Numerical Investigation of a Novel Microscale Swirling Jet Reactor for Medical Sensor Applications

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Abstract. A microscale swirler and corresponding reactor for a recent detection and analysis tool for healthcare applications, Fiber optic-surface plasmon resonance (FO-SPR), is presented in this study. The sensor is a 400 μm diameter needle that works as a detector for certain particles. Currently, the detection process relies on diffusion of particles towards the sensor and hence diagnostic time is rather long. The aim of this study is to decrease that diagnostic time by introducing convective mixing in the reactor by means of a swirling inlet flow. This will increase the particle deposition on the FO-SPR sensor and hence an increase in detection rate, as this rate strongly depends on the aimed particle concentration near the sensor. As the flow rates are rather low and the length scales are small, the flow in such reactors is laminar. In this study, robustly controllable mixing features of a swirling jet flow is used to increase the particle concentration near the sensor. A numerical analysis (CFD) is performed to characterize the flow and a detailed analysis of flow structures depending on the flow rate are reported.

1. Introduction

Fiber optic-surface Plasmon resonance (FO-SPR) is a recent detection and analysis tool with many promising applications in health care diagnostics [1]. The sensor is a 400 μm diameter needle that works as a detector for certain particles. Currently, the detection process relies on diffusion of particles towards the sensor and hence diagnostic time is rather long [1]. As the flow rates are low and the scales are small, the flow in such reactors is laminar. However, a previous study by Ogus et al. [2] shows that it is possible to achieve mixing and turbulent-like characteristics in low Reynolds number regimes by introducing swirl to the flow. This technique will be applied to the microscale reactor in this study.

Annular swirling jets have robust control capability over flows. The flow topologies that can be achieved by changing the inlet swirl are reported thoroughly in literature [2,3]. The challenge for FO-SPR is to increase mixing and particle concentration near the sensor. The swirl has influence on the flow field can meet this challenge. For instance, above a critical value of swirl rate, an isolated recirculation zone downstream of the nozzle appears, called vortex breakdown. Vortex breakdown can be defined as the abrupt widening of the jet core creating a spiral or bubble-like recirculation zone [4,5]. The reviews of Syred et al. [6] and O’Negro et al.[7] are one of the most comprehensive summaries of vortex breakdown and spiral type precessing vortex core studies, mainly related to swirl combustion systems. The nature of the onset of vortex breakdown is not fully understood yet. For a free jet annular or bulk flow jet, previous studies show that the vortex breakdown occurrence is correlated to critical swirl rates [6,8]. In previous studies, it was observed that the vortex breakdown flow state in these type of flows increases mixing [6,8]. There are several types of vortex breakdown. The annular jets with swirl are known to create a spiral type vortex breakdown with a single [10] or a
double helix [11]. This type of vortex breakdown, also known as the precessing vortex core (PVC), creates a helical structure inside the jet core. For a Reynolds number in the same order of magnitude, a single helical vortex is observed previously [12].

Enhance mixing in small scale flows, such as bioreactors, is a big challenge as the Reynolds numbers are low and a fully turbulent flow is not feasible to achieve. Using the features of the spiral vortex formation on a swirling jet flow may provide a solution to this problem. The mixing enhancement by vortex breakdown provided by swirl addition is discussed in this paper. By means of direct numerical simulations (DNS), the contribution of vortex breakdown and the PVC to mixing is studied. First, a mixing vessel is designed in the required length scale for the FO-SPR sensor. The vessel is fed by a swirl generator. Then, the fluctuation and precession frequencies are determined for different Reynolds numbers. These frequencies correspond to shedding and laminar instabilities. Turbulent frequencies are not observed. Auto correlation maps for different regions of the flow field are compared. For a further investigation of the flow field, 3D visualization of the vortices are acquired.

2. Swirler and vessel design.
To increase the mixing in small bioreactors, a flow chamber based on a 24 well plate vessel is designed. The design is aimed to work with flow injection methods working with standard syringe pumps for particle detection. The flow is injected from the inlet, shown in Figure 1, coming from the syringe pump. The fluid is transferred to a settling chamber to ensure uniform flow distribution. A microscale swirl generator is connected to this settling chamber and swirl is provided by 6 channels connected to an annular nozzle. The outer nozzle diameter is 3mm, with an inner body diameter of 1.8 mm. The system feeds inside a 15mm diameter to 15mm height vessel of a 24 well plate. Inside this vessel the FO-SPR sensor is planned to be placed for the diagnostics after determining the optimum location for better mixing.

![Figure 1](image)

**Figure 1.** The vessel and swirler design.(Cross section, \(D_s = 3\) mm, \(D_i = 1.8\) mm, \(D_{\text{vessel}} = 16\) mm, \(D_{\text{in}} = 1.6\) mm and \(D_s = 6.5\) mm)

3. Numerical Configuration
The simulations are done using the commercial solver Fluent [13]. Since, the Reynolds number is very low, the Navier – Stokes equations are solved directly using DNS without using any turbulence modelling. The governing equations are
\[
\frac{\partial u_i}{\partial x_j} = 0 ,
\]  
(1)

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad \text{and}
\]  
(2)

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}
\]  
(3)

where \( u_i \) and \( u_j \) are velocity components, \( \mu \) is the viscosity, \( \rho \) is the density, \( p \) is the pressure, and \( \tau_{ij} \) is the viscous stress. A structured numerical grid is constructed with a finer midcore region of the flow as high gradients are expected due to shear layers. Figure 2 shows the details of the numerical grid.

![Figure 2. Numerical grid details.](image)

The nature of the flow includes free shear layers that lead to very high gradients. To resolve these gradients, QUICK (Quadratic upstream interpolation for convective kinematics) discretization scheme for momentum has been used [14]. The segregated SIMPLE (Semi-Implicit Method for Pressure Linked Equations) is used for pressure velocity coupling. The discretization of the diffusion term is second order central differencing. A bounded second order implicit time discretization scheme is used for second order accuracy and numerical stability. For a valid DNS study, the spatial and temporal resolution should be taken into account separately. There are two main criteria for the temporal resolution. The first one is that the time step should be as small as to resolve the smallest time scale in the flow. A time step independence simulation is made for 1 ms and 0.5 ms. It is observed that the error between these time steps for second order statistics (root mean square) of centerline velocity is maximally 2.9\%, and for the mean velocities around 1.8\%. For this study, the time step is chosen to be 0.5 ms for Courant number concerns. The frequency of large scale instabilities such as jet core
fluctuation and the vortex precession is found to be around 2-3Hz. Therefore, the chosen time step is small enough to fully resolve these fluctuations.

To validate the DNS study, as well as the temporal resolution, the spatial accuracy should be taken into account. For the spatial resolution, the first criterion checked is the Courant–Friedrich–Lewy condition, \( \text{CFL} = u\Delta t/\Delta x \approx 1 \), which represents that in the flow field an imaginary Lagrangian particle travels less than or equal to one cell size distance. This condition is met inside the vessel areas within the area of interest.

As grid convergence study and to determine the spatial discretization errors, the grid convergence method suggested by Roache [15] is used. At least 3 reference solutions on three grids are required. These grids have approximately 900,000, 1,800,000 and 3,900,000 elements. Then, converged solutions of first and second order statistics on these grids are obtained. The converged solutions are analyzed to determine the grid convergence index, \( \text{GCI} = F_{s}e^{2}/(r^{p} - 1) \), where \( F_{s} \) is the safety factor for the grid convergence, which is 3 for 2 grid studies in 95% confidence interval, \( r \) is the grid convergence rate, \( p \) is the order of extrapolation (chosen as 2), and \( e_{12} = (g_{1} - g_{2})/g_{2} \) is the error between the two finest grids, with \( g \) being the solved flow parameter. As flow parameter, the maximum RMS values of axial velocity and velocity magnitude, as well as the means of these values are considered. For the maximum RMS values, the convergence index between finest (3.8 million cells) and 2nd (1.8 million cells) grids are 7% and the maximum error \( e_{23} \) is 2.9%. Therefore the 1.8 million cell grid is used for the rest of the study.

4. Velocity field results
As the aim of this study is to determine the regions and flow states with highest fluctuation values, i.e., regions with intensive mixing, mean flow fields for understanding the flow field and root mean square (RMS) of the axial velocity are reported as it resembles the inner and outer shear layer very clearly. Table 1 shows the mass flow rates, Reynolds and swirl numbers for each setting. The flow rates are limited by the syringe pump that the application requires to be used. The Reynolds number is calculated with the velocity measured on a line on the outlet of the nozzle based on the hydraulic diameter \( D_{H} = D_{o} - D_{i} \). The Reynolds numbers vary between two extremes, Re= 42, and Re = 168. The swirl rates are determined with the ratio of tangential momentum flux to axial momentum flux as

\[
S_{w} = \frac{\int_{D_{o}}^{D_{i}} 2\pi r U W r^{2} d r}{0.5 \int_{D_{o}}^{D_{i}} 2\pi (\rho U^{2}) r d r},
\]

where, \( U \) and \( W \) denote, respectively, instantaneous axial and tangential velocity components, and the overbar denotes time average of them. The swirl numbers that these flow rates produce also vary with Reynolds number as the swirl generator has a constant geometry.

Table 1. Swirl rates and Reynolds numbers reported in this study.

| Case | Mass Flow Rate (kg/s) | Nozzle Mean Velocity (m/s) | Reynolds number | Swirl rate |
|------|----------------------|--------------------------|----------------|-----------|
| Case 1 | 1.05x10^{-4} | 0.036035081 | 42 | 0.223 |
| Case 2 | 2.63x10^{-4} | 0.090373696 | 84 | 0.608 |
| Case 3 | 5.26x10^{-4} | 0.180747393 | 168 | 0.684 |
Figure 3 shows the mean axial velocity field results for these 3 cases. The first case doesn’t provide vortex breakdown. As mentioned before, the vortex breakdown requires a recirculation zone inside the core. However, for the second and third case, this recirculation zone is observed with a negative axial velocity present inside the jet core.

![Figure 3. Mean axial velocity fields [m/s]. (Left: Case 1, Middle: Case 2, Right: Case 3)](image)

Figure 4 shows the RMS of axial velocity fields for Case 2 and Case 3. Case 1 is not reported as it does not have significant fluctuations. The root mean square of the flow fields shows that the fluctuation values on these zones are concentrated at the inner and outer shear layer for the Re = 84 and Re = 168 cases (Case 2 and Case 3). Case 2 has a more homogeneous fluctuating velocity region in inner and outer shear layer. On Case 3 with double higher flow rate as the 2nd case, the highest fluctuations are observed in a complete different region compared to Case 2, where the jet loses its momentum. Fluctuations with similar magnitude on inner and outer shear layers, as in Case 2, still exist. The fluctuation magnitudes correspond to 10% of the maximum velocity for the second case as for the inner and outer shear layer of the Case 3. The highest fluctuations observed are around 25% of the maximum velocity for the third case. This suggests that this case might be better for mixing. Application wise, the needle sensor should be aimed to the location of maximal RMS velocity, where increased mixing and particle concentration is to be expected. This optimal location strongly depends
on the flow rate. To further understand the mixing behavior, the frequencies of these fluctuations also need to be determined. The frequency of fluctuations are obtained by a fast Fourier transform in a point inside the highest RMS region. Both cases show a very steady fluctuation around 2Hz. The fluctuations have a very periodic nature and turbulent mixing does not exist in these flow configurations. However, the existence of vortices should be proved if any exist. The vortices, with circulation, may trap the particles and enhance the particle concentration. The first analysis is to determine the autocorrelation mapping with 2-point correlations on a 2D plane with the velocity components as

\[
\rho_{ij}(t) = \frac{\langle u_i(z_1,t_1)u_j(z_1,t_1) \rangle}{\sqrt{\langle u_i^2(t) \rangle \langle u_j^2(t) \rangle}},
\]

where, \(u_i\) and \(u_j\) are the velocity deviation from the mean component and \(\langle \cdot \rangle\) denotes time averaging. This autocorrelation mapping is made in a point where the highest deviation magnitudes are observed for each case. The correlation maps for Case 2 shown on Figure 5 shows a non-isotropic behaviour when the radial (\(V_r\)) and the swirling (\(V_s\)) velocity components are compared. This behaviour is also reported by Freitag et al [16] for swirling flows with higher velocity, and is reported as most probably the result of a vortex breakdown spiral. To prove that this spiral type vortex is present in this state, a 3D visualization is required.

The correlation map for Case 3, shown in Figure 6 for the location with the highest RMS magnitude location, shows an isotropic behaviour on the contrary to the previous case. This suggests that the vortex that is present here, is not likely to be a spiral pattern type vortex. Also, the correlation maps for Case 3 are approaching to zero (from red to dark blue) in a slightly smaller distance than Case 2. This suggests that the vortices present in this case are smaller than the previous one, since this distance is a measure of the biggest scale of the vortex structure.

**Figure 5.** Autocorrelation Map for Case 2.
Figure 6. Autocorrelation Map for Case 3.

5. Vortex visualization

A further investigation on the vortex structures is made. This visualization gives more insight, not only for the position of the sensor, but also for the fundamental nature of the precessing vortex core or other flow features. For the visualization, the Q criterion described by Jeong and Hussain [17] is used. It is defined as $Q = 0.5(|\Omega^2| - |S^2|) > 0$, where the vorticity tensor ($\Omega$) dominates the strain rate tensor ($S$) that is derived by partitioning the second order velocity gradient tensor. The visualized cases are discussed in terms of the sensor application and the nature of the vortices.

The first case visualized is Case 1 with $Re = 42$ and $Sw = 0.22$. The vortex formation is extremely weak except just downstream the nozzle. Even though the robust location of this circulation bubble provides a good option for the sensor position, fluctuation values lower than 1% of the velocity are considered not to provide enough mixing. The visualization of the second case, with $Re = 82$ and $Sw = 0.6$, clearly shows the precessing vortex core or spiral vortex core. The spiral is visible both at the inner shear layer of the core and the outer shear layer. The oscillation frequency of the spirals has been determined as 2 Hz. The configuration provides a solution for mixing and a robust location for the sensor to place in order to obtain a higher particle concentration. The vortex structure shows an irregularity in vortex distribution. These vortices should be regularly shaped in ideal axisymmetric conditions [2]. The irregular shape is caused by the non-ideal conditions of the swirler design. This suggests that the designed swirler is not able to provide fully axisymmetric swirling velocity profiles.
Figure 7. Vortex Visualization for Case 1 (Yellow: $Q = 200$, Blue $V_y = 0$ m/s (axial) at an arbitrary instant)

Figure 8. Vortex Visualization for Case 2 (Green: $Q = 1000$, Blue $V_y = 0$ m/s (axial) at an arbitrary instant)
Figure 9. Vortex Visualization for Case 3 (Yellow: Q = 1000, Blue \( V_y = 0 \) m/s (axial) at an arbitrary instant)

The third case with the highest velocity and swirl rate, the vortex formation is not following the PVC formation pattern. The chaotic positions of the vortices might provide a better mixing resulting in higher fluctuation magnitudes as previously shown. Even though the fluctuation frequency stays the same as the previous case at 2Hz, the higher magnitude of the fluctuations is an advantage. However, if a very precise control of the vortex structures is desired, this flow rate is not sufficient. This result shows that the swirler design could be revised to provide a more regular flow on these Reynolds numbers. A previous study [2] shows for Reynolds number around 180, this type of flow creates robustly controllable flow fields at much higher frequencies. However, the irregularity is an advantage in maintaining higher fluctuation magnitudes.

6. Conclusion

For finding the optimum mixing characteristics for a FO-SPR sensor, a novel mixing tank is designed. The new design consists of a swirl generator feeding a single vessel of a 24 well plate. The swirling flow considered is investigated in term of vortex structures and fluctuation characteristics. An optimum position for the needle–like sensor is tentatively determined by investigating the behaviour of the flow features for different flow rates. The numerical analysis is made by a DNS approach with relatively low computing power as the flow velocities are very low. The resulting flow fields did not provide turbulent mixing. However, a fluctuation of 2 Hz frequency is obtained without using an external mechanical effect, just by controlling the flow. The precessing vortex core obtained, provides an optimum location for the needle like sensor. Also, for higher flow rates, an irregular vortex distribution is obtained that could be beneficial for mixing. The design is open to development by a more optimum swirler design, for a better control of the flow and to obtain higher fluctuation magnitudes at higher flow rates. The future research is to improve the swirler design to provide a more
regular flow field, determine the particle concentration ability of the PVC and validate the flow fields experimentally.

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