FLOW FIELD CHARACTERIZATION AND IMPINGING JETS STABILITY STUDIES IN RIM

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Abstract. The stretching properties of the flow in a RIM machine mixing chamber were investigated from a Computational Fluid Dynamics (CFD) 3D model coupled with Lagrangian tracking of passive material elements. The flow regimes and the jets’ impingement point position under unequal flow rates and different injectors’ diameters were also studied from Particle Image Velocimetry (PIV) experiments. Results show that the flow under certain conditions develops the ability to reorient trajectories and exponentially generate interfacial area, a feature of chaotic flows. Both simulations and experimental results show that Re ≥ 110 is the value that sets the transition from a steady laminar flow regime to a self-sustained laminar chaotic flow regime. An elastic analogue model of the jets’ behavior is also proposed to predict its impingement point. The good agreement between the PIV experiments and the model indicates that the jets’ kinetic energy feeding rate ratio is the key parameter to control mixing in RIM for formulations with stoichiometric and density ratios different from 1.

Keywords: RIM, Mixing, Chaotic Advection, Impinging Jets, CFD, PIV.

1. INTRODUCTION

Reaction Injection Molding (RIM) is an industrial process for the production of plastic parts where two or more viscous liquid monomers are injected and mixed in a cylindrical mixing chamber by opposed impinging jets. The mixture that leaves the mixing chamber is discharged into a mold where the polymerization occurs and the plastic part is formed. The mixing chamber is a cylinder with 1 cm diameter and 5 cm length, the injectors’ diameters are in the range of 1 – 2 mm and the mean residence time in the mixing chamber is in the range of 10 – 100 ms. An efficient mixing of the two monomers in the mixing chamber before entering the mold must be achieved in order to avoid zones of unreacted monomers that may lead to structural defects and the eventual rejection of the plastic parts [1]. The jets’ Reynolds number range of industrial practice goes up to 600.

Previous computational and experimental works [2, 3] have shown that mixing in RIM mainly occurs above a critical jets’ Reynolds number that marks the transition from a steady segregated laminar flow regime to a self-sustained laminar chaotic regime with strong mixing dynamics. It has also been shown that in equal injector diameter chambers the iso-momentum condition between the opposed jets is fundamental to ensure the continuous presence of the self-sustainable chaotic flow regime [4].

In this work the stretching properties of the flow in the RIM machine mixing chamber are studied from 3D (CFD) simulations and Lagrangian tracking of the position and deformation
of material spherical elements. The flow regimes and the jets’ impingement point position under unequal flow rates and different injectors’ diameters are further studied here from PIV experiments. An elastic analogue model of the jets is proposed to predict its impingement point.

2. FLOW STRETCHING PROPERTIES

2.1 3D CFD Model

The velocity, \( u \), and pressure, \( p \), fields of an incompressible fluid flow inside the RIM machine mixing chamber was modeled by solving the Navier-Stokes equations. The following boundary conditions were considered: fully developed parabolic velocity profile normal to the inlet surfaces; no slip condition at the walls (\( u = 0 \)); uniform and constant pressure at the outlet. The flow equations were solved with the finite-volume commercial CFD solver ANSYS Fluent™. A 3D geometrical flow domain was considered consisting of a cylindrical chamber with a diameter of \( D = 10 \) mm, a height of \( H = 50 \) mm. The injectors have a diameter of \( d = 1.5 \) mm and are placed at 5 mm from the top making an angle of 180º between each other. The computational grid consisted of 1.3 million prismatic elements with 0.15 mm of edge length. Initially, the simulations were performed at steady state and placing a shear-free planar central wall, normal to the injection direction, dividing the chamber in two. This procedure was taken to obtain an initial symmetric solution of the flow. The unsteady simulations were performed from the steady symmetric flow solutions by imposing a small and smooth perturbation to one of the inlets’ velocity profile. To ensure that the perturbation had no longer an effect on the flow, any analysis was only carried out after a flow time equal to three times the chamber residence time. Density, \( \rho \), of \( 10^3 \) kg/m³ and viscosity, \( \mu \), of 20 cP were assumed for the fluid, similar to the experiments.

2.2 Stretching Histories

The stretching properties of the flow were studied by tracking the position and deformation, in a Lagrangian point of view, of spherical material elements injected at the mixing chamber inlets and with infinitesimal initial radius \( |\delta X| \). Knowing the flow field from the CFD simulations, the position, \( X \), of the elements’ centroid can be determined by integrating the advection equation \( \dot{X} = u(X,t) \) for each element with initial position \( X_{t=0} = X \).

The tracked elements were considered to have the same physical properties of the remaining fluid, thus, not perturbing the flow. As the material spheres are advected, they rotate and stretch being continuously deformed into ellipsoids. The distance between the centroid and any point in the surface of an ellipsoidal element, \( \delta x \), is given by \( \delta x = F \cdot \delta X \), where the deformation tensor, \( F \), is obtained directly from the flow integrating \( \dot{F} = F \cdot \nabla u \) with \( F_{t=0} = I \) (identity tensor) as the initial condition [5]. The velocity gradient tensor was computed along the element trajectory. If a new coordinate system is chosen to be coincident with the principal axes of the deforming ellipsoid, the stretching of the \( i \)-th principal axis, \( \lambda_i \), can be calculated from the eigenvalues of the right Cauchy-Green strain tensor \( C = F^T \cdot F \) [6]. A long time average of the specific stretching rates is the equivalent, in Dynamical Systems theory, to the system’s Lyapunov exponents [5]. One positive Lyapunov exponent, \( \sigma \), is an indication that the flow is extremely sensitive to the initial conditions and that two initially close pair of particles will diverge exponentially with time as \( \delta x = \delta X \cdot e^{\sigma t} \), a characteristic of chaotic flows. Due to the finite time that the particles remain inside the reactor, the stretching properties of the flow were estimated from the average stretching of a group of advected material elements.
3. FLOW REGIMES AND IMPINGEMENT POINT POSITION

3.1 PIV Experimental Set-up and Methodology

The velocity field in an axial cut through the injectors of the mixing chamber was obtained from PIV experiments. Three different transparent Plexiglas mixing chambers with different injectors’ diameters were used: (1.5 mm, 1.5 mm), (2.5 mm, 2.5 mm) and (1.9 mm, 1.5 mm). All the chambers have a diameter of 10 mm and a length of 50 mm. The injectors are placed at 5 mm from the top making an angle of 180º between each other. The flow was seeded with 4 μm spherical nylon particles with a concentration that ensured at least 20 particles per interrogation zone. Care was taken to confirm that the particles follow the flow without disturbing it. The chambers were illuminated with a laser sheet and 16 bits black and white images of the particles field were captured. The velocity field was obtained by cross correlating a successive pair of images for interrogation zones of 64 pixels. The time between each pair of images was calculated so that the particles could move only 1/4 of the interrogation zone in that time interval. The seeded fluid was injected in the chamber from two pressurized tanks. The flow rate in each injector was controlled with two needle valves and measured in Coriolis flow meters. The fluid used in the experiment was a solution of water and glycerin with a density around 1.2×10³ kg/m³ and a viscosity of 20 cP at 24 ºC.

3.2 Elastic Analogue Model

To predict the impingement point position, x_{ip}, of the two opposed jets in the RIM machine mixing chamber an elastic analogue model is proposed. The model assumes that the two opposite jets behave like two springs that are forced to compress from an initial length equal to the mixing chamber diameter, D, to an equilibrium length, l. In this elastic system each competing spring applies a force to the other spring so that, in the equilibrium, Spring 1 has a length l_1 and Spring 2 a length l_2, with l_1 + l_2 = D. Considering the springs to behave ideally, the force applied to Spring 2 by Spring 1, F_{1→2}, and the applied to Spring 1 by Spring 2, F_{2→1}, can be related to the springs’ displacement by Hooke’s law

\[ F_{1→2} = k_1(D-l_1) = k_2 l_2 \quad \text{and} \quad F_{2→1} = k_2(D-l_2) = k_1 l_1, \tag{1} \]

where \( k_1 \) and \( k_2 \) are the springs’ constants, and can be considered to be a function of the injector diameter, jet velocity and the fluid physical properties. Since the two springs are in equilibrium, \( F_{1→2} \) must be equal to \( F_{2→1} \). Considering the equilibrium condition and combining the two terms of Equation 1, the springs’ constants ratio is equal to

\[ k_1/k_2 = l_1/l_2. \tag{2} \]

The springs’ compression will result in an increase of its elastic potential energy. The potential energy stored by Spring 1, \( \Delta E_{p1} \), and Spring 2, \( \Delta E_{p2} \), are given by the work performed by the forces along the compression length

\[ \Delta E_{p1} = \frac{1}{2} k_1 l_2^2 \quad \text{and} \quad \Delta E_{p2} = \frac{1}{2} k_2 l_1^2. \tag{3} \]
The potential energy stored by one spring can be assumed to be equal to the kinetic energy rate, $E_K$, of the opposed jet forcing the spring to compress. With this assumption, combining Equations 2 and 3 results in

$$\Delta E_{p,2}/\Delta E_{p,1} = \dot{E}_{K,1}/\dot{E}_{K,2} = k_1 l_1^2/(k_2 l_2^2) = l_1/l_2. \tag{4}$$

As the jets enter in the mixing chamber they expand and dissipate kinetic energy. The jets’ kinetic energy with the position inside the chamber can be estimated through the simplified model of a narrow axisymmetric jet model described by White [7]. The jet’s axial velocity, $u_x$, considering a point source of momentum is given by

$$u_x = 3J/(8\pi\mu x)\left[1 + C^2 r^2/(4x^2)\right]^{-2} \tag{5}$$

where $J = \pi/3 \rho u_{inj}^3 d^2$ is the jet momentum rate assuming a parabolic inlet velocity profile, $C = \sqrt{3\rho J/(16\pi\mu^2)}$ an integration constant, $u_{inj}$ the average injection velocity, and $r$ and $x$ the radial and axial positions, respectively. Combining Equations 4 and 5 results in

$$l_1/l_2 = \dot{E}_{K,1}(l_1)/\dot{E}_{K,2}(l_1) = 1/2\rho \int_0^\infty u_x(l_1, r) 2\pi r dr / \left(1/2\rho \int_0^\infty u_x(l_2, r) 2\pi r dr \right) \tag{6}$$

The distance from the point source of momentum until the injector’s inlet, $l^*_r$, is calculated from

$$1/2\rho \int_0^\infty u_x(l_r^*, r) 2\pi r dr = \pi/2 \rho d^2 u_{inj}^3.$$ 

With the above considerations the non-dimensional impingement point position, $\Phi$, can be estimated from

$$\Phi = \frac{x_p}{D/2} = \left[\left(\frac{Re_2 d_2}{10 D} + 1\right)\sqrt{\frac{\phi_k \frac{Re_1 d_1}{Re_2 d_2} - \left(\frac{Re_1 d_1}{10 D} + 1\right)}{\sqrt{\phi_k \frac{Re_1 d_1}{Re_2 d_2} + 1}}\right] \tag{7}$$

where $\phi_k = \rho d_1^2 u_{inj,1}^3/(\rho d_2^2 u_{inj,2}^3)$ is the jet’s kinetic energy feeding rate ratio at the inlet, and $Re = \rho d u_{inj}/\mu$ the jet’s Reynolds number.

4. RESULTS AND DISCUSSION

4.1 Stretching Histories

3D CFD simulations of the flow were performed for $Re = 100, 110, 200$ and $300$. Unsteady flow fields were obtained for $Re > 100$. A number of 344 particles were tracked from both inlets until the first particle came out. Figure 1 shows the average maximum stretching, $\lambda_{max}$, as a function of time and the cumulative distribution of the stretching experienced by the particles up to the moment the first element leaves the mixing chamber. Figure 1a shows that for $Re = 100$ and $110$, despite of the flow being unsteady for $Re=110$, the elements undergo, on average, a linear stretching with time. For $Re = 200$ and $300$ the average stretching increases nearly exponentially with time, an indication that the flow developed the ability to reorient the trajectories and improve mixing. Figure 1b shows that, in the studied range of Re, the average stretching experienced by the elements and the fraction of elements with higher deformation increases with Re.
4.2 Critical Reynolds Number

The transition of mixing regimes was also verified from experimental PIV results. An average kinetic energy of the velocity fluctuations was calculated from the velocity field as

\[
\langle k \rangle = \frac{1}{2} \sum_{i=1}^{2} \left( \vec{u}_i(x,t) - \overline{\vec{u}}(x) \right)^2.
\] (8)

Figure 2 shows the non-dimensionalised values of \( \langle k \rangle \) for the equal injector diameter chambers. As observed in the flow simulations (Figure 1), the PIV results show that for both designs a value of Re around 110 marks the transition from steady to an unsteady chaotic flow regimes. For the chamber with 1.5 mm diameter injectors a hysteretic behavior was observed for increasing and decreasing flow rates.

4.3 Jet Impingement Point Position

The jet’s impingement point position was determined from the PIV results at different Reynolds numbers and jets’ flow rate ratios for the studied mixing chamber designs. Figure 3 shows the non-dimensional impingement point position as a function of \( \Phi(K_D, \phi, D, d) \). The experimental results show good agreement with the proposed elastic analogue model, especially for Re up to 100 and for small deviations of the impingement point from the center of the chamber. The divergence of the experimental data from the model increases as Re increases or for impingement points close to the walls of the chamber, showing that this model, based in the simplistic narrow axisymmetric jet model, has limitations. The effect of the walls and additional dissipation due to the jets’ instability in the mixing regime has not
been considered. Nonetheless, the results indicate that the jets’ kinetic energy rate is the key parameter that determines its impingement point.

![Figure 3](image)

**Figure 3.** Jets’ impingement point position as a function for different injector diameters: a) (1.5 mm, 1.5 mm), b) (2.5 mm, 2.5 mm) and c) (1.9 mm, 1.5 mm).

5. **CONCLUSIONS**

From the Lagrangian analysis of the flow, the present work shows that only above a Reynolds number of 110 the flow develops the ability to reorient the trajectories and produce a nearly exponential average stretching of fluid elements with time. The exponential reduction of mixing scales is an indication that, in the mixing regime, the flow in the RIM machine mixing chamber is chaotic. Both simulations and experimental results show that Re ≥ 110 is the value that sets the transition from a steady laminar flow regime to a self-sustained laminar chaotic flow regime.

The PIV experimental results and its agreement with the elastic analogue model indicate that the jets’ kinetic energy feeding rate ratio is the key parameter to control mixing in RIM for formulations with stoichiometric and density ratios different from 1.

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6. **REFERENCES**


