A STUDY OF MIXING PERFORMANCE IN A MICROREACTOR USING COMPUTATIONAL FLUIDS DYNAMIC (CFD)

by

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LIST OF ABBREVIATIONS

CFD	Computational Fluid Dynamics
LF	Laminar Flow
PI	Process Intensification
SSIMM	Standard Slit Interdigital Micro Mixer
TDS	Transport of Diluted Species

LIST OF SYMBOLS

c	Concentration	mol/dm^3
D	Diffusion coefficient	m^2/s
D_h	Hydraulic Diameter	m
F	Volume force vector	N/m^3
p	Pressure	Pa
L	Length	m
w	Width	m
h	Height	m
R	Reaction	mol/(m^{3}s)
T	Absolute Temperature	K
v	Velocity	m/s
μ	Dynamic Viscosity	Pa.s
ρ	Density	kg/m^3
V	Volume	m^3
λ	Molecular diameter	m
D	Characteristic dimension	m
μm	Micrometer	
Å	Angstrom	
σ	Variance	
σ_{max}	Maximum variance	
N	Number of sampling point	
I_S	Intensity of segregation	
I_M	Mixing Intensity	

Re	Reynold Number
Pe	Peclet Number
Kn	Knudsen Number

KAJIAN PRESTASI PENCAMPURAN DALAM REAKTOR MIKRO MENGGUNAKAN PENGKOMPUTERAN DINAMIK BENDALIR

ABSTRAK

Bergerak menuju masa depan kejuruteraan kimia yang lebih sebagai tindak balas kepada perubahan keperluan and kehendak, memerlukan keseimbangan antara alam sekitar, keselamatan and kos dalam penghasilan sesuatu produk. Pertumbuhan proses intensifikasi dilihat sebagai satu jalan untuk mencapai matlamat ini. Reaktor mikro merupakan salah satu peranti terintensif yang terhasil daripada proses intensifikasi memerlukan pemahaman tentang ilmu asas supaya ianya boleh digunakan secara menyeluruh. Justeru itu, tujuan kajian ini dilakukan untuk mencirikan percampuran dan menilai prestasi percampuran dalam elemen pencampur milik Standard Slit Interdigital Micro Mixer (SSIMM) dengan konfigurasi saluran mikro yang berbeza. Penyiasatan ke atas kesan konfigurasi saluran mikro, halaju masuk dan pekali resapan terhadap keamatan pencampuran dilakukan dengan menggunakan simulasi pengkomputaran dinamik bendalir (CFD). Keputusan menunjukkan halaju masuk mempunyai kesan yang nyata kepada prestasi pencampuran yang diwakili oleh keamatan pencampuran dalam kajian ini. Halaju yang lebih tinggi menghasilkan kualiti pencampuran yang rendah. Halaju 1000 µm/s dan 10000 µm/s menunjukkan nilai keamatan pencampuran yang rendah dan pencampuran yang rendah di penghujung slit keluar. Pekali resapan yang tinggi menyebabkan proses pencampuran lebih cepat. Pencampuran berlaku serta merta pada pekali resapan $1.0\mathrm{x}10^{-8}$ m^2/s. Profil keamatan pencampuran milik saluran mikro yang beralun yang mewakili elemen pencampur dalam SSIMM menunjuk trend yang licin berbanding dua konfigurasi saluran mikro yang lain.

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ABSTRACT

Moving towards better future of chemical engineering in respond to the changing need and demand requires complementary of environmental, safety and cost in production of a product. The growth of process intensification has found to be the path to achieve this goal. Microreactor is one of the intensified equipment which is a product of process intensification, which requires understanding of the fundamental knowledge in order for it to be fully utilised. Therefore, the purpose of this study is to characterize mixing and to evaluate mixing performance of the Standard Slit Interdigital Micro Mixer (SSIMM) mixing element with different configurations of microchannel. Investigation on the effects of microchannel configurations, inlet velocity and diffusion coefficient toward mixing intensity was conducted using Computational Fluid Dynamics (CFD) simulation. The result showed that inlet velocity has significance effects on the mixing performance which represented by mixing intensity in this study. Higher inlet velocity resulted in lower mixing quality. The inlet velocity of 1000 µm/s and 10000 µm/s give low mixing intensity and incomplete mixing at the end of discharge slit position. High diffusion coefficient value gave faster mixing process. The mixing process occurred instantaneously at diffusion coefficient value of 1.0x 10^{-8} m^2/s.

The mixing intensity profile of corrugated microchannel which represents the mixing element of the SSIMM showed a smooth trend as compared to the other two microchannel configurations.

CHAPTER 1

INTRODUCTION

1.1 Future of Chemical Engineering

Nowadays, chemical and process engineering especially in the area chemical reactor engineering has to respond aptly to the changing need of chemical and related process industries in order to meet the market demands (Jean-Claude 2005; Charpentier 2002; Jean-Claude 2007). Producing high quality of product, at lower cost and at the same time managing the environment and safety issues is paramount and provides challenge in chemical industries. So, being a key to survival in globalization of trade and competition, the evolution of chemical engineering is thus necessary (Jean-Claude 2005).

In the frame of globalization and sustainability, the future of chemical engineering can be summarized by four main objectives: (1) a total multiscale control of the process (or the procedure) to increase selectivity and productivity; (2) a design of novel equipment based on scientific principles and new operation modes and methods of production: process intensification; (3) product design and engineering: manufacturing end-use properties with a special emphasis on complex fluids and solids technology; (4) an implementation of the multiscale and multidisciplinary computational chemical engineering modelling and simulation to real-life situations: from the molecule to the overall complex production scale into the entire production site (Jean-Claude 2005).

Focusing on the second objective, process intensification is a path to make this objective achievable (Jean-Claude 2007).

1.2 Process Intensification

The chemical, pharmaceutical and bio-based industries produce products that are essential for modern society. Nevertheless, these industries face considerable challenges because of the need to develop sustainable production methods for the future (Lutze et al. 2010).

Process intensification technology proposes substantially smaller, cleaner and more energy efficient technology which can be categorically divided into equipment and methods. While cost reduction was the original target for process intensification, it quickly became apparent that there were other important benefits, particularly in respect of improved intrinsic safety, reduced environmental impact and energy consumption. For example, in reducing production plant volume, the toxic and flammable inventories of intensified plant are correspondingly reduced, thereby making a major contribution to intrinsic safety. In addition, the cost of effluent treatment systems will be less, allowing tighter emission standards to be reached economically (Choe et al. 2003).

The high heat and mass transfer coefficients which can be generated in intensified equipment can be exploited to reduce the concentration or temperature driving forces needed to operate energy transformers such as heat pumps, furnaces, electrochemical cells etc. This enhances the equipment's thermodynamic reversibility and hence its energy efficiency (Ramshaw 1999). Process intensification technologies give these goals achievable together with the development of microsystems technology. The intensified equipment has a parallel function as microsystems technology with combination of chemistry which leads to micro process engineering that play important role in providing better future of engineering (Choe et al. 2003).

Microreactor is more commonly known in the field of process intensification and microsystems technology that has attracted significant interest in several years. Numerous plausible advantages of microreactors for the pharmaceutical and fine chemicals industries has been realised, thanks to their excellent capability for mixing and for thermal exchanges which increase yields and selectivity of reactions (Choe et al. 2003; Haverkamp et al. 1999; Lomel et al. 2006; Song et al. 2006).

Microreactors have two major advantages with respect to smaller physical size and the increase in numbers of units. Benefits from reduction of physical size became more apparent in chemical engineering aspects. The difference of physical properties such as temperature, concentration, density or diffusional flux increase with decreasing of linear dimension (Ponce-Ortega et al. 2012; Tsouris & Porcelli 2003). Consequently the driving forces for heat transfer, mass transport increase when using the microreactors. In addition, significant reduction in volume for microreactor as compared to conventional reactors lead to smaller hold up that increase process safety and improves selectivity due to shorter residence time (Ehrfeld et al. 2000; Moulijn et al. 2008).

Parallel units of microreactors in a system could lead to fast and cost saving whilst maintaining the high throughput. An increase in throughput in microreactors is achieved by a numbering-up approach, rather than by scaling-up. The functional unit of a microreactor for example the mixing element is multiply repeated. This technique guarantees that desired features of a basic unit are kept when increasing the total system size (Ehrfeld et al. 1999; Ehrfeld et al. 2000).

1.3 Problem Statement

The exponential increase of research in miniaturization and microfluidic applications highlights the importance of understanding the theory of microfluidic environment and their applications in the context of mixing. Since mixing has a decisive impact on the overall performance of micro reaction processes, there is increased desire for measuring and comparing mixing performance. In recent years, many researches on mixing characterization of T-shaped (Zhendong et al. 2012; Bothe et al. 2006) and Y-shaped (Bhagat et al. 2007; Shi et al. 2012) and other type of micromixers have been done via experimental and computer simulation approaches.

However, little information on simulation study was found with regards to Standard Slit Interdigital Micro Mixer (SSIMM) which is the micromixer used in this work. Comprehensive understanding of fundamental SSIMM is still incomplete and lacking which being agreed upon by several literatures that mentioned fundamental knowledge on the underlying mixing processes in interdigital mixers was so far not broadly accessible (Hessel et al. 2003; Hardt & Schönfeld 2003; Löb et al. 2006). Numerous experimental studies of SSIMM have been done in recent (Ehrfeld et al. 1999; Song et al. 2006; Löb et al. 2006; Haverkamp et al. 1999; Hessel et al. 2003; Panić et al. 2004). Hessel et al, (2003) managed to fabricate rectangular walls in their study to represent the slit-shaped structure which later was simulated by Hardt et al, (2003).

However none of the simulations resemble the geometric structure of mixing element of SSIMM was found in literatures so far. The unique feature of mixing element in SSIMM which has corrugated microchannel configuration has not been fully investigated yet. Owing to this situation, this research took the opportunity to construct the geometry of the mixing element of SSIMM and analysis via computational simulation. Additional geometry configurations were also constructed for the purpose of comparison. Investigation on the effect of inlet velocity, diffusion coefficient and microchannel configurations towards mixing and evaluation of the mixing performance of all the three geometry configurations were also included in this study.

1.4 Research Objective

1. To develop model geometry domain of the Standard Slit Interdigital Micro Mixer (SSIMM) mixing element that consist of corrugated microchannel and discharge slit together with another two geometry configurations.
2. To conduct a Computational Fluid Dynamics mixing simulation of the geometries domain based on mass and momentum conservation and convection-diffusion concept.
3. To evaluate mixing performance at different inlet velocities and diffusion coefficients and make comparison among the geometric configurations.

1.5 Scope of Study

In this work, a model of geometric domain of the Standard Slit Interdigital Micro Mixer (SSIMM) mixing element that consists of microchannel and discharge slit is developed together with another two geometry configurations. Geometric domain model consist of corrugated microchannel to represents the mixing element of

SSIMM with another two geometry configurations namely straight microchannel and T-shaped microchannel.

A Computational Fluid Dynamics mixing simulation of the geometries is conducted. The mixing simulation is based on mass and momentum conservation and convection-diffusion concept. The governing equations for this simulation are Navier Stokes equation and Convective-Diffusion equation. COMSOL Multiphysic software tool is used to simulate this mixing process.

A study of mixing characterization by numerical analysis is done by evaluating the mixing performance of the geometries configurations. Mixing performance is evaluated by mixing intensity in this study. Mixing intensity is calculated in respond to the change of inlet velocity and diffusion coefficient values. Finally, the simulation results are compared among the geometries configurations and literatures.

1.6 Thesis Organization

Chapter 1 describes the general knowledge of process intensification, microreactor and computational fluid dynamics. The research background together with the problem statement, research objective and research summary are also stated in this chapter.

Chapter 2 provides the review on process intensification, microreactor and mixing in microfludic. The literature review also covers types of microreactors with their different geometric configuration and principles of mixing characterization in a microreactor. Brief explanations about the Computational Fluid Dynamics (CFD) are also included.

Chapter 3 provides the methodology of the research which includes the project flow chart, simulation of the microreactor, the physical geometry dimensional and parameters used in this study. The introduction of data collection, verification and validation are also discussed.

Chapter 4 provides brief explanation on Computational Fluid Dynamics (CFD) simulation used in this research. The construction of the computational geometry structure domain and meshing of the micromixer were explained and discussed. The physical models together with the data interpretation are also have been briefly explained in this chapter.

Chapter 5 presents the result and discussion of this research. This chapter consist of four sections of result and discussion including the velocity, concentration and mixing intensity profile of the micromixer together with the comparison of the result.

Chapter 6 presents the conclusion that can be deduced from the research. In additional of recommendation of further improvement of the research are also included.