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A Study of the Flow Structures Generated by Oscillating Flows in a Helical Baffled Tube

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Abstract: Oscillatory baffled reactors (OBRs) are able to generate plug flow at laminar net flow conditions, providing appropriate oscillation conditions are selected. Mesoscale OBRs containing helical baffles exhibit wider “operating windows” (i.e. a broader oscillation intensity range) for plug flow than other baffle designs. It has been hypothesised that additional swirling in the flow provides another mechanism to limit axial dispersion. These swirling flows have previously been qualitatively identified, but in this study these flows were investigated both numerically and experimentally using CFD and PIV for the first time. The flow structures obtained via simulation (laminar solver) were visualised using isosurfaces of the Q-criterion and 3D streamlines. The characteristic feature of the flow is a helically shaped vortex that forms behind the baffle. Streamlines move both radially (wrapping around the vortex structure) and tangentially. Using the swirl number and analogous ‘radial’ number, a transition between vortex-dominated and swirl-dominated mixing was observed providing evidence that the hypothesis is valid. It was found that when the oscillation intensity is increased, the tangential motion of the flow increases faster than the increase in radial flow because the vortex sizes are bounded by the column diameter.

Keywords: Plug flow, swirl flow, helical coil, oscillatory baffled reactor, mesoscale

1 Introduction

Oscillatory flow inside a baffled tube leads to a cycle of vortex formation and dissipation during each flow reversal, producing axial and radial velocities of the same order of magnitude. Upon addition of a net flow, the baffled tube behaves as a large number of continuous well-mixed tanks-in-series, giving a good approximation to plug flow. Plug flow is a model condition where the cross-sectional velocity profile is constant, meaning any point in the transverse direction exhibits the same time history upon exiting the domain. The main practical application of such a condition is reaction engineering. Indeed, this plug flow behaviour has been exploited for the screening of reactions in flow in Oscillatory Baffled Reactors (“OBRs”), where the effects of multiple operating conditions have been determined in a single experiment [1].

Three dimensionless groups govern the hydrodynamics in the OBR. These are the net flow Reynolds number (Re_n), oscillatory Reynolds number (Re_o) and Strouhal number (St). Defined by equations 1–3 below, these groups define the net flow, oscillation intensity and eddy propagation respectively. Additionally, the velocity ratio (ψ) is sometimes used (equation 4). In these equations, v is the net flow velocity, ρ is the liquid density, D is the reactor diameter, μ is the liquid viscosity, f is the oscillation frequency and x_o is the oscillation amplitude.

$$Re_n = \frac{\rho v D}{\mu} \quad 1$$

$$Re_o = \frac{2\pi f x_o \rho D}{\mu} \quad 2$$

$$St = \frac{D}{4\pi x_o} \quad 3$$

$$\psi = \frac{Re_o}{Re_n} \quad 4$$

Plug flow has been characterised at “conventional scale” (≥ 25 mm diameters) [2] and mesoscale (~ 5 mm diameter) [3,4,5] using the tanks-in-series model. Here, the effective number of tanks-in-series (N) describes the plug flow quality. The velocity ratio, ψ , has been correlated to the plug flow response. For conventional scale orifice baffles, suitable plug flow can be achieved when $2 < \psi < 12$ [2]. Similarly, with mesoscale central and integral baffles (see Figure 1), conditions of $4 < \psi < 8$ [3] and $5 < \psi < 10$ [3] respectively produce suitable plug flow. The helical baffle conversely has a very wide operating range. It is able to produce a high level of plug flow [5] at velocity ratios of $5 < \psi < 250$. This is believed to be because an additional swirling motion is superimposed onto the oscillatory mixing. This swirling motion has been qualitatively identified in CFD studies by Solano *et al* [6] and Mazubert *et al* [7,8]. The latter study also confirmed that single helical ribbons provided the lowest axial dispersion compared to single orifice and disc-and-donut orifice baffles. However, no quantification of the swirling motion has been investigated, nor has any experimental validation of helical baffle flow patterns been attempted.

Figure 1 – Mesoscale OBR baffle geometries / (a) integral, (b) central, (c) helical, (d) sharp-edged helical, (e) sharp-edged helical with central rod, (f) wire wool [1]

Swirling flows are used in many industrial processes such as cyclone separators, combustors and heat exchangers. Typically, the tangential velocity component in a swirling flow in a plain tube can be categorised into core, annular and wall regions [9]. The core flow region undergoes a solid body rotation that is stabilised by centrifugal force, while the annular region is less stable and anisotropic because of free vortex behaviour [9]. Also, because of centrifugal forces, at some point downstream the pressure at the centre of the pipe reduces to the point where the flow collapses on itself, known as vortex breakdown. This process results in high recirculation at the centre of the domain [10]. A common method for characterising the swirl flow intensity is the Swirl number, S_n , given by equation 5 in its simplest form [10]. Here v_z and v_θ are the axial and tangential velocity components respectively, r is the radial position and R is the hydraulic radius of the tube of interest (5 mm for the meso-OBR). This equation describes the ratio of axial flux of angular momentum to the axial flux of linear momentum. Generally, the swirl is considered significant when $S_n > 0.4$.

$$S_n = \frac{\int v_z v_\theta r^2 dr}{R \int v_z^2 r dr} \quad 5$$

The vortices produced in the OBR upon each flow reversal resemble features of a turbulent flow. However, an important result from the numerous numerical studies reported for OBRs is the flow can be considered ‘laminar unsteady’. Ni *et al* [11,12] showed that the mixing is mainly governed by the resolved scale flow structures such as flow separation and vortex interactions. Therefore, the subgrid scale turbulent kinetic energy (TKE) has been observed to be much smaller in comparison to the resolved TKE, giving a corresponding turbulent integral length scale of the order of 1 mm. Consequently, laminar solvers are able to match the bulk flow patterns obtained using the large eddy simulation (LES) model as well as experimental particle image velocimetry (PIV) results. The term “laminar solver” described here is analogous to direct numerical simulation, where no additional subgrid scale models are used. Zheng *et al* [13] additionally showed that the frequency spectrum of the radial velocity component contains only two dominant frequencies. These relate to the boundary condition (oscillatory velocity) and formation of two vortex pairs per cycle (on the up and down

stroke of the oscillation). The authors argue a turbulent flow would produce a more stochastic frequency spectrum [13]. The most recent discussion about the use of laminar solvers in oscillatory flows was made by Nogueira *et al* [14], who argue that the laminar solver behaves as an implicit large eddy simulation (or ILES). Here, no subgrid scale model is used but instead, dissipation is provided solely by the model truncation error.

The mixing in OBRs observed from CFD has been quantified using the volume-averaged axial to radial velocity ratio (equation 6) [15], asymmetry index (equation 7) [13] and axial dispersion coefficient [15,16]. The axial dispersion coefficient can be obtained from the Péclet number, which itself can be calculated from the variance and mean residence time of a distribution of either particles [16] or a second fluid [15] patched into the simulation. In these equations, v is the velocity, V is the volume, σ^2 is the variance of a tracer distribution, t_m the mean residence time of tracer and Pe the Péclet number. The subscripts z , r and θ describe the axial, radial and tangential directions, while the subscript i refers to the cell (position within the full mesh).

$$v_R = \frac{\sum_{i=1}^I |v_{z_i}| V_i}{\sum_{i=1}^I |v_{r_i}| + |v_{\theta_i}| V_i} \quad 6$$

$$\eta = \frac{1}{2} \times \left(\frac{|v_z - v'_z|}{|v_z| + |v'_z|} + \frac{|v_r + v'_r|}{|v_r| + |v'_r|} \right) \quad 7$$

$$\frac{\sigma^2}{t_m^2} = \frac{2}{Pe} + \frac{8}{Pe^2} \quad 8$$

Particle image velocimetry (PIV) is a common technique used to quantify flow fields. By comparing digital images taken by a CCD camera of illuminated seeding particles (micron-scale) in a flow via specialised software (e.g. PIVlab), a velocity field can be constructed. For oscillatory flows, PIV has mainly been used to validate CFD simulations by qualitative comparison of the flow patterns or quantitative comparison of various metrics. For instance, Reis *et al* [17] studied the flow patterns in a mesoscale OBR containing smooth periodic constrictions and found the results obtained from 3D laminar, 3D LES and 2D laminar axisymmetric CFD simulations to be comparable to the PIV results. Here, the size, shape and positions of the eddies as well as the area- and time-averaged velocity profiles were compared. Other methods of validation have also been used, but these typically rely on qualitative comparison of the bulk flow fields and are therefore unreliable.

The aim of this study is to explore the flow behaviour of helically baffled meso-OBRs. This includes qualitative study of the flow patterns/structures, quantification of the swirl flow strength using equation 5, and assessment of the contributions of swirl flow and vortices to the plug flow quality.

2 Numerical Simulations

2.1 Geometry and Mesh

The helical baffle geometry shown in Figure 2 was studied. The diameter of the domain was 5 mm, while the helical coil had a 1 mm diameter, e , and 7.5 mm pitch, p . In dimensionless terms, the helical diameter and pitch selected were $e/D = 0.22$ and $p/D = 1.5$ respectively, giving a cross-sectional opening fraction of $S = 0.77$ (standard orifice baffles typically use $S = 0.2-0.4$ [1]). The total length of the domain was 45 mm, incorporating 6 full turns of the helical coil. This length was chosen because it was found in preliminary simulations that 1.5 turns was needed to establish the swirling flow, especially for increasing oscillation intensities ($Re_o > 50$). To suppress numerical errors at the baffle-tube wall contact point, a small section of mesh was trimmed (Figure 3a).

A uniform structured hexahedral mesh was created in ICEM CFD 15.0. A 2D mesh was first created at the outlet face using blocking and O-grids. This 2D mesh was then extruded by rotation to fully enclose the geometry. Figure 3a shows the face mesh while Figure 3b shows the resulting 3D mesh. The mesh had 2,440 face cells and 450 extrusion layers with rotation angles of 4.8° per layer, giving a total cell count of 1,098,000.

Figure 2 – Helical baffle geometry

Figure 3 – (a) 2D face mesh, and (b) 3D surface mesh

2.2 Model Configuration and Boundary Conditions

The laminar solver was selected for this study, with water (density: 998.2 kg/m³ and viscosity: 0.0010 Pa.s) used as the working fluid. Here, the standard continuity and Navier-Stokes equations for an incompressible flow were used (equations 9 and 10 respectively). Where, $\mathbf{v}_i$ is the velocity vector, $\mathbf{P}$ is the pressure field, ρ is the liquid density and μ is the liquid viscosity.

$$\frac{\partial(\mathbf{v}_i)}{\partial x_i} = 0 \quad 9$$

$$\frac{\partial(\mathbf{v}_i)}{\partial t} + \frac{\partial(\mathbf{v}_i \mathbf{v}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \mathbf{P}}{\partial x_i} + \frac{\mu}{\rho} \frac{\partial}{\partial x_j} \left(\frac{\partial \mathbf{v}_i}{\partial x_j} \right) \quad 10$$

The simulations were performed in FLUENT v15.0 using the finite volume discretisation scheme. The pressure-based solver was also used with a 2nd-order implicit time formulation. For discretisation, the least squares cell based gradient method was selected, with the PRESTO! scheme used for the pressure (suggested for swirling flows [18]) and the 2nd-order upwind scheme for the momentum terms (to provide numerical dissipation [14]). Finally, the SIMPLEC pressure-velocity coupling scheme was used with a skewness correction of 1 (necessary because of increased skewness in the mesh at the helical baffle-wall interface).

The inlet fluid velocity consisted of net and oscillatory components, and was defined using equation 11. Here, v_o is the superficial net flow velocity (defined from Re_n), and f and x_o are the oscillation frequency and amplitude respectively (defined from Re_o and St). This velocity was discretised and implemented as a velocity-inlet boundary condition in FLUENT using a user defined

function (UDF). An interval of 100 time steps per oscillation cycle was selected (the actual time steps used are shown in Table 1). Each simulation was run for 25 full oscillation cycles to ensure the results could be considered independent of the initial conditions.

$$v(t) = v_0 + 2\pi f x_o \sin(2\pi f t) \quad 11$$

The simulations were carried out using a 6-core Intel® Xeon® CPU E5-2620 v2 with a speed of 2.37 GHz. A typical simulation used 2500 time steps and took around 57 hours to complete (utilising 6 real cores and 4 logical cores). The data was exported in the post-CFD compatible format and imported into the results viewer in ANSYS for analysis.

2.3 Characterisation of Mixing

To characterise the swirling flow in the helically baffled geometries, the swirl number was used (equation 5). Analogously, the strength of the radial flow was also determined using equation 12. Here, the axial flux of radial momentum was compared to the axial flux of axial momentum. In the literature [15,19], the velocity ratio has instead been used to compare the axial and radial velocities. The advantage of equation 12 is the radial flow strength can be directly compared with the swirl strength. Thus, the relative contributions of vortex shedding and swirling on the plug flow quality can be deduced.

$$r_n = \frac{\int v_z v_r r \cdot dr}{\int v_z^2 r \cdot dr} \quad 12$$

To evaluate the swirl and ‘radial’ numbers several custom field functions were defined in FLUENT. Both geometries were created with the z-axis at the centre of the domain. Therefore, the tangential and radial velocity components were first calculated using equations 13 and 14 respectively. Here, x and y are the Cartesian distances along the x- and y-axes from the centre of the domain, and v_x and v_y are the x- and y-direction velocities. These directions are shown in Figure 2. Equations 15–17 then define the tangential, radial and axial momentum fluxes. At each converged time step during the simulations, the surface integrals of these custom field functions were evaluated and exported as a text file. The swirl and radial numbers were finally constructed using equations 18 and 19 respectively in Excel.

$$v_\theta = \frac{(xv_y - yv_x)}{\sqrt{x^2 + y^2}} \quad 13$$

$$v_r = \frac{(xv_x + yv_y)}{\sqrt{x^2 + y^2}} \quad 14$$

$$\theta'' = v_z v_\theta \sqrt{x^2 + y^2} \quad 15$$

$$r'' = v_z v_r \quad 16$$

$$z'' = v_z^2 \quad 17$$

$$S_n = \frac{\int_S \theta'' dA}{R \int_S z'' dA} \quad 18$$

$$r_n = \frac{\int_S r'' dA}{\int_S z'' dA} \quad 19$$

3 Particle Image Velocimetry, PIV

3.1 Experiment Set-Up

To validate the simulations, accompanying particle image velocimetry experiments were conducted. The meso-OBR used in these experiments was a glass tube with inner and outer diameters of 5 mm and 8 mm respectively. This tube could be fitted with a stainless steel helical coil, with thickness of 1 mm and 7.5 mm pitch. Stainless steel was used because glass could not be adequately manufactured into a uniform geometry.

Four sets of oscillation conditions were tested in this study corresponding to low and high intensity mixing as summarised in Table 1. C3000 series confluent PVM syringe pumps

(Tricontinent) were used to fill the meso-OBR (containing the helical coil described above) and apply oscillation at the base of the glass tube. The amplitude (centre-to-peak) was controlled by varying the volume of the displaced liquid, whilst the frequency was controlled by varying the speed and acceleration settings of the plunger. The syringe pumps were connected to the base of the meso-OBR via PTFE tubing and a custom-built Swagelok union (Figure 4), and controlled via text input commands using Sapphire Commander. Reasonably accurate sinusoidal waveforms could be generated using these syringe pumps, measured using a high-speed camera to track the position of the plunger over time. The supplementary materials document provides further details and an example waveform of the oscillations.

Table 1 – Oscillation conditions with corresponding Stokes numbers and time steps

	Re _o	St	x _o (mm)	f (Hz)	S _k (d _p = 5–30 μm)	Δt _{CFD} (ms)	Δt _{PIV} (ms)
1	126	0.2	2	2	0.02–0.13	5	1.90
2	188	0.13	3	2	0.03–0.19	5	1.50
3	503	0.1	4	4	0.10–0.58	1.5	0.90
4	565	0.13	3	6	0.09–0.51	2.5	0.55

The working fluid was deionised water, which was used at room temperature (~16–20 °C), and was seeded with silver-coated hollow glass microspheres ($\rho = 0.72 \text{ g/cm}^3$) with a particle diameter range of 5–30 μm. Ideally, seeding particles should be neutrally buoyant, inert and small enough to ensure the flow patterns are adequately followed whilst providing a good degree of light scatter from the laser sheet. The Stokes number, S_k (equation 20) was used to assess these requirements. In equation 20, τ_p is the particle relaxation time, v is the net flow velocity and d_c is the characteristic diameter of the particles. The particle relaxation time is determined using equation 21, where ρ_p and ρ_f are the densities of the particles and fluid respectively, g is gravitational acceleration, d_p is the particle diameter and μ_f is the liquid fluid viscosity. Ideally, the Stokes number should be much less than 1 in order for the tracer particles to follow the fluid streamlines. To determine the Stokes numbers for the four oscillation conditions used in this study, the velocity in equation 20 was replaced with the maximum oscillatory velocity during the oscillation cycle ($2\pi f x_o$). The resulting Stokes numbers are shown in Table 1.

$$S_k = \frac{\tau_p v}{d_c} \quad 20$$

$$\tau_p = \frac{(\rho_p - \rho_f) g d_p^2}{18 \mu_f} \quad 21$$

Illumination of the seed particles was achieved with a CFR-200 double pulsed Nd:YAG laser ($\lambda = 532 \text{ nm}$, 120 mJ per pulse) created by Big Sky Laser. The laser beam produced was directed through a light arm (TSI model 610015), which was connected to cylindrical/spherical lenses to diverge the beam and create a lightsheet with 1 mm thickness. In order to minimise laser light reflections and optical distortions, a Perspex viewing box was sealed around the column and filled with glycerol to match the refractive index of the glass tube. The illuminated test section (consisting of approximately 3 turns of the helical coil) was imaged using a TSI Powerview Plus 4MP camera (model 630059) with CCD sensors, which had a resolution of 8.14 μm/pixel. This camera was fitted with an AF Micro-Nikkor lens (105 mm, f/2.8D) with long pass optical filter screen (so only the laser wavelength could be detected), and was positioned approximately 10 cm from the viewing box. The camera was connected to a 64-bit frame grabber (Xcelera-CL PX4) to capture/digitize the images, while a synchroniser (TSI model 610035) was used to synchronise the laser pulses and image capture. Insight4G software (TSI) was used to acquire data. The positions of the meso-OBR with viewing box, laser sheet and camera are shown in Figure 4.

Figure 4 – Experimental particle image velocimetry (PIV) set-up showing the positioning of the laser sheet, glycerol-filled viewing box/meso-OB and camera

The experiment procedure was as follows. First, the meso-OB was primed using the syringe pumps. Here, the deionised water containing the seeding particles was transferred to the meso-OB from a small reservoir containing deionised water and the tracer particles. Then, the density of the particles was adjusted (by mixing the seeded reservoir prior to priming the meso-OB) so that approximately 15 particles could be observed in a 64x64 pixel area [20]. Next, fluid oscillation was started and the time difference between the two captured images was adjusted so that the tracer particles moved no more than approximately 16 pixels (one quarter of the initial 64x64 pixel integration area). The time differences used between a single set of image pairs are also summarised in Table 1. Finally, 700 image pairs were captured at each oscillation condition using the maximum sampling rate of 7.25 Hz (between each image pair).

As the laser could not be synchronised to the syringe pump, the oscillation cycle was constructed via stroboscopic sampling. For example, a 2 Hz oscillation frequency equates to an oscillation period of 0.5 s. With a 7.25 Hz sampling rate, the oscillation cycle times sampled would be $t = 0.138$ s, $t = 0.276$ s, $t = 0.414$ s, $t = 0.052$ s, etc. In this case, 29 phases of the oscillation cycle would be imaged, capturing ~24 oscillation cycles in total (for 700 image pairs). Each sequence of 29 images captured from 8 ‘real’ oscillation cycles could then be reordered to construct a single ‘virtual’ oscillation cycle. A slightly more detailed description of this process can be found in the supplementary materials.

All images were analysed using PIVLab1.4 [20]. For $Re_o \leq 188$, a 2-pass FFT deformation was used to generate the velocity vectors with an initial integration area of 64x64 pixels and step size of 32 pixels, and a second pass integration area of 32x32 pixels with step size of 16 pixels. For $Re_o \geq 188$, a 3-pass FFT deformation was applied, with subsequent integration areas and step sizes of 64x64 pixels (32 pixel step size), 48x48 pixels (24 pixel step size) and 32x32 pixels (16 pixel step size). These combinations were found to yield good resolution with minimal noise. Erroneous vectors were detected using a cross-correlation filter (between x and y velocities) and replaced via an interpolation.

Calibration was applied by selecting the tube diameter as a reference distance in the images and specifying the time difference (see Table 1).

The simulated and experimental velocity fields were compared at 8 phases of the oscillation cycle, corresponding to the points of maximum acceleration/deceleration, maximum velocity and flow reversal as shown in Figure 5. Approximately 24 oscillation cycles were captured in the PIV experiments for all oscillation frequencies under investigation. To reduce experimental noise, the flow patterns at each of these 8 oscillation cycle phases were averaged over 15 oscillation cycles. Not all captured cycles were used in the averaging procedure because some of the processed velocity fields were corrupted by localised noise, possibly due to erroneous laser scattering.

In addition to the description of the stroboscopic sampling method and explanation of the operation of the syringe pumps, full images of the flow fields and full summaries of the comparison data between the experimental and numerical flows are included in the supplementary materials. This includes video animations of particle injections into the simulations at low and high intensity oscillation conditions to aid visualisation.

Figure 5 – Visualisation of oscillation cycle phases

4 Results and Discussions

4.1 2D Velocity Fields

4.1.1 Helical Baffles

Figures 6 and 7 show the normalised velocity vector fields plotted along the meridional plane for a single baffle cavity (1 turn of the helical coil) at the lower oscillation intensities ($Re_o = 126-188$). The velocities were normalised against the highest velocity produced during the oscillation cycle, occurring at $t/T = 0.25$ around the baffle edges. In addition, the positions obstructed by the helical baffle have been added to aid visualisation, while transparent mask regions are used to show where data interpolation was required in the shadows behind the coils.

The simulated 2D flow patterns (upper rows of Figures 6 and 7) were largely similar to those previously reported by Solano *et al* [6]. Initially, at the point of maximum acceleration in the oscillation cycle ($t/T = 0.125$) the velocity is highest at the baffle edge because of acceleration through the baffle constriction. Then, at the point of maximum velocity ($t/T = 0.25$) these regions of higher velocity become stretched in the axial direction and start to coalesce. Next, at the point of maximum deceleration in the cycle ($t/T = 0.375$), a strong core flow forms and small regions of recirculation begin to form behind the baffles. Finally, at the point of flow reversal ($t/T = 0.5$) a strong vortex detaches from the baffle edge, which also reduces the intensity of the core flow. The flow patterns were highly repeatable between different baffle cavities for both the forward and backward

oscillation cycle and across multiple oscillation cycles. This shows that these flow conditions are helically symmetric. Additionally, these 2D flow fields show an apparent meandering path at the channel core, which is more noticeable at the point of vortex formation. This is a consequence of swirling generated by the helical coil.

Increasing the oscillation amplitude from 2 mm to 3 mm resulted in larger vortices upon flow reversal and an increased eddy detachment length from the baffle (approximately 44% longer). For the lowest oscillation intensity studied ($Re_o = 126$), the core flow produced velocities 37.5% higher than the recirculations, whereas at $Re_o = 188$ the core flow produced velocities 50% higher than the vortex regions. This suggests that axial dispersion increases faster than the radial/tangential flow for this change in amplitude.

The corresponding 2D flow patterns obtained from the PIV experiments at the lower oscillation intensities are shown in the bottom rows of Figures 6 and 7. These experimentally obtained flow fields generally matched the simulated results. Mainly, the vortices produced at the point of flow reversal were the correct size and shape, and had similar detachment lengths from the baffle edge. Additionally, the overall shape of the PIV fields generally matched the shapes of the simulated results, with meandering observable. The main differences were: (i) the velocity magnitudes at $t/T = 0.125$ were smaller in the experimental flow fields, and (ii) the experimental results showed gaps in the core regions of the experimental flow fields.

These differences can be attributed to restrictions of the experiment. The helical coil was constructed from stainless steel, which partially obstructed the view of the camera (these regions are highlighted in Figures 6 and 7). Additionally, shadows created behind the coil resulted in a secondary obstruction (observable in Figure 4). These regions were removed with a mask prior to analysis of the experimental results and interpolated for plotting. This data interpolation resulted in the reduced intensity of the velocity magnitude at the core of the flow because the calculation was slightly weighted towards these zero velocity regions.

Figure 6 – 2D normalised velocity magnitude contours and velocity vectors in the meridional plane / maximum corresponding velocity = 0.06 m/s / forward half of oscillation cycle / oscillation conditions: $Re_n = 0$, $Re_o = 126$, $St = 0.2$ ($x_o = 2$ mm, $f = 2$ Hz) / Top row shows CFD results and bottom row shows PIV results

Figure 7 – 2D normalised velocity magnitude contours and velocity vectors in the meridional plane / maximum corresponding velocity = 0.092 m/s / forward half of oscillation cycle / oscillation conditions: $Re_n = 0$, $Re_o = 188$, $St = 0.13$ ($x_o = 3$ mm, $f = 2$ Hz) / Top row shows CFD results and bottom row shows PIV results

Figures 8 and 9 show the normalised velocity vector fields for the higher mixing intensities investigated in this study ($Re_o = 503$ – 565). Here, the same phase-averaging procedure as the lower oscillation conditions was used, and again, visual aids have been added to the figures to show the position of the helical coil and data interpolation regions. In these figures, different flow features were observed compared to the lower mixing intensities ($Re_o = 126$ – 188). For instance, at the point of maximum acceleration in the cycle ($t/T = 0.125$), the velocity is more uniform over the cross-section of the domain. The regions with slightly higher velocity now occur near the channel wall, because the bulk flow is redirected there as a consequence of the larger vortices that formed during the previous cycle. The remnants of the vortices are also present at this stage of the cycle. At the peak oscillatory velocity ($t/T = 0.25$), the highest velocities are again found at the edge of the baffles. As in the lower mixing intensity results, these higher velocity regions are stretched axially. However, unlike the lower oscillation intensities small regions of recirculation are forming downstream of the baffles at this point. After the flow has reached maximum deceleration ($t/T = 0.375$), large vortices appear behind the baffles that then grow further in size at the point of flow separation ($t/T = 0.5$). These vortices fill the majority of the cross-section, reducing channelling at the centre of the column.

Apart from decreasing the helical symmetry, the higher mixing intensities ($Re_o = 503\text{--}565$) reduced the magnitude of the core flow and increased the swirl and radial flow strength. This is seen at 50% of the cycle. The velocity vectors at the centre of the column are pointed towards the column walls and increased meandering is observed.

The PIV results (bottom rows of Figures 8 and 9) again show a general agreement with the simulated flow fields. At $t/T = 0.125$, the PIV results correctly show that the higher velocities occur closer to the wall because of the redirection of the bulk flow from the larger vortex structures from the previous cycle. Additionally, the vortices at the point of flow reversal are comparable, showing the same attachment lengths and approximate sizes.

The main differences were observed at $t/T = 0.25$ and $t/T = 0.375$. Here, the reduced velocity magnitude at the core due to the interpolation of the velocity vectors is more pronounced than the lower oscillation intensity results (Figures 6 and 7). This could be because additional swirling is present; the Z-axis motion is not captured in the 2D images.

Figure 8 – 2D normalised velocity magnitude contours and velocity vectors in the meridional plane / maximum corresponding velocity = 0.25 m/s / forward half of oscillation cycle / oscillation conditions: $Re_n = 0$, $Re_o = 565$, $St = 0.13$ ($x_o = 3$ mm, $f = 6$ Hz) / Top row shows CFD results and bottom row shows PIV results

Figure 9 – 2D normalised velocity magnitude contours and velocity vectors in the meridional plane / maximum corresponding velocity = 0.24 m/s / forward half of oscillation cycle / oscillation conditions: $Re_n = 0$, $Re_o = 503$, $St = 0.1$ ($x_o = 4$ mm, $f = 4$ Hz) / Top row shows CFD results and bottom row shows PIV results

4.2 Validation of the Simulations

The simulations were validated by comparing the vortex structures observed in the two sets of flow fields. Specifically, the number of vortices, as well as vortex sizes/positions and the flow reattachment points to the wall were determined for both the simulated and experimental data. First, the vorticity and shear strain rate fields were computed using the antisymmetric and symmetric portions of the stress tensor, using equations 22 and 23 respectively. These equations were implemented using 2nd order accurate finite difference approximations. Then, the Q-criterion was calculated using equation 24. The vorticity is calculated as the curl of the velocity field and thus describes regions of rotation. The filtered Q-criterion ($Q > 1$) therefore describes regions in the flow where circulation dominates shear forces. Vortex properties (centre of mass and vortex area) were subsequently obtained from the Q-criterion field contours.

$$\omega_{i,j} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i} \right) \quad 22$$

$$S_{i,j} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \quad 23$$

$$Q = \frac{1}{2} (\omega_{i,j} \omega_{i,j} - S_{i,j} S_{i,j}) > 0 \quad 24$$

Figure 10 shows an example of the Q-criterion contours produced at the points of flow reversal (corresponding to maximum vortex size) for an oscillation intensity of $Re_o = 188$ and $St = 0.13$. The vortices appear to be slightly oval in shape. Figure 11 quantitatively compares the Cartesian coordinates of the centre of masses of these vortices for each of the four oscillation conditions studied. These coordinates were calculated as the mean of the x- and y-coordinates along the outer Q-criterion contour lines shown in Figure 10. On the assumption of uniform fluid density, this method ensured that the centres of mass were influenced by the shapes of the vortices allowing for further implicit comparison of the vortex shapes. Table 2 then summarises the average vortex areas between the two sets of flow fields for both the forward and reverse oscillation cycles. It is clear that the simulations are able to correctly predict the number and location of the vortex structures for a domain containing 3 turns of the helical coil (total length of 22.5 mm). Table 2 shows that the average vortex areas in the experimental flow fields are similar when accounting for the error.

Figure 10 – 2D Q-Criterion contours at the point of flow reversal | oscillation conditions: $Re_n = 0$, $Re_o = 188$, $St = 0.13$ ($x_o = 3$ mm, $f = 2$ Hz) | (a) simulated data [$t/T = 0.5$], (b) experimental data [$t/T = 0.5$] (c) simulated data [$t/T = 1$], (d) experimental data [$t/T = 1$]

Figure 11 – Vortex centre coordinates comparison between simulated and experimental data / (a) axial coordinate, (b) radial coordinate

Table 2 – Vortex areas calculated from the Q -Criterion contours / the errors represent the standard deviation of the areas calculated from the 6 main observable vortices in the flow fields

Oscillation Condition	Oscillation Cycle Phase	CFD Area (mm ²)	PIV Area (mm ²)
$Re_o = 126, St = 0.2$ ($x_o = 2$ mm, $f = 2$ Hz)	$t/T = 0.5$ (forward)	3.61 ± 0.25	2.71 ± 0.31
	$t/T = 1$ (backward)	4.43 ± 0.14	2.62 ± 0.86
$Re_o = 188, St = 0.13$ ($x_o = 3$ mm, $f = 2$ Hz)	$t/T = 0.5$ (forward)	4.79 ± 0.61	6.16 ± 1.18
	$t/T = 1$ (backward)	4.97 ± 0.35	3.51 ± 1.13
$Re_o = 565, St = 0.13$ ($x_o = 3$ mm, $f = 6$ Hz)	$t/T = 0.5$ (forward)	1.73 ± 0.71	2.74 ± 0.37
	$t/T = 1$ (backward)	2.44 ± 0.76	2.29 ± 0.88
$Re_o = 503, St = 0.1$ ($x_o = 4$ mm, $f = 4$ Hz)	$t/T = 0.5$ (forward)	3.49 ± 0.76	2.52 ± 1.12
	$t/T = 1$ (backward)	3.32 ± 0.81	1.87 ± 0.35

Wall attachment after flow separation causes an inversion of the wall shear stress from positive to negative values [21]. This is because wall attachment involves the flow splitting and flowing in opposite directions; therefore, the velocity gradient $\partial v_z / \partial r$ inverts. To assess whether the simulated data was able to correctly model the wall reattachment lengths, equation 25 was used to determine the wall shear in the CFD and PIV flow fields. Here, μ is the liquid viscosity, v_z is the axial velocity and r refers to the radial direction.

The wall shear stress profiles were calculated at a distance of 0.25 mm from the wall. Figure 12 summarises the wall shear stress profiles for each of the flow fields at the point of flow reversal. The other phases of the oscillation cycle are contained within the supplementary materials. It can be seen that the wall shear stress values of the PIV data generally matched the CFD results. Here, the peaks in wall shear stress were aligned for both data sets, and the points where the wall shear stress inverted from positive to negative values were approximately the same. The slight differences observed in Figure 12 are likely to be because of optical distortion effects and possible particle stagnation/inhomogeneity around the walls in the PIV data.

$$\tau_w = \mu \left(\frac{\partial v_z}{\partial r} \right) \bigg|_{r=0.00225} \quad 25$$

There were several technical difficulties in obtaining the flow fields via the PIV technique in this study. Primarily, the largest challenge was the complete imaging of the test section, owing to the slight obstruction of the laser sheet and blocking of the camera's view at any orientation of the helical baffles. This meant data interpolation was required to reconstruct some parts of the flow field, possibly leading to unavoidable erroneous results; these regains are highlighted in Figures 6–9. Therefore, it may be the case that the simulation methodology used in this study is the best approach to studying the flow patterns in oscillatory flows in the presence of helical baffles. Nevertheless, the flow patterns obtained via simulation were at the very least replicable in the experiments. Based on the similarities of the 2D velocity vector fields, wall shear stress profiles, and vortex numbers, sizes, shapes and locations, it can be concluded that the laminar solver available in Fluent is sufficient to describe the bulk flow patterns obtained in helically baffled meso-OBRs.

Figure 12 – Wall shear stress profiles at the point of flow reversal / forward half of the oscillation cycle ($t/T = 0.5$) / (a) $Re_o = 126$, $St = 0.2$ ($x_o = 2$ mm, $f = 2$ Hz), (b) $Re_o = 188$, $St = 0.13$ ($x_o = 3$ mm, $f = 2$ Hz), (c) $Re_o = 565$, $St = 0.13$ ($x_o = 3$ mm, $f = 6$ Hz), (d) $Re_o = 503$, $St = 0.1$ ($x_o = 4$ mm, $f = 4$ Hz)

4.3 Swirl and Radial Numbers

It is well known that oscillatory baffled reactors can operate with high degrees of plug flow at low net flow rates (well within the laminar regime), providing the correct operating range is selected [2,3]. Fundamentally, vortices that form behind the baffles on each flow reversal redistribute the flow in the radial direction, limiting the amount of axial dispersion that can occur. With helical baffles, a larger operating window for plug flow is reported [5]. It is proposed that the additional swirling motion created in the presence of the baffles further limits axial dispersion by also redirecting the flow in the tangential direction [5], creating more compact streamlines. To investigate this hypothesis, the swirl number and corresponding ‘radial’ numbers were computed during the simulations.

The swirl and radial numbers were obtained using equations 13–19. The surface integrals were computed on five different cross-sectional planes spaced evenly every 3.75 mm, centred on an axial position of 22.5 mm (centre of the simulated domain). The swirl and radial numbers obtained on each of these five cross-sections were averaged for each time step of the simulation. Then, orbital plots of the averaged swirl and radial number were created by plotting the swirl and radial numbers against the oscillatory velocity. Here, the corresponding oscillatory velocities were defined as the inlet boundary condition, $2\pi f x_0 \sin(2\pi ft)$.

Figure 13 – Swirl and radial numbers versus oscillatory velocity / (a) $Re_o = 126$, $St = 0.2$; (b) $Re_o = 188$, $St = 0.13$; (c) $Re_o = 565$, $St = 0.13$; (d) $Re_o = 503$, $St = 0.1$

For an oscillation intensity of $Re_o = 126$ and $St = 0.2$ (Figure 13a), the radial number is larger than the swirl number suggesting that vortex formation is chiefly responsible for minimising axial dispersion. The radial number has an absolute peak value of 0.3, with the sign changing during the forward and backward parts of the oscillation cycle. In contrast, the peak swirl number ($= 0.2$) is positive during both the forward and backward portions of the oscillation cycle. This is because the flow always rotates clockwise relative to the axial flow. However, the swirl number at the points of maximum oscillatory velocity is negative. This was found to be a consequence of counter-rotation in the flow, which is observable in the particle injection videos contained within the supplementary material. Here, the flow close to the boundary of the domain rotates with respect to the curvature of the helical coil, while the core flow is still rotating in the opposite direction from the previous cycle. Also, the peak values of the swirl and radial number do not coincide with the point of flow reversal (0 m/s), but are delayed slightly.

Increasing the oscillation amplitude from 2 mm to 3 mm ($Re_o = 188$ and $St = 0.13$) was found to increase the magnitudes of both the swirl and radial numbers, as shown in Figure 13b. Here, the shapes of the orbital plots remained the same suggesting the flow maintains the same general structure, but the swirl and radial strengths were closer in magnitude.

Figure 13c shows the effect of further increasing the oscillation frequency from 2 Hz to 6 Hz relative to Figure 13b, with an oscillation intensity corresponding to $Re_o = 565$ and $St = 0.13$. In contrast to the lower oscillation conditions, the flow is asymmetric and chaotic. The swirl number is also larger than the radial number, reaching an average peak of 0.4, and the peak radial and swirl numbers are no longer aligned with each other. Here the peak vortex strength occurs before the peak swirl strength. As discussed in Section 4.4, this occurs because the vortex structure becomes less coherent, while the net rotation provided by the helical coil remains.

Finally, Figure 13d shows the results obtained using $Re_o = 503$ and $St = 0.1$ (amplitude of 4 mm and frequency of 4 Hz). This represents a smaller oscillation frequency, but larger amplitude than the result in Figure 13c. Here the flow appears to be less chaotic but not symmetric. The swirl number is largest after the forward oscillation cycle, reaching a peak of ~ 0.55 . The radial number shows the opposite trend, with the largest peak occurring after the reverse cycle.

It can be seen between Figures 13c and 13d that there is a sudden onset of chaotic behaviour for only a small change in Re_o and St , characterised by varying flow patterns cycle-to-cycle. Roberts and Mackley [22] comparably described the development of asymmetric behaviour in oscillatory baffled flows as a period-doubling cascade. When Re_o is increased, the flow bifurcates from a one-cycle repeating pattern to two different patterns that repeat over two cycles. This appears to have occurred in the helical baffle simulations in this study using $Re_o = 503$. Here, the swirl and radial numbers reach different maxima during the forward and backward portions of the oscillation cycle. Roberts and Mackley [22] then describe further bifurcations that lead to four-, eight-, sixteen-, etc. cycle repeating patterns until a chaotic-like flow results where the periodicity is indeterminable, akin to the result in Figure 13c ($Re_o = 565$). In a 25 mm diameter column containing orifice baffles, the transition to these chaotic regimes was instead identified as approximately $Re_o > 200$ [22]. Mesoscale (5 mm diameter) OBRs containing smooth constrictions reportedly show stirred tank behaviour when $Re_o > 100$ [17]. However, it is unclear if this refers to either a breakdown in the plug flow performance only, or the specific onset of asymmetry between different oscillation cycles.

Zheng *et al* [13] identified that for low St (≤ 0.1), shear instabilities were responsible for the onset of chaotic flows when using orifice baffles (50 mm diameter), with a corresponding onset condition of $Re_o = 100$. Alternatively, for larger Strouhal numbers ($St \geq 0.5$), they found that interactions of eddies from different oscillation cycles produced a higher critical Re_o (≥ 200) for instability. Nevertheless, it is apparent that the transition to chaotic flow is delayed when using helical baffles ($Re_o > 503$). One possibility is swirling provides a centrifugal force that stabilises the core flow [9]. However, centrifugal forces can also lead to destabilisation near the wall regions in swirling flows [9], meaning further study is warranted to better understand the source of the bifurcations when using the helical baffles. Speculatively, there might be an oscillation intensity where the centrifugal stability inverts to an instability due to a change in the balance of inward acting (e.g. pressure gradient) and outward acting (centrifugal) forces.

Based on Figure 13 there appears to be a transition between vortex-dominated and swirl-dominated flow. Phan and Harvey [5] observed this behaviour experimentally when analysing the

plug flow quality using tracer pulse injections and the tanks-in-series model. They observed a transition point for a 4 mm oscillation amplitude and net flow of $Re_n = 7.2$ when increasing the oscillation frequency from 1–3 Hz. These results are shown in Figure 14a. Here, the variance was used to characterise the plug flow response, with smaller variances indicating favourable higher degree of plug flow (i.e. a narrower residence time distribution). As shown, the variance initially increases when increasing Re_o from 125 to 250 before decreasing.

The same conditions were repeated in this study to test the hypothesis that the wide plug flow operating range is a consequence of the more compact flow due to swirling. Figure 14b and c below show two metrics of the swirl and radial numbers. These metrics are the average enclosed areas of the swirl and radial number orbital paths (S_n and r_n vs oscillatory velocity plots), and the average peak value of swirl and radial number. The average area of these orbital plots accounts for the differences in the swirl and vortex strength over the whole oscillation cycle. The peak swirl and radial numbers instead describe the difference between the swirl and vortex strength at the point of flow reversal, where the vortices form. The enclosed area was calculated using the “polyarea” function in Matlab. For the swirl number, this required unfolding the shape of the orbital plot by flipping the forward oscillation cycle across the y-axis. The peak values of S_n and r_n were simply taken as the average absolute values of the two peaks produced during a single oscillation cycle.

Figure 14 – Evidence for vortex and swirl dominated flows at $Re_n = 7.2$, $St = 0.1$ ($x_o = 4$ mm) / (a) experimental tracer distribution variance [5], (b) average areas of swirl and radial numbers, (c) average peak swirl and radial numbers

As shown in Figures 14b and 14c, the swirl strength surpasses the radial flow strength when increasing the oscillation frequency from 1 to 2 Hz. This transition closely resembles the increase in variance of the experimental tracer distribution obtained by Phan and Harvey [5] (Figure 14a), implying that the swirling element to the flow is indeed responsible for the wide operating window for plug flow. This is also evident when analysing Figure 14c. It can be seen that the swirl number continues to increase as Re_o is increased from 377 to 503, whereas the radial number (related to the strength of the vortex) decreases. This was similarly observed in Figure 16 (Section 4.4) where the vortex was less coherent due to increased turbulence while a sense of swirl was still present.

4.4 Visualisation of Swirling Flow Structures (3D Flow Patterns)

To visualise the flow patterns obtained in the helically baffled domains, isosurfaces of the Q-criterion and 3D streamlines were plotted. As previously described, the Q-criterion is defined as the difference between the square of the vorticity and shear strain rate fields. Thus, filtering out the negative Q-criterion values allows the regions dominated by rotation to be observed. In the following

figures, the isosurfaces of Q-criterion define the centres of the vortex structures, while the streamlines show the shapes of the general flow fields.

Figure 15 shows the flow patterns produced at an oscillation condition of $Re_o = 126$ and $St = 0.2$ ($x_o = 2$ mm, $f = 2$ Hz) at 4 points during the forward part of the oscillation cycle (Figure 5 shows the corresponding phase positions). It can be seen that near the start of the oscillation cycle ($t/T = 0.125$), the dominant rotation in the flow field exists close to the surface of the helical coil. The corresponding streamlines are approximately parallel with minimal swirling present; this agrees with the swirl number results in the orbital plots (Figure 13a). At the next cycle position ($t/T = 0.25$) a vortex has started to form behind the baffle. Here, the Q-criterion isosurface has started to break away from the baffle edge while the streamlines behind the baffle have become more tangentially orientated. After the flow reaches maximum deceleration ($t/T = 0.375$), the vortex structure becomes clearer, with many of the streamlines now following an orbital path around the helically shaped vortex. Finally, at the point of flow reversal ($t/T = 0.5$) the vortex rapidly grows in strength, with the dominant structure in the flow field being a single helical vortex. The rotational symmetry of this flow condition is apparent.

In contrast, Figure 16 shows the flow patterns produced at a non-helically symmetric and more chaotic flow condition. Here, the corresponding oscillation conditions are: $Re_o = 565$, $St = 0.13$ ($x_o = 3$ mm, $f = 6$ Hz). At the start of the oscillation cycle ($t/T = 0.125$), there is still a large remnant of the vortex from the previous oscillation cycle. As discussed in the 2D velocity magnitude contours (Figure 8), these vortex remnants redirect the bulk flow towards the walls instead of through the centre of the column. At the point of maximum velocity in the cycle ($t/T = 0.25$), a helically shaped vortex is seen to be forming behind the baffle edge. Here, the Q-criterion isosurface at the centre of this rotation is still connected to the baffle edge, similar to the result in Figure 15b, but the vortex is larger than the lower oscillation intensity. There are also smaller pockets of recirculation at the centre of the domain. The vortex structure is more easily observable at $t/T = 0.375$ and $t/T = 0.5$. The streamlines at the point of flow reversal ($t/T = 0.5$) at this higher oscillation intensity are not as uniform as the results in Figure 15d, but the underlying vortex and swirling behaviour is still apparent. Based on the streamlines, the vortex at the higher oscillation condition appears to be less coherent than at the lower mixing intensity.

Figure 15 – Q -criterion isosurfaces (900 s^{-2}) and fluid streamlines (coloured by velocity magnitude) / oscillation conditions: $Re_n = 0$, $Re_o = 126$, $St = 0.2$ ($x_o = 2 \text{ mm}$, $f = 2 \text{ Hz}$) / forward half of the oscillation cycle: (a) $t/T = 0.125$, (b) $t/T = 0.25$, (c) $t/T = 0.375$, and (d) $t/T = 0.5$

Figure 16 – Q -Criterion isosurfaces ($20,000 \text{ s}^{-2}$) and fluid streamlines (coloured by velocity magnitude) | Oscillation conditions: $Re_n = 0$, $Re_o = 565$, $St = 0.13$ ($x_o = 3 \text{ mm}$, $f = 6 \text{ Hz}$) | forward half of the oscillation cycle: (a) $t/T = 0.125$, (b) $t/T = 0.25$, (c) $t/T = 0.375$, and (d) $t/T = 0.5$

Figures 15 and 16 show the types of flow structures obtained using ‘vortex-dominated’ and ‘swirl-dominated’ oscillation intensities. However, apart from the increased turbulence at the higher oscillation intensity, there is little distinction between these two regimes. Therefore, to further understand how the swirling motion affects axial dispersion, more detailed analysis of the streamlines was made. Here, fluid streamlines traced out by particles injected into the simulations were compared. The two oscillation intensities used for the comparison were $Re_o = 188$ and $Re_o = 565$, because these conditions used the same amplitude ($St = 0.13$). This means the differences between the streamlines can be attributed to the flow regime. The tracer particles were injected into the simulation after 12 oscillation cycles had been simulated to ensure independence of the initial conditions. Streamline coordinates corresponding to 10 full oscillation cycle were extracted for analysis. For both oscillation conditions, 2382 tracer particles were successfully tracked, and the average particle behaviour for a single oscillation cycle is considered.

Axial spread is minimised in the oscillatory baffled reactor by the addition of radial flow provided by the formation of vortices. It is proposed in the helically baffled OBR that swirling provides a further mechanism to limit axial dispersion [5]. Therefore, it was decided to track the rotational history and radial traversal history of the particle streamlines. This was achieved by first converting the Cartesian coordinates of the streamlines into polar coordinates (equations 26 and 27) and then calculating the cumulative rotational angle and radial distance travelled by each particle as they followed the streamlines. In the equations below, x and y are the x - and y -coordinates of the streamlines.

$$\theta = \tan^{-1}(x/y) \quad 26$$

$$r = \sqrt{x^2 + y^2} \quad 27$$

The resulting histograms of the cumulative axial, rotational and radial motion of the particles are shown in Figures 17a–c respectively. All results are approximately normally distributed. As shown in Figure 17a, the average axial spread of the tracer particles (non-dimensionalised using the column diameter) per cycle is almost identical for both oscillation intensities. Both distributions are centred on 3, implying the particles move a total distance of 15 mm in the axial direction during one full oscillation cycle. Therefore, the extra flow acceleration generated at $Re_o = 565$ must ‘dissipate’ solely in the cross-sectional plane in the form of swirling and radial motion.

Figures 17b and 17c show the average rotational and radial movement distributions in a single oscillation cycle. In Figure 17b, the distribution of rotational motion is shifted to higher angles for the higher oscillation intensity. Similarly, Figure 17c shows that the higher oscillation intensity produced larger cumulative radial movement overall (non-dimensionalised using the column diameter). These results agree with the swirl and radial numbers in Figure 13. I.e. the larger oscillation intensity produces larger radial motion (relative to the oscillatory velocity) and higher swirling.

It is clear, therefore, that the tangential motion of the fluid is intrinsically linked with the vortex structures. This can also be seen in Figures 15d and 16d where the streamlines are wrapped around a common rotating core (the helical vortex). Subsequently, Figure 17d was plotted which shows the ratio of the rotation of the particles (number of revolutions around the column) to radial distance travelled by the particles (non-dimensionalised using the column diameter). Here, the two distributions have similar means, but the data at $Re_o = 565$ is broader because of the chaotic flow condition (see Figure 13c). In addition, the distribution at $Re_o = 565$ has a noticeably higher right-handed skewness. This implies that the absolute swirling strength grows faster than the absolute radial flow strength upon increasing the oscillation intensity. This is because the upper size limit of the vortices bounded by the size of the column, whereas tangential movement has more room to develop. Presumably, the upper limit to tangential movement is linked to the pitch of the helical coil.

Figure 17 – Average characteristic axial, rotational and radial properties of fluid streamlines per oscillation cycle (collected from 10 oscillation cycles) / $St = 0.13$ ($x_o = 3$ mm) / $Re_o = 188$ ($f = 2$ Hz) & $Re_o = 565$ ($f = 6$ Hz) / (a) average axial motion during oscillation cycle (non-dimensionalised using the column diameter), (b) average cumulative rotation along the streamlines, (c) average radial distance travelled along each streamline (non-dimensionalised using the column diameter), and (d) ratio of number of revolutions around the column to non-dimensionalised radial motion

Therefore, degradation of plug flow can now be understood. In conventionally baffled columns (e.g. containing orifices), the production of vortices creates a radial motion that minimises the amount of axial dispersion that can take place. However, because the vortices are bounded by the column diameter while axial dispersion is limited only by the length of the column, increasing the oscillation intensity results in reduced plug flow quality (the radial motion is limited). In contrast, helical baffles promote both radial and tangential motion in the presence of oscillatory flow. Because the tangential motion is not as bounded as the radial motion, there still exists a mechanism to dissipate axial dispersion at higher oscillatory intensities.

5 Conclusions

For the first time, the flow patterns in a helically baffled tube subjected to an oscillatory flow have been experimentally validated using PIV. Qualitatively, the 2D velocity fields along a central plane show the same number and positions of eddies at low and high oscillation intensities. Quantitatively, the simulated vortex sizes and positions correctly match the experimental results. Additionally, wall shear stress profiles confirm the correct wall attachment distances after flow separation. It is concluded that the laminar solver available in Fluent is sufficient to describe the bulk flow patterns.

The flow was visualised using isosurfaces of Q-criterion and 3D streamlines. The characteristic flow structure observed was a helically shaped vortex behind the baffles. Increasing the oscillation amplitude increased the eddy size and detachment length. Increasing the oscillation frequency reduced the rotational symmetry and reduced channelling through the centre of the column.

The magnitudes of swirl and radial flow were also quantified. At low mixing intensities ($Re_o < 200$) with no net flow, the peak radial component of the flow was larger than the peak swirl number, suggesting vortex-dominated flow. For $Re_o = 126$ and $Re_o = 188$, the respective radial components were 74.2% and 21.1% greater than the swirl strength. As the oscillation intensity increased, the flow became “swirl-dominated”. This switch between vortex and swirl dominated mixing was also observed in the simulations where an additional net flow was applied ($Re_n = 7.2$). By matching the numerical data with plug flow data from the literature, and by analysing 3D streamlines, it was clear that the additional swirl element to the flow was responsible for the wide operating window for plug flow as originally hypothesised.

At low oscillation intensities, the swirl number was negative at the point of maximum velocity during the oscillation cycle. This is because the flow rotates clockwise near the surface of the baffles (same direction as the baffles), while the centre of the flow rotates anticlockwise due to inertial effects.

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Nomenclature

A	Cross-sectional area (m^2)
D	Oscillatory baffled column diameter (m)
D_f	Diffusivity/diffusion coefficient (m^2/s)
f	Oscillation frequency (Hz)
L	Characteristic length (m)
P	Pressure (Pa)
r	Radial position in column (m)
R	Oscillatory baffled column radius (m)
S	Open flow area (ratio of baffle constriction area to column area)
t	Time (s)
T	Oscillation period (s)
t_m	Mean residence time of tracer (s)
v_r	Velocity ratio
v_o	Superficial fluid velocity (m/s)
v_r	Radial velocity (m/s)
v_z	Axial velocity (m/s)
v_θ	Tangential velocity (m/s)
V	Volume (m^3)
x	Position in x-axis (m)
x_o	Oscillation amplitude (m)
y	Position in y-axis (m)
z	Position in z-axis (m)

Dimensionless Groups:

Pe	Péclet number ($= Lv_o/D_f$)
Re_n	Net flow Reynolds number ($= \rho v_o D/\mu$)
Re_o	Oscillatory Reynolds number ($= 2\pi f x_o \rho D/\mu$)
r_n	Radial number ($= \int v_z v_r r \cdot dr / \int v_z^2 r \cdot dr$)
S_n	Swirl number ($= \int v_z v_\theta r^2 \cdot dr / R \int v_z^2 r \cdot dr$)

St	Strouhal number ($= D/4\pi x_o$)
ψ	Velocity ratio ($= Re_o/Re_n$)

Greek Letters:

η	Asymmetry index
μ	Viscosity (Pa.s)
ρ	Density (kg/m ³)
σ^2	Variance of tracer distribution

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