Sodium Hydroxide solution
K	overall mass transfer coefficient, m/s	c	organic phase
k	mass transfer coefficient of the film, m/s	d	aqueous phase
Q	volumetric flow rate, m^3/s	org	organic phase
Re	Reynolds number	aqu	aqueous phase
r	reaction rate, $\text{mol}/\text{liter}/\text{s}$	0	initial condition
U	linear velocity, m/s	Superscript	
V	volume, m^3	$*$	Interfacial
We	Weber number		

generate a substantial specific surface. Annular flow appears while inertial force works more dominant than interfacial tension force. Interfacial tension force tends to reduce interfacial area, whereas inertial force breaks the shape and drags the interface in the flow direction. As the competitive nature between inertial and interfacial tension forces, annular flow can be destabilized by changing the flow rate of both phases and the flow rate ratio. Slug and droplet flows are extensively studied because of the ease of hydrodynamic control and potential applications in fine chemical synthesis. Operations in the slug flow regime have been demonstrated to become a valuable tool for increasing reaction performance limited by mass and heat transfer. Furthermore, the ease of slug dimensions control allows a more effective mass transfer process and reaction control, which is unachievable in batch and continuous stirred tank reactors (Ratchananusorn et al., 2011). In this case, two mechanisms are found to be responsible for mass transfer between liquid-liquid two-phase flow: first, internal circulations within the slug; second, gradient concentration between successive slugs leads to diffusion between phases. With its advantages, microfluidic systems are employed for increasing mass and heat transfer in many industrial purposes, such as the dehydration of bioethanol (Suerz et al., 2021), synthesis of ethyl methyl oxalate from diethyl oxalate (Ji et al., 2020), Biodiesel synthesis through transesterification (Wu et al., 2016; Tiwari et al., 2018; Mazubert, 2014; Jamil et al., 2016), fabrication of wrinkled protein microcapsules (Feng and Lee, 2019), and generation of gelatin emulsions and microcapsules (Yeh et al., 2013).

Compared to conventional systems, microdevices offer other advantages, such as effective mixing processes and process safety, mainly for processes employing hazardous and toxic chemicals such as nitration and polymerization. However, the microreactor performance still needs improvements, considering the potential occurrence of fouling in some chemical process applications due to chemical degradation, which is difficult to detect and clean because of the small diameter of the channel. The emergence of this problem will undoubtedly be troublesome when the scale-up process is carried out. Therefore, more in-depth and comprehensive studies regarding the scale-up process toward industrial capacity are still urgently needed (Jensen, 2017).

Flow behavior greatly determines the sustainability of the mass and heat transfer processes on the micro-scale. Mass transfer characteristics on a micro-scale differ from those on a macro-scale, mainly related to thin liquid film formation in a narrow space between the slug and channel wall and the diffusion process between phases. On a micro-scale, liquid films emerge in a more delicate dimension. Hence, the distance of molecular diffusion on a micro-scale becomes shorter and increases the mass transfer coefficient significantly. Some previous researchers have worked on the mass transfer phenomena in

microreactors. What distinguishes the current study from previous studies is the channel cross-section, channel material, and the liquid phase used. Previous studies employed channels with square (Dessimoz et al., 2008) and triangular cross-sections (Basher, 2021), while this study utilized circular cross-sections. The effect of channel materials was observed using glass tube (Dessimoz et al., 2008), PTFE (polytetrafluoroethylene) (Ghaini et al., 2010; Xu et al., 2013), PMMA (Kovalev and Yagodnitsyna, 2021), and PFA (Wang et al., 2020), while this study employed two different channel materials, i.e., silicone and PTFE. Sodium hydroxide-NBF ester was used as a liquid-liquid mixture (Ghaini et al., 2010), whereas the current study uses the liquid mixture of water-NaOH and CCl_3COOH -toluene as aqueous and organic phases. The tube cross-section, channel material, and different physical properties of the liquid determine the characteristics of the slug flow pattern generated. The various contact angles and liquid wettability on a channel wall affect the overall mass transfer coefficient (Wang et al., 2020; Liu et al., 2021; Antony et al., 2014).

The studies on mass transfer phenomena in microfluidic systems have been widely published (Zhang et al., 2019; Ratchananusorn et al., 2011; Wang et al., 2020; Liu et al., 2021; Zhang et al., 2012), but the previous results did not explain the correlation between slug dimensions and the mass transfer coefficient. In addition, previous studies have yet to study the impact of various channel materials on the mass transfer process between phases. Therefore, this work focused on exploring the liquid-liquid mass transfer phenomena regarding slug flow pattern and the influence of slug dimensions, channel material, volumetric flow rate, and the organic-to-aqueous flow rate ratio on the mass transfer coefficient.

2. Materials and methods

2.1. Material

The hydrodynamic of two-phase microfluidic systems has three different aspects to be considered: the first, the surface area to volume ratio; the second, the flow was characterized by a small Capillary number (C_a), which expresses that the influence of surface tension force is more predominant than viscous force in the system; and the third, micro-roughness and wettability channel wall exert significant influence to the formation of flow pattern. The two-phase flow pattern observed in the experiment consists of an aqueous and an organic phase. The aqueous phase involved a mixture of deionized water and NaOH (Fisher Scientific, $\geq 98\%$) with 0.1, 0.13, and 0.15 M concentration, and the organic phase comprised a mixture of toluene (Merck, $\geq 99.9\%$) and CCl_3COOH (strong acid) (Sigma Aldrich, $\geq 99\%$) with the concentration

of 0.4 M. Then, bromothymol blue was used as an indicator to facilitate flow observations. The physical properties of aqueous and organic phases at 25 °C are depicted in Table 1 below:

2.2. Equipment

The microchannel in this work has a 1 mm inside diameter and 15 cm long of PTFE and silicone materials. Two syringe pumps (NEM-ESYS high-pressure syringe pump type NEM-B203–01 B) were applied to ensure the stability of liquid flow along the channel. This pump can flow liquid with minimum and maximum debits in the range of 171.0 nl/min – 825 ml/min, maximum pumping pressure of 12 bar for 100 ml syringe, and liquid discharge in the field of 42.7 nl/min – 206 ml/min with a maximum pumping pressure of around 50 bar for a 25 ml syringe.

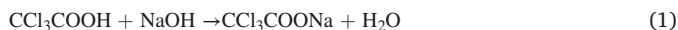
Visualization of the two-phase flow pattern was carried out by using a High-Speed Digital Camera (CCD HCC-1000) and an SMZ-10 microscope (Nikon) using image processing software NV 1000 (New Vision Technologies) and a light source (LED lamp), allowing slug shape and color changes detection to be observed clearly.

2.3. Method (continuous)

Principally, the experiment was carried out in three stages, i.e., slug formation in a microchannel, then visualizing slug flow pattern and measuring the slug length within a channel. Measuring slug length was conducted using a method depicted in Fig. 2. The ruler in Fig. 2 only intends to clarify the principle of the applied method. All measurements were conducted using the image processing software NV 1000 at ambient temperature and pressure (Figs. 1 and 3).

2.4. Analysis

To determine the overall mass transfer coefficient, neutralization was used as a reaction model with color change at pH 7 by bromothymol blue as an indicator. The reaction is instantaneous, thereby, controlled by mass transfer. The neutralization reaction takes place between CCl_3COOH and NaOH according to the stoichiometry as follows:



The reaction rate is expressed for the strong acid component CCl_3COOH ,

$$\frac{dN_{A,org}}{dt} = V_{A,org} \cdot \frac{dC_{A,org}}{dt} = -A_i \cdot K_L \cdot (C_{A,org} - C_{A,org}^*) \quad (2)$$

$N_{A,org}$ represents CCl_3COOH in the organic phase, while A_i is the interfacial area of two liquid phases. Eq. (2) can be expressed in another form by defining the holdup of the organic phase,

$$\varphi_{A,org} = \frac{V_{A,org}}{V_{mc}} = \frac{Q_{A,org}}{Q_{A,org} + Q_{A,aqu}} = \frac{1}{1+q} \quad (3)$$

$$q = \frac{Q_{A,aqu}}{Q_{A,org}} \quad (4)$$

where Q_{org} and Q_{aqu} are the volumetric flow rates of the organic and aqueous phases, respectively. Then, specific surface,

Table 1
Physical properties of aqueous and organic phases.

Fluids	ρ (kg/m ³)	μ (kg/m.s).10 ³	σ (N/m)
NaOH	2130	-	-
CCl_3COOH	1630	-	-
Toluene	887	0.5600	0.02785
Water	997	0.8937	0.07180

ρ = density, μ = viscosity, σ = surface tension (Melo-Espinosa et al., 2014).

$$a = \frac{A_i}{V_{mc}} \quad (5)$$

By substituting Eqs. (3) – (5) into Eq. (2), the following equation will be obtained:

$$\varphi_{A,org} \frac{dC_{A,org}}{dt} = -a \cdot K_L \cdot (C_{A,org} - C_{A,org}^*) \quad (6)$$

with K_L as the overall mass transfer coefficient. Because NaOH instantly neutralizes the CCl_3COOH molecule transferred to the aqueous phase close to the interface, the concentration of CCl_3COOH in the aqueous phase ($C_{A,aqu}$) can be assumed to be zero, so $C_{A,org}^* = m \cdot C_{A,aqu}^* = 0$.

$$\varphi_{A,org} \frac{dC_{A,org}}{dt} = -a \cdot K_L \cdot C_{A,org} \quad (6)$$

By integrating Eq. (6), the following volumetric mass transfer coefficient equation will be obtained:

$$K_L \cdot a = -\frac{\varphi_{A,org}}{\tau} \cdot \ln \left(\frac{C_{A,org}^0}{C_{A,org}^\tau} \right) = \frac{1}{\tau \cdot (1+q)} \cdot \ln \left(\frac{C_{A,org}^0}{C_{A,org}^\tau} \right) \quad (7)$$

$$\tau = \frac{A_{mc} \cdot L_\tau}{Q_{A,org}} \text{ and } C_{A,org}^\tau = C_{A,org}^0 - q \cdot C_{B,aqu}^0 \quad (8)$$

τ is the time required for a complete neutralization reaction. Eq. (7) was used to calculate the volumetric mass transfer coefficient of liquid-liquid two-phase flow in a microchannel.

3. Results and discussion

The hydrodynamics were studied in 1 mm inside diameter using PTFE and silicone tubes at various sodium hydroxide concentrations and the organic-aqueous flow rate ratios at various total flow rates ($Q_d + Q_c$) in the range of 30 – 40 ml/h. Among the liquid-liquid flow patterns that may be formed, slug flow exhibits the most stable characteristics. It has good potential for industrial applications involving mass and or heat transfer. Therefore, this study observed slug flow patterns focusing on mass transfer in microchannels with T-junction.

3.1. Liquid-liquid two phases flow pattern within a microreactor

Droplet, slug, and annular flow patterns were observed in the current study using circular channels. The flow pattern generated in a microfluidic system is greatly influenced by several factors, i.e., physical properties of fluid such as density, viscosity, surface tension, and contact angle. Channel diameter, material used, and experimental conditions such as pressure, temperature, and flow rate. Changes in channel shape and dimensions affect fluid flow, resulting in different flow patterns. The channel shapes often used in microfluidic systems are square, circular, and triangular under very fine diameters. However, the current experiment observed the mass transfer performance using a circular channel with a 1 mm inside diameter. On a micro-scale, the influence of gravitational forces becomes reduced; conversely, the performance of inertial, capillary, and surface tension forces becomes dominant and determines the formation of flow patterns. The dominance of each force can be sorted by determining dimensionless numbers (Reynolds, Capillary, and Weber numbers) because the magnitude of these numbers was affected by the performance of these forces. At constant temperature, the inertial force is primarily affected by the flow rate of the organic and aqueous phases. In contrast, the viscous force and surface tension are strongly determined by liquid density and viscosity. The density and viscosity will change at different concentrations. Changes in density and viscosity are more affected by the sodium hydroxide concentration than temperature because the operating temperature in this work was kept constant.

The droplet flow pattern was obtained when the flow rate of the

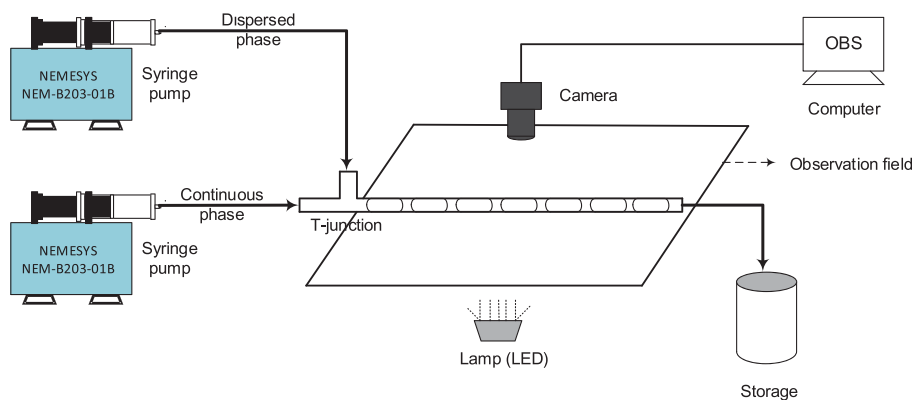


Fig. 1. Experimental setup.

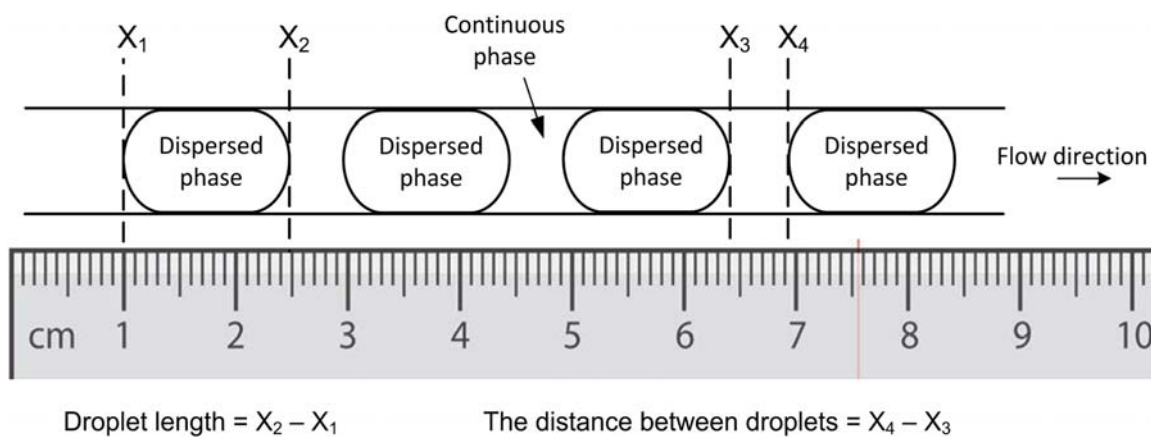
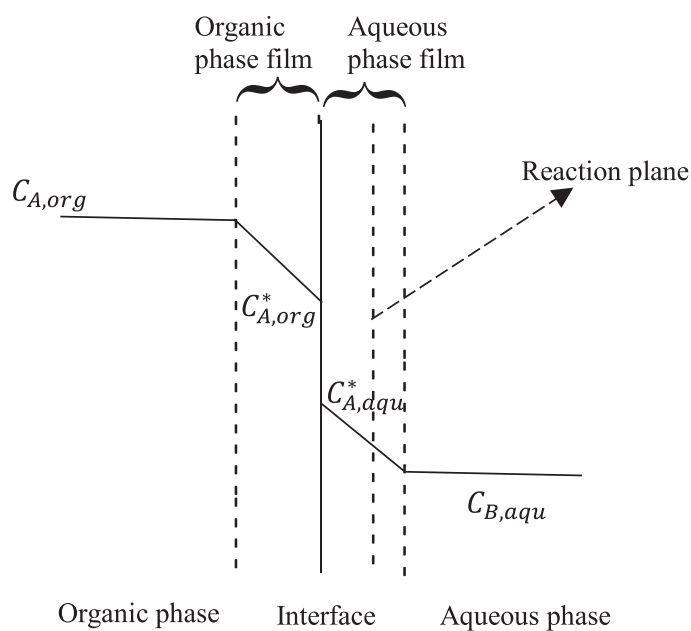
Fig. 2. The measuring method of droplet dimension and the distance between droplets. The horizontal positions of X_2 and X_1 indicate the droplet length, and the different positions of X_4 and X_3 show the distance between the droplets.

Fig. 3. Mass transfer mechanism between phases.

organic phase was too low compared to the aqueous phase, with a ratio of less than 0.6. Droplets appeared under a diameter smaller than the inner diameter of the channel. Meanwhile, an annular flow pattern emerged over a more substantial flow rate ratio of the organic-to-aqueous phase, i.e., more than 1.1. The slug flow pattern, which is the focus of the current study, was generated when the flow rate ratio of the organic to aqueous phases was 0.6 – 1.1 for both PTFE and silicon channels. The slug flow pattern emerged when the surface tension dominated inertial and viscous forces.

Fig. 4(a)–(d) present the slug flow pattern observed in the micro-channel. Sodium Hydroxide solution in the flow system formed droplets with a length over 1 mm dispersed in CCl_3COOH -toluene with a standard deviation below 12 % at the longest slug generated by the lowest sodium hydroxide concentration. At a total flow rate over 40 ml/h for the lowest sodium concentration (0.1 M), slug flow became unstable, indicated by the slug dimension emerging from 3 to several mm long. The slug length remained relatively constant for the total flow rate between 30 and 40 ml/h, with the dimensionless number presented in Table 3.

Slug flow observations using a high-speed camera have not detected any thin liquid films formed between droplets and channel walls. The outer surface of the dispersed phase is in direct contact with the channel wall. CCl_3COOH -toluene in both channels has much smaller contact angles than sodium hydroxide solutions. Therefore, CCl_3COOH -toluene has better wetting properties than sodium hydroxide solutions and is strengthened by the nature of immiscible liquids, causing the volume of the continuous phase in the narrow space between slug and channel walls to become very small because the continuous liquid will tend to be drawn out of this zone. The release of the liquid continuous from the narrow space caused the droplets of sodium hydroxide to come into direct contact with the channel walls. The measurement results of the contact angles of sodium hydroxide solutions and CCl_3COOH -toluene are presented in Table 2.

In a specific chemical process involving mass transfer, the presence of a thin liquid film in the narrow space between droplets and channel walls is advantageous. The formation of a thin liquid film will enhance the specific surface area, i.e., the ratio between surface area and volume of droplets, which is required for effective mass transfer between phases. In a thin liquid film, the mass transfer occurs at the interface between the organic and aqueous phases across the entire surface of the droplet. Conversely, if a thin liquid film does not appear within a flow system, the mass transfer will only occur at the interface of the head and tail of the droplets. In the current work, CCl_3COOH in the CCl_3COOH -toluene mixture diffused from organic to aqueous phases. The mass transfer occurred in one direction towards the aqueous phase because the sodium hydroxide solution did not diffuse toward the CCl_3COOH -toluene mixture. Furthermore, a neutralization reaction occurred between CCl_3COOH and sodium hydroxide solution with a high reaction rate at the aqueous phase interface. The reaction led to a color change from blue to yellow in the aqueous phase, which takes place at pH 7, indicating the end of neutralization.

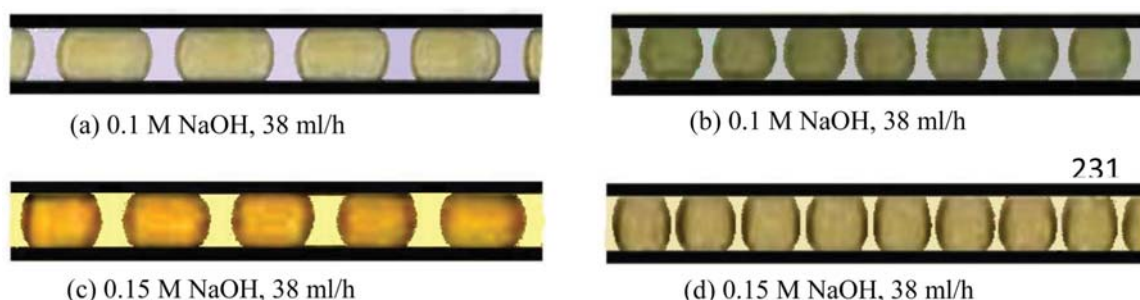


Fig. 4. (a) (c) Slug flow pattern within PTFE tube, (b) (d) within Silicone tube.

Table 2

The various contact angles of liquid mixtures in the PTFE and silicone channel.

Components	Contact Angles	
	PTFE	Silicone
Sodium Hydroxide solution (0.1 M)	91°	56°
Sodium Hydroxide solution (0.15 M)	92°	59°
CCl_3COOH -toluene (0.4 M)	12°	5°

Table 3

Dimensionless Numbers for slug flow observed.

Dimensionless Numbers			
Reynolds number organic phase, ($R_{e,d}$)	$\frac{\text{inertial forces}}{\text{viscous forces}}$	$R_{e,d} = \frac{D \cdot v_d \cdot \rho_d}{\mu_d}$	1.3117–1.7489
Reynolds number aqueous phase, ($R_{e,c}$)		$R_{e,c} = \frac{D \cdot v_c \cdot \rho_c}{\mu_c}$	0.0755–0.1006
Capillary number, (C_a)	$\frac{\text{viscous forces}}{\text{surface tension forces}}$	$C_a = \frac{\mu \cdot v}{\sigma}$ Volkel et al., (2008)	0.00375–0.1143
Weber number, (W_e)	$\frac{\text{inertial forces}}{\text{surface tension forces}}$	$W_e = \frac{v^2 \cdot D \cdot \rho}{\sigma}$ Volkel et al., (2008)	0.0049–0.0115

3.2. Dimensionless number

The Reynolds, Capillary, and Weber numbers are three important dimensionless numbers in the study of fluid flow. A comprehensive analysis of the dimensionless numbers was conducted to get an overview of slug formation within microchannels because, from these numbers, the predominant forces working in the microsystem can be identified.

Table 2 presents that the Reynolds number (R_e) of the organic phase is over one in the range 1.3117–1.7489, while the Reynolds number of the aqueous phase is less than one in the field 0.0755–0.1006. These values indicate that inertia force gave a more dominant influence than viscous force in the organic phase, and vice versa; viscous force has a more dominant effect than inertial force in the aqueous phase. The slightly different results exhibited by the Capillary number in these observations. The magnitude of the Capillary number (C_a) is less than one for both phases in the range of 0.00375–0.1143. These values characterized that in this flow system, surface tension exerts a more dominant influence in the organic and aqueous phases than viscous forces. A similar trend is described by Weber's number of the organic and aqueous phases, which exhibits a value of less than one in the range of 0.0049 – 0.0115. Weber number of less than one expresses that surface tension significantly influences organic and aqueous phases more than inertial forces. Knowing the predominant force working on each phase facilitates determining the flow rate ratio of the organic to

aqueous phases on slug flow generation (Yao et al., 2018).

For the organic phase, the predominant force in order from the largest to smallest is as follows: surface tension, inertial, and the smallest one is viscous force. In the same manner, the dominance force in order from the largest to smallest one for the aqueous phase is as follows: surface tension, viscous force, and minor inertia force. The influence of inertial forces increased with increasing fluid linear velocity of ρU^2 (U = fluid velocity). Furthermore, increasing fluid velocity bring to increasing the viscous forces affect on the liquid-liquid systems with a linear correlation at a specific viscosity, $\mu U/l$ (where μ = fluid viscosity; l = length characteristic). Then, if these forces are compared, the inertial force denotes a more considerable increase, which means that increasing the volumetric flow rate increases the Reynolds number significantly (see Fig. 5). As the flow rate ratio of the organic-aqueous phase grew, the dimensions of the slug appearing within the channel increased along with this ratio. A continuous enhancement of this ratio will be followed by an increase in slug dimension, eventually transitioning toward an annular flow pattern. Conversely, decreasing this ratio transforms slug to droplet flow, which is gradually less stable. Apart from viscous and inertial forces, surface tension forces also contribute to the slug length within the channel. Increasing interfacial tension force is favorable for slug formation, but a decreasing interfacial tension force tends to produce parallel flow in a microfluidic system. In industrial processes, the low stability behavior is undesirable because, under the low stability of processes, it will be difficult for an engineer to estimate many things related to process behavior, such as reaction conversion achievements, yields, production capacity, etc. Therefore, slug formation is more desirable and studied related to mass transfer in a microsystem. The slug formation with the smallest dimension and high stability is needed to generate a large specific surface area for effective mass transfer between phases.

The correlation of Reynolds number to Capillary and Weber number is denoted in Fig. 5. This figure also obviously exhibits the influence of inertial, viscous, and surface tension forces on microfluidic systems. The correlation curve of Reynolds number and Weber number provides information that the increase in Reynolds number due to an increase in inertial force is in line with the increase in the Weber number, shown on the vertical axis. Increasing the Weber number explicitly expresses that the influence of inertia force relative to the surface tension force will be greater. The correlation curve of the Reynolds number and Capillary number indicates the same trend. Enhancing Reynolds number is

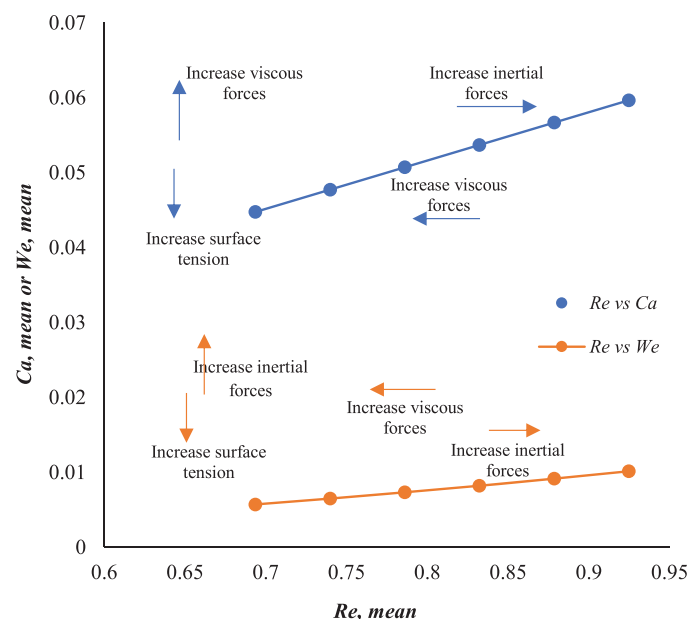


Fig. 5. The correlation between dimensionless numbers in the slug regime.

followed by an increase in Capillary number, which means that the viscous forces have a more considerable influence relative to surface tension forces.

3.3. Overall mass transfer coefficient

The volumetric mass transfer coefficient was determined using Eq. (7). Fig. 6(a)(b) depicts that the greater the total flow rate for the constant organic discharge, the greater the volumetric mass transfer coefficient obtained. These results indicate a similar trend to work conducted by Xu et al. (2013) (Zhang et al., 2019) and Wang et al. (2020) (Plutschack et al., 2017), which is, in this total discharge, T-junction will generate a smaller slug dimension with a more significant number of droplets appeared in the same channel length. The various flow rate ratios of the organic-aqueous phase were found to be an effective method for slug dimensions control. The increase in these ratios has led to an upward trend in the slug dimensions of the organic phase and a downward trend in the distance of successive slugs. The tiny dimension can provide a larger specific surface area (A/V) than the longer slug in a given channel length. The continuous increase in specific surface area brings up the higher volumetric mass transfer coefficient. Therefore, if the curves in Fig. 6(a) and (b) are compared, the volumetric mass transfer coefficient obtained on the tube with silicone material is higher than that for PTFE. This result aligned with the graphs in Figs. 8 and 9(a) and the trend of flow dimensions as illustrated in Fig. 4(a)–(d). These images present that the slug dimensions in PTFE have a longer dimension than the silicone channel (Fig. 7).

The concentration of the aqueous phase, sodium hydroxide, also determines the mass transfer coefficient. The utilization of a higher sodium hydroxide concentration ($C_{B,aq}$) with a constant organic phase concentration has enhanced the volumetric mass transfer coefficient (see Fig. 6(a) and (b)). Under these conditions, the final concentration of CCl_3COOH in the organic phase is getting smaller ($C_{A,org}$) since more CCl_3COOH is involved in neutralizing $NaOH$ (Eqs. (1) and (2)). The reaction occurred in the aqueous phase interface because the sodium hydroxide solution could not diffuse into the organic phase. Conversely, CCl_3COOH in the organic phase is able to diffuse (Xu et al., 2013) in the aqueous phase and dissolve in water. The occurrence of neutralization is indicated by a color change from blue to yellow in the aqueous phase, where the presence of yellow in the flow system denotes that the neutralization has been completed.

The influence of sodium hydroxide concentration on the mass transfer coefficient has been described by previous researchers (Xu et al., 2013; Dessimoz et al., 2008). From different points of view, they explained that the mass transfer coefficient increased due to the increasing sodium hydroxide concentration. This correlation is approached by the effect of sodium hydroxide concentration on the slug dimensions. As the aqueous phase's linear velocity (U_c) exceeds the organic phase (U_d), the slug had small sizes and generated a large specific surface area and a high volumetric mass transfer coefficient. These explanations will be relevant for some cases with large sodium hydroxide concentrations. Nevertheless, for the cases with moderate sodium hydroxide concentration, the change in liquid viscosity caused by changes in sodium hydroxide concentration in the mixture was insignificant (Yao et al., 2020). Hence, the chosen approach needs to be more precise in this situation. The profile of slug dimensions with variations in sodium hydroxide concentration is depicted in Figs. 8 and 9(a). The trend indicates that sodium hydroxide concentration is inversely proportional to the slug dimensions in the channel. The microchannel will generate the largest slug dimensions at the minor sodium hydroxide concentration. In this case, a smaller viscosity of the aqueous phase creates a lower hydrodynamic resistance. The lower hydrodynamic resistances and trend of inertial force to drag downstream surfaces were responsible for higher slug dimensions in a microflow system.

Fig. 7 describes the correlation of the volumetric mass transfer coefficient in a PTFE and silicone tube with various sodium hydroxide

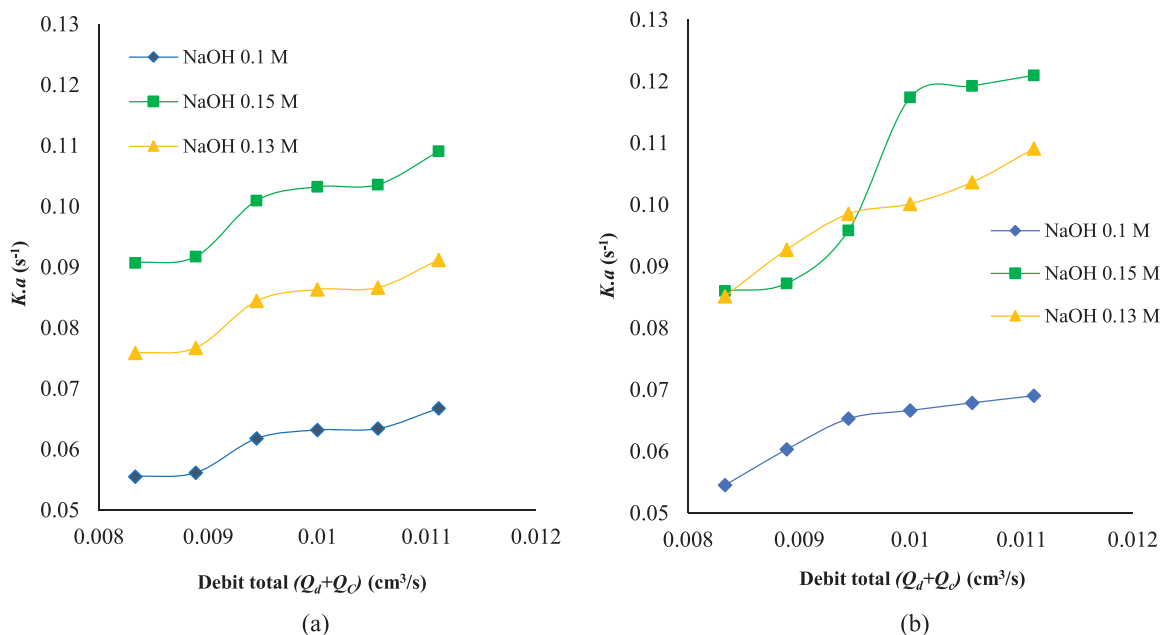


Fig. 6. (a) The effect of total discharge (with a constant debit of organic phase) to the volumetric mass transfer coefficient within PTFE channel, (b) Silicone channel.

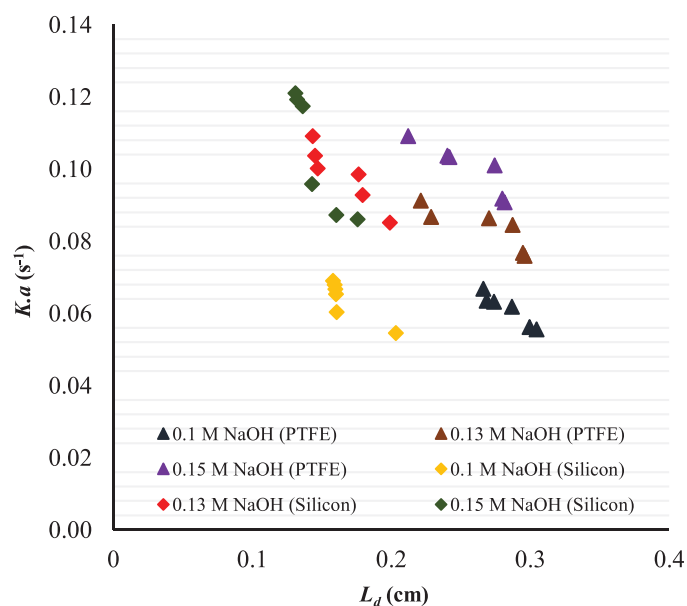


Fig. 7. The correlation between droplet length (L_d) and the volumetric mass transfer coefficient K_a .

concentrations (0.1, 0.13, and 0.15 M). The data points in Fig. 7 indicate at least two critical phenomena: first, there is a downward trend in the value of the volumetric mass transfer coefficient with increasing slug length, and second, a sharp reduction in mass transfer coefficient with a slight change in slug length was found to occur in silicone tubes. The trend denotes that a smaller slug will provide a considerable volumetric mass transfer coefficient (Fig. 7). When the operating parameter has a similar volumetric flow rate but applies different tube materials, different slug dimensions will be generated, and even the flow patterns formed can be different. Apart from being determined by the magnitude of the flow rate, these phenomena are also strongly influenced by the physical properties of each liquid phase, such as density, viscosity, and surface tension, as well as the liquid wettability to the channel walls. When the flow was put on the silicone channel, the organic phase

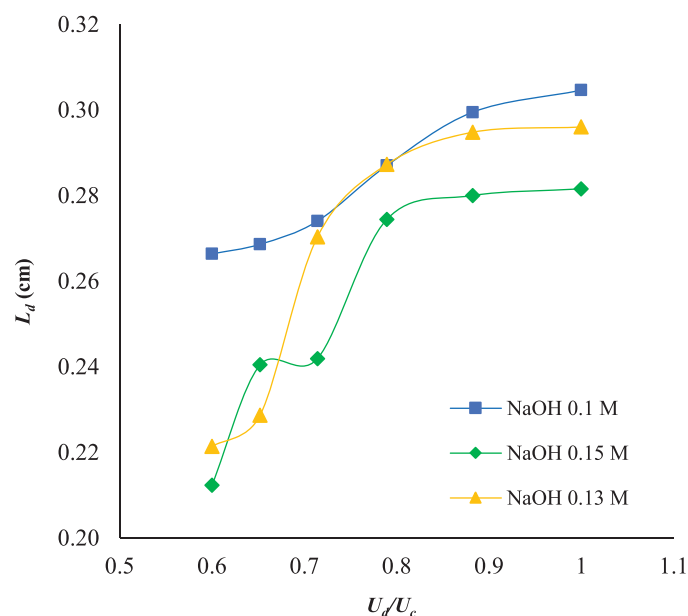


Fig. 8. The organic-to-aqueous phase linear velocity ratio (U_d/U_c) influences the droplet length (L_d) in the PTFE channel.

thoroughly wets the channel wall with a tiny contact angle (Prakash and Ghosh, 2021). In contrast, the organic phase forms a larger contact angle in the PTFE channel, indicating that it possesses poorer wetting properties than silicone. At a certain level, this flow behavior triggers the generation of different flow patterns.

From the experiments, the highest volumetric mass transfer coefficient obtained is 0.121/s, with a mass transfer rate of 0.0182 M/s. These values were at a concentration of 0.15 M NaOH with the rate of the organic and aqueous phase of 15 ml/hour and 25 ml/hour, respectively (total volumetric flow rate is 40 ml/hour), and this result was attained by using the silicone channel. The calculation assumes the slug shape is a cylinder with a hemispherical front and rear cap.

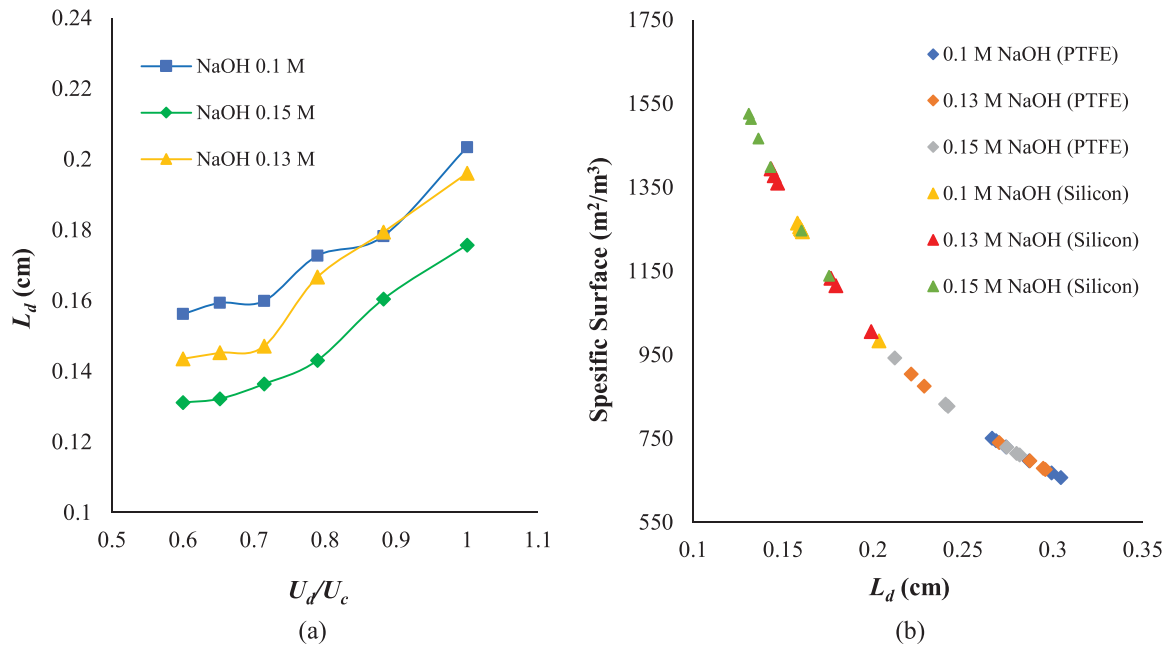


Fig. 9. (a) The effect of the organic-to-aqueous phase linear velocity ratio (U_d/U_c) on the droplet length in the silicone channel, (b) The correlation between droplet length (L_d) to the specific surface area on PTFE and silicone channels.

3.4. Mass transfer model under liquid-liquid slug flow

The mass transfer model under the slug flow pattern can be explained through two distinct mechanisms: i) the diffusion over the interface of both phases and ii) convection by internal circulation. Both mechanisms take place simultaneously with the different dominance of diffusion and convection depending on operating parameters. An increase in the linear velocity of the organic phase as a continuous phase leads to a decrease in the slug length, creating a larger interfacial area and significantly impacting diffusion between phases. Furthermore, the increasing linear velocity also increased internal circulation within the slug's body, enhancing mass transfer by convection.

If the mass transfer occurs via diffusion, the model can be derived by considering a stagnant microflow system. The detailed phenomena were explained by considering neutralization steps between CCl_3COOH and sodium hydroxide solution. Neutralizing sodium hydroxide solution with CCl_3COOH is an instantaneous reaction with the reaction plane located at the liquid film's aqueous phase. The reaction is controlled by the mass transfer of CCl_3COOH and sodium hydroxide solution. All CCl_3COOH compounds have run out at the reaction plane. It means no CCl_3COOH diffused to the bulk of the sodium hydroxide solution.

Changes in CCl_3COOH and sodium hydroxide concentrations will shift the reaction plane. At a steady state, the flow rate of sodium hydroxide toward the reaction zone is equal to the flow rate of CCl_3COOH toward the reaction zone (Fig. 10). Thus,

$$\begin{aligned} -r'_{A,org} &= -r'_{B,aqu} = k_{A,org} (C_{A,org} - C_{A,org}^*) = k'_{A,org} (C_{A,aqu}^* - 0) \cdot \frac{X_0}{X} \\ &= k_{B,aqu} (C_{B,aqu} - 0) \cdot \frac{X_0}{X_0 - X} \end{aligned} \quad (9)$$

Where $k_{A,org}$, $k'_{A,aqu}$, $k_{B,aqu}$ is the mass transfer coefficient of CCl_3COOH in the organic phase, aqueous phase, and mass transfer coefficient of sodium hydroxide in the aqueous phase, respectively, thereby, the mass transfer coefficient within the film correlates,

$$\frac{k_{A,aqu}}{k_{B,aqu}} = \frac{D_{A,aqu}/X_0}{D_{B,aqu}/X_0} = \frac{D_{A,aqu}}{D_{B,aqu}} \quad (10)$$

$$\frac{1}{K_{A,org}} = \frac{1}{k_{A,org}} + \frac{m}{k_{A,aqu} E_i} \text{ (Hatta Theory)} \quad (11)$$

If the system uses pure reactant CCl_3COOH , then $C_{A,org} = C_{A,org}^*$.

Another mechanism that accompanied the mass transfer diffusion in

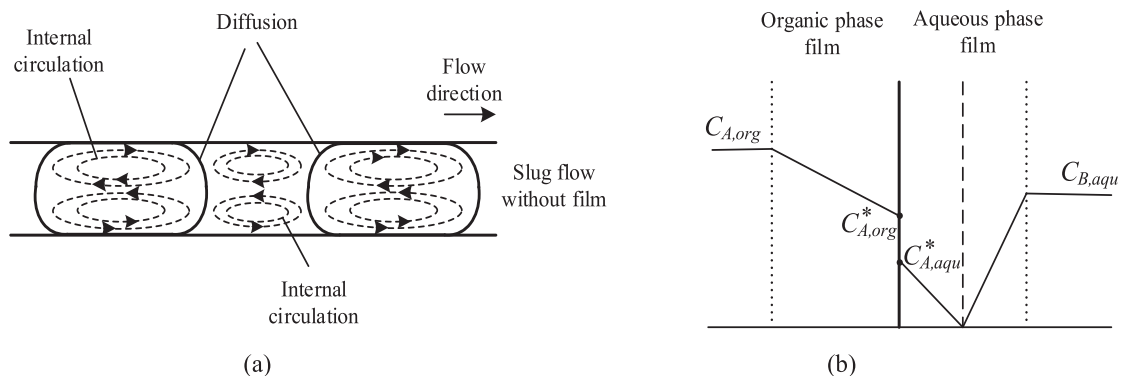


Fig. 10. (a) Mass transfer mechanisms (diffusion & convection) within slug flow, (b) Interface behavior for neutralization (Wang et al., 2017).

the microfluidic observed was convection by internal circulation. Convective mass transfer involves transferring materials between a liquid surface and a moving fluid or between CCl_3COOH -Toluene and sodium hydroxide solution that is relatively immiscible. The convective mass transfer took place under the influence of syringe pump performance. In this system, there was no density variation for both organic and aqueous phases because the temperature parameters remained constant during the flow observation, and the sodium hydroxide concentrations were relatively low. However, it should be noted that the influence of fluid density cannot be ignored at a higher concentration of sodium hydroxide. The transfer rate equation is reliable by

$$N_A = k_c(C_{AS} - C_A) \quad (12)$$

where N_A is the molar mass flux of CCl_3COOH species measured relatively to the fixed spatial coordinates; k_c is the convective mass transfer coefficient; C_{AS} is the concentration at the boundary layer; and C_A is the concentration at some arbitrary defined point in CCl_3COOH -Toluene. The mass transfer coefficient is related to the fluid properties, the hydrodynamic characteristics of the fluid, and the geometry of the preferred system.

The influence of internal circulating flow on mass transfer performance in slug flow can be explained using surface renewal theory. The theory developed by Danckwerts applies penetration theory, where the liquid is described as two areas, i.e., a well-mixed bulk area and an interfacial area, which is renewed so quickly, thus making this area behave like a thick film, as seen in Fig. 11. The dynamic nature of the liquid-liquid interfaces is the principal characteristic of this theory. The assumptions used in this theory are (1) the liquid components at the interface change randomly with fresh components from the well-mixed bulk area; (2) at any time, each liquid component at the interface has the same opportunity to be replaced by a new liquid component; and (3). mass transfer from one liquid to another occurs at the interface under unsteady state conditions. Therefore, the difference in liquid volume at the liquid-liquid interface is renewal due to turbulence around the interface, which is called surface renewal frequency (S).

For a liquid-liquid system like in the current work with the mass transfer taking place from liquid A to B, surface renewal theory states that the mass transfer coefficient on liquid A and B sides are in the surface renewal frequency (S) and molecular diffusivity of liquid A

toward B according (D_{AB}) to the following equation:

$$k_L = (D_{AB}S)^{0.5} \quad (9)$$

Eq. (9) obviously shows that an increase in surface renewal frequency (S) due to an increase in internal flow velocity in the slug flow at the liquid-liquid interfacial area will increase the mass transfer performance (k_L). The figure below exhibits a model of mass transfer phenomena between NaOH-water (aqueous phase) and CCl_3COOH -toluene (organic phase). The reaction occurred in the aqueous phase interface because the Sodium hydroxide solution could not diffuse into the organic phase. Conversely, CCl_3COOH in the organic phase is able to diffuse in the aqueous phase and dissolve in water.

4. Conclusions

Slug flow patterns were observed in the PTFE and silicone channels. In the microsystem, the gravitational force did not influence the flow formation. In the observed system, surface tension, inertial, and viscous force were the predominant forces influencing the flow system. Sodium hydroxide solution as an aqueous (dispersed) phase and CCl_3COOH -toluene as an organic (continuous) phase have better wettability in the silicone channel than the PTFE channels. The wettability of the sodium hydroxide solution on the channel wall determines the shape of the head and tail of the slug and the dimension. The slug on the PTFE channel indicates a more rounded head and tail shape with a larger contact angle. Channel material is one factor that influences the formation of flow patterns. In terms of operating conditions, using a higher total discharge, mainly for the volumetric flow rate of the aqueous phase lower than the organic phase, the microfluidic system will generate a smaller slug dimension and a larger specific surface area (A/V). A substantial specific surface area (A/V) will facilitate an upward trend on the volumetric mass transfer coefficient. The concentration of sodium hydroxide solution was also found to determine the slug dimensions. The trend exhibits that enhancing the sodium hydroxide concentrations decreases slug dimensions. In the current work, the highest distinctive character (A/V) is $100,282.563 \text{ m}^2/\text{m}^3$ with a volumetric mass transfer coefficient of $0.121/\text{s}$ and a mass transfer rate of 0.0182 M/s . This value was reached at a sodium hydroxide concentration of 0.15 M , an organic flow rate of 15 ml/hour , an aqueous flow rate of 25 ml/hour (total

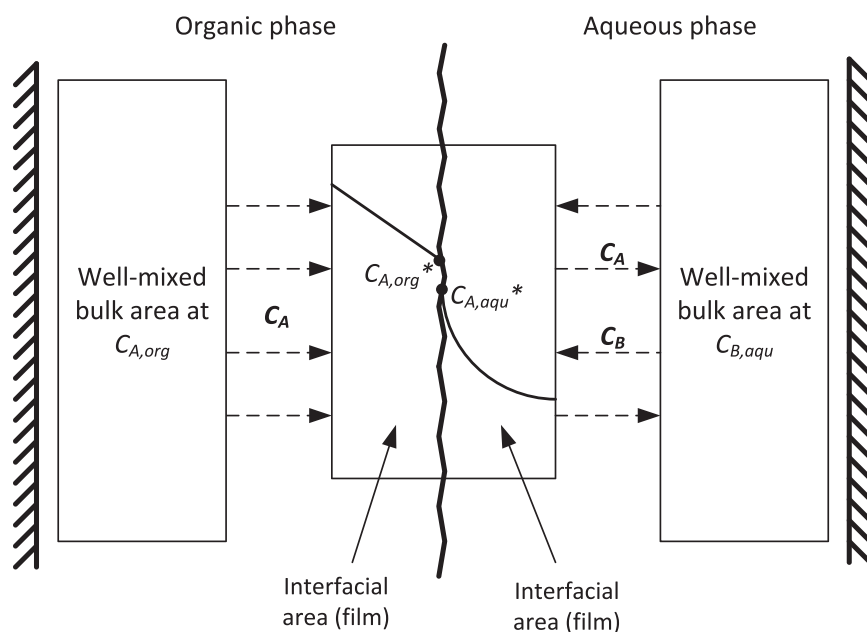


Fig. 11. Surface renewal theory as a model to approach mass transfer phenomena in acid-base neutralization between sodium hydroxide solutions and CCl_3COOH -toluene.

discharge of 40 ml/hour), and a circular silicone channel ($ID = 1$ mm). These experiments confirm that the slug dimensions, channel material, volumetric flow rate, and the organic-to-aqueous flow rate ratio influence the mass transfer coefficient.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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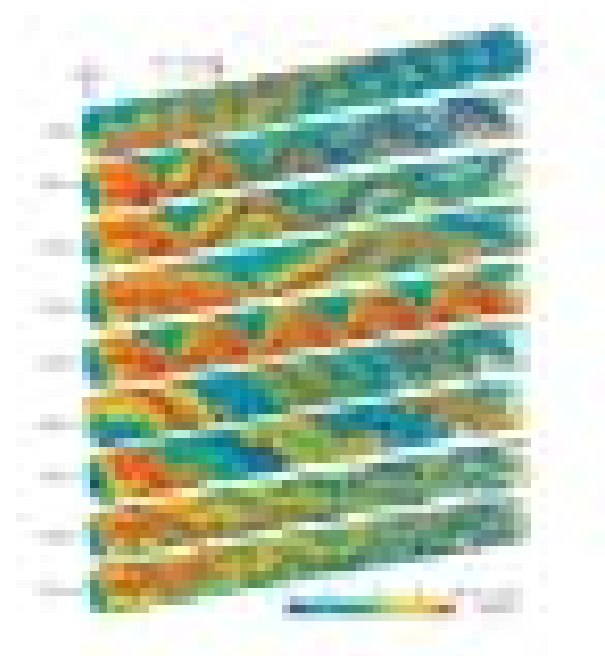


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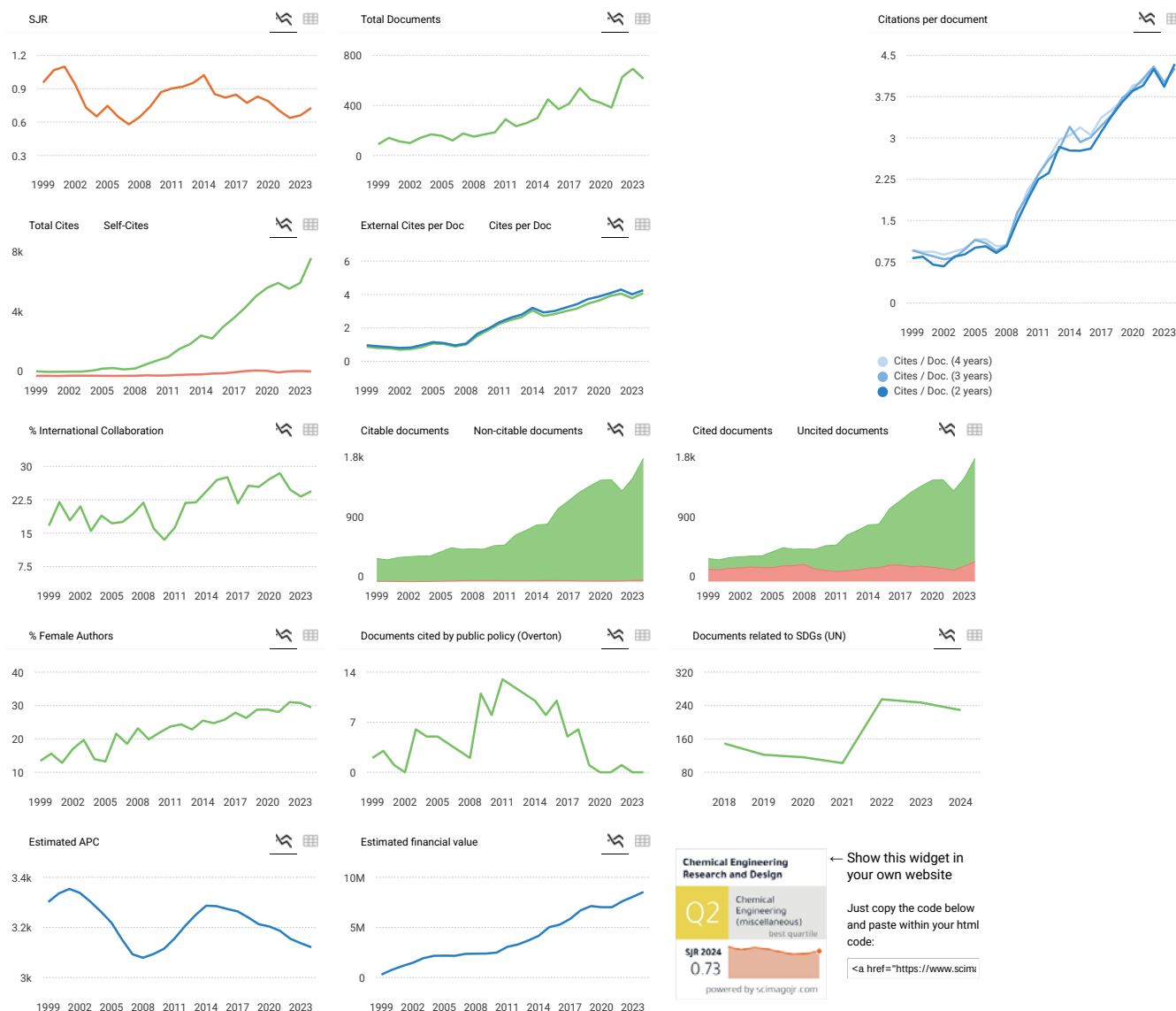
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