Turbulence in a microscale planar confined impinging-jets reactor

Ying Liu, a Michael G. Olsen b and Rodney O. Fox a

Received 20th October 2008, Accepted 15th December 2008
First published as an Advance Article on the web 29th January 2009
DOI: 10.1039/b818617k

Confined impinging-jets reactors (CIJR) offer many advantages for rapid chemical processing at the microscale in applications such as precipitation and the production of organic nanoparticles. It has been demonstrated that computational fluid dynamics (CFD) is a promising tool for “experiment-free” design and scale-up of such reactors. However, validation of the CFD model used for the microscale turbulence applications requires detailed experimental data on the unsteady flow, the availability of which has until now been very limited. In this work, microscopic particle-image velocimetry (microPIV) techniques were employed to measure the instantaneous velocity field for various Reynolds numbers in a planar CIJR. In order to illustrate the validation procedure, the performance of a particular CFD model, the two-layer $k$–$\varepsilon$ model, was evaluated by comparing the predicted flow field with the experimental data. To our knowledge, this study represents the first attempt to directly measure and quantify velocity and turbulence in a microreactor and to use the results to validate a CFD model for microscale turbulent flows.

Introduction

The confined impinging-jets reactor (CIJR) is of great industrial interest due to its ability to generate fast mixing, the timescale of which is on the order of milliseconds. 1–4 Confined impinging jets reactors are relevant to many chemical processes, including ultratine or nanoscale particle synthesis using liquid precipitation, hydrothermal synthesis, sol-gel processes, and many other processes. One particular promising application of the microscale CIJR is the manufacture of ultratine or nanoparticles for use in such applications as medical diagnosis and drug delivery, cosmetics, dyes, catalysts, and pesticides. 5,6 In a microscale CIJR the inlet streams are laminar, but the flow field inside the device can become highly turbulent due to the impinging jets. The unsteady nature of the flow field under conditions of rapid mixing makes experimental measurements extremely challenging. As discussed in detail elsewhere, 7 a computational fluid dynamics (CFD) approach that involves a two-layer $k$–$\varepsilon$ model 8 and a direct-quadrature-method-of-moments (DQMOM)-interaction-with-the-mean (IEM) model 9,10 has successfully reproduced (without adjustable parameters) the experimentally measured outlet conversion (i.e., non-local measurements) for a microscale CIJR with the fourth Bourne reaction system, suggesting that CFD can be a powerful tool for design and optimization of such reactors. However, the local velocity and species concentration fields predicted by the CFD model could not be validated since the experimental data were limited to overall conversion. Recent macroscale flow studies have shown that the two-layer $k$–$\varepsilon$ model is able to satisfactorily predict the turbulent flow fields in a macroscale confined planar-jet reactor 10 and confined planar-wake reactor, 11 with flow statistics such as mean velocity, turbulent kinetic energy, and dissipation rate predicted by the CFD model agreeing well with experimental data measured using particle-image velocimetry (PIV). Nevertheless, the performance of turbulence models for a CIJR with microscale dimensions in which the wall effects and the complexity of the flow due to the impinging jets are significant is still open to question. Therefore, we have measured the instantaneous velocity field on a plane in the flow using microPIV and validated a CFD model against the experimental data. To the authors’ knowledge, no similar attempt has been made for unsteady or turbulent flow in such a microscale device.

The theory and image analysis techniques of PIV have been summarized by Adrian, 12,13 and the design rules for optimizing the performance of the PIV system were first formulated by Keane and Adrian. 14 MicroPIV is a modification of PIV that is more suitable for measuring the flow field at the microscale. The first application of microPIV was demonstrated for steady flow by Santiago et al. 15 MicroPIV differs from its macroscopic counterpart primarily by the method of illumination. In PIV, measurements are taken on a plane illuminated by a thin laser sheet. In microPIV, the entire volume of the flow that is imaged by the microscope objective is illuminated, making the measurement depth, or depth of correlation, dependent on such diverse characteristics as the imaging optics, particle size, and emission wavelength, 16 and to a lesser extent, Brownian motion 17 and out-of-plane particle motion. 18

MicroPIV has been increasingly employed to measure the flow in many microfluidic devices. For example, qualitative measurements of the laminar to turbulent flow transition in microchannels and microtubes have been studied using microPIV by a number of researchers. 19–22 Other researchers have investigated quantitatively more complex flow geometries and conditions using microPIV. 23–26 In all these examples, the flow field was steady in time, making it possible to obtain accurate data by filtering spurious fluctuations caused by experimental error. In contrast, unsteady or turbulent flow fields are much more difficult to measure because the instantaneous velocity field measurement must be accurate. To our knowledge, quantitative measurement of turbulent flow fields in microscale planar CIJRs has not been reported before. In this work, microscopic particle-image velocimetry (microPIV) was employed to measure the instantaneous velocity field on a plane in the flow using microPIV. Nevertheless, the performance of turbulence models for a CIJR with microscale dimensions in which the wall effects and the complexity of the flow due to the impinging jets are significant is still open to question. Therefore, we have measured the instantaneous velocity field on a plane in the flow using microPIV and validated a CFD model against the experimental data. To the authors’ knowledge, no similar attempt has been made for unsteady or turbulent flow in such a microscale device.
dimensions for the microreactor are highly desired. Only those techniques that are able to ensure high precision of dimensions are acceptable.

3 If the microreactor consists of more than one piece, the adhesion of the pieces should not introduce any uncertainty in the dimensions of the channels. Moreover, the adhesion must be strong so that the microreactor is able to withstand high working pressures as the flow rate increases.

4 The two inlet channels should be aligned perfectly in order to ensure the impingement of the inlet jets.

5 The buildup of contaminants in the microreactor is almost inevitable. Therefore the microreactor is expected to be “disposable” and affordable.

Initially, we tried to fabricate the microreactor using polydimethylsiloxane (PDMS) replica molding. However, it was found that the PDMS microreactor deformed under high working pressures, altering the dimensions of the microchannel. We were therefore motivated to resort to a mechanical fabrication technique, electrical discharge machining (EDM).

EDM is one of the most accurate manufacturing processes available for creating two-dimensional shapes and geometries within parts and assemblies made of electrically conducting materials. It works by eroding material in the path of electrical discharges, leaving the cutting face clean and smooth. As the first step to fabricate the microreactor used in this study, the desired contour (see Fig. 1) was carved out by EDM on a 0.87 mm thick stainless steel plate. Two glass slides that form the top and bottom walls, respectively, were then bonded to the stainless steel plate by a double-sided silicon transfer adhesive film (Dielectric Polymers), the thickness of which is 0.02504 mm (as stated by the manufacturer). Thus, the depth of the resulting microreactor is 0.92 mm. The top glass slide has three small predrilled holes that hold the connectors for coupling the conduits to the microreactor.

Experimental apparatus and methodology

The experimental setup is schematically shown in Fig. 2. It consists of a flow-delivery system and a microPIV system. A reservoir, two microgear pumps (Console digital dispensing drive, Cole-Parmer Instrument Co.), two needle valves (Cole-Parmer Instrument Co.), and the microreactor are connected via flexible tubing (C-flex tubing, Cole-Parmer Instrument Co.) and form a closed flow-delivery system. The microgear pumps drive the fluid, which is ultrasonicated nano-pure water with dissolved fluorescent particles, at a rate controlled by the pump heads (0.092 ml/rev suction shoe gear pump heads, Cole-Parmer Instrument Co.). Nanopure water is more suitable than deionized water as the solvent in that its extremely low conductivity (18 mΩ-cm) helps reduce the agglomeration of the polystyrene seed particles. The reservoir supplies the inflow and collects the outflow. In this way, the particle solution circulates in the flow facility until all the desired microPIV images are obtained. About...
50 ml particle solution is held in the reservoir, limiting any temperature increase due to viscous heating. After each experimental run, the particle solution was replaced with nanopure water. Then the exact volumetric flow rates were determined by measuring the volume of outflow collected in a container for 5 mins. The inlet flow rates were balanced by adjusting the needle valves. It should be noted that the physical properties, such as density and viscosity, of the working fluid and nanopure water are very close since the density of the fluorescent particles is \( \rho = 1.05 \text{ g/cm}^3 \), and the working fluid contains a very small volume of the particles.

The microPIV system measures particle displacements in the microreactor, and the resulting velocity fields are two-dimensional. The microreactor is placed on the stage of an inverted biological microscope (Nikon model T-300 Inverted Microscope). By moving the microscope stage horizontally (in the \( x \)- and \( y \)-directions), the observed area can be changed without moving the lasers or the camera. The microscope stage can also be lowered or raised along the \( z \)-direction, changing the location of focal plane of the microscopic objective. The 532 nm laser beam from a New Wave Research Gemini PIV Nd:YAG laser system is expanded before being directed towards the microreactor by a dichronic mirror and passing through the objective. The 2 \( \mu \text{m} \) diameter fluorescent seed particles (nile red Fluospheres, Invitrogen Corporation) are excited by the laser light entering the microreactor through its bottom wall and fluorescence with a peak emission wavelength of 575 nm. The beamsplitter reflects the 532 nm laser light, but allows the emitted light to pass through. In this way, only fluorescence emitted by the particles reaches the CCD camera (12-bit LaVision Flowmaster 3S CCD). The laser and camera are connected to a host computer that controls the timing of laser illumination and image acquisition. Two images were captured per velocity field realization at a frame rate of 8 images/s. The corresponding velocity field was computed by dividing the image into small regions (called "interrogation windows") and using a cross-correlation technique to determine a velocity vector for each interrogation window.\(^{29,30}\) The timing between laser pulses was varied for the different flow rates investigated so that the particles travel approximately 1/4 of an interrogation window between exposures.

The concentration of the seed particles in the working fluid was computed by using

\[
C = \frac{N}{A(2Z_{\text{corr}})}
\]

where \( C \) is the number density of the fluorescent particles, and \( N \) denotes the number of particles in each interrogation volume. The typical value of \( C \) to minimize the number of "bad" velocity vectors is 5–10 particles per interrogation volume and is chosen to be 10 in this work.\(^{31}\) \( A \) and \( 2Z_{\text{corr}} \) represent the interrogation area and the depth of correlation, respectively. Given the numerical aperture (NA), the magnification \( (M) \), the wavelength (\( \lambda \)) of fluorescence emitted by the particles, and the particle diameter \( d_p \), the depth of correlation can be found using\(^{16,32}\)

\[
2Z_{\text{corr}} = 2 \left[ 1 - \frac{\sqrt{\epsilon}}{\sqrt{\epsilon} + \left( f^p d_p^2 + \frac{5.95(M + 1)^2 f^p}{M^2} \right)^{1/2}} \right]^{1/2}
\]

where \( \epsilon = 0.01 \). \( f^p \) is the focal number of the lens and can be related to NA by

\[
f^p = \frac{1}{2NA}
\]

In this study, a 4\( \times \) 0.2 NA objective was coupled with a 0.45\( \times \) coupler, yielding a total magnification of 1.8\( \times \) and a depth of correlation of 92 \( \mu \text{m} \). A sufficient seed particle density is required in order to obtain an accurate instantaneous velocity vector field. However, achieving a high seed particle density in microPIV
experiments can be more difficult than in PIV measurements\textsuperscript{10,11,33} and usually requires some sacrifice of spatial resolution.\textsuperscript{10,33} Interrogation windows of 16 × 16 pixels were chosen, corresponding to a spatial resolution of 57.5 \( \mu \)m in the \( x \)- and \( y \)-directions. Adjacent interrogation windows were overlapped by 50\%.

The experiments were performed for inlet jet Reynolds numbers ranging from 211 to 1003. Note that for these Reynolds number the flow in the inlet channels is laminar. The inlet jet Reynolds number \( \text{Re}_j \) is defined by the the inlet bulk velocity, \( u \), the hydraulic diameter of the inlet channel, \( d \), and the kinematic viscosity of nanopure water, \( \nu \), as

\[
\text{Re}_j = \frac{du}{\nu}
\]  

(4)

For each jet Reynolds number, up to 1500 instantaneous planar velocity field realizations were measured and analyzed.

The seed particles are expected to be small enough that their motion accurately reflects the local velocity. The effectiveness of

**Fig. 3** Mean velocity fields measured by microPIV (left) and predicted by the two-layer \( k-\varepsilon \) model (right) for \( \text{Re}_j = 211 \) (top), \( \text{Re}_j = 601 \) (middle) and \( \text{Re}_j = 1003 \) (bottom).
the seed particles can be quantified by introducing the particle Stokes number $St$ that characterizes the ratio of particle response time to the flow time scale:

$$St = \frac{\gamma r_p d_p^2}{12 \rho_f \rho_t}$$

(5)

In the equation above, $\gamma$ is a characteristic strain rate for the flow and can be approximated by $2u/W$, $\rho_t$ and $\rho_f$ are the fluid density and viscosity, respectively. For $Re_j = 1003$, $St = 2.9 \times 10^{-4}$, indicating that the inertia of the particles does not affect the experimental accuracy.  

**Simulation conditions**

The behavior of the planar CIJR was simulated using Fluent 6.2 with a steady-state flow solver. The 3-dimensional computational grid consisted of at least 20880 hexahedral cells, with more cells for grid-independent solutions at higher Reynolds numbers. For cases where the impinging jets generate a turbulent flow, the two-layer $k-\epsilon$ model, which is the standard $k-\epsilon$ model plus the enhanced wall treatment in Fluent 6.2, was employed to compute the turbulent kinetic energy and dissipation. For computational efficiency, the inlet and outlet length-to-width ratios, $L_1/w$ and $L_2/d$, were reduced to 4 and 2, respectively in the simulations. The laminar inlet boundary conditions for the two jets are assumed to be identical except for the sign of the $x$-component of velocity and were given by the outflow (computed separately) of a rectangular tube with $L_1/w = 30$. Our previous study has shown that the turbulence statistics near the impinging jets do not change significantly with $L_2/d$ unless the jet Reynolds number is high (that is, $Re_j > 1000$). For $Re_j = 211$, the flow is steady laminar flow everywhere in the device and no turbulence model was employed in the simulation. At higher Reynolds numbers, the flow near the impinging jets becomes unsteady and the turbulence model is used to compute the time-average (mean) velocity, the turbulent kinetic energy and dissipation.

**Results and discussion**

The flow field was measured for three inlet jet Reynolds numbers, 211, 601 and 1003. In the experiments, the objective was focused on the plane centered in the spanwise direction ($z$-direction). After some time to allow for the flow to reach a fully developed state, sample images were taken and the velocity vector field was calculated. The needle valves were adjusted carefully if the sample images indicated that the inlet jets were not well balanced. This procedure was repeated until the inlet jets met in the middle of the microreactor. Then up to 1500 realizations were captured for each jet Reynolds number and analyzed to extract the mean velocity and turbulent kinetic energy.

**Mean velocity field**

The image formed using the $4\times$ objective and $0.45\times$ coupling covers an area of $4.6 \times 3.68 \text{mm}^2$. The mean velocity fields measured by microPIV are compared with the mean velocity fields from CFD for $Re_j = 211$, 601 and 1003 in Fig. 3. They are in reasonable agreement, demonstrating that the steady-state CFD model is able to provide a good approximation for the mean velocity fields. Four recirculation areas exist in the flow, one pair above the impinging jets and one pair below. Each pair is located symmetrically with respect to the centerline of the chamber ($x = 0$). This is not surprising if one recalls that the volumetric flow rates of the inlet jets were balanced. The $x$-momentum diminishes quickly to zero once the inlet jets impinge, while the flow turns towards the
y-direction, leading the fluid to go up and down. The flow going up forms the recirculation zones above the impinging jets, while the recirculation zones below are generated by the flow going down. The impinging jets meet somewhere below $y = 0$, indicating that fluid tends to go to the outlet direction rather than the top of the chamber. In fact, velocities near the top of the chamber are very small and hence difficult to measure accurately. The length of the jets predicted by the two-layer $k-\varepsilon$ model is short and the $y$-momentum is high compared with their microPIV measurements (see Fig. 3 middle and bottom). This could be explained by a well-known behavior of the $k-\varepsilon$ model: it tends to overpredict the spreading rate of jets. In any case, given the relatively low Reynolds numbers in the experiments, we can conjecture that an unsteady flow solver such as large-eddy simulations might provide a better approximation of the mean velocity fields.

Fig. 4 shows the profiles of the $x$-component of the mean velocity ($\langle U \rangle$) as measured by microPIV and predicted by the CFD model on different $x$-planes. For $x = \pm 2$ mm, the computational results match the experimental data very well, most likely because the flow is laminar at these locations. At $x = 0$, $\langle U \rangle$ should be zero if the inlet flows rates are identical. It is shown by Fig. 4 that the flow rates for $Re_j = 1003$ (Fig. 4c) were

**Fig. 5** Instantaneous velocity fields as measured by microPIV for $Re_j = 601$ (left) and $Re_j = 1003$ (right).
well balanced, but for $Re_j = 211$ and $601$, the right inlet flow rate was slightly higher than the left inlet flow rate. This is because of the great difficulty in perfectly balancing the two inlet flow rates. However, based on the observed agreement relative to experimental errors seen for other flow quantities, this slight mismatch does not seem to be crucial.

Some instantaneous planar velocity fields, as measured by microPIV, are displayed in Fig. 5. For $Re_j = 211$, the instantaneous velocity field is very similar to the time-averaged velocity field (see Fig. 3), indicating that the flow is laminar and the velocity fluctuations are very small. The flow field shows stronger fluctuations at $Re_j = 601$ and $1003$ (Fig. 5) and some small turbulent eddies can be observed in the flow. The flow being turbulent at these two highest Reynolds numbers is consistent with large eddy simulations of an axisymmetric confined impinging jet reactor that showed the flow to be turbulent at $Re = 700$.\(^{38}\)

Figure 5 also shows that the inlet jets significantly flap about at $Re_j = 601$ and $1003$. Since the set points for the gearpumps and needle valves remained constant through the entire experimental run, it is likely that the movement of the flow in the impinging area is

---

**Fig. 6** Turbulent kinetic energy measured by microPIV (top) and predicted by the two-layer $k$-$\varepsilon$ model (top) for $Re_j = 601$ (left) and $Re_j = 1003$ (right). The profiles of turbulent kinetic energy at $x = 0$ are also compared (bottom). Line: microPIV; symbols: CFD.
very sensitive to instabilities that arise at the flow inlets at medium to high Reynolds numbers. Note that the large-scale flapping motion is not explicitly captured by the steady-state turbulence model, and instead it is lumped into the turbulent kinetic energy field.

Turbulence statistics

The turbulent kinetic energies predicted by the two-layer $k$–$\varepsilon$ model for $Re_j = 611$ and 1003 are compared with the experimental data in Fig. 6. We should reiterate that obtaining quantitative data for turbulence statistics in microscale devices is extremely challenging and requires careful control of all sources of experimental error. From Fig. 6, it can be seen that the CFD model roughly captures the essential features appearing in the experimental data. The turbulent kinetic energy has a peak value at the center of the impingment area, as expected. Generally speaking, the zone of intense turbulence is limited to a small region near the impingment point compared with the total volume of the planar CIJR. Therefore, the fluid from the inlets can easily bypass the impingment zone. This behavior was also observed in the original CIJR.7

The magnitude of the predicted turbulent kinetic energy differs from the experimental data to some extent, most likely due to the low Reynolds number and the large-scale flapping motion observed in Fig. 5. For example, the maximum value predicted for $Re_j = 611$ is $0.53 \, m^2/s^2$, which is higher than the measured value of $0.37 \, m^2/s^2$. In contrast, the maximum value predicted for $Re_j = 1003$ is $1.3 \, m^2/s^2$, which is lower than the measured value of $1.75 \, m^2/s^2$. These discrepancies can be attributed to the fact that the $k$–$\varepsilon$ model is parameterized for high-Reynolds-number turbulence. It is apparent that at $Re_j = 611$ the turbulence is not fully developed, and hence $Re_j$ is not high enough for the model to work with great accuracy. When the jet Reynolds number was increased to 1003, the turbulence model should be expected to do a better job, and yet it slightly underpredicts the measured velocity fluctuations. This discrepancy is due to the intense flapping of the impinging jets at the highest Reynolds number (see Fig. 5). The two-layer $k$–$\varepsilon$ model is unable to account explicitly for the flapping, resulting in the computed turbulent kinetic energy being lower than the measured value. Nevertheless, the overall performance of the two-layer $k$–$\varepsilon$ model is satisfactory as a first approximation of the flow. Further improvements are likely possible using an unsteady flow solver (e.g., large-eddy simulation) but at a much higher computational cost.

Conclusions

In this study, microPIV and CFD procedures were employed to study a planar microscale CIJR with inlet jet Reynolds numbers ranging from 211 to 1003. The technique for microreactor fabrication were discussed. The investigated microreactor consists of three pieces, a stainless steel plate precisely cut by EDM and two glass slides, that are bonded by adhesive film. The microPIV measurements were carried out using a $4 \times 0.2 \, NA$ objective and $2 \, \mu m$ fluorescent particles. Flow statistics such as the mean velocity and turbulent kinetic energy were computed from the microPIV velocity fields, and these data were then used to validate the two-layer $k$–$\varepsilon$ model.

The overall agreement between the CFD predictions and the experimental data for mean velocity and turbulent kinetic energy is satisfactory, but essential physics such as jet flapping are not captured by the steady-state CFD model. The inlet jets flap significantly at a high inlet jet Reynolds number, resulting in a turbulent kinetic energy larger than the CFD prediction. CFD model predictions can likely be improved by using an unsteady model such as large-eddy simulations, but at much higher computational cost. Nonetheless, this study represents the first attempt to validate a CFD model against quantitative experimental data for the unsteady velocity field in a turbulent microscale reactor.

Acknowledgements

The authors gratefully acknowledge the support from the National Science Foundation. This work has also benefited from our interaction with Dr. Hao Li at Argonne National Laboratory.

References

16 M. G. Olsen and R. J. Adrian, Exp. Fluids, 2000, 29, S166.