Numerical Simulation of Fluid Mixing in the Ribbed Microchannels

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ABSTRACT
Micromixers have received much interest as essential part of microfluidic devices. Therefore, enhancement of mixing quality has gained a lot of attention in recent years. In the present study, improvement of mixing quality for two different miscible liquids is considered in passive micromixers. Numerical approach is based on a second order finite volume Jameson scheme in order to solve two dimensional incompressible Navier-Stocks and mass transport equations by implementing artificial compressibility. Mixing quality is influenced by Reynolds and Schmitt numbers as well as size and location of the ribs. Diffusion mechanism has the main role for mixing in micro scale fluid flows; therefore, increasing Peclet number leads to extend mixing time. In order to enhance mixing quality, ribs are used in different locations through the microchannel which cause more instability in the fluid flow and leads to a better mixing. The Reynolds number is constant while the Schmitt number is in the range of 10 to 100. However, in order to laminar fluid flow, ribs just have an influence near itself and faraway, mixing mechanism return to earlier state. Therefore, in low Reynolds numbers they have no effective influence. When Reynolds number increase, flow instability that is created by different ribs leads to a better mixing.

INTRODUCTION
The importance of microfluidic and nanofluidic devices has increased in the recent years. In order to complicate and costly construction of devices in the small scales, need to modeling and simulation of phenomena before construction is appeared necessary. Microfluidic devices have diverse parts which do special task. Micromixers play a significant role in micro chemical processing and are employed in a multitude of tasks, including blending, emulsification and suspension, as well as for chemical reaction and also in combination with integrated heat exchangers. Due to the small dimensions of the microchannels, the flow is mostly laminar and mixing is therefore limited by molecular diffusion. Some biological analysis requires to be completely mixed before the reaction has carried out considerably; therefore, simulation and optimization of micromixer with minimum mixing time or length before construction is necessitated.

Due to the relatively young age of microreactor engineering, common design rules for micromixers have not yet been developed. However, one can see that apart from their minute size, microreactors are just continuous laminar flow reactors, which suggests that design approaches for mixing in microchannels could be dealt with in a similar manner to that of laminar mixing in macro scale pipe flow. In the laminar flow, the streamlines are parallel and there is no convective mixing in the radial or tangential directions. Thus in order to disturb the flow and facilitate mixing in laminar pipeline flow, in-line devices or static mixers is inserted into the microchannel. The design of micromixers, which are comparatively similar devices at a much smaller scale, can be looked at in the same manner, whereby the aim is to provide sufficient spatial and temporal mixing as fast as possible.

Over the past few years, several studies using different types of micromixers have been performed with the focus on characterizing the micromixer performance using various experimental techniques, such as fluorescent microscopy and special chemical reactions, as well as computational fluid dynamic simulations to draw species trajectories [1-7].

In the present work, numerical simulation of fluid mixing in the two dimensional micromixers using finite volume Jameson scheme is investigated. Therefore, two dimensional Navier-Stocks equations are solved by applying artificial
compressibility method to couple continuity with momentum equations. In order to disturb flow field to increase mixing quality, ribs are added to different location of the microchannel.

**NOMENCLATURE**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>Coordinates along microchannel length ($\mu m$)</td>
</tr>
<tr>
<td>y</td>
<td>Coordinates along microchannel width ($\mu m$)</td>
</tr>
<tr>
<td>t</td>
<td>Time (s)</td>
</tr>
<tr>
<td>V</td>
<td>Velocity vector (m/s)</td>
</tr>
<tr>
<td>u</td>
<td>Velocity in x – direction (m/s)</td>
</tr>
<tr>
<td>v</td>
<td>Velocity in y – direction (m/s)</td>
</tr>
<tr>
<td>p</td>
<td>Pressure (kPa)</td>
</tr>
<tr>
<td>m</td>
<td>Mass fraction</td>
</tr>
<tr>
<td>h</td>
<td>Microchannel width ($\mu m$)</td>
</tr>
<tr>
<td>L</td>
<td>Microchannel Length ($\mu m$)</td>
</tr>
<tr>
<td>m̅</td>
<td>Mean mass fraction</td>
</tr>
<tr>
<td>a</td>
<td>Artificial velocity (m/s)</td>
</tr>
<tr>
<td>G</td>
<td>Mass flux ($kg/m^2 s$)</td>
</tr>
<tr>
<td>D</td>
<td>Diffusion coefficient ($m^2/s$)</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>Sc</td>
<td>Schmidt number</td>
</tr>
<tr>
<td>Pe</td>
<td>Peclet number</td>
</tr>
<tr>
<td>Kn</td>
<td>Knudsen number</td>
</tr>
<tr>
<td>l_s</td>
<td>Intensity of segregation</td>
</tr>
<tr>
<td>l_m</td>
<td>Intensity of mixing</td>
</tr>
</tbody>
</table>

**Greek Symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nabla$</td>
<td>Gradient ($\mu m$)</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Viscosity (Pa·s)</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density ($kg/m^3$)</td>
</tr>
<tr>
<td>$\rho^*$</td>
<td>Artificial density ($kg/m^3$)</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Artificial compressibility factor ($m^2/s^2$)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Mass fraction variance</td>
</tr>
</tbody>
</table>

**Subscript and superscript**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>j</td>
<td>Species</td>
</tr>
<tr>
<td>n</td>
<td>Number of species</td>
</tr>
<tr>
<td>*</td>
<td>Nondimensional variable</td>
</tr>
<tr>
<td>wall</td>
<td>Wall</td>
</tr>
<tr>
<td>max</td>
<td>Maximum value</td>
</tr>
</tbody>
</table>

**MICROCHANNEL GEOMETRY**

Figure 1 illustrates the microchannel geometry with different locations of the ribs.

Two fluids enter to the microchannel from two separate and parallel entrances. Two ribs with one-fifth height of microchannel width are located in the different places. The real width and height of microchannel are,

$$h = 100 \mu m,$$
$$L = 2000 \mu m$$

**GOVERNING EQUATIONS**

To simulate mixing in the ribbed microchannels, following assumptions are used:

- Laminar flow
- Two dimensional Steady State
- Incompressible fluids
- Binary mixture

To simulate mixing phenomena, flow field must be solved simultaneously with mass transport equations of each species. Continuity and momentum equations are decoupled; therefore, they must be related by using a suitable method. One of the most appropriate ways is to use artificial compressibility [8].
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0
\]

In which, \( \rho \) is artificial density that relate to pressure by artificial velocity using artificial state equation.

\[
\frac{\partial p}{\partial t} = \beta \nabla \cdot (\rho V) = 0
\]  

Where, \( \beta \) is artificial compressibility factor that varies between 0.1 to 10. Therefore, continuity become as follows that is related to momentum equation by time derivative of pressure.

\[
\frac{\partial \rho V}{\partial t} + (V \cdot \nabla) \rho V = -\nabla p + \nabla (\mu \nabla V)
\]

Mass fraction is defined as a fraction of mass of species to mixture mass, \( m_j = \rho_j / \rho \); therefore, in the binary system,

\[
\sum_{j=1}^{n} m_j = 1 \Rightarrow m_1 + m_2 = 1
\]

By using Fick's low, mass flux in the binary system is,

\[
G_{\text{diff}} = -\rho D \nabla m
\]

It means that diffusive flux operates in the opposite direction of mass fraction gradient. Therefore, mass transport equations become [9],

\[
\frac{\partial \rho m_j}{\partial t} + \nabla \cdot (\rho m_j V) = D \nabla \cdot (\rho \nabla m_j)
\]

Governing equations must be solved simultaneously in time to reach steady state. Mixture properties are depended on place; thus, physical properties should be computed at each time step by means of mass fractions.

\[
\rho = \sum_{j=1}^{n} m_j \rho_j, \quad n = 1,2
\]

\[
\mu = \sum_{j=1}^{n} m_j \mu_j, \quad n = 1,2
\]

By using mean physical properties of mixture, mean entrance velocity and Microchannel width and defining,

\[
V^* = \frac{V}{h}, \quad t^* = \frac{u}{h}, \quad \rho^* = \frac{\rho}{\bar{\rho}}, \quad \mu^* = \frac{\mu}{\bar{\mu}}
\]

\[
I_s = \frac{\sigma^2}{\sigma_{\text{max}}}
\]

Where mean values are,

\[
\bar{\rho} = \frac{1}{n} \sum_{j=1}^{n} \rho_j, \quad \bar{\mu} = \frac{1}{n} \sum_{j=1}^{n} \mu_j, \quad \bar{u} = \frac{1}{n} \sum_{j=1}^{n} u_j
\]

Nondimensional governing equations by eliminating star are obtained as follows,

Continuity equation:

\[
\frac{\partial \rho}{\partial t} + \beta \nabla \cdot (\rho V) = 0,
\]

Momentum equations:

\[
\frac{\partial \rho V}{\partial t} + (V \cdot \nabla) \rho V = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot (\mu \nabla V),
\]

And mass transport equations:

\[
\frac{\partial \rho m_j}{\partial t} + \nabla \cdot (\rho m_j V) = \frac{1}{\text{Pe}} \nabla \cdot (\rho \nabla m_j)
\]

These equations must be solved by proper boundary conditions. In order to small Knudsen number which is defined by fraction of mean free path to width of microchannel, no slip boundary condition for velocity can be utilized on the walls. By using characteristic method, boundary conditions at the inlet and outlet are obtained. In low Reynolds numbers, velocity field in the inlet and pressure field at the outlet should be assumed. Also, mass fraction is known in the inlet and in the absence of blowing, suction and chemical reaction, mass flux at the wall becomes,

\[
G_{\text{wall}} = -\rho D \nabla m_j = 0
\]

**INTENSITY OF MIXING**

To consider micromixer efficiency, diverse methods exist which two of them are:

1. Mass fraction profile

Mass fraction profile illustrates mass fraction variations in microchannel cross section. Value of zero shows mass nonentity and value one illustrates that whole of the cell is filled by certain species.

2. Intensity of mixing

A common definition of the mixing quality is based on the Danckwert’s intensity of segregation [10] that defined by,
\[
\sigma_s^2 = \frac{1}{\nu} \int_V (m - \overline{m})^2 dV \tag{18}
\]

Where, \( \sigma_s^2 \) is the maximum possible variance. Unfortunately, there is no general definition for \( \sigma_s^2 \). But, for the binary systems, it can be defined as,

\[
\sigma_{\text{max}}^2 = \overline{m}(1 - \overline{m}) \tag{19}
\]

Since it varies with time and space, it cannot be used for defining a mixing time or a mixing length. In this case, the variance at the initial time or at the entrance can be utilized.

Based on the Danckwert's intensity of segregation, a measure for the intensity of mixing \[3\] can be deduced as follows,

\[
I_m = 1 - \sqrt{\overline{I_s}} = 1 - \frac{\sigma}{\sigma_{\text{max}}} \tag{20}
\]

Where, \( I_m \) reaches value of 1 for homogenous mixture and it becomes zero for segregated mixture.

**NUMERICAL SIMULATION**

Finite volume Jameson method is utilized to simulate fluid flow and mixing in the ribbed microchannel. In order to couple pressure to other conservative variables in incompressible flow, artificial compressibility is added to the continuity equation then unsteady governing equations should be solved over time to reach steady state. In the case of variant properties of binary mixture governing equation should be solved simultaneously; however, in the case of constant mixture properties, conservative equation of each species can be solved after fluid flow equations \[11\].

In this investigation after solving fluid flow and mass transport equations, intensity of mixing is computed for different cases along microchannel which can be used to compare mixing of two fluids.

**GRID INDEPENDENCY**

To consider the effect of the grid size on the results, the grid was verified to result in grid-independent results. For instance, mass fraction profiles are calculated for case (c) at \( \text{Re} = 50 \) and \( \text{Sc} = 10 \). Grid sizes of \( 31 \times 200 \), \( 41 \times 275 \) and \( 51 \times 300 \). This grid-independence is illustrated graphically in Figure 2. Therefore, the intermediate grid \( (41 \times 275) \) was chosen.

**COMPARISON OF VARIANT AND CONSTANT PROPERTIES SOLUTION**

To consider influence of mixture properties on flow fiel, simulation is performed for straight channel for binary mixtures with constant and variant physical properties.

Three pair fluids are picked that their properties are shown in Table 1 and Table 2 \[9\].

<table>
<thead>
<tr>
<th>Mixture</th>
<th>Schmidt number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water &amp; HCl</td>
<td>381</td>
</tr>
<tr>
<td>Water &amp; Ethyl alcohol</td>
<td>1005</td>
</tr>
</tbody>
</table>

**Table 1- Two pair Fluid**

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Density ( (\text{kg/m}^3) )</th>
<th>Viscosity ( (\text{Pa.s}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>998</td>
<td>( 1.002 \times 10^{-3} )</td>
</tr>
<tr>
<td>HCl</td>
<td>1180</td>
<td>( 1.9 \times 10^{-3} )</td>
</tr>
<tr>
<td>Ethyl alcohol</td>
<td>772</td>
<td>( 1.53 \times 10^{-3} )</td>
</tr>
</tbody>
</table>

**Table 2- Physical properties**

Velocity profiles for variant physical properties are shown as dashed lines in Figure 3.
Because the values of fluids properties are close together, their velocity profiles are similar to constant properties mixture ones. Thus, mixing of variant properties are close to constant properties ones, so to simulate fluid mixing in the ribbed microchannels constant properties of binary mixture is assumed. Simulation is performed for constant Reynolds number and two Schmidt numbers for each.

RESULTS AND DISCUSSIONS

Velocity vectors and streamlines in the straight microchannel are shown in Figure 4.

Velocity vectors and streamlines in each case near the ribs location are shown in Figure 5. Vortices are formed after each rib which helps to increase mixing of two fluids.

In addition to velocity vectors and streamlines, vortices are formed which affect mixing quality of two fluids.

Pressure drop in each case is shown in Figure 6. It is clear that for microchannel with ribs on the walls, pressure drop is less than other conditions.
To compare circumstance of mixing in the different geometries, mass fraction contours of fluid that enters from upper entrance is shown in Figure 7 (a), (b) in the case of \(Re = 50\) and \(Sc = 10, 100\).

Figure 7(a)- Mass fraction contours of upper fluid in the case of \(Re = 50\) and \(Sc = 10\)

Figure 7(b)- Mass fraction contours of upper fluid in the case of \(Re = 50\) and \(Sc = 100\).

Mass fraction profiles of upper fluid are illustrated for \(Re = 50\) and \(Sc = 10\) in Figure 8.

Figure 8- Mass fraction profiles of upper fluid at the outlet for \(Re = 50\) and \(Sc = 10\)

In order to high diffusivity of two fluids in each other, mixing quality in the outlet of the microchannel are similar. Also, Mass fraction profiles of upper fluid are illustrated for \(Re = 50\) and \(Sc = 100\) in Figure 9.

Figure 9- Mass fraction profile of upper fluid at the outlet for \(Re = 50\) and \(Sc = 100\)

Intensity of mixing in \(Re = 50\) and \(Sc = 10, 100\) is shown in Figure 10 and Figure 11.

Main effect of ribs especially center ribs expect to be seen in near the ribs region and by going away from these regions the effect of the ribs are going to be neglected. Thus, the center ribs cause a jump in the intensity of the mixing which is illustrated in Figure 10 and 11. This phenomenon happens because of formation of the vortices beyond the ribs and decreasing the velocity that leads to increase molecular diffusion.
CONCLUSION

Flow field and mixing of binary mixture is simulated by using finite volume Jameson scheme with artificial compressibility. Variant properties mixture is compared with constant properties mixture in the straight channel that shows if physical properties of two fluids are close together then constant properties assumption is reliable. Simulation is performed for straight and ribbed microchannels. Pressure drop and velocity vectors are shown in related diagrams. Also, Intensity of mixing diagrams are illustrated for $Re = 50$ and $Sc = 100$.

In the cases (b and c) using ribbed microchannel lead to decreasing intensity of mixing in location of the ribs, because velocity are increasing and diffusion is reducing. After rib symmetry of flow is ruined so mixing quality based on diffusion raise up. In the cases (d and e) take advantages of ribs lead to peak severely because vortices are formed behind the ribs which lead to increasing diffusion of two fluids in each other. In spite of all these facts, after the ribs because the flow regime is laminar, intensity of mixing is dropped suddenly.

Comparison of all cases shows that intensity of mixing in different ribbed channel is tend to be the same at the outlet of the microchannel; however, locating ribs at the middle of microchannel cause to higher pressure drop along the microchannel.

Finally, it is clear that inserting the ribs in the microchannel in the low Reynolds numbers is not appropriate method to enhance intensity of mixing; however, in higher Reynolds numbers, ribs can disturb flow field and instability creation causes better mixing.

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