A CFD Investigation of Mixing Profiles within a Micro-Coiled Flow Inverter

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Abstract

Background/Objectives: Due to the low Reynolds number (Re) in microfluidic domain, the predominant laminar flow might inhibit effective mixing in micro-Coiled Flow Inverter (mCFI). Fluid dynamics within the mCFI was simulated with Computational Fluid Dynamics (CFD) software to investigate the mixing profile. Methods/Statistical Analysis: Fluid flow was simulated with the software FLUENT with Species Transport (ST) setting, to replicate the mixing of two water bodies. Geometry of the mCFI was designed with a tubing diameter of 0.5 mm and curvature ratio of $\lambda = 10$. Fluid flow rate was adjusted to attain $25 \leq \text{Re} \leq 250$. Findings: A mixing time of 0.59s was achieved with Re=250. However complete mixing was still achievable even in Re=25 albeit with a longer mixing time. Application/Improvements: Flow inversion is improved the mixing condition in micro-structured tubing, in enhancement of the diffusive mixing in microfluidics.

Keywords: Flow Inversion and Computational Fluid Dynamics (CFD), Micro-Coiled Flow Inverter (mCFI), Reynolds Number

1. Introduction

Coiled Flow Inverter (CFI) is an existing tubing configuration proved to improve mixing¹ and thermal distribution² through the formation of secondary flow within a fluid domain. Fluid flow in a coiled tube succumbs to a centrifugal force that acts outwards from the centre of curvature³. However, there exist confined regions which fluid resume laminar flow and can only escape through diffusion. CFI is constructed based on the principle of complete flow inversion. The geometry of a CFI consists of 90 degree bends at equal intervals of length in coiled tube geometry, designed to induce Dean vortices rotating corresponding to the 90 bending ⁴. CFI has already been proven as an efficient device for mixing of two liquid in the process industry⁵. Through an investigation of the velocity field and scalar concentration distribution of liquid in CFI, it was concluded that CFI exhibited significant increase in mixing of two liquid as compared to a straight tube and helical mixing element.

In recent years, CFI has been scaled down to micro-dimensions as a three-dimensional microfluidic device for process intensification⁶, highlighting its main potential as a micro heat exchanger. Micro-Coiled Flow Inverter (MCFI) was constructed from tubing with internal diameter of equal or less than 1 mm. Results showed that MCFI offers higher thermal merit, with up to 4 fold heat transfer enhancement as compared to straight tube with similar heat transfer area, achievable through a precise adjustment of the Reynolds number and Prandtl number. The heat transfer coefficient was increased by 38.5% as compared to micro helical coil. Characterization of residence time distribution curve from different MCFI reactor setup also found that the shape of the reactor had negligible effect on the axial dispersion⁷. Hence, MCFI structures can be fabricated with specific considerations in place requirement or field application.

MCFI has also been applied in a liquid-liquid extraction system along with other capillary setups for single-stage extraction, implemented through the generation of slug flow⁸. MCFI presented high extraction efficiencies in an n-butyl acetate/acetone/water test system of up to 20% in comparison to straight capillaries, as the dean vortices in slug flow patterns provided enhanced liquid-liquid mass transfer.

Due to the low Reynolds number (Re) in micro-
channels, the predominant laminar flow might inhibit effective mixing in MCFI. Mixing within a microfluidic domain depends solely on molecular diffusion to achieve a uniform spatial distribution in solute concentrations. To date, the mixing profile of two miscible liquid in a MCFI has not been reported. In the present work, a Computational Fluid Dynamics (CFD) study performed in tubing with circular cross-section and it is constructed into a MCFI to examine the mixing of two miscible fluids under laminar flow conditions.

2. Materials and Methods

CFD analysis was carried out with the software FLUENT in ANSYS 15 to examine the feasibility and mixing efficiency of the MCFI operations. In this study, a liquid-liquid flow system of water-based dyes was considered and it was let to interface in the MCFI.

Assuming the fluid properties of the dye were negligible as a result of dilution, the simulation was carried out with the properties of liquid water.

2.1 Governing Equations

Species Transport model (ST) model was used to solve the conservation equations for chemical species. This model predicts the local mass fraction of each species by solving the convection-diffusion equation for the \( i \)th species.

Conservation equation:

\[
\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{j}_i + R_i + S_i
\]  

(1)

Where the letters \( \rho, Y, \vec{v}, \vec{j}, R \) and \( S \) indicates respectively the density, local mass fraction of species, velocity vector, diffusion flux of species, the net rate of production of species \( I \) by chemical reaction and the rate of creation by addition from the dispersed phase. Suffix \( i \) refers to each separate species.

In this study, the liquid-liquid laminar mixing of dyes was non-reactive as no consumption or production of any species was involved. Thus, species transport was dominated by mass diffusion due to the diffusion flux, \( \vec{j} \) due to concentration and temperature gradient. The modelling of mass diffusion was achieved utilizing Ficks Law, i.e. the dilute approximation method.

Diffusion flux:

\[
\vec{j}_I = -\rho D_{I,m} \nabla Y_I - D_{I,T} \frac{\nabla T}{T}
\]

Where \( D_{I,m} \) is the mass diffusion coefficient for species \( I \) in the mixture and \( D_{I,T} \) is the thermal diffusion coefficient.

2.2 Geometry Design

MCFI geometry was constructed with the software SolidWorks, consisting of four straight coils connected in subsequence with 90 degree bends in between as shown in Figure 1. The inner tubing diameter (\( d_i \)) is 0.5mm and the loop diameter (\( D_c \)) of 5mm, which corresponded to a curvature ratio of 10.

The curvature ratio (\( \lambda \)) is the ratio of \( D_c \) over \( d_i \). As the \( \lambda \) of current MCFI was fixed, different values of Re were achieved through an adjustment of flow rate. The small diameter of the MCFI tube led to laminar flow as the Re values were well in the laminar region.

2.3 Grid System

Model equations were applied to a non-uniform, unstructured grid topology for computations. Three different mesh sizes constructed from hexahedral cells were generated with the Mesh component in the ANSYS workbench as shown in Figure 2. The number was varied by the maximum face size.

Figure 1. Geometry design of MCFI with \( \lambda = 10 \).

Figure 2. Cross-section grid topology at the MCFI inlet, extended throughout the geometry.
Grid independence was checked for the pressure drop within the MCFI. Table 1 presents a comparison of the predicted results at different grid size for a fully developed laminar fluid in coiled tube. At a mesh size of 514 x 2869 (cross section x axial) elements, solution convergence was observed.

| Cell density          | Pressure drop (kPa) |
|-----------------------|---------------------|
| 324 x 2869            | 1.732               |
| 514 x 2869            | 1.743               |
| 514 x 4782            | 1.743               |

### 3. Results and Discussion

As a lack of data on mixing profile in a MCFI persists, the velocity profile at different bends was generated with the present computational method and compared to results of available literature for validation. Fluid flow was simulated in MCFI with Re=434, d=0.5 mm and λ=10. Predicted results of the horizontal and vertical centreline in Figure 3 are showed. The good agreement with the numerically computed results is reported in literature.

3.1 Velocity Profile

Laminar flow in a circular cross-section tube exhibits a parabolic velocity profile. Figure 4 shows the velocity profile within the MCFI for fluid flow with three increasing Re value. For Re=25, the velocity profile was parabolic with a maximum velocity at the middle of the tube without noticeable rotation after 90° bends.

![Figure 4. Velocity profile for fluid flow in MCFI.](image)

As the Re increased to Re=125, the velocity profile skewed according to the coil configuration, rotating 90° from arm n=1 to n=4 of the MCFI. The region of maximum velocity gradually moved towards the outer wall of the tube. For Re=250, the shape of the region of maximum velocity had stretched slightly sideward and orientate along the curvature of the wall.

3.2 Visualisation of Fluid Flow

ST simulation was initialized with half of the inlet as the entry for the red dye and half the inlet as the entry for the blue dye. Mixing of the fluids caused the mass fraction value of dyes to decrease.

Figure 5 shows the visualisation of fluid flow within the MCFI. It can be observed that throughout the helical coil (first half loop φ=180°, full loop φ=360°), a secondary flow was exerted on the fluid such that fluid with low velocity near the outer wall moves along the upper and lower halves while fluid far from the wall with high velocity moves to the outer wall. After each 90° bend,
the secondary flow rotated in accordance to the velocity profile.

3.3 Mixing Profile

Ideal mixing was indicated by a mass fraction of 0.5 signifying that a cell contained equal parts of red dye and blue dye. Through an evaluation of the tube cross-section, the percentage of cells that achieved a value of 0.5 represented the percentage of fluid mixing.

![Cross-sectional mass fraction contour.](image)

Figure 5. Cross-sectional mass fraction contour.

Referring to Figure 6, it can be perceived that the mixing curves had shoulders which corresponded to the 90° bends of MCFI, whereby after each bend a significant increment of mixing rate was observed. Along with the increase of Re, this increment appeared more prominent. This observation confirmed that the presence of 90° bends improved the rate of mixing, brought on by flow inversion.

When Re was further increased to 250, the gradual increment presented in previous mixing plots diminished. Instead, the mixing rate increased exponentially to achieve complete mixing, resembling a sigmoidal curve.

![Mixing plot for (top) Re=25, (middle) Re=125, and (bottom) Re=250 in comparison to straight tube and straight coil.](image)

Figure 6. Mixing plot for (top) Re=25, (middle) Re=125, and (bottom) Re=250 in comparison to straight tube and straight coil.

For comparison, fluid mixing in straight tube and straight coil was also simulated. Mixing time \( \theta_{95} \) for the MCFI for Re=25, 125 and 250 respectively were 7.08s, 1.20s and 0.59s, whereas dyes in straight tube and straight coil were unable to achieve complete mixing with tube length equivalent to the construction of MCFI.

4. Conclusion

Secondary flow was observed in the simulation of fluid flow in MCFI. Higher Re led to better mixing through
a process of flow inversion. A mixing time of 0.59s was achieved with Re=250, however complete mixing was still achievable even in Re=25 with a longer mixing time. In order to achieve higher Re, the fluid flow rate had to be increased. This leads to a high liquid flow volume and pressure build-up within the microchannel, which might be unfavourable for microfluidic applications. Thus, thorough considerations are needed to balance out the requirements for rapid mixing with amount of reactant consumption for a mixing operation.

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