CFD STUDY ON MIXING PERFORMANCE IN VARIOUS MICROCHANNEL GEOMETRIES

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CFD STUDY ON MIXING PERFORMANCE IN VARIOUS MICROCHANNEL GEOMETRIES

by

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LIST OF ABBREVIATIONS

CFD	Computational Fluid Dynamics
LF	Laminar Flow
PI	Process Intensification
TDS	Transport of Diluted Species

LIST OF SYMBOLS

c	Concentration
D	Diffusion coefficient
D_h	Hydraulic Diameter
F	Volume force vector
I_M	Mixing Intensity
p	Pressure
L	Length
w	Width
h	Height
R	Reaction
Re	Reynold Number
T	Absolute Temperature
v	Velocity
µ	Dynamic Viscosity
ρ	Density
Å	Angstrom

KAJIAN PENGKOMPUTERAN DINAMIK BENDALIR (CFD) PADA PRESTASI PERCAMPURAN DI DALAM PELBAGAI GEOMETRI MIKRO SALURAN

ABSTRAK

Reaktor mikro ialah sebuah elemen dalam proses intensifikasi di mana, peralatan intensif seperti reactor mikro memerlukan pemahaman tentang ilmu asas supaya ianya boleh digunakan secara menyuluruh. Pencampuran dalam reaktor mikro sangat dipengaruhi oleh tingkah laku hidrodinamik dan dengan itu, meningkatkan keperluan untuk mempunyai pandangan mengenainya. Dalam geometri mikro, kesan likat bendalir menjadi dominan, dan aliran mikro biasanya jatuh dalam rejim lamina. Dalam ketiadaan pergolakan, pencampuran bendalir menjadi semata-mata bergantung kepada resapan, yang merupakan proses molekul yang perlahan. Akan tetapi, pencampuran cecair secara cepat dan lengkap adalah sangat penting untuk kebanyakan proses di dalam kejuruteraan kimia, Kualiti pencampuran menentukan prestasi keseluruhan sistem mikrofluidik dan ia adalah masalah yang paling mencabar yang memerlukan penjelajahan lanjut. Dalam kajian ini, bendalir aliran, intensiti pencampuran dan kejatuhan tekanan saluran mikro diselidiki antara bilangan Reynolds (0.1 <Re <120) melalui model tiga dimensi pengkomputeran dinamik bendalir (CFD). Dua aspek saluran mikro, sudut masuk dan jenis alur akan disiasat dalam kajian ini. Keputusannya memberikan beberapa maklumat berkaitan fenomena perpindahan terhadap pencampuran yang terjadi di dalam saluran mikro. Dari segi sudut masuk, saluran berbentuk T menunjukkan pencampuran yang lebih baik daripada saluran Y- dan Anak Panah untuk semua nombor Reynolds yang diuji dan intensiti pencampuran berkurangan dengan peningkatan nombor Reynolds. Dari segi alur, saluran berbentuk T dengan alur ke dalam menunjukkan pencampuran

prestasi yang jauh lebih baik berbanding saluran berbentuk T dan saluran berbentuk T dengan alur ke luar. Ini adalah disebabkan alur masuk yang menyebabkan gangguan aliran dan membentuk sekunder aliran atau vorteks, yang membawa kepada pembesaran ruang antara cecair untuk meningkat penyerapan dan masa pertembungan antara cecair yang menyebabkan kecekapan pencampuran yang lebih besar. Sedangkan pencampuran di saluran T dan saluran T dengan alur keluar berkurangan dengan peningkatan nombor reynolds disebabkan oleh tidak adanya gangguan dalam medan aliran, dengan itu berkuranglah kecekapan pencampuran. Keputusannya juga mendedahkan bahawa penurunan tekanan bergantung sepenuhnya pada nombor Reynolds. Semakin tinggi nombor Reynolds, semakin tinggi kejatuhan tekanan semua saluran mikro, dan saluran berbentuk T dengan alur masuk mempunyai tekanan tertinggi kejatuhan berbanding saluran mikro yang lain.

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ABSTRACT

Microreactor is an element of Process intensification (PI) where intensified equipment such as a microreactor requires the understanding of fundamental knowledge in order for it to be fully utilised. Mixing in microreactor is greatly influenced by its hydrodynamic behaviour and thus, increases the need to have insights on it. In micro-geometries, the fluid viscous effect becomes dominant, and micro-flow typically falls in the laminar regime. In the absence of turbulence, the fluid mixing becomes purely dependent on diffusion, which is a slow molecular process. On the other hand, in many chemical engineering processes, fast and complete mixing of relevant fluids is of crucial importance. The mixing quality may determine the performance of the whole microfluidic system and it is the most challenging problems which needs further exploration. In this work, fluid flow, mixing intensity (I_M) and pressure drop of microchannels were investigated over a range of Reynolds number ($0.1<Re<120$) via three-dimensional Computational Fluid Dynamics (CFD) model. Two aspects of microchannel, inlet angles and types of grooves will be investigated in this research. The results obtained provide some insight of transport phenomena on mixing that occurred in a microchannel. T-shaped channel showed better mixing than Y- and Arrow-shaped channel at all Reynolds number (Re) tested and mixing intensity decreases with an increase of Re. T-shaped channel with inlet grooves showed far better mixing performance compared to T-shaped channel and T-shaped channel with outlet grooves as the I_M for inlet grooves

reached more than 0.8 at all Re tested. This is due to the inlet grooves that causes flow disruption and forms secondary flow or vortices, which led to an enlargement of the fluids interface for increased diffusion and residence time thereby causing greater mixing efficiency. T-channel and T-channel with outlet grooves reached I_M less than 0.4 for Re>10 at the end of the mixing channel due to the absence of disruption in the flow field, thereby decreasing the mixing efficiency. In terms of time scale evaluation, diffusion is dominant at Re = 0.1 where the residence time is 3s and complete mixing is achieved for all the geometries. Compared to Re = 120 where the residence time is 0.0025s, advection is dominant and complete mixing only achieved in T-shaped channel with inlet grooves. The results also revealed that pressure drop is totally dependent on Re. The higher the Re, the higher the pressure drop for all micro channels, and T-shaped channel with inlet grooves exhibit the highest pressure drop compared to the other microchannels.

CHAPTER ONE

INTRODUCTION

1.1 Chemical Engineering Challenges

The chemical engineering field encounters many challenges in today's changing world. In United States (U.S.) for an example, almost 14 thousand chemical industries manufactures transform raw materials into more than 70,000 compounds, which are used to produce daily basis products, including plastics, paper, paints, cleaners, adhesives, pharmaceuticals, cosmetics, textiles, building materials, food packaging, appliances, and electronic devices. As presented in Figure 1.1, the conversion of raw materials to commodity chemicals, then to intermediates which span various sectors of the U.S. economy in areas of textiles, safe food supply, transportation, housing, recreation, communications, and health and hygiene products and goods (PNNL, NRE 2004).

Huge amount of energy supply is needed to run those chemical industries which consequently increase the pollution to the environment and operating cost. Thus, the need for environmental friendly and cost effective processes is very significant as the chemical industries are growing larger and larger by days. World issues such as the greenhouse effect and the supply of energy are moving the industry towards more efficient processes in terms of energy, cost and raw material consumption. Process intensification which offers potential benefits to the future of chemical engineering by increasing transfer rate and safety resulting from low hold-ups has found to be the path to overcome those issues.

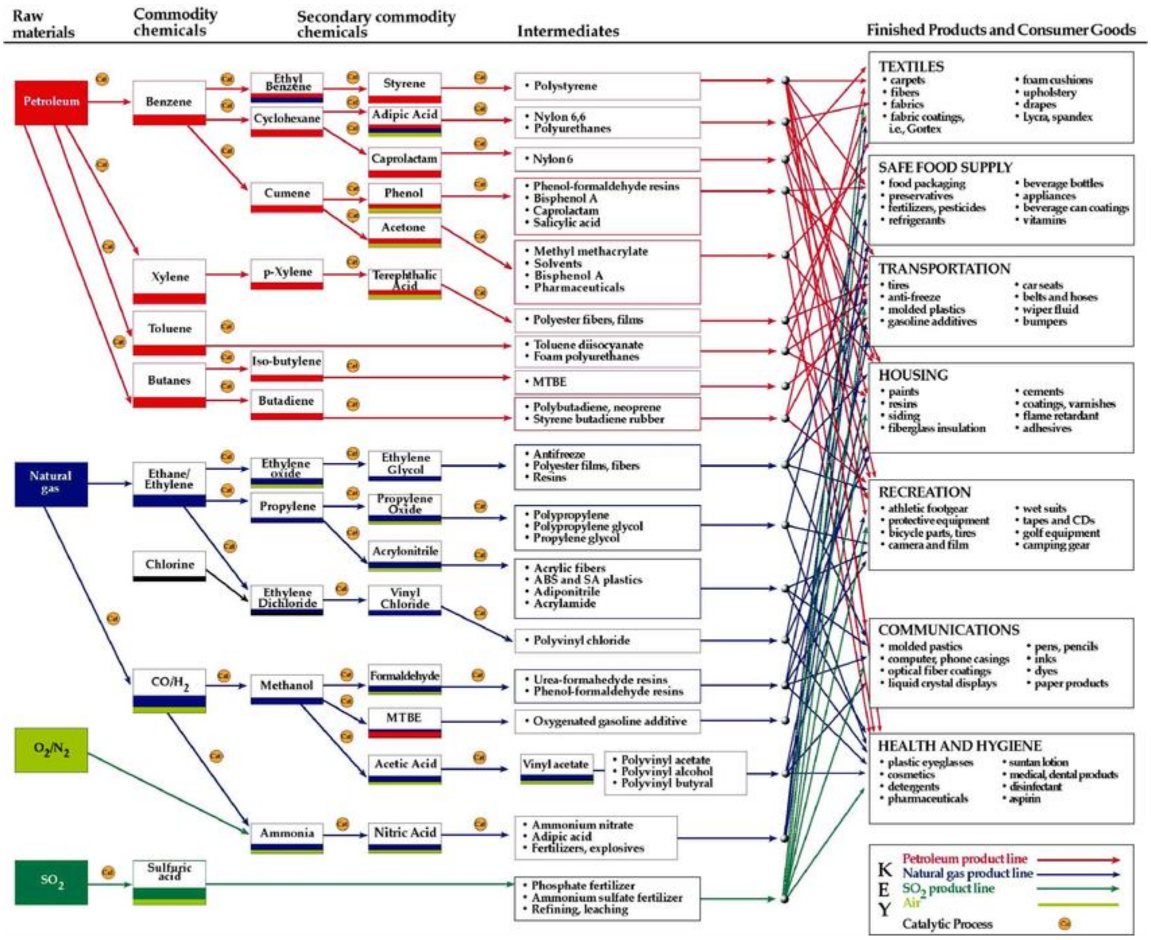

Figure 1.1: Chemical manufacturing pathways (PNNL, NRE 2004)

1.2 Process Intensification

Process intensification is a concept proposed to improve chemical processing by decreasing the ratio of equipment size to production capacity, energy consumption and waste production (Ehrfeld et al. 2000). For example, size of unit operations decreases, thus enhancing heat and mass transfer which in turn improves the process and intrinsic safety. Together, the cost of waste treatment systems also will be reduced. In addition, energy efficiency can be enhanced by the utilization of high heat and mass transfer coefficients generated by the intensified equipment (Ramshaw 1999). It can be used to reduce the concentration or temperature driving forces needed to operate energy transformers such as heat pumps and furnaces. As a result, compact, clean, cheaper, safe, environmental friendly, and energy efficient technology can be achieved (Ehrfeld et al. 2000). Process intensification technologies make these goals feasible together with the evolution of micro systems technology. Micro reactors are an example product of merging both technologies, which are the process intensification technologies and micro systems technology.

1.2.1 Micro Reactor

A micro reactor or micro structured reactor or micro channel reactor is a device in which chemical reactions take place in a confinement with typical lateral dimensions below 1 mm; the most typical form of such confinement are micro channels (Arbor & Brakel 2002). Some of the applications using micro channel reactors are the production of chemicals such as vinyl acetate, acrylonitrile, ethylene oxide and acrylic acid through partial oxidation reactions. Micro reactors are also used for syngas and biodiesel production using biogas reforming processes and Fischer-Tropsch synthesis, respectively. Furthermore, it is also used for production of H_2O_2 (Gokhale et al. 2005). Owing to the small dimensions of micro reactors compared to macroscopic devices, micro reactors have a very high surface to volume ratio, which accelerate the rate of reactions. Process safety is another beneficial outcome of miniaturized equipment. This is due to the small amount of chemicals releases and could be controlled easily if micro reactors were to fail or an exothermic runaway reaction occurred. Furthermore, a lesser amount of waste produced due to the small amount of chemicals used in the micro reactors is also environmentally friendly (Arbor & Brakel 2002).

Replication of micro reactors used in laboratory for scaling-up to production would remove expensive design as only one engineering sequence would be required. By numbering-up approach, failed units can be changed easily without interfering with other equipment, which is both a maintenance and economic advantage (Arbor & Brakel 2002). This method guarantees that desired configurations of a basic unit are secured when increasing the whole system size (Ehrfeld et al. 2000). The most imperative of these categories is the taking of the numbering-up approach rather than scaling up approach which recently increased the attention worldwide for its simplicity, less costly reproduction and assembly (See Figure 1.2).

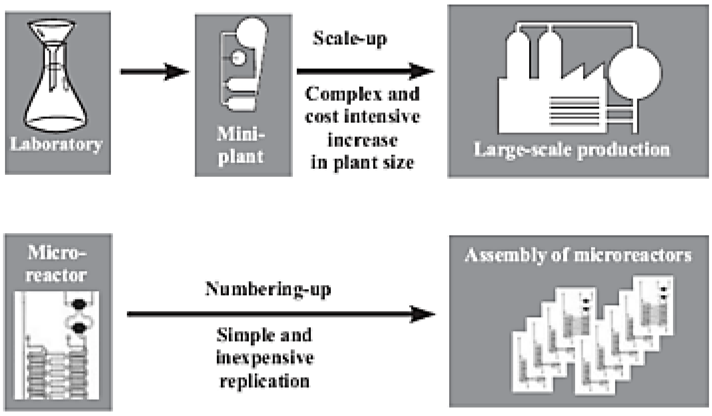

Figure 1.2: Simplified scheme illustrating scale-up versus numbering-up strategies (Ehrfeld et al. 2000)

The promising advantages of micro reactor are deniable. Therefore, the process inside the micro reactor also must be taken into account in order to produce valuable products. The system in the micro reactor which deals with fluids is called microfluidic. The microfluidic system determines the performance of the whole micro reactor system because it is the platform where chemical reactions take place.

1.2.2 Microfluidic system

Microfluidics is the term that is used to describe flow in devices having dimensions ranging from millimeters to micrometers such as micro reactors and capable of handling volumes of fluid in the range of nano- to microliters (10^{-9} – 10^{-6} l) (Ottino & Wiggins 2004). Microfluidic system has received recent attention as the increased availability of fabrication methods and integrated flow configurations have made it more readily accessible. It is designed to exploit the fluid mechanics of laminar flows in small geometries, reducing the cost, time, and infrastructure needed in comparison to macroscale geometries (Bhagirath Chawan et al. 2013). However, laminar flows make mixing particularly difficult for the effective functioning of microfluidic devices, because of their low Reynolds numbers (Jeon & Shin 2009).

1.3 Problem Statement

The exponential increase of research in microfluidic applications highlights the importance of understanding the theory of microfluidic environment and their applications in the context of mixing. Since mixing has a significant 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 straight T-shaped (Zhendong et al. 2012), T-shaped with wavy mixing channel (Afzal & Kim 2014), T-shaped channel with obstruction (Alam et al. 2014) and other type of T-shaped channel micro mixers has been studied via experimental and computer simulation approaches.

However, little information on both experimental and simulation study was found with regards to T-shaped micro channel or other inlet-shaped micro channel with inlet and outlet grooves which is the main interest in this work. Comprehensive understanding of grooves micro channel based on mixing characterization in precise geometry coupled with fine CFD simulations in micro channels is still lacking.

Furthermore, none of the simulations resemble the direct comparison of geometry structure of T-shaped micro channels with inlet and outlet grooves were found in literatures so far. Owing to this situation, this research took the opportunity to construct the geometry and analysis via simulation to get clearer understanding on the flow dynamics occurred in the micro channel with grooves. For comparison purpose, investigation on the effect of micro channel configurations and Reynolds number towards mixing and pressure drop in the micro channels were also included in this study.

1.4 Research Objective

i. To develop different geometry configurations using Comsol Multiphysics software.
ii. To evaluate flow, mixing and pressure drop in each microchannel geometry configuration over a range of Reynolds number.
iii. To determine the best geometry configuration for better fluid mixing.

1.5 Scope of study

The scope of the current research project is focusing on the mixing performance study of micro channel reactors. Our strategy is to compare different configuration of micro channels based on different inlet angles (T, Y and Arrow) and type of grooves (inlet and outlet). The hypothesis of this study is, difference Reynolds number (Re) will results in different flow regimes, mixing lengths, mixing time, mixing qualities and pressure drops based on the different micro channels configuration.

The range of Re studied is from 0.1 to 120 chosen based on various researches previously conducted in CFD for micro channel reactor related work. Comsol Multiphysics software was used for the entire research work from the development of geometries to the result analysis. Direct solver was used to solve the simulation work. The effect of geometry configurations towards mixing performance in microchannel was conducted based on the five geometries chosen; T-shaped micro channel, Y-shaped micro channel, Arrow-shaped micro channel, T-shaped micro channel with inlet grooves and T-shaped micro channel with outlet grooves. The cross section of the channels is a square with 0.1mm side length and the whole length of the mixing channel is 3mm. Every channel was meshed with fine type of mesh. The mixing performance evaluation is based on the results obtained from the simulation which are velocity profile, velocity streamline and concentration profile. Further analysis of the result is the evaluation of the value of mixing intensity, mixing time and pressure drop. Finally, the best geometry is chosen from the overall evaluation.