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A fundamental investigation of scaling up turbulent liquid-phase vortex reactor using experimentally validated CFD models

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A fundamental investigation of scaling up turbulent liquid-phase vortex reactor using experimentally validated CFD models

by

Zhenping Liu

A dissertation submitted to the graduate faculty in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Co-majors: Chemical Engineering; Mechanical Engineering

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Iowa State University
Ames, Iowa
2016
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DEDICATION

I would like to dedicate this dissertation to my parents, sister and Daisy without whose support I would not have been able to complete this work.
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CHAPTER 1. GENERAL INTRODUCTION

The production of uniform-sized nanoparticles has potential application in a wide variety of fields, but is still a challenge. One main reason that many lab-scale manufactured nanoparticles have not appeared in industry is because there is lack of control on physical properties and surface functionality of nanoparticles during massive production. Recently, a process called "Flash Nanoprecipitation (FNP)" has been developed to produce nanoparticles with controlled size and high drug-loading rate.[48] In FNP, fast mixing is required to make sure that solvent and non-solvent mix homogeneously so that competitive precipitation of organics and polymer could result in functional nanoparticles with narrow size distribution.[82] A multi-inlet vortex reactor (MIVR) has been developed to provide fast mixing for the FNP. The MIVR includes four inlets which are tangential to the mixing chamber of reactor.[57] The MIVR has the operational advantage of providing different inlet-flow momentum and configurations compared to other reactors used in the FNP such as confined impinging jet reactor (CIJR). Former studies have already shown its ability of providing fast mixing and successfully producing functional nanoparticles in the FNP. However, until now all previous investigations about the MIVR only focused in its micro-scale (dimensions in millimetre).

While the micro-scale MIVR does show great promise in the production of functional nanoparticles, the small dimensions and correspondingly small output of the micro-scale MIVR limit its usefulness to producing functional nanoparticles for applications requiring small production run such as high-value pharmaceutical agents. Some applications such as nanoparticle used in pesticides and cosmetics may require larger production run than the micro-scale MIVR can provide, making it economically unrealistic based on the relatively high capital and operating costs needed for a large number of reactors operating in parallel. For this reason, in the study we are interested in investigating the feasibility of scaling up the FNP process to
a macro-scale MIVR capable of generating large quantities of functional nanoparticles, both rapidly and economically, and consequently developing experimentally verified computational fluid dynamics (CFD) models that can be used as design tools for further optimizing reactor design and operation parameters to produce customized functional nanoparticles. To accomplish this investigation, a macro-scale MIVR has been built with optical access. Non-intrusive, optical-based measurement techniques including particle image velocimetry (PIV) and planar laser-induced fluorescence (PLIF) were used to measure flow field and mixing, and related CFD models, specifically turbulence models were validated and developed for optimizing the MIVR and future model development of the FNP process.

1.1 Flow velocity and mixing evaluation of the macro-scale MIVR

In the past two decades, with the advancement of flow visualization method, laser-based measurement techniques such as PIV and PLIF have become very popular in determining flow velocity and passive scalar transport. As a non-intrusive and whole-field measurement technique, PIV is superior to traditional point-wise measurement technique such as laser doppler velocimetry (LDV) and hot-wire probe. In PIV the fluid is seeded with tiny tracer particles which follow the flow faithfully. A pulsed thin laser sheet is used to illuminate the flow and images (usually two) recording the motion of tracer particles are captured by a camera. By analysing the displacement of tracer particles the flow velocity can be estimated. In current study, stereoscopic PIV (SPIV) is used to measure velocity field in the MIVR. SPIV uses two cameras instead of just one in regular PIV so that all three components of velocity can be measured. PLIF has been used to measure the mixing inside the reactor. In PLIF, a fluorescent dye is added to the flow, which can emit fluorescence light when excited by the laser. Through measuring the fluorescent light intensity, the concentration of dye in local position can be estimated, thus mixing in the flow can be measured.
1.2 Turbulence modelling

In CFD the governing equations of flow motion are solved numerically. In most cases CFD needs to deal with turbulence in the flow which is a complex phenomenon and not well understood yet. For most practical flow direct resolving all the turbulence scale is too expensive, thus turbulence model is frequently used in CFD. Commonly the Reynolds-averaged Navier-Stokes (RANS) approach and large eddy simulation (LES) approach are used in CFD. However, it is found very challenging to apply common-used RANS and LES approach to study the flow in the MIVR. This difficulty is mainly due to the dominant flow motion in the MIVR, which is swirling. In the micro-scale MIVR there is transitional swirling flow while highly turbulent swirling flow exists in the macro-scale MIVR. Swirling motion can alter turbulence field by streamline curvature effect and usually is not considered in common-used RANS model. LES is a better choice for simulating swirling flow. However, it requires very fine mesh near the wall. For wall-bounded flow in complex geometry such as the MIVR, LES is found very expensive. When coarse mesh was used in the LES, its prediction accuracy was compromised. Transition is also a challenging phenomenon to model in CFD. All these difficulties in CFD require more advanced approach. Hybrid RANS/LES approach is thus considered here where RANS model is mainly used to predict flow near the wall and LES model is used to predict flow elsewhere. In current study, we have applied and developed hybrid RANS/LES model for comparison with experimental data and prediction of the complex swirling and transitional flow inside the MIVR.

1.3 Dissertation organization

The remaining of this dissertation is organized as follows: Chapter 2 presents a vortex model development for describing the mean velocity field in the macro-scale MIVR. This study reveals the physics of flow phenomenon in the macro-scale MIVR and provides a simple method to predict its mean velocity. In Chapter 3 the flow characteristic in the macro-scale MIVR are analysed in detail. This study helps us understand the flow field in the macro-scale MIVR and how flow behaviour changes when the MIVR is scaled up. A follow-up CFD study on
the flow field is presented in Chapter 4, with good match to the experimental data. A hybrid RANS/LES method called dynamic delayed detached eddy simulation (DDES) is used in the CFD study and this method is found very promising in predicting turbulent swirling flow. Chapter 5 takes a look at the turbulent mixing in the macro-scale MIVR. The passive scalar mixing is measured by using PLIF technique. This study provides useful measurement about turbulent mixing in the macro-scale MIVR which is directly related to its application in the FNP. In Chapter 6 we come back to the micro-scale MIVR and developed a hybrid RANS/LES model to predict its transitional flow field, with good agreement to previous measurement. This study can help build a more accurate model for predict the FNP within the micro-scale MIVR (which is the main application of MIVR now). Finally, summary and future work directions are given in Chapter 7.
CHAPTER 2.  A BATCHELOR VORTEX MODEL FOR MEAN VELOCITY OF TURBULENT SWIRLING FLOW IN A MACRO-SCALE MULTI-INLET VORTEX REACTOR

A paper modified from a publication in *Journal of Fluids Engineering*  

Zhenping Liu, Rodney O. Fox, James C. Hill and Michael G. Olsen

Abstract

The velocity field in a macro-scale multi-inlet vortex reactor used in the Flash Nanoprecipitation process for producing functional nanoparticles was investigated using stereoscopic particle image velocimetry. Based on the experimental data, a simple model was proposed to describe the average velocity field within the reactor. In the model, the axial and azimuthal velocities could be well described by the combination of two co-flowing Batchelor vortices. In this model, six dimensionless coefficients are identified by non-linear curve fitting, and their dependence on Reynolds number can be linearly described. This simple model is able to accurately predict the mean velocity field within the confined turbulent swirling flow based purely on Reynolds number.

2.1 Introduction

The multi-inlet vortex reactor (MIVR) was originally developed for use in the Flash Nanoprecipitation (FNP) process for manufacturing functional nanoparticles and has been proven

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2Primary researcher and author

3Corresponding author
effective due to its ability of providing rapid fluid mixing and insensitivity of inlet stream momentum[57]. FNP produces mono-disperse functional nanoparticles through rapid mixing of a saturated solution and a non-solvent[48]. The MIVR has been used in FNP to produce pesticide nanoparticles for agricultural use[61] and drug-loaded polymeric nanoparticles for the pharmaceutical industry[82].

Previous work on the MIVR has focused on micro-scale MIVRs (dimensions on the order of millimetres). Liu et al.[57] studied turbulent transport phenomenon in a micro-MIVR, and found that changing the inlet arrangement causes only a minor change of the performance of the MIVR, and adequate micro-mixing was achieved within the MIVR when Reynolds number was higher than a threshold of 1600. Cheng et al. and Shi et al.[12; 84] have measured both the two dimensional laminar and turbulent velocity field within the micro-MIVR using microscopic particle image velocimetry. While the micro-scale MIVR does show great promise in the production of functional nanoparticles, some applications (e.g., nanoparticle use in pesticides and cosmetics) may require larger production runs than the micro-scale MIVR can provide. For this reason, a scaled-up MIVR (dimensions on the order of centimetres) is of great interest, and could potentially generate large quantities of functional nanoparticles, both rapidly and economically.

The macro-scale MIVR (Figure 2.1) consists of four inlets, one reaction chamber, and one outlet. The four inlets are tangentially aligned to the reaction chamber with a 90 degree angular array around the outlet tube. Each inlet has a square cross section of 25.4 mm side length

Figure 2.1  Dimensions of the multi-inlet vortex reactor.
and 870 mm overall length. The outlet is located on the top center of the chamber. The cross section of the outlet is circular with 25.4 mm diameter and its length is 1067 mm. The reaction chamber is 25.4 mm in height and 101.6 mm in diameter. The dimensions of the macro-reactor are approximately 16 times larger than its micro-counterpart[12; 84]. Four individual streams enter the reaction chamber, mix and undergo spiral motion towards the outlet. As the Reynolds number, i.e., the inlet velocity, of the MIVR increases, the flow inside the reaction chamber becomes a turbulent swirling flow[84]. This type of swirling flow is common in everyday life as well as industrial applications (e.g. bath drain vortices, tornadoes, gas cyclone separators). Simple vortex models such as the Lamb-Oseen vortex model and the Batchelor vortex model provide useful methods to describe the velocity field of these swirling flows[80; 5]. For complex swirling flows, linear combinations of vortices can also yield analytical expressions of the velocity field[91].

In the current work, the three-dimensional velocity field inside the reaction chamber was measured by stereoscopic particle image velocimetry (SPIV)[77]. Based on the experimental results, a simple model consisting of two co-flowing Batchelor vortices is found able to describe the average velocity of this turbulent swirling flow. This model helps reveal the flow physics inside the macro-scale MIVR.

2.2 Experimental Apparatus and Methodology

The experimental flow facility is shown in Figure 2.2. Water is used as the working fluid. The four feed tanks hold a maximum of 1893 litres of water, and water is recycled among the four tanks. Four feedback control valves (Fisher Inc.) provide stable flow rates with accuracy of 0.005 L/s. Free stream turbulence intensities in each inlet of the MIVR were reduced by a ∼ 11 cm long flow conditioner consisting of screens and honeycombs. For the present study, each inlet of the MIVR had the same flow rate. In order to test the influence of Reynolds number on the velocity field, four flow rates of each inlet, 0.08 L/s, 0.12 L/s, 0.16 L/s and 0.2 L/s were investigated, which correspond to a bulk inlet Reynolds numbers 3290, 4935, 6580 and 8225.
respectively. The bulk inlet Reynolds number is defined as\[84\]

$$Re = \frac{d_h U_j}{\nu}$$

(2.1)

where $d_h$ is the hydraulic diameter of the inlet, $U_j$ is the bulk inlet velocity and $\nu$ is the kinematic viscosity of water.

SPIV was used to measure velocity fields inside the reaction chamber. The measurement position was fixed at the middle height of the reaction chamber, and the measured area is near the reactor center where most of the out-of-plane motion occurs (Figure 2.1). In order to minimize the refraction and reflection of laser light on the complex surface of reaction chamber, four water-filled zones were constructed around the reaction chamber (Figure 2.1). The flow was seeded with $\sim 11.7\mu m$ diameter hollow glass spheres and illuminated by a double-pulsed Nd:Yag laser (New Wave Research Gemini) with a 1.5 mm Laser sheet thickness. Two 12-bit double-frame CCD cameras with 1280*1024 pixel resolution were used to capture the SPIV images in a frequency of 4 Hz. The effective view angle of two cameras is about 80 degrees due to the refraction between the water-air interfaces.
A two-level calibration plate (LaVision GmbH) was used for in situ calibration. This volumetric calibration method does not require facilities to move the calibration plate[77], which is usually time-consuming and can easily introduce extra errors. The calibration grids are a high precision dot pattern with 2.2 mm dot diameter, 10 mm dot spacing and 2 mm dot level separation. Due to the confined geometry of the MIVR, a mock reactor sharing identical geometry to the real reactor was used to hold the calibration plate. A technique called self-calibration[98] was applied to minimize the registration error[95] caused by the deviation between the location of the laser sheet and calibration plate surface. After implementing the self-calibration technique, the average deviation of plate to laser sheet is found to be about 0.078 mm, which is about 5% of the thickness of the laser sheet. For each Reynolds number, 5000 SPIV image pairs were obtained. Velocity vector computation was completed by using the commercial PIV software package Davis 7.2 (LaVision GmbH). Velocity was computed by a multi-pass cross correlation interrogation. The final interrogation window is 32*32 pixels with 50% overlap, corresponding to a 0.6 mm velocity vector spacing.

![Diagram](image)

Figure 2.3  (a)The location of inlet measurement, (b) contour of $u_x$ at 1/2 height of inlet and (c) comparison between average velocity at 3/4, 1/2 and 1/4 height.

Besides the SPIV measurement of the chamber, the middle part of one inlet has also been measured by regular two-dimensional PIV where 3/4, 1/2 and 1/4 height of the intersection was investigated. As the four inlets are under the same control condition, the measurement of one inlet is thought enough to represent all four inlet conditions. The measured location and results can be seen in Figure 2.3(a). As it is expected, average velocity at 1/2 height does not
change as flow moves along the channel, indicating that flow has already been fully developed. Average velocity at 3/4 and 1/4 height is found to be of the same magnitude, showing that inlet flow is symmetrical with respect to the middle plane. The profile of velocity at 1/4 and 3/4 height is found to have a defect in the center. This finding is consistent with the contour of mean stream-wise velocity obtained by large eddy simulation[66]. The turbulent intensity is found to be about 10 percent of the mean velocity along the center-line and about 16 percent of the mean velocity close to the wall.

2.3 Postprocessing of the Velocity Field

The SPIV interrogation software computes velocity in Cartesian coordinates, i.e., $u_x, u_y, u_z$. Because the flow inside the MIVR is strongly swirling, a cylindrical coordinate consisting of radial, azimuthal and axial velocity, i.e., $u_r, u_\theta, u_z$ is more convenient to describe the velocity field. One problem related to the cylindrical coordinate is its undetermined origin point which is the center of swirling flow (also called as vortex center). The center of this swirling flow is unsteady, with a random or precession wandering motion. For significant wandering motion of the vortex center, the average velocity obtained at a fixed coordinate will become smeared[44]. Thus, it is important to investigate the wandering motion of swirling flow before choosing the appropriate post processing method. For the flow within the MIVR, a single vortex center is observed for all realizations. The determination of the vortex center is then based on the center of mass approach proposed by [44; 56]. In detail, the magnitude of axial vorticity $\omega_z$ over in-plane velocity [equation (2.2)] is calculated which has its maximum value at the vortex center. Then, the vortex center is calculated as the mass center of all position with value larger than 0.95 of the maximum vorticity which cover the entire vortical system.

$$R = \frac{\sum W_i r_i}{\sum W_i} \quad (W_i \geq 0.95W_{max})$$

where $R$ and $r_i$ is the position vector.

For the flow within the MIVR, it is found that the wandering motion of vortex center of 5000 instantaneous velocity realization is random and confined in a small area (about 5% of the chamber diameter) for all investigated Reynolds numbers (figure 2.4). As the time-averaged
velocity profile obtained at a fixed coordinate could well represent the key flow features for a small wandering motion[44], the average velocity in the results presented here was calculated based on a fixed coordinate rather than a moving coordinate which puts the instantaneous vortex center as its origin.

Figure 2.4  Time average velocity field at Re=3290. The in-plane velocity is shown in vectors and the axial velocity is shown in contour.

The time-averaged velocity profile is calculated as the ensemble average of 5000 velocity realizations. One example of mean velocity field is shown in figure 2.4, where the Reynolds number is 3290. It is found that the out-of-plane motion only becomes significant near the center of the reaction chamber. Far away from the outlet, the flow is well constrained by the top and bottom walls, resulting in an almost two-dimensional flow. When the flow moves close to the vortex center, axial and azimuthal velocities first increase, and then decrease. Figure 2.5 shows the three velocities as functions of radial position. The Error bars represent the standard deviation of 29 velocities extracted from polar angles ranging from 0 degree to 360 degree, showing the variation of time-averaged velocities along the azimuthal direction. The dotted line in figure 2.5 shows the averaged velocities of these 29 samples. It is found that the radial, azimuthal and tangential velocity could be well represented by its average value due to
the small scatter around the dotted lines.

Figure 2.5  Velocity components as a function of radial position within the reactor at Re=3290.

2.4 Analytical Vortex Model

The simplest vortex model for a viscous fluid is the Rankine vortex model which characterizes the swirling flow as a forced vortex in its core, surrounded by a free vortex. The discontinuity of gradient at the interface between the forced and free vortex makes the Rankine vortex model non-physical for real applications. However, the concept of a free and forced vortex region could still be applied to the flow in the MIVR. A more physical-based vortex model is the Lamb-Oseen vortex model which arises as an exact solution of the Navier-Stokes equations for the initial condition [80]

\[
\begin{align*}
    u_z(r, 0) & = \Gamma_0 \delta(x) \delta(y) \\
    u_{\theta} & = \frac{\Gamma}{2\pi r} \left(1 - \exp\left(-\frac{r^2}{4\nu t}\right)\right)
\end{align*}
\]  

(2.3)

The exact solution of the Lamb-Oseen vortex is

\[
\begin{align*}
    u_z(r, 0) & = \frac{\Gamma_0}{4\pi \nu t} \exp\left(-\frac{r^2}{4\nu t}\right), u_{\theta} = \frac{\Gamma}{2\pi r} \left(1 - \exp\left(-\frac{r^2}{4\nu t}\right)\right)
\end{align*}
\]  

(2.4)

where \(\Gamma\) is the circulation contained in the vortex, and \(\nu\) is the kinetic viscosity. A similar expression to describe a viscous vortex is the Batchelor vortex model, in which flow far down
stream of a single trailing axis has a similarity solution[5]

\[ u_\theta = \frac{\Gamma}{2\pi r} [1 - \exp\left(-\frac{U_r^2}{4\nu_z}\right)] \] (2.5)

\[ u_z = \frac{BU^2}{8\nu_z} \exp\left(-\frac{U_r^2}{4\nu_z}\right) \] (2.6)

where \( U \) is free stream velocity, and \( B \) is a constant coefficient. Equations (2.5) and (2.6) are obtained from Navier-Stokes equations based on the assumption that axial velocity \( u_z \) has a small change around the free stream velocity \( U \).

The radial velocity is negligible for both the Lamb-Oseen and batchelor vortex model. Based on the expression of their solutions, the batchelor vortex model describes steady, axisymmetric two-dimensional flow, while Lamb-Oseen model applies for unsteady one-dimensional flow. Susan-Resiga et al.[91] studied the swirling flow downstream of a Francis turbine Runner and found that its axial and azimuthal velocity profiles could be well described by superposition of two counter-flowing batchelor vortices and a solid body motion. The idea of superposing different vortex models is very useful in obtaining analytical expressions of velocity fields. For example, in the turbulent swirling flow of a straight pipe, the azimuthal velocity could be expressed as the sum of several forces and free motions[50]. For the mean velocity within the MIVR, it is found that the azimuthal and axial velocities can be well described by the expressions derived by Susan-Resiga et al.[91]

\[ \bar{u}_\theta(r) = \Omega_0 r + \frac{\Omega_1 R_1^2}{r} [1 - \exp\left(-\frac{r^2}{R_1^2}\right)] + \frac{\Omega_2 R_2^2}{r} [1 - \exp\left(-\frac{r^2}{R_2^2}\right)] \] (2.7)

\[ \bar{u}_z(r) = U_0 + U_1 \exp\left(-\frac{r^2}{R_1^2}\right) + U_2 \exp\left(-\frac{r^2}{R_2^2}\right) \] (2.8)

where \( \Omega_0, \Omega_1 \) and \( \Omega_2 \) are characteristic angular velocities, \( R_1 \) and \( R_2 \) are characteristic vortex radii, and \( U_0, U_1 \) and \( U_2 \) are characteristic axial velocities. When the axial and azimuthal velocities are normalized by the inlet velocity \( U_j \), and dimensionless radial position \( r^* \) is set as \( r/r_0 \), the equations (2.7) and (2.8) can be further written into dimensionless forms

\[ \frac{\bar{u}_\theta(r)}{U_j} = V_0^* r^* + \frac{V_1^* R_1^2}{r^*} [1 - \exp\left(-\frac{r^*}{R_1^2}\right)] + \frac{V_2^* R_2^2}{r^*} [1 - \exp\left(-\frac{r^*}{R_2^2}\right)] \] (2.9)
\[
\frac{\overline{u}_z(r)}{U_j} = U_0^* + U_1^* \exp(-\frac{r^2}{R_1^*}) + U_2^* \exp(-\frac{r^2}{R_2^*})
\] (2.10)

where \( V_0^*, V_1^* \) and \( V_2^* \) are dimensionless characteristic tangential velocities, \( R_1^* \) and \( R_2^* \) are dimensionless characteristic vortex radii, and \( U_0^*, U_1^* \) and \( U_2^* \) are dimensionless characteristic axial velocities. For analytical expressions of \( \overline{u}_\theta \) and \( \overline{u}_z \) in the equations (2.9) and (2.10), eight unknown coefficients need to be identified. These eight coefficients are fitted simultaneously by the non-linear fitting function of OriginPro 9 (OriginLab), where the Levenberg-Marquardt (L-M) algorithm was used to adjust the parameter values in an iterative procedure. The rigid body rotation term \( V_0^* \) is found much smaller than \( V_1^* \) and \( V_2^* \). For example, in the case of \( \text{Re}=3290 \), \( V_0^* \) is found to be -0.42 while \( V_1^* \) is 49.57 and \( V_2^* \) is 158.92. For all the investigated Reynolds number, \( V_0^* \) is less than 1 percent of \( V_1^* \) and \( V_2^* \) and thus is neglected in the following model. It is worth noting that the characteristic axial velocity \( U_0^* \) cannot be ignored here because it represents the axial velocity far away from the vortex center which is very small yet not zero. The average flow field can be viewed as the combination of two Batchelor vortices without the rigid body motion term. One more constraint can be added to the coefficients in equation (2.9) and (2.10). According to the measurement of the inlet (Fig. 2.3), the average velocity \( u_x \) at 3/4 and 1/4 plane is found to be almost identical to each other, indicating that the velocity profile is symmetrical with respect to the middle plane of the chamber. Thus, considering a mass balance, the total volume of fluid passing through the center plane of the reaction chamber must be equal to 1/2 of the total inlet flow rate, which gives

\[
\int_0^R 2\pi r \overline{u}_z \, dr = -\frac{q}{2} \tag{2.11}
\]

where \( R \) is the radius of the reaction chamber and \( q \) is the total volumetric flow rate (L/s). Substituting equation (2.10) into (2.11), the dimensionless integral form can be written as

\[
\int_0^1 \left( U_0^* + U_1^* \exp(-\frac{r^2}{R_1^*}) + U_2^* \exp(-\frac{r^2}{R_2^*}) \right) dr = -\frac{q}{2\pi U_j R^2} \tag{2.12}
\]

Upper integral limit \( U_1^* \exp(-\frac{1}{R_1^*}) + U_2^* \exp(-\frac{1}{R_2^*}) \) are assumed to be zero when characteristic vortex radius \( R_1^* \) and \( R_2^* \) are found much smaller than 1. Integration of equation (2.12) gives the following constraint that relates the dimensionless coefficients \( U_0^*, U_1^*, U_2^*, R_1^* \) and \( R_2^* \)

\[
U_0^* + U_1^* R_1^2 + U_2^* R_2^2 = -\phi = -\frac{q}{2\pi U_j R^2} \tag{2.13}
\]
Considering the volumetric flow rate \( q = 4a^2U_j \) where \( a \) is the side width of an inlet, \( \phi \) is constant and equal to 0.159.

Thus, equations (2.9) and (2.10) are further simplified to include only six parameters

\[
\frac{\overline{u_\theta}(r)}{U_j} = \frac{V_1^* R_1^*}{r^*} \left[ 1 - \exp\left(\frac{-r^*}{R_1^*}\right) \right] + \frac{V_2^* R_2^*}{r^*} \left[ 1 - \exp\left(\frac{-r^*}{R_2^*}\right) \right] \tag{2.14}
\]

\[
\frac{\overline{u_z}(r)}{U_j} = -\phi - U_1^* R_1^* - U_2^* R_2^* + U_1^* \exp\left(\frac{-r^*}{R_1^*}\right) + U_2^* \exp\left(\frac{-r^*}{R_2^*}\right) \tag{2.15}
\]

Figure 2.6 Coefficients at different Reynolds number and the corresponding linear fit curve, (a) \( V_1^*, V_2^* \), (b) \( R_1^*, R_2^* \) and (c) \( U_1^*, U_2^* \).

Figure 2.7 Comparison of the vortex model to experimental data at \( \text{Re}=3290 \), (a) \( \overline{u_\theta} \) and (b) \( \overline{u_z} \).
All the coefficients at different Reynolds numbers are shown in figure 2.6. The fitting error is plotted as the error bar which is found to be very small (most of the error bars are smaller than the corresponding dot diameter), showing that analytical expressions (2.14) and (2.15) are capable of describing the average velocities in the MIVR well over the large range of Reynolds numbers investigated. Figure 2.6 also shows the effect of Reynolds number on the six coefficients. The trend of these coefficients with Reynolds number could be linearly described. When $\bar{u}_\theta$ and $\bar{u}_z$ are scaled by $U_j$, the principal Reynolds number dependence has already been removed. Thus, the variation of these dimensionless coefficients indicates the non-linear effect of Reynolds number which could be well predicted by linear functions in the investigated range from 3290 to 8225. Velocity fields for other Reynolds numbers could be interpolated based on these linear functions.

The batchelor vortex represented by the characteristic values $R_1^*, V_1^*$ and $U_1^*$ can be called Vortex1, and the other Vortex can be called Vortex2. One typical profile of azimuthal and axial velocity for $Re=3290$ is shown in figure 2.7, where experimental data are also plotted for comparison. Overall, the experimental data are well described by the proposed vortex model. The contributions of the two batchelor vortices to the final velocity profile are also plotted in figure 2.7. The physical meaning of the combination of these two vortices could be explained by considering the main contributing phenomena in the swirling flow. Far away from the vortex center, the flow is in the free vortex region and driven by inlet momentum. In the forced vortex region, the viscosity becomes more significant. As flow velocity increases, the pressure is expected to decrease. Flow recirculation occurs due to the drop in pressure at the vortex center. Two types of flow motion happen inside the reaction chamber, i.e., exiting and recirculation. Vortex1 possesses negative characteristic axial velocity, representing flow moving towards the outlet. Vortex2 has positive characteristic axial velocity, meaning it contributes to a recirculation of flow back into the reactor. Because recirculation just happens in a small area near the vortex center, Vortex 1 has a larger vortex radius and smaller characteristic tangential velocity than Vortex 2. The exiting and recirculating flow due to the inlet momentum and low pressure at the vortex center justify the usage of the combination of two Batchelor vortices to represent the velocity field.
2.5 Conclusion

The velocity field within the reaction chamber of a macro-scale multi-inlet vortex reactor has been measured by stereoscopic PIV. The unsteady wandering motion of the vortex center was found to be confined near the center of the reactor. Thus, the ensemble averaged velocity was calculated based on a fixed vortex center position. While the radial velocity was found to be very small for all the radial positions, the average azimuthal and axial velocities were described by the proposed vortex model. In the model, two Batchelor vortices are combined. One vortex is viewed as the contribution of inlet momentum, and the other vortex models flow recirculation back into the reactor. Six model coefficients for these two vortices were found by curve fitting stereoscopic particle image velocimetry data. The fitting errors are found to be very small over the investigated Reynolds number. The coefficients of this combination could be well described by linear functions of the Reynolds number. The proposed analytical expression combined with the linear relationship between these coefficients and Reynolds number provides a simple model to describe and predict the average axial and azimuthal velocity within the reactor based solely on Reynolds number.
CHAPTER 3. FLOW CHARACTERISTICS IN A MACRO-SCALE MULTI-INLET VORTEX REACTOR

A paper modified from a publication in Industrial & Engineering Chemistry Research

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Abstract

The micro-scale multi-inlet vortex reactor (MIVR) has been developed for use in Flash NanoPrecipitation (FNP), a technique to generate functional nanoparticles. A scaled-up MIVR is motivated by the desire for a higher output of nanoparticles than the micro-scale reactor can provide. As the first step of this scaling process, the flow characteristics in a macro-scale MIVR have been investigated by stereoscopic particle image velocimetry (SPIV). The studied Reynolds numbers based on the inlet geometry range from 3290 to 8225, resulting in a turbulent swirling flow within the reactor. The flow in the mixing chamber is found to be unstable with a wandering vortex center. The vortex wandering is constrained to a small area near the center of the reactor and has little effect on the mean velocity field. However, the measured turbulence kinetic energy (TKE) and Reynolds stresses are found to be sensitive to the vortex wandering. The flow characteristics of the macro-scale MIVR are compared with the micro-scale MIVR in terms of swirl ratio and micro-mixing time. It is found that the swirl ratio and micro-mixing time of the flow increases as the MIVR is scaled up, indicating a flow with stronger swirl yet less mixing effectiveness in the scaled-up reactor.

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3.1 Introduction

Functional nanoparticles are of great scientific and industrial interest for their unique size-related properties and have a wide application in various areas, such as dyes, pesticides, and pharmaceuticals[39]. However, it is still challenging to produce functional nanoparticles in a relatively easy and inexpensive way. Flash NanoPrecipitation (FNP) has been developed to produce functional nanoparticles with a narrow particle size distribution[48]. In the FNP technique, functional nanoparticles are formed by rapidly mixing supersaturated organic active and copolymer anti-solvent, resulting in organic active precipitation and particle growth where the growing particle size of the organic active is frozen by deposition of block copolymer on its surface[48]. Mixing time in the FNP technique should be short enough to provide an uniform starting time for the precipitation. Two mixer geometries, the Confined Impinging Jet Reactor (CIJR)[60] and the Multi-Inlet Vortex Reactor (MIVR)[57] have been developed to meet the high demand of rapid mixing in FNP. While the CIJR is limited by the requirement of equal momenta of solvent and anti-solvent streams, the MIVR is insensitive to the equality of the momentum from each stream, allowing the final fluid phase to be anti-solvent dominant, which increases the stability of nanoparticles by depressing the rate of Ostwald Ripening[57]. Thus far, there have been many applications using the MIVR to produce functional nanoparticles.[61; 82; 1; 3; 69]

In order to help understand the nanoprecipitation mechanism within the MIVR, mixing performance and flow characterization have been investigated in previous studies. Liu et al.[57] evaluated the mixing performance of a micro-scale MIVR by using a competitive reaction and computational fluid dynamics (CFD). Cheng et al.[12] measured flow velocity in the mixing chamber of a micro-scale MIVR by micro-PIV and compared the measurement with large eddy simulation. Shi et al.[84] further presented detailed velocity measurements within the micro-scale MIVR to reveal the mean velocity field and turbulence characteristics. Using these data, a comparison has been performed by Bensaid et al.[6] to validate turbulence models against experimental data collected for the MIVR. Simulation results from both Cheng and Bensaid demonstrated good agreement with micro-PIV measurements when the flow is laminar. How-
ever, the comparison becomes worse when the flow is turbulent, where there is a large variation between experimental and simulation results in terms of mean velocity and turbulence kinetic energy. To study mixing and reaction, Cheng et al.[11] integrated a population balance equation with FNP kinetics into the CFD simulation. Their results show that the FNP process in the micro-scale MIVR is macro-mixing dominated, and the mixing is limited by the geometry of the reactor, although increasing the Reynolds number can result in a more homogeneous flow and improve the particle size distribution slightly. The laminar and turbulent mixing performance of the micro-scale MIVR was experimentally investigated by laser induced fluorescence with confocal laser scanning microscopy, and the mixing is found to be incomplete even at its highest investigated flow rate[85; 86]. Nevertheless, although the mixing performance of the MIVR is found to be incomplete, applications of the MIVR on FNP have made successful production of nanoparticles with narrow size distribution[61; 82; 1; 3; 69]. These can be explained by two reasons: 1) The mixing performance of the MIVR is determined by many factors, and it can be improved, for instance, by increasing the flow rate; 2) Considering the application of the MIVR to FNP, nanoparticle size distribution is not only determined by the mixing performance, but also by the concentration of polymeric stabilizer[61; 82]. For the same mixing condition, the particle size can be decreased by adding more stabilizers.

Despite the scalability of the MIVR in the FNP technique, most previous research has focused on the micro-scale reactor (dimensions on the order of millimeters). While the micro-scale MIVR does show great promise in the production of functional nanoparticles, some applications such as the use of nanoparticles in pesticides and cosmetics, require larger production runs than the micro-scale MIVR can provide. A scaled-up MIVR could potentially generate large quantities of functional nanoparticles in a both efficient and economical way. Some previous work does exist on scaling up the CIJR used in the FNP. The scale-up criteria for the CIJR has been investigated by Johnson et al.[49], where a second-order competitive reaction set was used as a chemical ruler to correlate the mixing time with reactor geometry and Reynolds number. Marchisio et al.[68] utilized CFD and a simple precipitation model to explore the role of turbulent mixing on particle formation in the CIJR and derived related scale-up criteria. However, to the knowledge of the authors, there has been no research on scaling up the MIVR. In the
current paper, the flow characteristics within a scaled-up MIVR (dimensions on the order of centimeters) are investigated for the first time using stereoscopic particle image velocimetry (SPIV).

The scaled-up MIVR operates at a much higher Reynolds number than its micro-scale counterpart, resulting in a turbulent swirling flow in the mixing chamber. Although the configuration has not been studied before, some characteristics of the flow are similar to other swirling flows, and comparison with these swirling flows can enhance the understanding of the current investigation. Turbulent swirling flow exists in a wide range of fluid equipment such as cyclone separators, swirl combustors, engines with swirl inlets, etc. Swirling flow is known for the unsteady nature of its vortex center, which can be a random or precessing motion[41; 44]. In a turbulent swirling flow, the measured fluctuations can be enhanced by the vortex wandering motion which is called pseudo-fluctuation[34]. An inappropriate processing method for experimental data without considering the vortex wandering can smear the mean velocity field and exaggerate the turbulent fluctuations in the flow[44]. Previous experimental work on the MIVR has not considered the influence of wandering motion on the calculated flow features.[12; 84] In the current paper, this influence is investigated extensively by comparing the results with and without considering the wandering motion, providing a better understanding of the flow turbulence inside the MIVR.

The previous micro-PIV measurements in the micro-scale MIVR can only resolve two-dimensional velocity fields, while flow inside the MIVR is essentially three dimensional, especially close to the center of reactor. To overcome previous two-dimensional measurement limitations, the three-dimensional velocity field within the macro-scale MIVR is investigated by stereoscopic particle image velocimetry (SPIV). SPIV employs two cameras to image the flow and extract all three components of flow velocity in a plane[77]. Based on the SPIV measurement, the flow characteristics in the macro-scale MIVR are analyzed extensively. In the current paper, the influence of the wandering vortex center on the mean field and turbulence statistics such as turbulence kinetic energy (TKE) and Reynolds stress are discussed first. Then, comparison in terms of normalized mean velocity and TKE is made between different inlet Reynolds numbers to investigate the Reynolds number effect. The flow characteristics in the macro-scale MIVR
are finally compared with that in the micro-scale MIVR to provide a better understanding how the flow changes as the reactor is scaled up.

Figure 3.1  Geometry of the multi-inlet vortex reactor.

3.2  Experimental section

3.2.1  Experimental Apparatus

The experimental set-up shown in figure 3.1 is designed to provide four independent inlet steams to the MIVR. The working fluid is water at room temperature. Each tank can contain a maximum of 1893 litres of liquid (500 Gallons). Flow from two feed tanks is powered by two pumps (Mach pumps Inc.) and sent to the four inlets of the MIVR through four automatic control valves (Fisher Inc.). Each control valve provides a stable flow with accuracy around 0.5% for the investigated flow rate. Before the flow enters the reactor, the free steam turbulence intensity at each inlet of the MIVR is reduced by an ~ 11cm long flow conditioner containing 3.175 mm cell size honeycomb and screen grids. Flow exiting the reactor is pumped into two collection tanks and can be recycled back into the two feed tanks.
Figure 3.2  Geometry of the macro-scale MIVR. (a) Top view; (b) side view.

The macro-scale MIVR is made of acrylic glass to provide for good optical access. As shown in figure 3.2(a) and 3.2(b), the reactor consists of four inlets, one outlet, and one mixing chamber. The four inlets are tangential to the mixing chamber in a 90 degree angular array. The outlet is located on the top center of the chamber. The cross section of the inlets are square in shape, 25.4 mm in width, and 870 mm in length. The cross section of the outlet is round with 25.4 mm diameter and 1067 mm length. The mixing chamber has a 25.4 mm height and 101.6 mm diameter. The dimensions of the macro-scale MIVR are about 16 times larger than those of the micro-scale reactor studied by Cheng et al.[12] and Shi et al.[84]. However, due to different manufacturing methods, the macro-scale MIVR is similar yet not geometrically scaled up to its micro-counterpart.

There are two common ways of defining the Reynolds number for the MIVR[84]. One way of defining Reynolds number is based on one inlet and applied to the case where all four inlets have the same flow rate. The other type of Reynolds number is based on the diameter of the mixing chamber which is used in the case where four inlets have different flow rates. In the current study, each inlet of the MIVR has been set up with the same flow rate, as previous studies have found the mixing performance to be insensitive to the inlet configuration[57]. The investigated Reynolds number of the MIVR based on the bulk velocity of one inlet is 3290 ~ 8225, corresponding to 52640 ~ 131600 when it is based on the mixing chamber. In the following sections, the Reynolds number $Re_j$ is used, which is based on one inlet.
3.2.2 Swirl Ratio

Swirl ratio is introduced here to quantify the swirl strength of flow inside the MIVR. The swirl ratio is typically used in tornado-like vortex flow and defined as the ratio of angular momentum to radial momentum. Although the swirl ratio is an important parameter for determining the characteristics of Tornado-like vortices\cite{14}, it is not universally defined from one investigation to another. Here, the definition of swirl ratio used in Haan et al.\cite{37} is adopted which is written as

\[ S = \frac{\pi r_c^2 V_c}{Q} \]  \hspace{1cm} (3.1)

where \( V_c \) is the maximum azimuthal velocity, \( r_c \) is the radial position at which \( V_c \) occurs, and \( Q \) is the volumetric flow rate through the system. For the flow in the MIVR, Equation 3.1 can be further simplified as

\[ S = \pi r_c^* V_c^* \]  \hspace{1cm} (3.2)

in which \( r_c^* \) is the radius normalized by chamber radius, and \( V_c^* \) is the velocity normalized by bulk inlet velocity \( U_j \). The swirl ratio \( S \) depends on the shape of the measured azimuthal velocity profile. As azimuthal velocity within the MIVR in four planes has been measured, a mean swirl ratio can be obtained by averaging the value from each plane.

\[ \overline{S} = \frac{1}{4} \sum_{i=1}^{4} \pi r_{ic}^* V_{ic}^* \]  \hspace{1cm} (3.3)

3.2.3 Stereoscopic Particle Image Velocimetry

SPIV was used to measure the velocity field inside the mixing chamber. The measured planes are located at the 1/4, 1/2, 3/4 and 7/8 height of the chamber along the z-direction. The 1/8 height was found difficult to measure because it is close to the bottom of the chamber, and there is a strong optical interference from seed particles depositing on the bottom. The flow was seeded with hollow glass spheres with diameter of 11.7\( \mu \)m at a concentration of 5.88\( g/m^3 \). The flow was illuminated by a double-pulsed Nd:Yag Laser (New Wave Research Gemini). The thickness of the laser sheet was 1.5 mm. In order to minimize the refraction and reflection of the laser sheet on the curved surface of the chamber, four water filled zones were constructed around the chamber (figure 3.2(a)). The time delay between the two laser pulses was chosen
carefully so that average movement of particles was approximately 5~8 pixels, and out-of-plane particle motion was controlled to be less than 25% of the laser sheet thickness[95]. Two 12-bit double-frame CCD cameras (LaVision Flowmaster 3S) were used to capture the PIV images at a frequency of 8 Hz. The camera resolution was 1280 × 1024 pixels with a pixel size of 6.7 µm. The viewing angle of the two cameras was set at nearly 90 degrees so that the measurement uncertainty in determining out-of-plane motions would be the same as in-plane motions[95]. The accuracy of a stereoscopic PIV measurement relies on the implementation of a proper calibration. A general reconstruction technique based on a two-level calibration plate (LaVision GmbH) was applied here. This volumetric calibration method does not need facilities for moving the plate during calibration which is usually time-consuming and can easily introduce extra errors. The calibration grids use a high precision two-level dot pattern with 2.2 mm dot diameter, 10 mm dot spacing, and 2 mm level separation. Due to the confined geometry of the MIVR, a mock reactor was used to hold the calibration plate, and an initial third-order mapping function was generated. After that, a self-calibration technique[98] was applied to correct the initial mapping function based on images taken for the real reactor to minimize the registration error which is found to play a dominant role in the accuracy of SPIV measurement[95]. The area near the center of the reaction chamber was investigated (figure 3.2(a)) rather than a plane covering the entire chamber, because most out-of-plane motions were found to occur near the center. For each Reynolds number 5000 image pairs were captured and analysed by a commercial PIV software package Davis 7.2 (LaVision GmbH). A detailed introduction about stereoscopic PIV vector computation can be found in Calluaud et al.[9]. Multi-pass correlation techniques were used to compute vectors, resulting in a final interrogation window size measuring 32 × 32 pixels with 50% overlap, corresponding to a 0.6 mm vector spacing. Although a smaller interrogation window such as 16 × 16 pixels can provide more resolved information, it has an unacceptably high noise level.

3.2.4 Post-processing Method

As mentioned in the introduction, the average velocity field and turbulence statistics can be affected by the wandering motion of the vortex center. It is therefore important to track
For the flow in the MIVR, a single vortex center is observed for all realizations. The center of mass approach proposed by Ingvorsen et al.\cite{44} is adopted here to identify the vortex center. In detail, the function $W$, i.e., the magnitude of axial vorticity $W_z$ divided by in-plane velocity magnitude is calculated, and this should have its maximum value at the vortex center. The vortex center $\vec{R}$ is computed as the center of mass of all positions with $W_z$ larger than 0.95 of the maximum $W$ (Equation 3.4). The position of the vortex center is calculated for 5000 instantaneous velocity fields. One typical result of the wandering motion of vortex center is shown in figure 3.3 where the measurement is taken at four planes when $Re=3290$. Figure 3.3 is a scatter plot depicting all of the measured vortex center locations. It is found that the wandering motion of the vortex center before choosing an appropriate processing method.

Figure 3.3  Wandering motion of the vortex center at four planes when $Re=3290$. 

![Figure 3.3](image_url)
wandering motion of vortex centres is well constrained within a circle whose diameter is about 5% of the chamber diameter. The wandering range of the vortex center is found to be similar for all measurement planes. Using the measured locations of the instantaneous vortex center, two methods are applied here to investigate the effect of wandering motion on the ensemble-averaged velocity, TKE, and Reynolds stress. The first method (referred to as Method One) is to calculate these statistical features in a fixed frame centred at the geometric center of the reactor. In the second method (referred to as Method Two), each instantaneous result is transformed to a new frame where its vortex center is set as the origin. Interpolation based on a first-order Taylor expansion is used to make sure all measured points have the same coordinate after the transform. Statistical features are then determined based on the new set of 5000 instantaneous fields. Calculations using Method Two are limited to within 15% of the chamber diameter because the wandering motion has little influence on the velocity far away from the vortex center.

$$\vec{R} = \frac{\sum W_i \vec{r}_i}{\sum W_i}, \quad W = \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \sqrt{u_x^2 + u_y^2}$$  \hspace{1cm} (3.4)
al.[84] extracted velocity profiles along one line across the center of the measured plane. While this one-dimensional extraction can represent important features of the mean velocity field, it omits information from other orientations of the extraction segment and causes an asymmetric feature of velocity, especially the radial velocity, which cannot be observed in related simulation work[12; 6]. An alternative method of extracting information for a single profile is to consider values along different azimuthal angles. In practice, this is achieved by using more than one line across the measured plane. As it is shown in figure 3.4(a), 39 lines radiating from the vortex center can be used to divide the ensemble-averaged velocity field into several samples. Time-averaged velocities $u_r, u_\theta$ and $u_z$ along each line are then averaged together, providing a single profile of mean velocity and fluctuations. In figure 3.4(b), the dotted line shows the mean value of these 39 samples, and the error bars represent the standard deviation of velocities from polar angles ranging from 0 degree to 360 degrees, showing the variation of mean value with azimuthal direction. In this way, profiles of the radial, azimuthal and axial velocities are represented as functions of radial position only, making it easy to make comparisons for different flow conditions. It is found that these three velocities can be well represented by their average values due to the small scatter around the dotted lines, indicating that the ensemble-averaged velocity field is nearly axisymmetric.

3.3 Results and Discussion

3.3.1 Ensemble-average features of flow in the MIVR

Figure 3.5 shows example instantaneous and ensemble-averaged SPIV measurement results at all four measured planes for a Reynolds number of 3290. It can be seen that the instantaneous velocity shown in the left hand figure shows irregularities compared to the smooth streamlines in the right hand figure for the averaged velocity, indicating that flow has already become turbulent at $Re = 3290$. The streamlines in all the velocity fields reveal that the flow undergoes a spiral motion towards the center and a single vortex center is observed for all measurement planes. The pattern is clearer in the ensemble-averaged velocity fields. Far away from the vortex center, streamlines show that flow approaches the center through the spiral motion. Near the vortex
Figure 3.5 Typical instantaneous velocity fields at the four measurement planes (left) and corresponding ensemble-averaged velocity (right) when Re=3290. The magnitude of velocity is indicated by the colored contour. The solid lines are streamlines based on in-plane velocities.
center, the streamlines resemble concentric circles, indicating that the core-region is similar to a potential vortex where radial velocity becomes negligible.

Ensemble-averaged velocity is obtained using both Method One and Method Two previously introduced in the Post-processing section. To compare average velocity in different measurement planes, the radial, azimuthal, and axial velocity profiles are extracted from the SPIV measurements using the averaging method mentioned in the Post-processing section. These three velocities are then normalized by the bulk inlet velocity $U_j$. Figure 6 shows the comparison of these three velocities for the 1/4, 1/2, 3/4 and 7/8 planes. It is found that none of the ensemble-averaged velocities display any significant change between the use of Method One or Method Two. This finding reveals that the wandering motion of vortex center has little effect on the ensemble-averaged velocity, which is consistent with the finding in Ingvorsen et al.’s study[44] that ensemble-averaged velocity profiles of swirling flow obtained at a fixed frame could well represent the key flow features for a small wandering motion.

![Figure 3.6](image-url) Comparison of normalized mean velocity by Method One and Method Two when Re=3290. (a) Normalized mean radial velocity $\langle u_r \rangle / U_j$; (b) Normalized mean azimuthal velocity $\langle u_\theta \rangle / U_j$; (c) Normalized mean axial velocity $\langle u_z \rangle / U_j$.

Figure 3.6(a) shows normalized mean radial velocity $\langle u_r \rangle / U_j$ as function of radial position for all four planes. The radial velocity is much smaller in magnitude compared to the other two velocities $\langle u_\theta \rangle / U_j, \langle u_z \rangle / U_j$, and thus, its measurement uncertainty is higher compared to
the other two velocities, especially near the vortex center where a larger standard deviation is observed. In cylindrical coordinates, negative values of \( \langle u_r \rangle / U_j \) mean the direction of velocity is towards the center. For the 1/4, 1/2, 3/4 and 7/8 measurement planes, the radial velocity is found to be negative at positions far from the center. This is understandable due to conservation of mass, because flow from the inlets needs to exit through the outlet located at the center. This trend becomes much clearer for the 7/8 plane where the magnitude of \( \langle u_r \rangle / U_j \) starts to increase until it comes close to the edge of the exit (\( r/R_0 = 0.25 \)). As the flow approaches the center, \( \langle u_r \rangle / U_j \) at all planes begins to decrease and even becomes positive suggesting a recirculation zone near the center of the reactor. The largest positive \( \langle u_r \rangle / U_j \) is found in the 1/4 measurement plane.

Figure 3.6(b) shows the normalized mean azimuthal velocity \( \langle u_\theta \rangle / U_j \) for all four planes. The distribution of \( \langle u_\theta \rangle / U_j \) is nearly axisymmetric because its standard deviation is quite small. It can be seen that \( \langle u_\theta \rangle / U_j \) is almost the same for the different planes in terms of shape and magnitude, indicating that top and bottom walls of the chamber have little effect on this component of velocity. The profile of \( \langle u_\theta \rangle / U_j \) is similar to what is described by a simple vortex model such as the Lamb-Oseen vortex model or the batchelor vortex model[5]. Far from the vortex center, \( \langle u_\theta \rangle / U_j \) is in the free vortex region and is driven by the inlet momentum. As the flow moves towards the center, \( \langle u_\theta \rangle / U_j \) increases because of conservation of angular momentum. However, \( \langle u_\theta \rangle / U_j \) cannot increase infinitely as dissipation due to turbulence becomes significant close to the center. For radial distances smaller than a certain value, dissipation dominates the flow, and \( \langle u_\theta \rangle / U_j \) starts to decrease until it becomes zero in the vortex center.

Figure 3.6(c) shows the normalized mean axial velocity \( \langle u_z \rangle / U_j \) for all four planes. Far from the center, \( \langle u_z \rangle / U_j \) is found to be negligible, indicating that out-of-plane motion only becomes significant near the center of the MIVR, and thus flow far from the center can be assumed to be two-dimensional. It is also found that the area with apparent out-of-plane motion becomes larger for measurement planes closer to the top wall, indicating more flow exiting the chamber through top planes (once again, simply a consequence of conservation of mass). At radial locations close to the chamber center, \( \langle u_z \rangle / U_j \) starts to decrease and even becomes negative very close to the center. The negative magnitude of \( \langle u_z \rangle / U_j \) is further indication of back flow
near the reactor core (a recirculation region). This deficiency of axial velocity in the center is also observed in other confined turbulent vortex flows and can be affected by the diameter of the outlet[25]. It is observed that the profiles of $\langle u_\theta \rangle / U_j$ and $\langle u_z \rangle / U_j$ have identical peak magnitude locations and similar shapes for all measurement planes. This behaviour can be explained by the batchelor vortex model in which a change in the axial velocity must be accompanied by a change in the azimuthal velocity[5]. Recent work has shown that the mean velocity in the MIVR can be described by the superposition of two batchelor vortices [62].

![Image of mean flow pattern](image)

Figure 3.7 Mean flow pattern when Re=3290. The axial velocity is shown by the contour plot.

A visualization of the mean flow pattern in the mixing chamber of the MIVR is shown in figure 3.7. Due to optical access constraints, the X-Z plane shown in figure 3.7 has not been measured. Instead, it is constructed based on the information from X-Y planes. In practice, the velocity at four intersection lines between the X-Z plane and the measured plane, i.e., the X-Y plane, can be obtained from the SPIV measurement at the 1/4, 1/2, 3/4 and 7/8 planes. Based
on the information of velocities for these four planes, the velocity field in the X-Z plane has been constructed. Streamlines in the X-Y plane show that the flow moves toward the center in a spiral motion. Streamlines in the X-Z plane reveal how flow from the horizontal inlets comes to the vertical outlet. In detail, flow from the inlet first slowly moves towards the center and then accelerates as it escapes from the chamber. It can be seen that there is a small region of back flow in the vortex center. Most of the out-of-plane motion happens near the center area, and it is found that part of the back flow is reverted towards the exit by the outflow. The vortex flow is stabilized by the inlet momentum and centrifugal force, producing a pear shape of streamlines near the center at X-Z plane where flow goes outwards near the 1/4 plane and then inwards near the 3/4 and the 7/8 planes.

### 3.3.2 Turbulence Characteristics of Flow in the MIVR

Turbulence kinetic energy (TKE defined in Eq. (3.5)) is calculated using the measured root-mean-square velocity fluctuations.

\[ TKE = \frac{1}{2}\langle u'_i u'_i \rangle \]  

(3.5)

It is important to provide correct measured TKE as a reference for related CFD work. However, for flow in the MIVR, the measured TKE can be affected by the vortex wandering, resulting in a much higher measured TKE than the real turbulent fluctuation. That is because the instantaneous velocity near the center can be significantly changed by the vortex wandering. This change, referred to as pseudo-fluctuation, is more like a structure motion than a turbulent fluctuation and is due to the instantaneous unequal momenta of inlet flows\[34\]. This pseudo-fluctuation can contaminate the measured TKE in swirling flow, making it difficult to know the real turbulence strength inside the flow.

To investigate the influence of the pseudo-fluctuation on the measured TKE, Method One and Method Two are adopted here to calculate the TKE at all four measurement planes. The TKE is normalized by \( U_j^2 \). For both results, the TKE contour is found to be nearly axisymmetric in the measured plane and is presented in figure 3.8 in a way similar to that for the mean velocities. The TKE calculated by the two methods is found to be almost the same.
Figure 3.8  Comparison of normalized TKE by Method One and Method Two when Re=3290.
when the dimensionless radius $r/R_0$ is larger than 0.05, indicating that vortex wandering only affects the TKE in a small region near the center. When $r/R_0$ is smaller than 0.05, the TKE calculated by Method Two becomes smaller than that by Method One. This is because the wandering motion of the vortex center is eliminated by Method Two. The reduced percentage of the maximum TKE ranges from 17% to 30% for all four measurement planes. This finding shows that calculating the TKE without considering the vortex wandering will overestimate its value by up to 30%. The TKE by both methods begins to decrease with increasing plane height. For example, the maximum normalized TKE at the 1/4 plane is calculated to be 19 by Method Two, whereas it decreases to 7.57 at the 7/8 plane. It can be seen that TKE far away from the vortex center is quite small compared to that in the center. As the flow approaches the center, the TKE increases significantly. This non-uniform distribution of TKE suggests that most turbulent mixing happens near the center area where velocity fluctuations are strong.

![Figure 3.9](image1)

Figure 3.9 Comparison of normalized Reynolds normal stress by Method One and Method Two when $Re=3290$. (a) $\langle u'_r u'_r \rangle / U_j^2$; (b) $\langle u'_\theta u'_\theta \rangle / U_j^2$; (c) $\langle u'_z u'_z \rangle / U_j^2$.

These trends in the TKE can be further analysed by considering the distribution of normalized Reynolds normal stresses, i.e., $\langle u'_r u'_r \rangle / U_j^2$, $\langle u'_\theta u'_\theta \rangle / U_j^2$, $\langle u'_z u'_z \rangle / U_j^2$, which are shown in figure 3.9. It is found in figure 3.9 that only the in-plane Reynolds normal stresses, $\langle u'_r u'_r \rangle / U_j^2$
and \( \langle u'_r u'_r \rangle / U_f^2 \) show apparent differences between Method One and Method Two, indicating that only \( \langle u'_r u'_r \rangle / U_f^2 \) and \( \langle u'_q u'_q \rangle / U_f^2 \) are significantly affected by the wandering motion of the vortex center. These two Reynolds normal stresses calculated using Method Two have a value deficiency in the center and their profile is flatter than that found by Method One, especially in the 3/4 and 7/8 planes. The Reynolds normal stress \( \langle u'_z u'_z \rangle / U_f^2 \) shown in figure 3.9(c) is nearly the same in the two processing methods. It is found that \( \langle u'_r u'_r \rangle / U_f^2 \) and \( \langle u'_q u'_q \rangle / U_f^2 \) have approximately the same magnitude at the different measurement planes, whereas \( \langle u'_z u'_z \rangle / U_f^2 \) shows a clear decreasing trend from the 1/4 plane to the 7/8 planes and always has its maximum value in the center. Moreover, the Reynolds normal stress \( \langle u'_r u'_q \rangle / U_f^2 \) is found to be dissimilar to \( \langle u'_r u'_r \rangle / U_f^2 \) and \( \langle u'_q u'_q \rangle / U_f^2 \) with respect to the shape and magnitude of its curve along the radial coordinate, indicating that the turbulent fluctuations inside the MIVR are highly anisotropic.

The normalized Reynolds shear stresses, i.e., \( \langle u'_r u'_q \rangle / U_f^2 \) and \( \langle u'_r u'_z \rangle / U_f^2 \) and \( \langle u'_q u'_z \rangle / U_f^2 \) have also been compared between Method One and Method Two. Figure 3.10 shows the comparison of Reynolds shear stress at the 1/2 measurement plane when the Reynolds number is 3290. As the Reynolds shear stresses are not symmetric, they are presented in a contour plot. Although the two methods produce similar structures of shear stress, Method Two seems to provide more reasonable results with \( \langle u'_r u'_q \rangle / U_f^2 \) and \( \langle u'_r u'_z \rangle / U_f^2 \) being more symmetrical than those from Method One. Overall, the Reynolds shear stress is much smaller than Reynolds normal stress, indicating a weak correlation between the different fluctuations. \( \langle u'_r u'_q \rangle / U_f^2 \) is a measure of the fluctuation correlation between radial velocity and azimuthal velocity, which has negative and positive zones alternately located around the vortex center. \( \langle u'_r u'_z \rangle / U_f^2 \) has a similar alternating structure in the center whereas it is further surrounded by a negative zone outside. Unlike \( \langle u'_r u'_q \rangle / U_f^2 \) and \( \langle u'_r u'_z \rangle / U_f^2 \), \( \langle u'_q u'_z \rangle / U_f^2 \) is dominated by negative values with two negative zones located near the center. All the Reynolds shear stresses are found to have significantly non-zero values only near the center, which is consistent with the distribution of TKE and Reynolds normal stress.

In swirling flow, the turbulence field is typically anisotropic due to strong streamline curvature effects. For example, the turbulence field in a stirred tank has been evaluated based
Figure 3.10 Comparison of normalized Reynolds shear stress ($\langle u'_r u'_\theta \rangle / U_j^2$, $\langle u'_r u'_z \rangle / U_j^2$, $\langle u'_\theta u'_z \rangle / U_j^2$ (from top to bottom)) by Method One (left) and Method Two (right) when $Re=3290$. 
on PIV measurements, and the flow close to the impeller tip is found highly anisotropic[26]. The Reynolds stresses presented in figure 3.9 and 3.10 show that flow inside the MIVR is also highly anisotropic. For the strong swirling flow within the MIVR, it is valuable to determine the degree of anisotropy of the turbulence. Based on Reynolds stress results in the 1/2 measurement plane calculated by Method Two when Re=3290, two independent invariants, i.e., the quantities $\xi$ and $\eta$, are used here to characterize the Reynolds stress anisotropy, which is defined by Equation 3.6[76].

$$6\eta^2 = -2II_b, 6\xi^3 = 3III_b$$

(3.6)

where $II$ and $III$ are the second and third invariants of the normalized anisotropy tensor $b_{ij}$.

$$b_{ij} = \frac{\langle u_i' u_j' \rangle}{\langle u_k' u_k' \rangle} - \frac{1}{3} \delta_{ij}$$

(3.7)

Figure 3.11 shows the distribution of $\xi$ and $\eta$ (black points) in the Lumley triangle at 1/2 plane when Re=3290.

Figure 3.11 shows the distribution of $\xi$ and $\eta$ in the Lumley triangle[76]. It is found that the Reynolds stress in the 1/2 plane is far from the 3-D isotropic region; instead, most of the results are located near the center of the Lumley triangle, further confirming the anisotropic characteristic of the investigated flow.
Figure 3.12 Normalized TKE, mean axial velocity, and mean azimuthal velocity at the 1/2 plane (from top to bottom) as Reynolds number changes from 3290 to 8225.
3.3.3 The Effect of Reynolds Number

The Reynolds number is an important parameter for predicting the mixing performance of the MIVR. Previous researchers have claimed that sufficient mixing is achieved in the micro-scale MIVR when the Reynolds number based on the reaction chamber reaches 1600\cite{57}. Further increasing the Reynolds number will not improve the mixing performance significantly, and the mixing is limited by the geometry of reactor\cite{11}. For the macro-scale MIVR, it is necessary to investigate the influence of Reynolds number on the flow characteristics so as to provide guidelines for selecting the operating Reynolds number. As mentioned previously, four Reynolds numbers based on the inlet ranging from 3290 to 8225 have been investigated. Normalized mean azimuthal velocity $\langle u_\theta \rangle / U_j$, axial velocity $\langle u_z \rangle / U_j$ and $TKE/U_j^2$ can be compared for these Reynolds numbers. One typical result for the normalized mean velocity in the 1/2 measurement plane is shown in figure 3.12. As $\langle u_\theta \rangle$, $\langle u_z \rangle$ and TKE are scaled by $U_j$, the linear dependence on the Reynolds number is removed; thus the variation between different curves represents the non-linear influence of Reynolds number. $\langle u_\theta \rangle / U_j$ at different Reynolds numbers overlaps over most of the curve. Still, there is a change in the peak value of $\langle u_\theta \rangle / U_j$ where higher Reynolds number leads to higher peak value. Similar trends are observed for $\langle u_z \rangle / U_j$ where both the positive and negative maximum values increase as the Reynolds number increases. In terms of normalized TKE, the curves begin to overlap with each other when the Reynolds number is larger than 3290. The trends of $\langle u_\theta \rangle / U_j$, $\langle u_z \rangle / U_j$ and $TKE/U_j^2$ suggest that flow characteristics become more linearly dependent on Reynolds number with increasing Reynolds number. With higher Reynolds number, deviation from linear dependence should become even less significant.

3.3.4 Flow Patterns in the Micro-scale and Macro-scale MIVR

An interesting question in the current study is how the flow characteristics in the macro-scale MIVR compare with those in the micro-scale MIVR. Previous micro-PIV measurements for the micro-scale MIVR provide two-dimensional velocity fields at the 1/4, 1/2 and 3/4 measurement planes over a range of Reynolds numbers from 53 to 240\cite{84}. These measured
Figure 3.13 Comparison of normalized azimuthal velocity $\langle u_\theta \rangle / U_j$ between the micro-scale MIVR and the macro-scale MIVR.
Reynolds numbers correspond to laminar flow when $Re=53$ and $Re=93$, and turbulent flow when $Re=240$. In the laminar regime, the vortex center was found to be steady, whereas the vortex center wandered significantly in the turbulent regime. This finding reveals that the phenomenon of vortex wandering is related to the turbulent fluctuations in the flow. Figure 3.13 shows the comparison of normalized azimuthal velocity between the micro-scale MIVR and the macro-scale MIVR. Far from the vortex center, the normalized azimuthal velocities for $Re=240$ and $Re=3290$ are similar to each other. This is understandable as radial momentum flux should be equal to the inlet momentum flux near the outside wall of the mixing chamber. Swirl ratio is used here to relate flow in the two reactors. As it is defined in Equation 3.3, the swirl ratio for $Re=240$ is found to be 0.12 whereas it is 0.24 for $Re=3290$. Further examination reveals that swirl ratio in the macro-scale MIVR is weakly related to Reynolds number. Church et al.[14] classified tornado-like vortices based on the swirl ratio and provided qualitative observation of vortex configurations where the flow has moderate swirl when the swirl ratio is between 0.1 and 0.5. This observation based on swirl ratio predicts well the flow characteristic in the macro-scale MIVR, including the appearance of back flow in the center and a single-celled vortex core of flow. The swirl ratio in the micro-scale MIVR is only half of that in the macro-scale MIVR. For the case of the micro-scale MIVR, the swirl ratio of 0.12 indicates that the central core has a smooth, laminar appearance and that maximum axial velocity occurs on the central axis. As the swirl ratio is increased to 0.24 for the macro-scale MIVR, the reduced axial velocity in the center extends towards the bottom of the reactor, back flow appears, and the range of vortex wandering motion increases. Vortex breakdown is also predicted to exist in flows with moderate swirl ratio. However, this is not observed in the mixing chamber of both reactors, likely due to the confined geometry.

### 3.3.5 Micro-mixing Time in the Macro-scale MIVR

For a mixing sensitive technique like FNP, the mixing time of the reactor should be less than the nucleation and growth time of a nanoparticle. Thus, it is interesting to know how fast the mixing can occur in the macro-scale MIVR. Micro-mixing time is usually used to characterize mixing within a reactor[49; 57; 11]. Johnson et al.[49] defined a characteristic mixing time of
the CIJR as

$$\tau_m = \frac{1}{4} \left( \frac{\nu}{\epsilon} \right)^{1/2} \quad (3.8)$$

where $\nu$ is the kinematic viscosity of water and $\epsilon$ is the turbulence dissipation rate. Liu et al.[57] and Cheng et al.[11] modelled the micro-mixing time of the micro-scale MIVR as

$$\tau_m = \frac{TKE}{C_\phi \epsilon} \quad (3.9)$$

where $TKE$ is turbulence kinetic energy, and $C_\phi$ is the nominal value of the mechanical-to-scalar time scale ratio which is approximately 2 for the high Reynolds number flow here[11]. The two definitions of micro-mixing time in Equation 3.8 and 3.9 actually define the time-scales of eddies of different sizes in turbulent flow. Equation 3.8 is often referred to the Kolmogorov time-scale for eddies in the Kolmogorov scale. Equation 3.9 is sometimes referred to the integral time-scale for the larger, more energetic eddies[23]. The micro-mixing time defined by Equation 3.8 will be smaller than that defined by Equation 3.9. Turbulence dissipation rate is essential for both definitions and can be estimated from the experimental data. Because the resolved velocity spacing in the SPIV measurement is larger than the Kolmogorov scale, the turbulence dissipation rate is estimated by a large eddy PIV method.[83] In the large eddy PIV method, the dissipation rate can be estimated from the resolved strain rate tensor $\overline{S}_{ij}$ and the modelled sub-grid-scale (SGS) tensor $\tau_{ij}$.

$$\epsilon = 2C_s^2 \Delta^2 \langle |\overline{S}| \overline{S}_{ij} \overline{S}_{ij} \rangle \quad (3.10)$$

where $C_s = 0.17$ is the Smagorinksy constant and $\Delta = 8.22 \times 10^{-4} m$ is the low-pass filter width. The resolved rate tensor $\overline{S}_{ij}$ can be written as

$$\overline{S}_{ij} = \frac{1}{2} \left( \frac{\partial \langle u_j \rangle}{\partial x_i} + \frac{\partial \langle u_i \rangle}{\partial x_j} \right) \quad (3.11)$$

The gradient of in-plane velocity along the axial direction was not measured by SPIV and is assumed to be zero in the dissipation estimation, as the mean velocity field is found to be similar in different measurement planes. Vortex wandering is eliminated by using Method Two for the estimation of the turbulent dissipation rate. Figure 3.14(a) shows the Kolmogorov time scale $\tau_{sm}$ at the 1/2 measurement plane as a function of radial position, where $\tau_{sm}$ at different Reynolds numbers are compared. $\tau_{sm}$ decreases as the flow moves towards the center of the
reactor, and it decreases as the Reynolds number increases at all positions. Figure 3.14(b) presents the integral time scale $\tau_{lm}$ at the 1/2 measurement plane and shows a similar distribution as $\tau_{sm}$. However, as the Reynolds number increases from 3290 to 8225, $\tau_{lm}$ first increases and then decreases. The trend of $\tau_{lm}$ with Reynolds number is caused by the competition between turbulent kinetic energy and turbulent dissipation rate as both of them tend to increase as Reynolds number increases. A typical value of $\tau_{lm}$ in the macro-scale MIVR at Re=3290 ranges from 5 ms to 50 ms, whereas it ranges from 1 ms to 6 ms for the micro-scale MIVR at Re=240[11]. The increase of the modelled micro-mixing time suggests that the macro-scale MIVR will have a less effective mixing performance than the micro-scale MIVR with regard to the FNP technique. An important scale-up question is whether the mixing time can be decreased by increasing the Reynolds number. Figure 3.14(a) and 3.14(b) show that the Kolmogorov time scale and integral time scale all decrease as Reynolds number increases. However, this decrease is less significant for higher Reynolds number, indicating that the time-scale is becoming independent of Reynolds number. The integral time scale ranges from 2.8 ms to 26.6 ms for the highest investigated Reynolds number (Re=8225), which is still larger than those of the micro-scale MIVR.
3.4 Conclusion

An experimental investigation was performed to quantify the turbulent swirling flow within a scaled-up multi-inlet vortex reactor (MIVR). The flow characteristics were investigated using stereoscopic particle image velocimetry (SPIV). Four measurement planes in the mixing chamber were investigated for Reynolds numbers ranging from 3290 to 8225. The influence of vortex wandering on the mean velocity field and turbulence characteristics was assessed by using two different processing methods. Method One, which calculates velocity statistics in a fixed frame, was used as a control group for Method Two, where the vortex wandering was eliminated by keeping the instantaneous vortex center at the coordinate origin. Reynolds number effects were investigated by comparing flow characteristics at different Reynolds numbers. The main findings of the current work are as follows:

1. Turbulent swirling flow in the MIVR is unstable with its vortex center wandering in a small region whose diameter is about 5% of the chamber. The mean velocity field is found to be the same using either Method One or Two, indicating that the ensemble-averaged velocity is insensitive to the small wandering motion of the vortex center. The mean velocity field shows that flow from the inlet undergoes a spiral motion towards the center of the mixing chamber where most of the axial motion occurs. A recirculating back flow is observed near the center and is visible in all the measurement planes.

2. It is found that measured TKE and Reynolds stress are sensitive to the small wandering of the vortex center. The maximum value of TKE calculated by Method Two is reduced by 17% to 30% at all four measurement planes compared to that by Method One. Detailed analysis of the Reynolds normal stress shows that the vortex wandering only affects the in-plane normal stresses. Method Two is also found able to provide more reasonable Reynolds shear stress measurements than Method One. As the vortex wandering produces pseudo-fluctuations, it is important to separate the wandering from the turbulent fluctuations. The Reynolds stress tensor is found to be highly anisotropic; thus related CFD work using an isotropic turbulence model may fail to capture the correct flow characteristics in the MIVR. Reynolds number effects are observed for all investigated Reynolds numbers in terms of mean velocity and TKE.
However, this effect decreases as the Reynolds number increases.

3. Swirl ratio is used to describe the swirling strength of the flow. The swirl ratio of flow in the macro-scale MIVR is found to be insensitive to the Reynolds number. Flow characteristics in the reactor can be described as a function of swirl ratio. The swirl ratio is found to be 0.12 for the micro-scale MIVR and 0.24 for the macro-scale MIVR. The small swirl ratio makes flow in the micro-scale reactor have a laminar-appearing central core and no back flow in the center of the reactor. As the swirl ratio increases, as in the macro-scale MIVR, a recirculating back flow appears in the center, and the vortex wanders around a larger region near the reactor center.

4. The scaled-up reactor also has a corresponding increase in theoretical micro-mixing times, suggesting it to be less mixing effective than the micro-scale MIVR for such processes as Flash Nanoprecipitation. However, further studies of mixing, including those with FNP, need to be made in order to determine the effectiveness of the macro-scale MIVR.
CHAPTER 4. DYNAMIC DELAYED DETACHED EDDY SIMULATION OF A MULTI-INLET VORTEX REACTOR

A paper modified from a publication in *AICHE Journal* ¹

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Abstract

The multi-inlet vortex reactor (MIVR) has been used for flash nanoprecipitation to manufacture functional nanoparticles. A validated computational fluid dynamics model is needed for the design, scale-up, and optimization of the MIVR. Unfortunately, available Reynolds-averaged Navier-Stokes methods are unable to accurately model the highly swirling flow in the MIVR. Large eddy simulations (LES) are also problematic, as excessively fine grids are required to accurately model this flow. These dilemmas led to the application of the dynamic delayed detached eddy simulation (DDES) method to the MIVR. In the dynamic DDES model, the eddy viscosity has a form similar to the Smagorinsky sub-grid viscosity in LES, which allows the implementation of a dynamic procedure to determine its model coefficient. Simulation results using the dynamic DDES model are found to match well with experimental data in terms of mean velocity and turbulence intensity, suggesting that the dynamic DDES model is a good option for modelling the turbulent swirling flow in the MIVR.

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4.1 Introduction

Chemical reactors for rapid mixing have been investigated intensively as they are required in certain precipitation reactions, including semi-batch stirred tank precipitators and impinging jet precipitators.[32; 4; 67] The multi-inlet vortex reactor (MIVR) was originally designed as a microscale chemical reactor used to produce functional nanoparticles in the flash nanoprecipitation (FNP) technique where rapid mixing is required.[57] The MIVR achieves fast mixing of streams from different inlets by inducing turbulent swirling flow into the reactor. The reactor consists of four inlets, one mixing chamber, and one outlet. Due to the arrangement of the inlets and the mixing chamber, the MIVR can provide good mixing at high Reynolds numbers and its mixing performance is insensitive to inlet flow rates of the individual streams, a superior feature compared to another reactor developed for the FNP technique, i.e., the confined impinging jet reactor (CIJR).[49; 59; 18] A natural question, which has not been answered, concerning the microscale MIVR is if it can be scaled up to larger dimensions without sacrificing its mixing performance.[68] In order to answer this question, a scaled-up prototype of the MIVR has been built and investigated experimentally using stereoscopic particle image velocimetry (SPIV).[64] The experimental measurements reveal a number of interesting phenomena about the complex swirling flow in the MIVR. For example, a wandering motion of the vortex center was found to exist in the flow, and this wandering motion affects the measured turbulence kinetic energy and Reynolds stresses significantly. Despite the abundant information provided by the SPIV measurements, the understanding of the true three-dimensional structure of flow inside the reactor is still limited. Important parameters such as turbulent dissipation rate can only be obtained through approximations. A reliable numerical simulation of the scaled-up reactor is thus necessary to gain deeper understanding of the fundamental flow physics. Moreover, such simulations can be used to optimize the design and performance of the reactor.

The flow motion inside the MIVR is a turbulent swirling flow. Turbulent swirling flows play a very important role in industrial applications such as gas-particle separation, combustion and fluid mixing. However, the turbulence in swirling flow is difficult to model. These challenges are mainly caused by significant streamline curvature existing in swirling flow. Streamline
curvature affects turbulence structure by adding additional rate of strain into the flow, which in turn produces significant changes in turbulence kinetic energy production and distribution. These extra strain rates include lateral divergence, normal divergence, bulk compression, and rotation of whole flow system about the rotation (z) axis.[7] In the MIVR, flow undergoes helical motion towards the outlet. The sudden contracting geometry in the outlet of the MIVR also produces lateral and normal divergence. Thus all the additional strain rates except bulk compression will exist in the flow field of the MIVR, which makes successfully simulating the flow difficult.

Large eddy simulation (LES) is usually able to produce satisfactory results for the mean velocity and turbulent structure for turbulent swirling flow.[96; 65; 55] Cheng et al. and Ben-said et al. have used LES to simulate the flow in the microscale MIVR.[6; 12] However, LES becomes very expensive when simulating the wall-bounded flow in the MIVR as the Reynolds number increases greatly in the scaled-up reactor. With limited computational resources, it is impractical to apply LES in analysing scaled-up processes in the MIVR due to the fact that a large number of cases need to be run with different parameters for design and optimization. Alternatively, Reynolds-averaged Navier-Stokes (RANS) simulations with curvature correction in the eddy-viscosity models, or second-moment closure models, are popular options for simulating turbulent swirling flow. A few applications using an eddy-viscosity model with curvature correction include Cheng et al. who used the flux Richardson number to represent the effect of longitudinal curvature and proposed an algebraic formation for the eddy viscosity in the k-epsilon model[10], Petterson Reif et al. applied curvature correction to the v2-f model based on calibration in rotating homogeneous shear flow [75], which was further used to model tip vortex flows and reasonable agreement of mean velocity field was achieved with experiments.[22] Compared to the eddy-viscosity model, second-moment closures are inherently capable of capturing rotational and swirl effects as they contain exact terms for rotation effects in the Reynolds-stress equations. Hu et al. utilized an IPCM (isotropization of production and convection model) Reynolds-stress model with modified coefficients to model the swirling flow in a cyclone separator.[42] Jakirlic et al. performed a systematic survey of the performance of second-moment closures in a range of rotating and swirling flows. Though superior to eddy-
viscosity models, second-moment closure models were still found to be unable to predict some key features such as capturing the transition from a free vortex to solid-body rotation in a long straight pipe with a weak swirl, or reproducing the normal stress components in the core region.[46]

The main problem with models using modified eddy viscosity is that they may only work for particular cases because these model coefficients are specifically tuned for a certain case. Hybrid RANS/LES is a promising method, which is able to improve the performance of RANS models while requiring less computational resources compared to LES.[45] Detached eddy simulation (DES) falls into the category of hybrid RANS/LES methods. DES was originally developed to avoid the high grid requirement in LES by employing RANS in the near-wall region and an eddy-resolving simulation in regions away from the wall.[89] The original DES method could have artificial grid-induced separation when the eddy-simulation mode took place inside the boundary layer where the resolved Reynolds stresses have not replaced the modelled Reynolds stress.[71] Delayed DES (DDES) was then proposed to solve this issue by using a shielding function to prevent the model from switching to eddy simulation near boundary layers.[88] Recently, Reddy et al. developed a new variant of the DDES model by clipping the length scale to the eddy viscosity in the model, making the eddy simulation more similar to LES.[78] Furthermore, Yin et al. implemented a dynamic procedure to compute the coefficient used in the eddy simulation, resulting in the dynamic DDES model. This dynamic DDES model adapts its coefficient according to how well turbulence is resolved, thus maximizing the resulting eddy-simulation region.[100] Recent advances in the DDES model provide a powerful tool for simulating turbulent swirling flows, which can possess the accuracy of LES while having a computational cost closer to RANS. In the current study, the dynamic DDES method is used to simulate flow inside the MIVR. A precursor simulation was first run to obtain the fully developed flow for the inlets of MIVR. Both steady and unsteady inlet conditions were tested for the simulation. The simulation results are validated by comparison with our SPIV measurements.
4.1.0.1 Experimental Setup and Measurement Method

The experimental set-up shown in figure 4.1 depicts how the flow field inside the MIVR was measured using SPIV. Individual inlet steams are pumped to the four inlets of the MIVR, and their flow rates are controlled by four automatic control valves. The MIVR is made of acrylic glass to provide optical access from all directions. As shown in figure 4.2, the four inlets are tangentially aligned to the chamber. The cross section of the inlets is square measuring 25.4 mm in width and 870 mm in length. The outlet is a round pipe with 25.4 mm diameter and 1067 mm length. The mixing chamber is 25.4 mm in height and 101.6 mm in diameter.

Measurements were taken in the mixing chamber and inlets using SPIV. The flow was seeded with hollow glass spheres and illuminated by a double-pulsed Nd:YAG laser. Two 12-bit double-frame CCD cameras were used to capture images for the SPIV measurements. A detailed description of the related experimental work can be found in Liu et al.[64] Experimental data at four Reynolds numbers were collected. However, only Reynolds number 6580 based on the inlet geometry will be used in this study as the main purpose is to evaluate the dynamic...
DDES model for flow inside the MIVR. Thus, evaluation of the Reynolds number influence on the mixing performance of the MIVR is outside the scope of this paper, but will be addressed in future work.

4.2 Modelling Approach

4.2.1 Dynamic DDES model

The dimensionless filtered Navier-Stokes equations can be expressed as (repeated indices imply summation)

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0$$ (4.1)

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial \overline{u}_i}{\partial x_j} \right) - \frac{\partial \tau_{ij}}{\partial x_j}$$ (4.2)

where $\tau_{ij}$ is the Reynolds-stress tensor in the RANS mode and turbulent sub-grid stress (SGS) tensor in the LES mode, and it is modelled as

$$\tau_{ij} = 2\nu_T S_{ij} - \frac{2}{3} k \delta_{ij}$$ (4.3)

where $S_{ij}$ is the mean strain-rate tensor. The dynamic DDES model[100] is based on clipping the production rate of the k-ω RANS model. In the DDES model, the turbulent eddy viscosity term in the k-ω model is replaced by the production of the square of the length scale and $\omega$. When using the RANS length scale, the simulation runs in a RANS mode. However, if the
length scale is the LES length scale, the simulation runs in an LES mode. Except for the wall area, the selection of the mode is determined by the magnitude of the RANS and LES length scales and, in principle, the smaller length scale is used. A shielding function is employed to ensure that the RANS mode will always be selected in the near-wall region. Here, the $k$-$\omega$ RANS model\cite{99} given by

\[
\frac{Dk}{Dt} = 2\nu_T |S|^2 - C_\mu k \omega + \nabla [(\nu + \sigma_k (k/\omega)) \nabla k]
\]  \hfill (4.4)

\[
\frac{D\omega}{Dt} = 2C_\omega 1 |S|^2 - C_\omega 2 \omega^2 + \nabla [((\nu + \sigma_\omega (k/\omega)) \nabla \omega]
\]  \hfill (4.5)

is used with the standard constants: $C_\mu = 0.09, \sigma_k = 0.5, \sigma_\omega = 0.5, C_\omega 1 = 5/9, C_\omega 2 = 3/40$.

The only change in the current DDES model compared to the traditional RANS mode is the turbulent viscosity appearing in equation 4.4, which is defined by

\[
\nu_T = l_{DDES}^2 \omega, l_{DDES} = l_{RANS} - f_d max(0, l_{RANS} - l_{LES}), l_{RANS} = \frac{\sqrt{k}}{\omega},
\]  \hfill (4.6)

where $V$ is the cell volume, $h_{max} = max(dx, dy, dz)$ is the maximum cell spacing, and $f_d$ is the DDES shielding function. It is worth mentioning that the equation for the grid size $\Delta$ helps alleviate the log layer mismatch problem. For this purpose, the shielding function is defined by

\[
f_d = 1 - \tanh((8r_d)^3), r_d = \frac{k/\omega + \nu}{\kappa^2 d_w^2 \sqrt{U_{i,j} U_{i,j}}},
\]  \hfill (4.7)

where $\nu$ is the kinematic viscosity, $\kappa$ the von Krmn constant, $d_w$ the wall distance, and $U_{i,j}$ the velocity gradient tensor (repeated indices imply summation).

A dynamic procedure gives the empirical constant $C_{DES}$ of the eddy simulation adaptively. This procedure also ensures that $C_{DES}$ becomes a default number as the dynamic procedure is likely to fail on coarse meshes where the inertial range has not been resolved. Specifically, the dynamic procedure is defined as follows:

\[
C_{DES} = max(C_{lim}, C_{dyn}), C_{dyn}^2 = max(0, 0.5 \frac{L_{ij} M_{ij}}{M_{ij} M_{ij}}),
\]  \hfill (4.8)

\[
M_{ij} = \Delta^2 \frac{\omega S_{ij}}{\omega S_{ij}} - \Delta^2 \frac{\omega S_{ij}}{\omega S_{ij}}, L_{ij} = \hat{\omega}_i \hat{\omega}_j - \hat{\omega}_i \hat{\omega}_j
\]

\[
C_{lim}^2 = C_{DES}^0 \left[1 - \tanh(\alpha \exp(\frac{-\beta h_{max}}{L_k}))\right], L_k = \left(\frac{\nu^3}{\epsilon}\right)^{1/4},
\]  \hfill (4.9)

\[
\epsilon = 2(C_{DES} h_{max})^2 \omega |S|^2 + C_\mu k \omega, C_{DES}^0 = 0.12, \alpha = 25, \beta = 0.05
\]
The dynamic DDES model was implemented into the open-source computational fluid dynamics (CFD) code OpenFOAM. A second-order, backward-difference method was used for time integration. Gradients were discretized with second-order accuracy, accounting for non-orthogonal corrections. The divergence scheme for \( k \) and \( \omega \) is limitedLinear, which is a central scheme with the Sweby limiter [93]. The divergence terms for other variables are discretized using a second-order central scheme. The Laplacian scheme is second-order accurate. The generalized geometric-algebraic multi-grid (GAMG) solver is used as the linear system solver for the pressure equation and the Gauss-Seidel algorithm is used for other variables including velocity, \( k \) and \( \omega \). The solution for the system of partial conservation equations was obtained, at each time-step, by solving iteratively, to a specified tolerance of the residual norm.

### 4.2.2 \( k-\omega \) SST model with curvature correction

In addition to the dynamic DDES model, a \( k-\omega \) model with curvature correction was also used in simulations of the MIVR. The \( k-\omega \) SST model with curvature correction[2] is based on the idea that the model should behave close to second-moment closures (SMC) under a swirling or systematic rotating situation. The original SST variant of the \( k-\omega \) model[70] can be written as

\[
\frac{Dk}{Dt} = 2\nu_T|S|^2 - \beta^* k\omega + \nabla[(\nu + \sigma_k \nu_T)\nabla k] \tag{4.10}
\]

\[
\frac{D\omega}{Dt} = 2\gamma|S|^2 - \beta\omega^2 + \nabla[(\nu + \sigma_\omega \nu_T)\nabla \omega] + CD_\omega \tag{4.11}
\]

where the eddy viscosity is \( \nu_T = C_\mu k/\omega \) with \( C_\mu = 1, \beta^* = 0.09, \sigma_k, \gamma, \beta \) and \( \sigma_\omega \) are blending terms between the \( k-\omega \) and \( k-\epsilon \) models and \( CD_\omega \) is the cross-diffusion term. Considering the curvature effect, the eddy viscosity coefficient has the form

\[
C_\mu^* = C_\mu(\alpha_1(|\eta_3| - \eta_3) + \sqrt{1 - \min(\alpha_2\eta_3, 0.99)})^{-1} \tag{4.12}
\]

where \( \eta_1 = S_{ij}^* S_{ij}, \eta_2 = \Omega_{ij}^* \Omega_{ij}^* \) and \( \eta_3 = \eta_1 - \eta_2 \). \( S_{ij}^* \) is the dimensionless rate of strain and \( \Omega_{ij}^* \) is the dimensionless rate of rotation. \( \alpha_1 = 0.04645, \alpha_2 = 0.25 \) and \( C_\mu^* \) is limited to a maximum value of 2.5 to avoid excessive turbulent diffusion. More information regarding the dimensionless rate of strain and rotation can be found in [75; 2; 24]. The simulation using the
modified k-ω SST model was run as an unsteady RANS simulation. It is worth mentioning that the primary focus of current paper is on the dynamic DDES model. Results predicted by the modified k-ω SST model are mainly used for comparison. Accordingly, the following contents are primarily about simulation using the dynamic DDES model, and thus concern the dynamic DDES model unless the modified k-ω SST model is mentioned explicitly.

4.2.3 Boundary and inlet conditions

The investigated Reynolds number is 32,000 based on the outlet geometry (round tube) of the reactor and the bulk flow rate. All four inlets have the same flow rates. The simulated geometry of the MIVR is shown in figure 4.3. The outlet pipe has been made long enough to encompass any recirculation zones that may exist in the outlet. As the inlet channel in the experiment is about 870 mm long and is long enough for the inlet flow to fully develop, the inlet condition is modelled as fully developed for the reactor simulation. To obtain this developed inlet flow profile, a precursor simulation using a 160 mm long square duct was first conducted. The outflow is mapped back to the inlet so as to reach fully developed condition with relatively low computational cost. In each inlet, the bulk Reynolds number is 6580 and the dynamic DDES model is used as a turbulence model where grid resolution near the wall regions is fine enough so no wall functions must be used.

The velocity field in the middle section of the inlet channels has been measured using PIV. These experimental data are used to validate the simulation results. It is well known that flow in a square duct has mean secondary flow patterns near its corners, which are caused by the anisotropy and inhomogeneity of Reynolds stresses.[43; 66] Although these secondary velocities are usually only 1%-3% of the stream-wise velocity, they significantly alter the momentum and scalar transport phenomenon near the wall. Thus, it is important for the turbulence model to capture this secondary pattern. As shown in figure 4.4, eight vortices are predicted near the corners in the contours of mean velocity, indicating the secondary flow pattern is successfully reproduced by using the dynamic DDES model. In figure 4.4 the mean velocities in both the X and Y directions are compared with PIV results along the profile across the inlet center and overall good agreement is observed. Note that the cross-stream velocity is much smaller
Figure 4.3  Simulation domain.

Figure 4.4  Comparison of mean streamwise (left) and spanwise (center) velocity components between PIV measurement and dynamic DDES model, and contour of mean streamwise velocity (right).
than the stream-wise velocity, and these small velocities can be difficult to measure with PIV. Despite this difficulty, simulation and experiment are seen to agree very well. Figure 4.5 shows a comparison of the Reynolds stresses. Again, there is overall good agreement between CFD and PIV.

Figure 4.5 Comparison of Reynolds stresses (left: xx, center: yy, right: xy) between PIV measurement and dynamic DDES model.

Once the fully developed flow profile is obtained, two types of inlet conditions can be applied to the MIVR. One inlet condition technique is to map a slice of the precursor inlet simulation onto the inlets of MIVR. Using this technique, the simulation of the MIVR will have a steady inlet condition. It is easy to implement this boundary condition, but the potential disadvantage is that it may not provide the correct fluctuation level for the inlets. The second technique is to generate an unsteady inlet condition based on the profile given in the precursor simulation, which can still preserve the essential properties of the flow. For this purpose, the digital filter method of Klein et al is used.[51] This method has also been used to simulate flow in a confined jet reactor using LES.[73; 52] For fluctuating inlet conditions, this turbulent inlet method can give a good estimation of the inflow profile. The turbulent inlet velocity is constructed based on the mean velocity and Reynolds stresses obtained from the precursor simulation as follows:

\[ U_i = \bar{U}_i + a_{ij} U_j \]  

(4.13)

where \( \bar{U}_i \) is the mean inflow velocity, \( U_j \) is a provisional three-dimensional signal that possesses
prescribed two-point statistics, and

$$a_{ij} = \begin{bmatrix} \sqrt{R_{11}} & 0 & 0 \\ R_{21}/a_{11} & \sqrt{(R_{11} - a_{21}^2)} & 0 \\ R_{31}/a_{11} & (R_{32} - a_{21}a_{31})/a_{22} & \sqrt{(R_{33} - a_{31}^2 - a_{32}^2)} \end{bmatrix}$$

(4.14)

$$U_j(m,n) = \sum_{i'=-N_x}^{N_x} \sum_{j'=-N_y}^{N_y} \sum_{k'=-N_z}^{N_z} b(i',j',k') \Re(i',m+j',n+k')$$

(4.15)

where $\Re$ is a series of three-dimensional random fields and the filter coefficient $b$ has the form

$$b(i,j,k) = b_i b_j b_k$$

(4.16)

By assuming the autocorrelation function of $U_j$ to have the same form as homogeneous turbulence, the filter coefficient can be approximated as

$$b_k \approx \overline{b_k} / (\sum_{j=-N}^{N} \overline{b_j^2})^{1/2}, \overline{b_k} = \exp(-\pi k^2 / 2n^2)$$

(4.17)

The length scale in each dimension should be provided as input values with $L_x = n_x \Delta x, L_y = n_y \Delta y$ and $L_z = n_z \Delta z$. To guarantee the approximation accuracy of the filter coefficient, the dimension of the random fields should satisfy $N_a = 2n_a, a = x, y, z$. This turbulent inlet method has been implemented into OpenFOAM and applied to all four inlets of the MIVR in the unsteady inflow case.

At the outlet, boundary conditions for most terms are zero gradient except for the pressure, since the outlet pipe in the experiment is long enough (about 1000 mm) to have flow field fully developed. The pressure condition in the outlet has a fixed mean value, which allows for radial variation of pressure due to the swirling motion. The no-slip boundary condition is applied on the walls. The low-Reynolds-number wall function implemented in OpenFOAM was used for turbulent kinetic energy near the wall as the mesh size cannot guarantee y-plus less than 1 everywhere.
4.3 Results and Discussion

4.3.1 Instantaneous velocity profiles

The streamlines of one typical instantaneous flow field from the simulation are presented in figure 4.6. The flow in the MIVR moves mainly in a helical motion. As can be seen in the streamlines at $Z=0.06$ m, this swirling motion is preserved quite well by the confined geometry and does not significantly dissipate as flow moves through the reactor. Vortex breakdown does not occur in the simulation domain. This phenomenon is different from the case where swirling flow enters a sudden expansion area. In a sudden expansion area, swirling motion decays much faster, and vortex breakdown is usually observed downstream of the expansion.[96; 65] The center of the swirling motion, i.e., the vortex center, also wanders around just as has been observed in other swirling flows.[44] This wandering movement is found to be a small random motion rather than a preceding motion and no distinct frequency exists. In the streamlines at $X=0$ m, a low velocity area is observed near the center region where a recirculation appears. In other corner locations, small recirculation zones are also observed.

4.3.2 Mean velocity profiles

Figure 4.7 shows the contours of the shielding function, $f_d$, and the eddy-simulation region in the center slice of the simulation results. As is expected, the shielding function is close to zero near the wall and returns to one when it is away from the wall. This result guarantees the...
Figure 4.7  Dynamic DDES shielding function and eddy simulation branch on the center slice.
RANS mode will always be used near the wall. However, the selection of eddy-simulation mode away from the wall is determined by the ratio of the LES length scale, $C_{DES}\Delta$, over the RANS length scale, $\sqrt{\bar{k}}/\omega$. For the current CFD work, not every location away from the wall has a grid fine enough to turn on the eddy-simulation mode, especially near the bottom of the outlet region. Although these RANS locations can be eliminated by further refining the mesh size, the main consideration here is to achieve accurate CFD predictions without consuming excessive computational resources, and thus such a grid refinement was not found to be necessary.

Figure 4.8 shows the radial distributions of the time-averaged radial, axial, and azimuthal velocity components at three measurement planes, $z/H = 1/4$, 1/2 and 3/4. The error bar at each point indicates the variance of the mean result that comes from performing this time average along different azimuthal angles. Simulation results using the dynamic DDES model with steady (DDES_S) and unsteady (DDES_T) inlets are compared with SPIV measurement. Overall, reasonable agreement is observed between simulations and experimental measurements. The dynamic DDES model with unsteady inlet conditions gives a better prediction for the mean velocity field, especially the radial velocity at the 1/4 plane. This is expected, as the unsteady inlet condition is closer to the physical situation and is thus usually recommended in an eddy simulation. The $k-\omega$ SST model with curvature correction did a fairly accurate job predicting the mean velocity in the region away from the center. However, near the reactor center,
the azimuthal velocity is significantly underestimated and the declining trend of axial velocity cannot be captured. The RANS modelling tends to predict premature laminarization of the flow by adding excessive turbulent diffusion. The flow in the chamber is dominated by the azimuthal velocity, where peak radial velocity is much smaller than the other two components, and axial velocity is almost zero away from the center region \((r/R_0 > 0.3)\). Based on the distribution of the azimuthal velocity, flow can be divided into two main regions, a forced vortex region and a free vortex region. Near the reactor center, the azimuthal velocity corresponds to a forced vortex. Outside of the location of the peak azimuthal velocity, the azimuthal velocity resembles a free vortex. It is observed that the mean axial velocity has similar profiles as the azimuthal velocity.

It has been previously found that the mean azimuthal and axial velocity profiles can be well represented by a simple model combining two Batchelor vortices.\cite{62} This gives a physical description of the swirling flow in the MIVR as combinations of canonical vortex flows. The peak location of the azimuthal velocity is slightly underestimated, that is, it is found to be closer to the reactor center by the dynamic DDES model, indicating a higher swirling ratio in the experimental results. This deficiency may be attributed to the RANS part of the dynamic DDES model being an eddy-viscosity model and this tending to cause premature laminarization in swirling flow.\cite{46} When a laminar-like solution is obtained in the CFD simulation, the swirling ratio decreases, which causes a smaller peak location of the azimuthal velocity profile. The underestimated swirling ratio also helps explain the relatively large negative axial velocity in SPIV results as back flow is closely related to swirling ratio \cite{14}.

Figure 4.9 shows the velocity magnitude of flow inside the MIVR. Due to the confined geometry, no vortex breakdown is observed, and the swirling pattern of flow persists in the whole domain of the outlet pipe. Furthermore, the iso-surface of \(U_z = -0.1 \text{ m/s}\) clearly shows the existence of a recirculation zone in the center of the reactor, which extends from the reactor bottom to the outlet pipe. The appearance of this recirculation zone can be explained by the pressure distribution in the flow. It is shown in figure 4.9 that the density normalized mean pressure has the lowest value near the lower center area of the chamber. This negative pressure attracts flow from both the inlets and the outlet, helping to form the back flow in the reactor.
Figure 4.9  Velocity magnitude (left) with iso-surface of axial velocity $U_z = -0.1$ m/s and normalized mean pressure contour in the center slice (center: DDES, right: k-omega).

center. The modified k-ω SST model predicts a much higher pressure in the center, suppressing the appearance of this back flow. Another recirculation area is also identified near the corner of the outlet entrance, which is caused by the sudden turning of the flow there.

4.3.3 Turbulence intensities

Figure 4.10 shows the radial distribution of normalized turbulence intensity components at three measurement planes, $z/H = 1/4$, 1/2 and 3/4. Again, the error bar at each point represents the variance of the mean result calculated along different azimuthal angles. The dynamic DDES model with steady (DDES_S) and unsteady (DDES_T) inlet conditions give almost the same predictions, indicating the fluctuation of inlet flow has little impact on the turbulence intensity of flow inside the chamber. Overall, reasonable agreement is observed between the simulation using dynamic DDES model and experimental results. The predicted radial and azimuthal turbulence intensities show good agreement with SPIV data. However, the axial turbulence intensity is underestimated in the simulations, especially near the reactor
center. This discrepancy could be caused by the measurement noise in SPIV and the unsolved vortex core motion in simulation. Near the center of the reactor, the gradients of azimuthal and axial velocity become large, and in such high-gradient regions, the SPIV measurement could have high correlation noise.[95] This correlation noise could explain why high turbulence intensity is observed in the center area. When vortex core motion is not well captured, the predicted turbulent intensity will also deviate from experimental data. The $k$-$\omega$ SST model with curvature correction gives almost identical results as the dynamic DDES model in the region away from the center ($r/R_0 > 0.2$). However, it underestimates the turbulence intensities significantly near the center. The wandering motion of the vortex center and anisotropic features of turbulence seem to be the reasons causing the failure of the RANS simulation.

The measured turbulence intensity in the current swirling flow can be attributed to both the pure turbulence phenomena and coherent structure bulk motion, i.e., precessing vortex core phenomenon or vortex wandering motion. The coherent structure motion tends to increase the measured turbulence intensity near the center of swirling flow. This contribution can be removed by freezing the vortex wandering motion during the calculation of turbulence intensity.[64] It is found that the vortex wandering motion mainly increases the radial and azimuthal turbulence intensities near the center. This finding suggests that the turbulence intensity near the vortex center should decrease if only the pure turbulence phenomenon is
considered. This argument actually agrees with the streamline curvature effect on turbulence intensity. Turbulence will be stabilized in the forced vortex region by the mean velocity distribution while being destabilized in the free vortex region by the centrifugal force.[40] just like the prediction by the k-ω SST model with curvature correction.

Figure 4.11 shows contours of resolved Reynolds normal stress and modelled turbulent kinetic energy. The highest Reynolds stress is primarily concentrated near the reactor center. However, for the stress $R_{zz}$, its value decays rapidly as flow advects downstream. The highly anisotropic feature of the turbulence is also observed as the contour of $R_{zz}$ is significantly different from $R_{rr}$ and $R_{tt}$. The resolved Reynolds stress is much larger than the modelled TKE, indicating that most of turbulence intensity is captured by the eddy-simulation mode. This actually is to be expected as the eddy-simulation mode can reduce the shortcomings of the RANS model, enabling the dynamic DDES model to accurately predict the key features of the turbulent swirling flow in the MIVR.
4.4 Conclusions

Turbulent swirling flow in the MIVR is affected by both vortex wandering motion and streamline curvature, which makes a successful simulation difficult. In the current study, a dynamic DDES model was applied to model this flow. Both steady and unsteady inlet conditions are used and a small improvement of predicting the mean velocity is observed in the unsteady inlet case. Overall, the simulation results agree quite well with the experimental results in terms of the mean velocity and turbulence intensities. The recirculating back-flow occurring at the center of MIVR is also captured by the dynamic DDES model. The existence of back-flow is likely caused by the scale-up process and has not been reported previously in the microscale MIVR. The recirculation in the larger reactor could potentially cause a wider particle size distribution in the FNP technique and thus future work is needed to optimize the geometry of MIVR to eliminate the back mixing at the center. For comparison, a k-ω SST model with curvature correction has been used to simulate flow in the MIVR. Even with the curvature correction, the k-ω SST model is unable to accurately predict the flow field near the reactor center. As the vortex wandering and anisotropic turbulence features exist there, it is not surprising that the RANS model fails. The superior performance of the dynamic DDES model confirms that it can reduce the drawbacks inherent to the RANS model and can be a good alternative for studying complex turbulent swirling flows.
CHAPTER 5. TURBULENT MIXING IN THE CONFINED SWIRLING
FLOW OF A MULTI-INLET VORTEX REACTOR

A paper under review in AICHE Journal

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Abstract

Turbulent mixing in the confined swirling flow of a multi-inlet vortex reactor (MIVR) was investigated using planar laser induced fluorescence (PLIF). The investigated Reynolds numbers based on the bulk inlet velocity ranged from 3290 to 8225, and the Schmidt number of the passive scalar was 1250. Measurements were taken in the MIVR at three different heights (1/4, 1/2 and 3/4 planes). The mixing characteristics and performance of the MIVR were investigated using instantaneous PLIF fields and point-wise statistics such as mixture fraction mean, variance, and one-point concentration probability density function (PDF). It was found that the scalar is stretched along velocity streamlines, forming a spiral mixing pattern in the free-vortex region. In the forced-vortex region, mixing intensifies as the turbulent fluctuations increase significantly there. The mixing mechanisms in the MIVR were revealed by identifying specific segregation zones. At Re=8225 the mixing in the free-vortex region was dominated by both large-scale structures and turbulent diffusion, while in the forced-vortex region mixing is dominated by turbulent diffusion.

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5.1 Introduction

Turbulent mixing of passive scalars is important in the chemical process industry, as it affects chemical reactions, precipitations, etc. Although the transport of a passive scalar is governed by the convection-diffusion equation, which is linear in the scalar concentration, mixing of passive scalars in turbulent flows is far from simple, as a wide range of scales are involved and the cascade paradigms used for the velocity field often fail when applied to the scalar.[97] For flows with high Schmidt number (Sc) (the ratio of momentum diffusivity to mass diffusivity), the Batchelor scale characterizing the smallest scalar eddies is much smaller than the Kolmogorov scale (i.e., the smallest turbulent scale) so that the scalar field contains much more fine-scale structure than the velocity field.[30] The existence of fine-scale structures makes experimental resolution and direct numerical simulation of turbulent mixing in liquids difficult.[21] It is found that a sheet-like topology can be sustained in the scalar dissipation rate field while line-like structures must decay exponentially in time.[8] All of the molecular-scale mixing occurs in the sheet-like structures and such structures suggest a degree of universality in the fine structure.[19] In addition to the study of turbulent mixing at small scales so that some universal features can be identified, investigations may also focus on practical applications of turbulent mixing where the distribution of concentration with regard to time and location is of importance.

The study of turbulent mixing has benefited greatly from developments in laser-based flow diagnostic techniques such as Planar Laser Induced Fluorescence (PLIF). Compared to traditional point-wise measurements, PLIF can provide the two-dimensional mixing structure of a scalar field. The non-intrusive nature of PLIF also makes it a suitable tool to provide high-quality measurements of scalar transport in turbulent flows. In a typical PLIF experiment, the concentration field of fluorescent dye is determined through measuring its fluorescence intensity using CCD cameras. A detailed review on PLIF in liquids can be found in the review paper by Crimaldi[15] where the principles, set-up and applications of PLIF are explained. PLIF has been widely applied in our group to investigate turbulent mixing in turbulent shear flows[8; 28; 29], confined impinging jet flows[36; 94] and other geometries. Much of the progress in the study of turbulent mixing has been confined to canonical flows such as grid/isotropic
turbulence, channel flow and free-shear flow. There are relatively few studies focusing on turbulent mixing of swirling flow at high Schmidt number. Turbulent swirling flow is common in industrial applications and streamline curvature in the swirling flow can significantly modify the turbulence field. This unique feature of turbulent swirling flows compared to other canonical flows makes the investigation of its mixing process of interest. Swirling flow has long been used in combustion applications to enhance mixing and stabilize the flame.

The idea of enhancing mixing by confining swirling flow has been adopted to develop a novel continuous reactor called the multi-inlet vortex reactor (MIVR) for nanoparticle production. In the MIVR, swirling flow is formed by four tangential jets entering a short cylindrical reactor, and high turbulence intensity is generated near the reactor center by confining outflow with a small outlet. Unlike the mixing in most combustion applications, mixing of the swirling flow in the MIVR occurs in a contracted geometry without a sudden expansion section. Thus, the commonly observed vortex breakdown in combustion applications does not exist in the swirling flow of the MIVR, and random vortex wandering is found near the reactor center. Mixing of the swirling flow in the MIVR occurs in the liquid phase, which has a much higher Schmidt number than for gas flow; thus requiring much higher resolution for fully resolving its smallest length scales. Investigating turbulent mixing of swirling flow in the MIVR can benefit its application in Flash Nanoprecipitation (FNP) as the MIVR has been widely used in the FNP process to produce functional nanoparticles due to its ability to provide rapid mixing of solvent and anti-solvent. Thus, studying turbulent mixing of a passive scalar in the MIVR is of both fundamental and practical importance.

The presence of swirl can enhance mixing drastically. Mixing in swirling flow with a sudden expansion is found to be equally fast at all levels of swirl while measured fluctuation intensities indicate a much higher unmixedness at low swirl. The mixing process can be decomposed into two components: coarse-scale mixing by precession and large-scale eddy shedding, and fine-scale mixing due to turbulence in the flow. The study of a swirling recirculating flow with shows that the vortex region forms large coherent structures which lead to a pronounced inhomogeneous scalar field, and the mixing process is strongly modified by the precessing vortex core. Mixing of swirling flow in the MIVR was first investigated by Liu et al. using
computational fluid dynamics (CFD) and competitive fast reactions where only global mixing efficiency can be obtained. The mixing pattern in the MIVR was also qualitatively visualized using the reaction of iron nitrate and potassium thiocyanate.[82] Shi et al.[85] used laser induced fluorescence with a confocal laser scanning microscope to study mixing in a microscale MIVR under laminar flow conditions. Mixing in the MIVR has also been investigated through coupling CFD with the quadrature-based moments method.[57; 11; 6] Previous experimental and computational work has contributed greatly to understand the mixing of swirling flow in the MIVR. However, there is still no quantitative local concentration field available for the turbulent mixing regime, and validating the local mixing behaviour predicted by CFD with turbulence models has not yet been possible.

In the current work, turbulent mixing of swirling flow in the MIVR is quantitatively investigated using PLIF. Using the measurement, instantaneous concentration fields, mixture fraction mean and variance, and single point probability density function have been analysed for three different measurement planes inside the MIVR at four different Reynolds number. These results provide abundant information for understanding the physics of turbulent mixing in this confined swirling flow as well as data for future CFD model validation.

5.2 Experimental Setup and Measurement Method

Figure 5.1 shows the experimental apparatus, which is designed to provide four independent inlet streams to the MIVR. The MIVR is made of transparent acrylic so that the illuminating laser sheet can pass through it. The working fluid is deionized water at room temperature. Flow from two supply tanks is pumped into the four inlets of the MIVR where the flow rate can be adjusted using four automatic control valves (Fisher Inc.). A detailed description of the apparatus can be found in Liu et al.[64] The flow in the chamber of the MIVR is illuminated by a double-pulsed Nd:YAG laser (New Wave Research Gemini). The thickness of the laser sheet is 1 mm. One 12-bit CCD camera (LaVision Imager Intense) was used to capture images at a frequency of 8 Hz through the bottom of the MIVR. A Nikon lens with 50 mm focal length was used for the CCD camera and f-number of the lens is set to be 5.6. A long-pass optical filter that blocked light with wavelength shorter than 542 nm was mounted in the camera lens.
so that reflected and scattered laser light did not interfere with the fluorescence measurement.

Figure 5.1  Schematic of experimental setup.

Figure 5.2 shows the set-up of the PLIF experiment and the measurement locations. The dimensions of the MIVR are also presented in the figure 5.2. The fluorescent dye Rhodamine 6G was used as the passive scalar. Two inlets were fed with water while the other two were fed with water containing Rhodamine 6G with a concentration of 45 g/L. The concentration level of Rhodamine 6G was carefully selected so that the local intensity of the fluorescent light was proportional to the local intensity of the excitation source and the local concentration of the fluorescent dye.[29] Because the fluid in each experimental run passes through the reactor only a single time before the tanks must be refilled, new dye was used for each experimental run, and thus photobleaching of the dye was not a concern. Deionized water was used in each experiment, and the water was examined before each experiment to confirm the absence of chlorine that could potentially damage the dye. The shot-to-shot variation of the laser power was found to be approximately 2%.[58] Thus, it was not necessary to calibrate the PLIF images based on the shot-to-shot laser power variation. Each PLIF image was calibrated to eliminate the non-uniform energy distribution of laser sheet based on the procedure described by Feng et
The three PLIF measurement planes were located at the 1/4, 1/2 and 3/4 height of the chamber along the z-direction. The investigated Reynolds number is defined based on the bulk velocity of one inlet, as all four inlets have the same flow rate. Hydraulic diameter of single inlet is used as characteristic length scale for Reynolds number. Four Reynolds numbers were investigated in the experiment ranging from 3290 to 8225. For each case, 5000 instantaneous PLIF images were captured for analysis.

![Figure 5.2 PLIF setup and geometry of MIVR. (a) Top view. (b) Side view.](image)

The smallest length scale of turbulent mixing is known as the batchelor scale and can be estimated as $\eta_B = \eta/\sqrt{Sc}$, where $\eta$ is the Kolmogorov scale. Rhodamine 6G has a Schmidt number of approximately 1250 in water. The Kolmogorov length scale can be estimated based on previous stereoscopic Particle Image Velocimetry measurements. Figure 5.3 shows the estimated batchelor scale at the 1/2 plane for different Reynolds numbers. The other two measurement planes were found to have similar results as the 1/2 plane and are thus not reported here. For all four Reynolds number cases, the estimated value of $\eta_B$ was found to be between 0.25\(\mu\)m and 2.0\(\mu\)m. Based on the calibrated image size and pixel size of the CCD camera, the in-plane spatial resolution of the PLIF measurement was found to be 30\(\mu\)m, and the diffraction-limited spot size for the optical system was 8.89\(\mu\)m. Moreover, the spatial resolution in the z-direction was determined by the laser thickness which is 1.0mm. Thus, the final resolution of the PLIF measurements was determined to be 1.0mm in the measurement plane and in the z-direction.

Overall, the PLIF measurement resolution is much larger than the batchelor scale of scalar
Figure 5.3 Estimated Batchelor scale at plane at different Reynolds number.

field, and thus the smallest mixing scales cannot be fully resolved. The measured results thus represent a spatial filtering of the total scalar field. The mixture-fraction mean should not be affected by the limited resolution, while the measured variance will be slightly lower than the actual variance and the instantaneous mixing structure will be less sharp. A model scalar spectrum can be used to estimate the sub-grid scalar variance [30] and it is found to be approximately 10% of the resolved variance over most of the measurement plane.

5.3 Results and Discussions

5.3.1 Visualization of passive scalar field

The mean velocity of turbulent swirling flow in the MIVR can be described using a batchelor vortex model:[62]

$$\bar{u}_\theta(r) = \frac{V_1 R_1^2}{r} \left[ 1 - \exp\left( -\frac{r^2}{R_1^2} \right) \right] + \frac{V_2 R_2^2}{r} \left[ 1 - \exp\left( -\frac{r^2}{R_2^2} \right) \right]$$  (5.1)
\[ u_z(r) = U_0 + U_1 \exp\left(-\frac{r^2}{R_1^2}\right) + U_2 \exp\left(-\frac{r^2}{R_2^2}\right) \]  

(5.2)

where the model can be viewed as the combination of two Batchelor vortices. \( R_1, V_1 \) and \( U_1 \) are the characteristic values of one vortex, and \( R_2, V_2 \) and \( U_2 \) are for the other vortex. \( U_0 \) depends on the inlet flow rate, and \( U_1, U_2, R_1, R_2 \). Based on the mean velocity fields, the turbulent swirling flow in the MIVR can be divided into two regions, i.e., a free-vortex region \( (r/R_0 > 0.2) \) and a forced-vortex region \( (r/R_0 < 0.1) \) where \( R_0 \) is the radius of MIVR chamber and \( r \) is the distance from the reactor center.\[62] The turbulence intensity in the forced-vortex region is much higher than in the free-vortex region.\[64] As passive scalar transport is strongly dependent on the turbulence field, it is natural to describe the scalar field separately in these two regions. Figure 5.4 shows typical results for the instantaneous passive scalar from the 1/2 plane where several interesting features can be identified. First, a large-scale vortical structure can be identified in the scalar field within which fluid of different concentrations mixes spirally in the free-vortex region, while an almost homogeneous scalar field without apparent unmixed regions forms in the forced-vortex region. It is observed that unmixed fluid is stretched into thin layers as the flow spirals towards the reactor center and some of these layers preserve their shape well until they enter the forced-vortex zone. As the Reynolds number increases, the local unmixed region in the free-vortex region is reduced from large bulk shapes at \( \text{Re}=3290 \) to thin-strip shapes at \( \text{Re}=8225 \). It is expected that the size of the local unmixed scalar in the free-vortex region could be further reduced at even higher Reynolds number. As would be expected, the instantaneous scalar field clearly shows that the swirling flow has a much better mixing performance in the forced-vortex region than in the free-vortex region. The passive scalar is expected to be well mixed as it approaches the reactor outlet located in the forced-vortex region. Both the turbulence field and the vortex wandering motion contribute to the enhanced mixing in the forced-vortex region.

Figure 5.5 shows some interesting local structures of the instantaneous scalar field in the plane (\( \text{Re}=8225 \)). The grids in figure 5.5 indicate the in-plane resolution of the measurement (30\( \mu \text{m} \)). It should also be noticed that the out-of-plane resolution will be the laser thickness (1\( \text{mm} \)), which is much larger than the in-plane resolution. Regions of unmixed fluid exist in
Figure 5.4  Typical instantaneous passive scalar fields for 1/2 plane at different Reynolds numbers.
the free-vortex region, but they are short lived and tend to decay as they approach the reactor center. These unmixed fluid strips undergo numerous mixing mechanisms\[20; 92; 17\], such as engulfment (figure 5.5a), stretching (figure 5.5b) and penetration by surrounding fluid (figure 5.5c). In the free-vortex region, the passive scalar field is far from homogeneous and isotropic because of the low turbulence intensity there, and most of the mixing is due to advective mechanisms of laminae folding and stretching. However, in the forced-vortex region, the local unmixed regions nearly disappear (figure 5.5d) due to the high turbulence intensity and vortex wandering motion present there, and the mixing is dominated by turbulent scalar dissipation and molecular diffusion (i.e., micro-mixing).

Figure 5.5 Zoomed views of typical local mixing structures for 1/2 plane at Re=8225: (a) engulfment, (b) stretching, (c) penetration, (d) uniform.

5.3.2 Mixture-fraction mean and variance

Mixture fraction mean is an important statistical feature in the study of inhomogeneous passive scalar mixing as many closure models are based on the gradient of the mixture fraction
mean. The typical profile of ensemble-averaged mixture fraction mean \(< \xi >\) of the swirling flow in the MIVR is presented in figure 5.6 for \(\text{Re}=8225\). The mixture-fraction mean is based on an ensemble of 5000 instantaneous images. In our previous study, the velocity field inside the MIVR has already been measured by using stereoscopic particle image velocimetry.\([64]\) Using these stereo PIV data, the mean velocity field is plotted in front of the mixture fraction mean field as streamlines. The mixture fraction mean is aligned with the mean velocity streamlines fairly well. This can be explained by the fact that the convection term of the passive scalar transport is dominant in the free-vortex region as the turbulence intensity there is low. The mixture fraction mean contour in figure 5.6 provides a clear picture of the mixing structure in the MIVR. A spiral structure of the mixture fraction mean is observed at all three planes as the passive scalar swells towards the center. A large gradient of mixture fraction mean exists in the free-vortex region, while a near uniform mean is found in the forced-vortex region. This mean structure indicates that flow from different inlets of the MIVR does not fully mix until it reaches to the center.

Figure 5.7 shows the mixture fraction variance \(< \xi'^2 >\) at \(\text{Re}=8225\). Compared to the mixture fraction mean contour, the mixture fraction variance in the MIVR is symmetric around the center of the swirling flow. The magnitude of mixture fraction variance decreases moving from the free-vortex region to the forced-vortex region. When a passive scalar is perfectly mixed, the mixture fraction variance approaches zero. This trend further confirms that the mixing level in the MIVR increases as the flow approaches the center. Mixing level also increases from the 1/4 plane to 3/4 plane as the 3/4 plane has the largest low variance region. The main reason that mixing level improves from the 1/4 to the 3/4 plane is that much of inlet flow is displaced towards the bottom of the reactor before it enters the center area of the reactor.\([?]\) The passive scalar tracer is advected by the velocity field so fluid in planes near the reactor bottom, such as the 1/4 plane contain more unmixed scalar (and thus higher variance) than planes near the top of the reactor such as the 3/4 plane, because the unmixed scalar near the reactor bottom becomes more well mixed by the turbulence at the center of the reactor as it rises towards the reactor exit, thus the variance will decrease as fluid travels to planes closer to the outlet such as the 3/4 plane. Again, the results of both mixture fraction mean and variance only represent
Figure 5.6  Mixture fraction mean profiles at 1/4, 1/2 and 3/4 planes (from top to bottom) for Re=8225, streamlines are based on mean velocity field measured by previous experiment.
the resolved scales and their accuracy can be affected by the PLIF resolution.

Considering the symmetrical shape of the mixture fraction variance, its value can be represented by using data from one-dimensional profiles taken through the center of the measurement domain. In this way, the variance at different Reynolds numbers can be easily compared. Figure 5.8 shows the comparison of scalar variance at different Reynolds numbers. When the Reynolds number reaches 6580, the measured mixture fraction variance becomes Reynolds number independent, indicating that further increasing Reynolds number should not improve the mixing significantly. A similar trend was observed in a study on mixing in a micro-scale MIVR, where the mixing is not improved beyond Reynolds numbers larger than 1600.[57] The reason for this is that mixing in the MIVR is controlled by both macro-mixing and micro-mixing.[11] Micro-mixing is related to turbulence level, thus it can be improved by increasing Reynolds number. However, macro-mixing is controlled by the geometry of reactor and will not improve due to the change of Reynolds number. In current experiment, it is noticed that when Reynolds number is larger than 6580, further increasing Reynolds number does not improve mixing level significantly, indicating that macro-mixing becomes dominant and determines the threshold of mixing in the MIVR. The dashed lines in figure 5.8 further highlight the difference in mixing in the forced-vortex and free-vortex regions. In the forced-vortex region \((r/R_0 < 0.1)\) the variance can be represented by a line with slope equal to zero. In the free-vortex region \((r/R_0 > 0.2)\) a line with slope equal to -0.135 is found to represent the trend of variance observed in all three measurement planes well.

At high Reynolds number, a separation of mixing scales generally exists. The large-scale motions are mainly influenced by the geometry of the reactor while the small-scale motions are determined by the energy dissipation rate and viscosity.[57] Large-scale segregation (LSS) in the reactor can be described by introducing an LSS variance:

\[
\langle \xi'^2 \rangle_{LSS} = (\langle \xi \rangle - \bar{\xi})^2
\]  

(5.3)

where \(\bar{\xi}\) is the average mixture fraction after complete mixing, which is equal to 0.5. Here we define different segregation zones based on the value of the LSS variance \(\langle \xi'^2 \rangle_{LSS}\) and scalar variance \(\langle \xi'^2 \rangle\) as following:
Figure 5.7  Mixture fraction variance profiles at 1/4, 1/2 and 3/4 planes (from top to bottom) for Re=8225.
Figure 5.8  Comparison of mixture fraction variance profiles at 1/4, 1/2 and 3/4 planes (from top to bottom) for different Reynolds number.
\[\langle \xi'^2 \rangle_{LSS} > \sigma^2 \text{ and } \langle \xi'^2 \rangle < \sigma^2 \text{ [Large-scale segregation (LSS) zone]}\]
\[\langle \xi'^2 \rangle_{LSS} < \sigma^2 \text{ and } \langle \xi'^2 \rangle \geq \sigma^2 \text{ [Small-scale segregation (SSS) zone]}\]
\[\langle \xi'^2 \rangle_{LSS} \geq \sigma^2 \text{ and } \langle \xi'^2 \rangle \geq \sigma^2 \text{ [LSS&SSS zone]}\]

The cut-off standard deviation \(\sigma = 0.045\) was found suitable to describe the segregation zones. In the original study\[57\], the cut-off value was selected based on acid-base concentration ratio in the inlet stream. In current study, the previous cut-off value is used as a starting point for determining a new, more appropriate value. The final value is then chosen so that segregation zone can be clearly observed. Figure 5.9 presents the segregation zones at three planes for \(Re = 8225\). The red contour represents the SSS zone and the blue contour represents the LSS&SSS zone. No LSS zone was found present in the measurement plane, indicating that mixing in the MIVR is controlled by both macro-mixing and micro-mixing. Another reason that no LSS zone is observed is that current PLIF measurements only cover the center area of the MIVR, where the turbulence intensity is higher, and mixing is better. In regions away from the reactor center, LSS zone should exist, as far from the reactor center, turbulence intensities are much lower. As Reynolds number primarily tends to improve micro-mixing level, at lower Reynolds numbers the SSS zone will become smaller. This can be clearly shown in figure 5.10, a plot of segregation zones for \(Re = 3290\). This helps to explain the better mixing observed at \(Re = 8224\) compared to the lower Reynolds number. This distribution is consistent with the results from Liu et al.\[57\] In the reactor, mixing of swirling flow in the forced-vortex region is determined mainly by turbulent diffusion where the energy dissipation rate and viscosity play important roles. In the free-vortex region, the mixing of swirling flow is determined by both the large motions imposed by the geometry of the reactor in addition to weaker turbulent diffusion, and relatively poorer mixing can be observed.

### 5.4 One-point composition PDF

The one-point concentration probability density function (PDF) provides information on the distribution of the passive scalar within the flow, quantifying the time-independent mixing properties and local statistical information. Thus, it is important to study the PDF for the turbulent mixing of the swirling flow. As there are over one million points available in the
Figure 5.9 Distribution of segregation zones defined by $\sigma = 0.045$ at 1/4, 1/2 and 3/4 planes (from top to bottom) for Re = 8225.
Figure 5.10  Distribution of segregation zones defined by $\sigma = 0.045$ at 1/4, 1/2 and 3/4 planes (from top to bottom) for Re = 3290.
measurement plane (the pixels in the CCD camera image), it is convenient to limit analysis to a few representative points. The first step in selecting representative PDF points is to check if symmetric locations in the flow generate similar PDFs. If such symmetry exists, then PDFs at points along one line in the flow field could be sufficient to represent the whole measurement plane. Figure 5.11 shows the comparison of PDFs at typical symmetrical locations. The locations of the selected points are shown in the same figure. It is found that the PDFs at symmetrical points \((b, b', f, f', g, g')\) are almost identical to each other, demonstrating that symmetrical locations in the flow field do indeed yield similar PDFs.

Based on this symmetry, the PDFs at five points (point a-e) along the radius in the \(x\)-axis direction are presented in figure 5.12 for measurements at the 1/2 plane for \(Re=8225\). Figure 5.12 shows that as the distance from the center of the reactor increases, the shape of the PDF becomes broader. A broad distribution indicates a higher fluctuation of the passive scalar field and less complete mixing. The observed features of the PDFs with respect to location are as expected, i.e., the passive scalar is better mixed in the forced-vortex region than the free-vortex region.

In previous mixing studies in other geometries,\([58; 74]\) a beta function was found to represent the PDFs well. The beta function is defined as

\[
f(\xi) = \frac{\xi^{\alpha-1}(1 - \xi)^{\beta-1}}{\int_0^1 \xi^{\alpha-1}(1 - \xi)^{\beta-1} d\xi}\]

(5.4)

where \(\alpha = \langle \xi \rangle \left[ \langle \xi (1-\xi) \rangle / \langle \xi^2 \rangle \right] - 1 \), \(\beta = \alpha \left[ 1 - \langle 1/\xi \rangle \langle \xi \rangle \right] \). To determine if the beta function accurately models mixing in the swirling flow in the MIVR, the beta function based on the mixture fraction mean and variance is compared with the measured PDFs in figure 5.12. It is seen that the beta function can generally represent all the PDFs quite well, especially for the PDF at point a. It is believed that the performance of the beta function depends on the dominant mixing mechanisms, and it works best when turbulent diffusion dominates. It has been shown in previous sections that the forced-vortex region is dominated by turbulent diffusion, while mixing in the free-vortex region has contributions from both turbulent diffusion and large-scale structure. The importance of the large-scale structures to mixing in the free-vortex region explains the deviation of the beta function from the measured PDFs.
Figure 5.11 Comparison of probability distribution function (PDF) at different symmetrical points.
Figure 5.12  Probability distribution function (PDF) and fitted beta function at different symmetrical points (a-e) on 1/2 plane for Re=8225.
5.5 Conclusions

Planar laser induced fluorescence (PLIF) was used to visualize and quantify passive scalar transport in the turbulent swirling flow of a multi-inlet vortex reactor (MIVR). Two flow regions can be identified in the turbulent swirling flow, i.e., a free-vortex region \( (r/R_0 > 0.2) \) and a forced-vortex region \( (r/R_0 < 0.1) \). Scalar statistics including mixture fraction mean, variance, and probability density function (PDF) were calculated based on ensembles of instantaneous passive scalar images. The mixing structure of the swirling flow within the MIVR was found to consist of a spiral motion of the passive scalar in the free-vortex region and a nearly homogeneous mixing region in the forced-vortex region. Mixing in the free-vortex region is controlled by both turbulent diffusion and large-scale flow structures. In the forced-vortex region, mixing is dominated by turbulent diffusion, and here overall better mixing level is observed. The beta function based on the measured mean and variance was found to represent the measured PDFs quite well, especially in the forced-vortex region. These data represent the first passive scalar measurement of turbulent mixing in this swirling flow and could be valuable in validating CFD simulations for turbulent mixing in the MIVR.
CHAPTER 6. A DDES MODEL FOR TRANSITIONAL FLOW IN A MICRO-SCALE MULTI-INLET VORTEX REACTOR

A paper in preparation

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Abstract

The object of current work is to verify a new delayed detached eddy simulation (DDES) model for simulating transitional flow in a micro-scale multi-inlet vortex reactor (MIVR). The DDES model is based on k-ω model. Low Reynolds number correction is applied to the k-ω model so that RANS part of the DDES model can take care of low Reynolds number flow. By limiting the dissipation rate in the k-equation, LES part of the DDES model behaves as one-equation sub-grid model. The proposed model was first validated by simulating a separation-induced-transition flow case where results agree well with previous LES data. Applying the model to simulate both laminar and transitional flow in the micro-scale MIVR also produces good prediction of mean velocity, turbulent intensity and mixing pattern of passive scalar with respect to experimental data. It is demonstrated that the proposed DDES model is capable of simulating transitional flow in complex geometry such as the micro-scale MIVR. The simulation results also help us understand the flow and mixing pattern in the micro-scale MIVR, and provide guidances to optimize the reactor for its application of producing functional nanoparticles.

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6.1 Introduction

Manufacturing nanoparticles as drug delivery platform requires reproducible, scalable and stable formulation process. Anti-solvent precipitation such as Flash NanoPrecipitation (FNP) has been proven to be one of the robust and scalable process.[18] Multi-inlet vortex reactor (MIVR) is a novel continuous confined geometry developed for controlling functional nanoparticle formation in the FNP.[57; 61] The MIVR for producing functional nanoparticles is usually built in millimetre scale. As there are also studies on scaling up the MIVR[62; 64; 63], the reactor is called micro-scale MIVR here to avoid any potential confusion. Compared to other precipitation geometry such as confined impinging jet reactor (CIJR), the micro-scale MIVR has the flexibility of controlling mixing ratios of solvents through various combination of inlet flow rates as all streams contribute independently to the mixing in the chamber.[57] Many applications have been reported as successfully producing functional nanoparticles by using the micro-scale MIVR, proving the applicability of MIVR in anti-solvent precipitation process.[61; 82; 27; 6; 1; 69]

The design and optimization of the micro-scale MIVR for nanoparticle production could be greatly enhanced by developing reliable computational models. Computational fluid dynamics (CFD) has been used to understand the flow characteristic and nanoparticle formation inside the micro-scale MIVR.[57; 12; 11; 13; 6] Unlike most of micro-scale chemical reactors which work in the laminar flow region, mixing in the micro-scale MIVR is enhanced through introducing turbulence into the flow. However, the introduction of turbulence makes development of computational models for the micro-scale MIVR difficult. Before developing any advanced computational models regarding to mixing and particle precipitation, flow field inside the micro-scale MIVR such as the mean velocity and turbulent statistics has to be correctly predicted. In previous study, Cheng et al. and Bensaid et al. applied both Reynolds Average Navier-Stokes (RANS) and Large Eddy Simulation (LES) approach to simulate the turbulent flow inside the micro-scale MIVR with comparison to the microscope particle image velocimetry (micro-PIV) data.[12; 6] Shi et al. further studied the turbulence field of the micro-scale MIVR in detail by using the micro-PIV technique.[84] Previous simulation provides some understanding about
the flow field. However, in previous study no rigorous comparison has been made between the micro-PIV data and CFD results. The applied turbulence model such as k-\(\varepsilon\) model doesn’t provide very good prediction about the distribution of mean tangential velocity and turbulent statistics. Liu et al. pointed out that RANS and LES approach may both fail to predict the turbulent swirling flow in a scaled-up MIVR.[63] For RANS approach, it is inherent unable to predict transitional and swirling flow well because most of RANS model is developed for high turbulent flow case and curvature effect is not considered as well. The reasons that LES fails is mainly because mesh resolution cannot be guaranteed in the computational domain.

Considering flow inside the micro-scale MIVR, for most of its applications it falls into transitional flow region, i.e., both laminar and turbulence flow exists inside the reactor. Specifically, laminar flow is introduced into the reactor (Reynolds number (Re) is usually far below 1000 in the inlet.), and flow becomes turbulent when it comes to the outlet. Transitional flow is difficult to predict by using both RANS and LES approach. The ability of LES to predict transitional separation flow has been investigated with particular emphasis on the response to free-stream-turbulence.[54] It is found that LES yields a credible representation of transition induced by a combination of free-stream turbulence and separation. However, inadequate mesh resolution and the use of SGS modelling reduce the accuracy of LES prediction. For most of engineering flow, LES is still very expensive. To provide affordable prediction tool, RANS models for transitional flow have been developed, which mainly includes two categories, i.e., low Reynolds number (low-Re) turbulence model and intermittency-based model. By adding low Reynolds number correction to regular turbulence model, the transition behaviour of flow can be predicted at the right location.[99] However, Menter et al. pointed out that low-Re turbulence model is not capable of capturing influence of factors that affect transition behaviour such as separation.[53; 72] The intermittency-based model has then been developed to avoid disadvantages of low-Re turbulence model by using local variables and empirical correlation.[72] Recently, Ge et al. developed an intermittency model without using external data correlation.[33] Nevertheless, in the RANS model for transitional flow, a priori knowledge of transition location or empirical correlations has to be known, limiting its ability of predicting flow away from its original test case.[81]
It is very challenging for RANS approach to have a good prediction to the transitional swirling flow in the micro-scale MIVR. The main concern for LES is its comparable high computational cost caused by fine mesh, especially near the wall. Detached Eddy Simulation (DES) approach is a promising alternative method which improves the prediction of RANS approach while requiring less computational resources compared to LES approach.[90] The original DES model rested on Spalart-Allmaras model could have practical issues such as artificial grid-induced separation and logarithmic-layer mismatch. Delayed DES was proposed to solve the artificial grid-induced separation by using a shielding function to prevent the RANS mode switching to LES mode near boundary layers.[88] DDES can also rest on other two-equation RANS model to improve its performance in the RANS part.[35] In the DDES approach, the logarithmic-layer mismatch can be alleviated by modifying the length scale in the eddying regions.[78] Recently, DDES with dynamic procedure has been developed and applied to simulate the turbulent swirling flow in a scaled-up MIVR with good agreement between simulation and experimental results.[100; 63]

There are still not many study on using DDES for transitional flow. A new DDES model is proposed in current study to simulate the transitional flow within the micro-scale MIVR. In the new DDES model, low Reynolds number k-ω model is used in its RANS mode. When mesh is fine enough away from the wall region, the RANS mode will switch to LES mode with one equation sub-grid model. In the following part of the paper, the new DDES model is first derived. Then, the new DDES model was first tested by simulating a separation-induced-transition flow case where previous pure LES results will be used to validate DDES results. Finally, the new DDES model will be used to model the transitional flow in the micro-MIVR at different Reynolds number where experimental data will be used to validate the DDES model.

### 6.2 Model formation

The idea of the DDES model is to use low Reynolds number k-ω model in laminar flow region and LES in turbulent flow region. The low-Re k-ω model is derived by Wilcox[99] and proven to work well for low Reynolds number flow. LES with one equation eddy model is used in high Reynolds number flow. The ability of the DDES model in predicting transition
behaviour of flow is dependent on the low-Re k-ω model. Separation and streamline curvature effect in the flow can be handled by LES part of the DDES model. The following contents show the derivation process of the DDES model.

The dimensionless filtered Navier-Stokes equations for incompressible flow can be expressed as (repeated indices imply summation)

\[
\frac{\partial \overline{u}_i}{\partial x_i} = 0 \quad (6.1)
\]

\[
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = - \frac{\partial \overline{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial \overline{u}_i}{\partial x_j} \right) - \frac{\partial \tau_{ij}}{\partial x_j} \quad (6.2)
\]

where \( \tau_{ij} \) is the Reynolds-stress tensor in the RANS approach and turbulent sub-grid stress tensor in the LES approach, and it is modelled as

\[
\tau_{ij} = 2(\nu + \nu_T) S_{ij} - \frac{2}{3} k \delta_{ij} \quad (6.3)
\]

where \( \nu \) is the molecular viscosity, \( \nu_T \) is the turbulent viscosity which need be modelled, \( S_{ij} \) is the filtered strain-rate tensor, and \( k \) is the turbulent kinetic energy in RANS approach and sub-grid scale kinetic energy in LES approach. The original k-ω RANS model[99] for modelling the turbulent viscosity can be written as

\[
\frac{Dk}{Dt} = 2\nu_T |S|^2 - C_\mu k \omega + \nabla[(\nu + \sigma_k \nu_T) \nabla k] \quad (6.4)
\]

\[
\frac{D\omega}{Dt} = 2C_\omega 1 |S|^2 - C_\omega 2 \omega^2 + \nabla[(\nu + \sigma_\omega \nu_T) \nabla \omega] \quad (6.5)
\]

where \( \nu_T = k/\omega \) and constants in the k-ω model are

\[
C_\mu = 0.09, \sigma_k = 0.5, \sigma_\omega = 0.5, C_\omega 1 = 5/9, C_\omega = 3/40. \quad (6.6)
\]

To improve its ability of predicting transitional flow, low Reynolds number correction can be applied to the original k-ω model.[99] Low Reynolds number correction is applied through modifying turbulent viscosity, \( C_\mu \) and \( C_\omega 1 \) in the k-ω model.

\[
\nu_T = \alpha^* \frac{k}{\omega}, \alpha^* = \alpha_0^* + \frac{Re_T}{R_k}, C_\mu = 0.09 \frac{5/18 + \left( \frac{Re_T}{R_\beta} \right)^4}{1 + \left( \frac{Re_T}{R_\beta} \right)^4}, C_\omega 1 = \frac{5 \alpha_0^* + Re_T/R_\omega}{9 \left( 1 + \frac{Re_T}{R_\omega} \right)} \quad (6.7)
\]

Constants for the low Reynolds number correction are

\[
R_\beta = 8, \alpha_0 = 1/10, R_\omega = 2.7, \alpha_0^* = 1/40, R_k = 6. \quad (6.8)
\]
Turbulent Reynolds number $Re_T$ is introduced here to represent the intensity of local turbulence. The relationship between $Re_T$ and $\alpha^*, C_\mu, C_\omega$ can be seen in figure 6.1. It is shown that the low-Re correction is dependent on $Re_T$, and all three modified coefficients will return to its original value at high Reynolds number when $Re_T$ is approximately larger than 100. The definition of $Re_T$ will be discussed later.

![Figure 6.1 Dependence of $C_\mu$, $\alpha^*$ and $C_\omega$ on turbulent Reynolds number $Re_T$.](image)

Although it can be used to predict flow in channel and boundary layer applications, the $k$-$\omega$ model with low Reynolds number correction is still criticized for not capable of capturing factors such as separation and streamline curvature that affect transition.[53; 72] Instead of using correlation-based RANS model, we propose a DDES model based on the low Reynolds number $k$-$\omega$ to take care of factors that affect transition. The basic idea is to apply LES in the high turbulence region so that factors such as separation and streamline curvature can be captured, and apply low Reynolds number $k$-$\omega$ model in the laminar region to predict the onset of transition. The proposed DDES model is based on the low Reynolds number $k$-$\omega$ model where the dissipation in the $k$-equation is clipped by using length scale $\ell_{DDES}$.

$$\frac{Dk}{Dt} = 2\nu_T|S|^2 - \frac{\sqrt{k^3}}{\ell_{DDES}} + \nabla[(\nu + \sigma_k\nu_T)\nabla k] \quad (6.9)$$

The DDES length scale $\ell_{DDES}$ is defined as

$$\ell_{DDES} = \ell_{RANS} + f_{d\text{max}}(0, \ell_{RANS} - \ell_{LES}), \ell_{RANS} = \frac{\sqrt{k}}{C_\mu \omega}, \ell_{LES} = C_{DES}\Delta \quad (6.10)$$

The DDES shielding function $f_d$ is defined as

$$f_d = 1 - tanh([8r_d]^3), r_d = \frac{\nu_T + \nu}{\kappa d_w^2 \sqrt{U_{i,j}U_{i,j}}} \quad (6.11)$$
where $\kappa$ is the von Kármán constant, $d_w$ the wall distance, and $U_{i,j}$ the velocity gradient tensor (repeated indices imply summation). $\Delta$ is an appropriate measure of grid size and is defined as

$$\Delta = f_d V^{1/3} + (1 - f_d) h_{\text{max}}$$

(6.12)

where $V$ is the cell volume and $h_{\text{max}} = \text{max}(\Delta x, \Delta y, \Delta z)$ is the maximum cell spacing of local grid. The definition of $\Delta$ helps alleviate log layer mismatch in the DDES model.[78] When the DDES length scale $\ell_{\text{DDES}}$ is equal to RANS length scale $\ell_{\text{RANS}}$, the k-equation returns to its RANS mode. When $\ell_{\text{DDES}}$ is equal to LES length scale $\ell_{\text{LES}}$, the k-equation will return to one equation eddy model in LES which is written as

$$\frac{Dk}{Dt} = 2C_k \sqrt{k \Delta} |S|^2 - C_e \frac{\sqrt{k^3}}{\Delta} + \nabla[(\nu + \nu_T) \nabla k]$$

(6.13)

where $C_k$ is 0.094 and $C_e$ is 1.048. To mimic the one equation eddy model in LES, $C_{\text{DES}}$ is chosen to be 0.95 so that the dissipation part in the DDES model is close to the one equation eddy model. To make sure the DDES model has the same turbulent production as LES, turbulent eddy viscosity $\nu_T$ is rewritten as

$$\nu_T = (1 - \Phi) \sigma^*_k + \Phi$$

(6.14)

where $\Phi$ is the index showing the region of LES mode and is defined as

$$\Phi = \frac{\ell_{\text{RANS}} - \ell_{\text{DDES}}}{\ell_{\text{RANS}} - \ell_{\text{LES}}}$$

(6.15)

$\sigma_k$ can be rewritten as $\sigma^*_k$ so that the diffusion part of k-equation will be equal to the one equation eddy model as well.

$$\sigma^*_k = (1 - \Phi) \sigma_k + \Phi$$

(6.16)

Unlike previous DDES model that mimic Smagorinsky sub-grid model in its LES part, one equation eddy model is used in the LES mode of the new DDES model. The main advantages of this change are that k-equation is consistently used in the DDES model and assumption about local equilibrium of energy transfer that deriving Smagorinsky model can be dropped.

In the original low Reynolds number correction, $Re_T$ is defined as $k/(\omega \nu)$ which only represents the model part of turbulence. In the DDES model k-equation will also be used to model
sub-grid kinetic energy. In that case the original definition of $Re_T$ will give value representing sub-grid turbulence level, which further cause incorrect low Reynolds number correction. Thus, when considering both low Reynolds number correction and DDES approach, the definition of $Re_T$ has to be modified to include both the resolved and model part of turbulence. The new definition of $Re_T$ should provide a more accurate estimation of local turbulence level. One way is to include the resolved turbulent kinetic energy into $Re_T$. However, estimation of resolved turbulent kinetic energy requires time average of flow field, making current simulation depend on historic results. This will make the whole simulation unstable. In the DDES model we propose to use the total turbulent dissipation rate $\epsilon$ to estimate $Re_T$.

$$Re_T = \frac{\epsilon}{\omega^2 \nu}, \epsilon = 2(C_{DES} h_{max})^2 \omega |S|^2 + k \omega$$  \hspace{1cm} (6.17)

The first part of $\epsilon$ is an estimation of dissipation rate in LES mode based on Smagorinsky model. Similar form has also been used in other study to estimate $\epsilon$.\cite{83, 100} The second part of $\epsilon$ is the model part. When turbulent dissipation rate is all modelled, the new $Re_T$ becomes the same as its original definition.

The DDES model was implemented into the open-source computational fluid dynamics (CFD) code OpenFOAM\cite{47}. In the following test cases, a second-order, backward-difference method was used for time discretization. Gaussian finite volume integration with central differencing for interpolation was selected for spatial discretization. The Sweby limiter was used in the convection terms of the $k$ and $\omega$ equations.\cite{93} The equivalent of the Rhie & Chow scheme was applied in the divergence term for velocity to remove two-delta waves in the laminar region of transition simulations.\cite{79} Gradients, divergence and laplacian scheme are all second-order accurate. The generalized geometric-algebraic multi-grid solver is used as the linear system solver for the pressure equation and Gauss-Seidel algorithm is used for other variables including velocity, $k$ and $\omega$. The solution for the system of partial conservation equations was obtained, at each time-step, by solving iteratively to a specified tolerance of the residual norm.
6.3 Results and Discussions

6.3.1 Test case: Separation Induced Transition

Before applying the new DDES model to simulate flow in the micro-scale MIVR, it is first tested by a separation-induced-transitional flow case. The geometry of the test case is shown in figure 6.2 where laminar flow enters a flat plane with a bump on its top side. Laminar flow undergoes separation after the bump due to adverse pressure gradient and becomes turbulent. Detailed introduction about the flow can be found in Lardeau et al.’s study.[54] In their study LES was used to simulate the flow. The simulation in current paper uses the same domain size and mesh. 1% inflow disturbance is generated by using Klein’s method.[51] The separation and transition features of this flow as well as the availability of LES prediction make it a good test case for the new DDES model.

Figure 6.2 Geometry and boundary condition of the separation-induced-transition flow case.

Figure 6.3 shows the prediction of skin-friction $C_f$ and separation bubble size by the new DDES model. The results are compared with data from LES with dynamic Smagorinsky model.[54] Overall, the prediction based on the new DDES model agree well with the LES results. It is demonstrated that the new DDES model is able to predict transition and separation features of the test flow with same accuracy as LES. Figure 6.4 shows the prediction of mean velocity at different y-coordinate location by the DDES model, all in close agreement with corresponding LES data. Figure 6.5 shows the prediction of Reynolds stress by the new DDES model. Again good agreement with LES data is observed overall. At $y/L=0.5$ the Reynolds stress $uu$ is underestimated. As only resolved Reynolds stress is considered in the comparison, this underestimation could be explained by the fact that not all turbulence is resolved at
$y/L=0.5$. Figure 6.6 shows the region of RANS and LES mode in the computational domain. It is found that the transition between RANS and LES mode approximately start at $y/L=0.4$ where separation starts. Most LES mode exists in the separation region while RANS mode is near the wall and in other laminar flow area. That distribution is under expectation and prove the advantage of using the DDES model for the separation-induced-transitional flow.

Figure 6.3 Comparison of $C_f$ (a) and separation bubble size (b) between DDES and LES.

Figure 6.4 Comparison of normalized mean velocity between DDES and LES: (a) $x/L=0.4$ and $x/L=0.5$, (b) $x/L=0.6$ and $x/L=0.7$. 
Figure 6.5  Comparison of Reynolds stress between DDES and LES: (a) x/L=0.4, (b) x/L=0.5, (c) x/L=0.6, (d) x/L=0.7.

Figure 6.6  Region of RANS and LES mode in the separation-induced-flow case.
6.3.2 Transitional Flow in Micro-scale MIVR

6.3.2.1 Validation of the DDES model

In this section, the DDES model is used to simulate flow in the micro-scale MIVR. The geometry of micro-scale MIVR is the same as that in the experimental study by Shi et al.[84]. In the experimental investigation, micro-particle-image-velocimetry (micro-PIV) was used to measure turbulence in the micro-scale MIVR. Three Reynolds number cases were studied, i.e., Re=53, Re=93 and Re=240. The Reynolds number is defined based on characteristic inlet velocity $U_j$. Flow at three location were measured, i.e., 1/4, 1/2 and 3/4 plane in the reactor chamber. In the experiment it was found that flow in the micro-scale MIVR is laminar when Re=53. Turbulence starts to show up when Reynolds number increases to 93. Much stronger turbulence appears in the reactor center and outlet at Re=240. Figure 6.7 shows the geometry and mesh used in current simulation. In the DDES model, no refined mesh is needed near the wall as RANS mode will be used there. That is also one of the motivation to apply DDES approach instead of LES for simulating flow in the micro-scale MIVR. Using the same post-processing technique presented in Liu et al.’s study about the macro-scale MIVR[64], velocity field in the micro-scale MIVR is described in cylindrical coordinate as radial, azimuthal and axial velocity, i.e., $u_r, u_\theta, u_z$. Both experimental and simulation data are averaged along different angles in the plane, assuming that flow is axis-symmetrical.

![Figure 6.7 Geometry and mesh of the micro-scale MIVR.](image)

All three Reynolds number cases are simulated by using the new DDES model. As low Reynolds number correction has already been added, the new DDES model can be applied to
the laminar flow case as well, thus no switch to laminar model is needed. Figure 6.8 shows the prediction of mean velocity at Re=53 with comparison to experimental data. The radial velocity $u_r$ is well predicted while azimuthal velocity $u_\theta$ is a little underestimated. It seems that the new DDES model produces excess turbulent viscosity even with low Reynolds number correction, which smooths the swirling pattern of flow and underestimates the magnitude of azimuthal velocity. Figure 6.9 shows the comparison of mean velocity at Re=93 between the DDES model and experimental data. The prediction of azimuthal velocity becomes better as flow becomes more turbulent and the DDES model is thus more suitable. The mismatch of radial velocity near the center could be caused by the measurement uncertainty in the experiment because its magnitude becomes very small there. Figure 6.10 shows the comparison of mean velocity at Re=240. A good match between DDES model and experimental data is observed. At Re=240 transition from laminar to turbulence has already occurred inside the micro-scale MIVR. Highly turbulent fluctuation near the reactor has been experimentally observed. However, previous study using RANS or LES simulation have not shown good prediction for this fluctuation.[12; 6] Actually, the main disadvantage of applying common RANS model such as k-\(\epsilon\) model to the micro-scale MIVR is that turbulent intensity is significantly underestimated in the reactor center. Figure 6.11 presents the prediction of turbulent intensity at Re=240 by the new DDES model, which matches the experimental measurement quite well with consideration of measurement uncertainty and noise. Both simulation and experiment confirm that turbulent fluctuation in the MIVR is concentrated in the reactor center. The same phenomenon is also found in the study about the macro-scale MIVR.[64]

6.3.2.2 Flow field in the micro-scale MIVR

It is interesting to see how the behaviour of flow changes in the micro-scale MIVR when Reynolds number increases. Streamlines based on mean velocity $u_r, u_z$ at different Reynolds number is shown in Figure 6.12. When Reynolds number increase from 53 to 240, recirculation regions appear in the reactor chamber and move towards the bottom and top side. It is found that as Reynolds number increases, more flow from the inlet tends to enter the outlet through top and bottom side of the reactor. This feature is adverse to the mixing performance of the
Figure 6.8  Comparison of normalized mean velocity at Re=53 between DDES and experiment:
(a) $\langle u_r \rangle / U_j$, (b) $\langle u_\theta \rangle / U_j$.

Figure 6.9  Comparison of normalized mean velocity at Re=93 between DDES and experiment:
(a) $\langle u_r \rangle / U_j$, (b) $\langle u_\theta \rangle / U_j$. 
Figure 6.10  Comparison of normalized mean velocity at Re=240 between DDES and experiment: (a) $<u_r>/U_j$, (b) $<u_\theta>/U_j$.

Figure 6.11  Comparison of normalized turbulence intensity at Re=240 between DDES and experiment: (a) $<u'_r>/U_j$, (b) $<u'_\theta>/U_j$.  

micro-scale MIVR as flow from different inlets can escape into the outlet through the wall without interaction. Figure 6.13 shows the change of turbulent Reynolds number $Re_T$ along with Reynolds number. $Re_T$ represents local turbulence level and depends on mesh size because resolved turbulence level is considered. The discontinuity feature of $Re_T$ in the center region is caused by mesh refinement there. At $Re=53$ $Re_T$ is steady and close to 1 as flow is laminar. Unsteady feature of $Re_T$ starts to appear in the outlet at $Re=93$. $Re_T$ becomes fully turbulent when Reynolds number reaches to 240. This finding is consistent with the experiment by Shi et al.[84] Most of high $Re_T$ exists in the outlet of the micro-scale MIVR rather than the chamber, indicating most of local mixing actually happens in the outlet region of the micro-scale MIVR.

Figure 6.12 Effect of Reynolds number on mean flow field in the micro-scale MIVR: (a) Re=53, (b) Re=93, (c) Re=240.

Figure 6.13 Effect of Reynolds number on turbulent Reynolds number $Re_T$: (a) Re=53, (b) Re=93, (c) Re=240.

The mean velocity and turbulent intensity field at $Re=240$ are further illustrated in figure 6.14. Contour in $y$-$z$ plane is plotted as flow is axis-symmetrical. It is found that flow from inlets enter the outlet mainly through the bottom and top wall area (figure 6.14a), same as
the finding in figure 6.12. Figure 6.14b also indicates that in the middle of chamber most of flow is close to irrotational where tangential motion is dominant. $u_z$ is positive everywhere except near the corner region, showing that no back flow exists in the reactor center (figure 6.14c), while back flow is observed when the reactor is scaled up[63]. It is noticed that $u_z$ is much higher than $u_\theta$ in the reactor chamber. But the magnitude of $u_z$ drop sharply after flow enter the outlet. That is because swirling flow tends to create low pressure zone in the center of outlet, causing the decrease of axial velocity. The confined geometry and swirling motion helps form the distribution of $u_z$, also causing high turbulent intensity $u_z'$ near the bottom of outlet(figure 6.14f). High turbulent intensity $u'_r, u'_\theta$ is observed in the center of reactor chamber (figure 6.14d and 6.14e). However, the high turbulent intensity doesn’t necessarily enhance the mixing in the center because unsteady motion of vortex center contributes partly to the turbulent intensity. The contribution of vortex wandering to turbulent statistics was also discussed in our previous paper. It is found that 17% - 30% of turbulent kinetic energy in the macro-scale MIVR can be reduced if vortex wandering is eliminated.[64] By assuming that turbulent intensity is isotropic if vortex wandering is not considered, the magnitude of $u'_r, u'_\theta$ should be the same as $u_z'$. Considering their peak value, it is estimated that about 60% of $u'_r, u'_\theta$ is increased near the center because of vortex wandering. This estimation also helps explain the sudden increase of $u'_r, u'_\theta$ at $-0.1 < r/R_0 < 0.1$ in figure 6.11.

6.3.2.3 Passive scalar mixing in the micro-scale MIVR

To further understand how the flow behaviour affect mixing performance of the micro-scale MIVR, passive scalar mixing is studied here. When turbulence field is correctly predicted, it is relatively easy to model bi-variable passive scalar transport in the reactor. The governing equation of passive scalar can be written as

$$\frac{\partial \overline{C}}{\partial t} + \frac{\partial (\overline{u_j C})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( (D + D_T) \frac{\partial \overline{C}}{\partial x_j} \right)$$

(6.18)

where $\overline{C}$ is the filtered concentration of passive scalar, $D$ is molecular diffusivity of passive scalar tracer and turbulent diffusivity $D_T$ is equal to $\nu_t/Sc_t$. $Sc_t$ is turbulent Schmidt number which is usually assumed to be 0.85 in RANS approach and 0.4 in LES approach.[30] In the
Figure 6.14 Mean and turbulent intensity contour at Re=240: (a) $u_r$, (b) $u_\theta$, (c) $u_z$, (d) $u'_r$, (e) $u'_\theta$, (f) $u'_z$. 

$u_r$, $u_\theta$, $u_z$, $u'_r$, $u'_\theta$, $u'_z$
new DDES model, $S_{ct}$ is defined as

$$S_{ct} = 0.85(1 - \Phi) + 0.4\Phi$$

so that in the DDES model $S_{ct}$ can be 0.85 in its RANS mode and 0.4 in its LES mode.

Passive scalar mixing in the micro-scale MIVR has already been measured by using confocal laser scanning microscopy.[85] In the experiment Rhodamine 6G was used as passive scalar tracer. The bi-variable mixing in the micro-scale MIVR is measured. Two opposing inlet streams are ethanol and another two contain Rhodamine 6G. The same set-up is used in the simulation where zero value of passive scalar represents ethanol and one hundred value represents Rhodamine 6G. The limitedLinear scheme in OpenFOAM is applied to the convection term in equation 6.19 so that realizable value of passive scalar is guaranteed.

Figure 6.15 shows the contour of scalar mixing at 1/2 plane with Re=53, 93 and 240. The simulation results of the DDES model is shown in figure 6.15a-c and experimental results are shown in figure 6.15d-f. The prediction of the new DDES model with passive scalar transport agree quite well with experiment where the inner ”tai-chi” pattern is reproduced at Re=53 and 93. As the confocal scanning technique fails to provide meaningful full field image at Re=240, mixing pattern at Re=240 can only be revealed by the simulation. It is found that the inner ”tai-chi” collapse at Re=240 though unmixed fluid still exists there. Figure 6.16 gives a clear view how passive scalar mixes in the micro-scale MIVR at Re=53, 93 and 240. Unmixed scalar enter the inner region through the bottom of reactor and then undergoes spiral motion until diffusion smooths the concentration difference. As Reynolds number increase, turbulence diffusion apparently enhance the mixing and passive scaler is well-mixed when it enters the outlet. Still, there is unmixed scalar in the chamber and further increasing Reynolds number may eliminate them. Study about flow field and mixing at higher Reynolds number than 240 is needed in future work.

6.4 Conclusions

A new DDES model is proposed in current study to predict transitional flow in the micro-scale MIVR which has been applied to produce functional nanoparticles in the Flash Nanoprecip-
Figure 6.15  Comparison of passive scalar mixing between DDES ((a) Re=53, (b) Re=93 (c) Re=240) and experiment ((d) Re=53 (e) Re=93 (f) Re=240).

The new DDES model was first tested by using a standard separation-induced-transition-flow case. Good agreement between the DDES model and pure LES model is observed in terms of transitional features, mean velocity and turbulent intensity of the flow, proving the ability of the proposed DDES model in predicting complex transitional flow. The DDES model was then applied to model the flow at Re=53, 93 and 240 in the micro-scale MIVR, including both laminar and transitional flow case. Overall, the simulation results agree quite well with the simulation data in terms of mean velocity and turbulent intensity, validating the proposed
Figure 6.16  Effect of Reynolds number on passive scalar mixing: (a) Re=53, (b) Re=93, (c) Re=240.
DDES model in modelling complex transitional flow. The simulation results of the micro-scale MIVR also provide us a deeper understanding about the flow in the micro-scale MIVR. It is found that flow from different inlets mainly go through the bottom and top part of the reactor into outlet, indicating flow tend to bypass each other in spiral motion instead of colliding together. By comparing the passive scalar mixing between the simulation and experiment, it is confirmed that the existence of unmixed fluid in the center of the reactor is also caused by the bypass motion of flow. However, with increasing turbulence level, the unmixed fluid can be significantly reduced. Nevertheless, the finding in current paper shows the optimization of the MIVR is necessary to improve its mixing performance, especially near the bottom of the reactor.
CHAPTER 7. SUMMARY AND FUTURE DIRECTIONS

7.1 Summary

In the dissertation, a fundamental investigation on scaling up the multi-inlet vortex reactor has been performed by using both experimental and computational methods. First, a macroscale MIVR with good optical access has been built in our lab, and a platform has been set up to provide flow test for the reactor. Laser-based diagnostic techniques including stereoscopic PIV (SPIV) and planar laser induced fluorescence (PLIF) have been used to measure flow velocity and turbulent mixing in the MIVR. The studied Reynolds number based on the inlet geometry range from 3290 to 8225, indicating a turbulent swirling flow in the MIVR. Based on the experimental velocity data, in Chapter 2 a batchelor vortex model has been derived to describe mean velocity field of the macro-scale MIVR. In the model, the mean axial and azimuthal velocities could be described by using a combination of two co-flowing batchelor vortices, where six dimensionless coefficients are identified by nonlinear curve fitting, and their dependence on Reynolds number are found to be linear. Based on the mean velocity field, turbulent swirling flow in the MIVR was found divided into a free-vortex region and a forced-vortex region. Beside predicting mean flow in the MIVR, the batchelor vortex model can also be extended to other turbulent swirling flow.

A detailed analysis of flow characteristic in the macro-scale MIVR has been performed in Chapter 3. It was found that turbulent swirling flow in the macro-scale MIVR is unstable with its vortex center wandering in a small region whose diameter is about 5% of the reactor chamber. The influence of vortex wandering on the mean velocity, Reynolds stress and turbulent kinetic energy (TKE) was assessed by using two different post-processing methods. In Method One, the velocity statistics are calculated in a fixed frame. In Method Two, the vortex wandering
is eliminated by moving the instantaneous vortex center to the coordinate origin. The mean velocity is found insensitive to the small wandering motion of vortex center. However, the measured TKE and Reynolds stress are found sensitive to the small wandering of vortex center. The maximum value of TKE calculated by Method Two is reduced by 17% to 30% compared to Method One. As the vortex wandering produces pseudo-fluctuations, this finding shows the importance of separating the wandering motion from turbulent fluctuation in estimating mixing performance of the MIVR. The swirling ratio of flow in the macro-scale MIVR is found twice larger than the micro-scale MIVR, explaining why backflow appears in the macro-scale MIVR, not in the micro-scale MIVR. The scaled-up MIVR also has an increase in the theoretical micro-mixing time, indicating it to be less mixing effective than the micro-scale MIVR for the FNP.

Turbulent swirling flow in the macro-scale MIVR was found affected by both vortex wandering and streamline curvature. In Chapter 4 a dynamic DDES model was applied to predict this flow when common-used RANS and LES approach are found inappropriate either due to immature model or high computational cost. Overall, the CFD simulation results agree quite well with previous SPIV data. The recirculating back flow occurring at the center of MIVR is captured by the dynamic DDES model. The superior performance of the dynamic DDES model confirms that it can reduce the drawbacks inherent to the RANS model and can be a good alternative for studying turbulent swirling flow in complex geometry such as the MIVR.

Turbulent mixing of passive scalar in the macro-scale MIVR has been investigated using PLIF. The investigated Reynolds number based on the bulk inlet velocity ranges from 3290 to 8225, and the Schmidt number of the passive scalar is 1250. The mixing characteristics of the MIVR were investigated using instantaneous PLIF fields and point-wise statistics such as mixture fraction mean, variance, and one-point concentration probability density function. The passive scalar field is affected by the velocity field. In the free-vortex region, the passive scalar concentration is stretched along velocity streamlines, forming a spiral mixing pattern and the mixing is dominated by large-scale structures and turbulent diffusion. In the forced-vortex region, mixing of passive scalar becomes much better as turbulent fluctuation becomes higher there, and the mixing is dominant by turbulent diffusion.
After studying the flow and mixing in the macro-scale MIVR, we come back to the micro-scale MIVR and develop a better CFD model for its transitional swirling flow. The new CFD model is a DDES model based on low Reynolds number k-ω model. By limiting the k-equation, LES part of the DDES model behaves as one equation sub-grid model. The proposed model was first validated by simulating a separation induced-transition flow case where results agree well with previous LES data. Applying the model to simulate both laminar and transitional flow in the micro-scale MIVR also produces good prediction for both mean velocity and turbulence intensity. These simulation results also help us understand the flow and mixing pattern in the micro-scale MIVR, and provide guidance for optimizing the reactor for its application in the FNP.

7.2 Future directions

Through the study in previous chapters, we have acquired the fundamental knowledge of the flow field and mixing phenomenon in both the micro-scale and macro-scale MIVR. A few points can be addressed in the future work.

1. More advanced experiment can be conducted to the macro-scale MIVR such as simultaneous SPIV and PLIF. By measuring velocity and concentration at the same time, new results such turbulence flux can be obtained which are valuable to validate scalar mixing model.

2. Since CFD models have already been validated for both the micro-scale and macro-scale MIVR, parameter study about mixing performance of the MIVR during the scale-up process can be conducted so that researcher using MIVR for the FNP can have a better reference for their experiment.

3. A validated model for the FNP process could be developed based on the new turbulence model coupled with population balance model. This would include other computational methods such as quadrature method of moments to predict nanoparticle formation in the MIVR.
BIBLIOGRAPHY


