Numerical Investigation of the Effect of Flow Geometry on Mixing a Viscous Polymer Melt

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ABSTRACT

Mixing enhancement is an important consideration when designing materials processing devices. There are a variety of mixing elements used in industry, with little consensus as to what differentiates a good mixing section from a poor one. However, good mixing is important to obtain homogeneity of the material structure and temperature profile in materials processes. This paper presents a numerical analysis of the role of flow geometry on mixing of polymer melt. Several cooling screw geometries, typical of those used by the extrusion industry, were used to assess mixing, by studying polymer melt flow and heat transfer in the screw channels.

1. INTRODUCTION

Extrusion is a manufacturing process used to create objects of a fixed cross-sectional profile. In the polymer extrusion process, a solid plastic is continuously fed into a heated chamber, melted and carried along by a feed screw within. A tandem extrusion system, as shown in Figure 1, includes a secondary extruder, which consists of a cold barrel and a cooling screw within, for cooling and homogenizing to produce high volume quality product at a low and constant temperature, to feed an extrusion die. The die (connected to the end of the cooling extruder) accomplishes the nucleation and cell growth functions when the system is used for microcellular polymer processing system, and the shaping function of a sheet processing system.

Optimization both of the equipment and of the extrusion process itself would enable more efficient use of raw materials and energy. Although the polymer melt is premixed in the first extruder, the mixture in the second extruder needs to be further mixed to achieve effective cooling and to homogenize the temperature distribution. The technological challenge of obtaining good mixing can be addressed by systematically examining different screw geometries.

In industrial processes, mixing is a unit operation that involves manipulating a heterogeneous physical system, to make it more homogeneous [1]. Mixing in an extrusion process is complicated due to the flow patterns in the extruder and the rheological complexity of polymer melts. Since polymer melt has a very low thermal conductivity, the heat transfer in an extrusion process is governed by flow pattern, and thus mixing can be evaluated by studying the heat transfer in the extruder. On the other hand, good mixing is usually achieved by providing sufficient distribution and dispersion, and mixing can be evaluated by studying the flow field.

Mixing is often described in terms of two mechanisms, defined as distributive and dispersive. Distributive mixing depends on the affine deformation of fluid particles, and involves stretching, dividing and reorienting the flow of a liquid in order to eliminate local variations in material distribution and produce a more homogeneous mixture. Dispersive mixing is characterized by the number of times that fluid particles break and coalescence [1]. These then define strategies that can be used to improve mixing. Distributive mixing can be achieved by providing convoluted flow paths that split and reorient the flow repeatedly, while dispersive mixing can be achieved by passing a mixture through small regions that lead to intense deformation. Therefore, mixing can be estimated by studying the flow and heat transfer within a few typical screw geometries that yield different flow patterns. This goal can best be achieved by developing a numerical model based on physical laws and assumptions to predict the melt flow and heat transfer behaviors in response to a given screw geometry.

As the use of tandem extrusion lines to produce quality microcellular foams has expanded, there has emerged an increased interest in designing better cooling screws. All cooling screws currently in widespread use have been designed to provide a varying flow pattern, to improve mixing. For example, the Turbo-Screw, designed by Fogarty et al. [2], includes small holes on the flights to create extra flow paths; Rauwendaal [3] developed the High Heat Transport (HHT) screw with segmented multi-flights to divide the flow field into smaller fields; the Barr Energy Transfer (ET) screw [4, 12] was designed with different channel depths to further deform the melt. Although these designs all claim to be superior to a standard screw, it is not clear to what extent they enhance mixing. This paper presents a study of the effect of screw geometry on mixing in a cooling extruder, by numerically modeling the flow and heat transfer in screw channels, for a standard screw geometry, and for geometries that are representative of improved designs.

2. METHODOLOGY

2.1 Conservation Laws

Polymer melt flow in a cooling extruder is assumed to be steady state, incompressible and comply with conservation laws for mass, momentum and energy, that are in the form of a set of partial differential equations:

Continuity equation:

$$\nabla \cdot u = 0 \tag{1}$$

Momentum equation:

$$\rho \frac{Du}{Dt} = \nabla \cdot \sigma + \rho g \tag{2}$$

Energy equation:

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = \nabla \cdot (D \nabla T) + \Phi \tag{3}$$

u is the velocity vector, σ is the stress tensor, ρ is fluid density, g is gravitational acceleration, T is temperature, D is thermal diffusivity, and Φ represents the viscous reheating. Equations (1), (2) and (3) can be simplified by the constitutive relationship between the stress and the properties of the flow, and non-dimensionalized by introducing a characteristic velocity U, length L, and temperature T. that lead to the following dimensionless quantities:

$$\mathrm{Re}_N = \frac{\rho U L}{\mu_N} \tag{4}$$

$$\beta = \frac{\mu_N}{\mu(\dot{\gamma})} \tag{5}$$

$$Pe = \frac{UL}{K} \tag{6}$$

Re_N is the Reynolds number at a reference viscosity μ_N, β denotes the relative magnitude of the reference viscosity to the local viscosity, and Pe is the Peclet number which indicates the relative importance of advection to diffusion. The polymer melt is modeled as a purely viscous fluid, where the shear-rate and temperature dependent viscosity of the polymer melt is described via a modified power-law model:

$$\mu(\dot{\gamma}) = m(\dot{\gamma})^{n-1} e^{-b(T-T_b)} \tag{7}$$

m is the consistency index (unit of $Pa \cdot s^n$), n is the power-law index, b is a constant, and T_b is a reference temperature. The dimensionless governing equations then become:

$$\nabla \cdot u = 0 \tag{8}$$

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla P + \frac{1}{\mathrm{Re}} \nabla \cdot \left\{ \mu \cdot \left[(\nabla u) + (\nabla u)^T \right] \right\} \tag{9}$$

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = \frac{1}{Pe} (\nabla^2 T) + f \tag{10}$$

The above equations are difficult to solve numerically due to the non-linear relationship between the stress and the rate-of-strain. For molten polymer flow, the Reynolds number is very small, usually in the range of 10^{-4} to 10^{-2} [4], so the flow field is governed by diffusion. On the other hand, the typical Peclet number is large due to the low thermal diffusivity of polymer melt; typically the thermal diffusivity is in the range of 10^{-6} to 10^{-7} m^2/s, that leads to a Peclet number on the order of 10^7, which makes heat transfer advection dominated, and leads to a temperature field within a screw channel that is characterized by a large interior region effectively insulated from the screw and barrel by a thin thermal boundary layer. Therefore, it is important to improve fluid mixing to ameliorate this temperature inhomogeneity.

Most problems in fluid dynamics and heat transfer require solution of coupled systems of equations, i.e., the dominant variable of each equation occurs in some of the other equations. For extrusion processing, the velocity and temperature fields are coupled by viscosity and shear-reheating terms in the governing equations. For this work, the flow was calculated by assuming an isothermal condition, and the energy equation solved subsequently, thereby decoupling the flow and heat transfer equations.

2.2 Numerical Algorithm

The governing equations (8), (9) and (10) are spatially discretized using a Galerkin finite element approach in conjunction with P2-P1 tetrahedral Taylor-Hood elements [5] that have ten nodes for velocity and temperature, and four nodes for pressure. A finite element solver for three-dimensional non-Newtonian fluid flow and advection-diffusion heat transfer has been developed based on two existing finite element codes [6, 7] to address flow and heat transfer modeling. The unknown velocity, pressure and temperature fields can be expressed in terms of the shape functions ϕ_j and ψ_j and the nodal velocity, pressure and temperature values u_j, p_j and T_j:

$$u\,(or\,\mathrm{T}\,) = \sum_{j=1}^{N} u_j\,(or\,T_j\,)\,\phi_j \tag{11}$$

$$p = \sum_{j=1}^{N_p} p_j \psi_j \tag{12}$$

where there are $N = 10$ degrees of freedom for velocity and temperature in each co-ordinate direction, and $N_p = 4$ degrees of freedom for pressure. Following the Galerkin spatial discretization, the governing equations can be written in semi-discrete form as:

$$[M]\frac{d\{u\}}{dt} + [S]\{u\} + [L]^T\{p\} = \int_\Gamma (-p\vec{n}\cdot\vec{x} + \frac{\partial u}{\partial n})\,d\Gamma \tag{13}$$

$$[L]\{u\} = 0 \tag{14}$$

$$\frac{\partial\{T\}}{\partial t} = D\{T\} + C\{T\} + f \tag{15}$$

where $\{u\}$, $\{p\}$ and $\{T\}$ are the vectors of nodal velocity, temperature and pressure values, $[M]$, $[S]$ and $[L]$ are elemental matrices, $D = \frac{1}{Pe}\nabla^2 T$ is the diffusion operator, $C = -u\cdot\nabla$ is the advection operator, Γ is the boundary of the elemental volume Ω, and $\vec{x}$ is the unit vector in the x_i direction, where $i = 1, 2, 3$ represent the *x, y,* and *z* directions.

The shear strain rate dependent viscosity of a non-Newtonian fluid leads to a full coupling of the velocity components if an explicit treatment is used for the viscous term. An approach was adopted in this study that decouples the different velocity components, yet still conserves the stability of the implicit scheme for the viscous term [7]. When the advection term dominates the heat transfer problem, most conventional numerical schemes, including the standard Galerkin finite element method, suffer from wiggles in the solutions. Therefore, stabilization is necessary for the numerical scheme. The stabilization approach in this study is the semi-Lagrangian method [7], that takes advantages of a Lagrangian method that is unconditionally stable, yet avoids the mesh motion associated with a pure Lagrangian scheme.

2.3 Boundary Conditions

Since the flow geometry has a periodic flow channel with a large L/D (Length/Diameter) ratio, a periodic inflow/outflow boundary condition was implemented to simulate fully developed flow, in a way that conserved the initially-specified volumetric flow rate. For the heat transfer modeling, a Dirichlet temperature condition was implemented at the barrel and a zero heat flux was assumed at the screw root.

3. RESULTS AND CONCLUSIONS

3.1 Screw Geometries

A standard screw geometry and three specially designed screw geometries, all illustrated in Figure 2, were studied. Figure 2(b) shows a multiple-flights screw with holes through the flights; Figure 2(c) shows a screw with segmental multi-flights; Figure 2(d) shows a multiple-flights (two flights) screw with two different channel depths. These geometries were spatially discretized and then studied by numerically modeling the flow and heat transfer in the screw channels. Figures 3 and 4 illustrate the finite element meshes for screws 2 and 3 respectively.

The material considered in this study is WB130HMS polypropylene (PP), which is a linear hydrocarbon polymer. The PP was assumed to be processed in a cooling extruder at $190^o C$, with the polymer melt flow rate controlled by the screw speed. A summary of material data used for the calculations, and the operating conditions considered, are listed in Table 1.

3.2 Flow Field

3.2.1 Velocity Field

Four flow simulations were carried out for PP melt in the channels between an outside barrel and the screw element 1, 2, 3 and 4 respectively. The melt velocity fields within the screw channels were calculated, the velocity contour levels and vector fields were plotted, and streamlines were traced. Figure 5 illustrates the axial velocity at cross sections of those screw channels. Compared to the more complex screw channels, the conventional cooling screw (screw element 1) yields the simplest flow pattern. Screw element 2, which is a design similar to the Turbo-screw, has a deeper channel depth and the three flights split the flow field into three parts; in addition, the holes on the flights provide extra flow paths with a high velocity at the centre of the holes. Screw element 3, with its multiple segmented flights (this is a design similar to the HHT screw), also generates a more complicated flow pattern, as the segmented flights force the melt to flow back and forth axially, which would contribute to distributive mixing. Screw element 4 was designed with two flights and different channel depths, a simplified version of the Barr ET screw. The velocity profile indicates that the flow patterns in the two channel depths are different, because the fluid stretches as the melt crosses from one channel to the other.

To further inspect the velocity distribution, the velocity vector fields were also plotted for each case, as shown in Figure 6. The vector fields clearly indicate that compared to a normal screw channel in which the melt rotates and shears as the screw rotates, the screw elements with multiple flights, like 2 and 3, yield more complex motions between the multiple channels, and the melt also reverses direction axially. The vector field for screw element 4 shows that the flow interacts across the channels of different depth, although the shallow channel in particular has a flow field that is very similar to that in the standard screw.

Figure 7 shows streamlines for all four simulations. For the standard screw, the streamlines across the screw channel are simple and straight. Across the channel of screw 2, vortices form due to the particular configuration of that screw element, while the different channel depths of screw 4 yield a flow field that is stretched intensely while passing through the channel, and so provides an extra deformation of the melt flow. The simulation results clearly indicate that the more complex flow patterns in screws 2, 3 and 4 are advantageous to mixing, and as a result, we surmise that they are superior to a standard screw.

3.2.1 Pressure Field

One of the important measures of an extrusion process is throughput. There are usually two components of flow in an extruder: the drag flow and the pressure flow [1]. The drag flow arises from the relative motion of the liquid (due to the rotating screw) and stationary barrel. The pressure flow arises from the back pressure caused by the build-up of pressure in the extruder during the extrusion process, but is a negative contribution to flow, and so reduces the throughput. As the pressure flow is a major function of the flow geometry, the pressure profiles for the four simulation cases are plotted in Figure 8, to compare the performance of the screw geometries considered. For the standard screw, the pressure rises along the channel (note that the jump in pressure midway along the element is due to the presence of the screw flight), and the overall rise in pressure is close to a value we measured experimentally (although we provide no details of that experiment here). For this case, as given by the operating conditions listed in Table 1, the pressure contributes negatively to the overall throughput for the standard screw. The pressure profiles of the other screws are different: the pressure along screw 4 contributes to a positive throughput; for screws 2 and 3, the pressure varies little between inlet and outlet, and so has little effect on throughput, which indicates that drag flow in these two channels dominates.

3.3 Mixing Evaluation

Recent developments in the field of dynamic systems have led to an approach to the understanding and study of the kinematics of fluid mixing. A mathematical framework for the analysis of mixing systems, by simultaneously considering shear strain and the orientation of fluid elements, has been advanced by Ottino *et al.* [9], and has shown how local stretch rates can be used to quantify kinematic mixing efficiency by use of a local mixing efficiency

$$e = \left| \frac{D : nn}{\sqrt{D : D}} \right| \qquad (16)$$

n is the normal direction of the interfacial area, which can be defined as $n_i = u_i / \sqrt{u_j u_j}$, and D is the rate of the deformation tensor. The duration of time that a polymer fluid element remains inside an extruder is the residence or dwell time. The average residence time of the polymer through the extruder is equal to the total channel volume divided by the volumetric output rate. Figure 9 shows the local mixing efficiency in the four screw channels. These results indicate that except for the regions located around the flights, the values of the local mixing efficiency in these channels are small (close to zero), which means that most of the stress is generated at the tips of the screw flights, that cause fluid particles to break down, and so these areas lead to dispersive mixing. Moreover, the value of the mixing index in a standard screw is smaller than the values for the other three cases, which implies that mixing in the channel of a standard screw is not good because mixing is induced only by unidirectional shear flow, which is the least effective mixing mechanism. On the other hand, screw 4 shows the highest value of efficiency, which implies that the dispersive mixing is best in this screw channel. This is because screw 4 has different channel depths, and thus the flow particles are stretched more when they pass between different depths, adding to the deformation of the melt. Figure 10 shows the average residence time for the four screws: the time for a standard screw is about 30 seconds, while screw 2 has the longest residence time.

3.4 Heat Transfer

Figure 11 illustrates temperature profiles across the screw channels for the four screw elements. These results show that due to the low thermal diffusivity of polymer melt, all the heat coming from the melt accumulated in the first extruder is carried along when melt flows in the cooling extruder. Only a very thin thermal boundary layer forms, and a small amount of heat is transmitted to the cooled barrel. Since shear reheating was not considered, the effect of screw geometry on heat dissipation from shearing was not included. On the other hand, although the flow fields of these four cases are different, the heat transport is limited due to the limited heat conduction between melt particles. Therefore the temperature profiles for these cases are similar, which implies that cooling is not sufficient if only the extruder barrel works as a cooling device. It should be re-emphasized that if shear reheating was considered, and because the inner region of the melt is insulated from the screw and barrel surface, the temperature would be higher in the center of the screw channel. This high temperature region is the major deficiency of the standard cooling screw: improving that, by eliminating this region, is of crucial importance when considering extruder design.

3.5 Conclusions

A finite element analysis for solving three-dimensional polymer melt flow and heat transfer in four cooling screws has been carried out, to investigate the effect of screw geometry on mixing. Polymer melts have a very limited capability to diffuse heat. Therefore, homogeneity in an extruder can be only achieved by providing sufficient mixing of the melt particles, which can be obtained by diversifying the flow pattern by using special screw geometries. The diversified flow patterns can be obtained by using multi-flights or by using elements to provide extra flow paths to divide and reorient the flow. In general, better homogenization is possible by the use of multiple-flight screws; using slots (holes) on flights generally yields a certain improvement in redistributing the melts; and using different channel depths will improve dispersive mixing by providing extra deformation to the melt.

Although homogenous melt distribution can be obtained by providing good mixing, cooling is limited if the only heat transfer path is through the barrel. This study provides a tool for the subsequent design of an optimal technical solution for the elements of an extruder.

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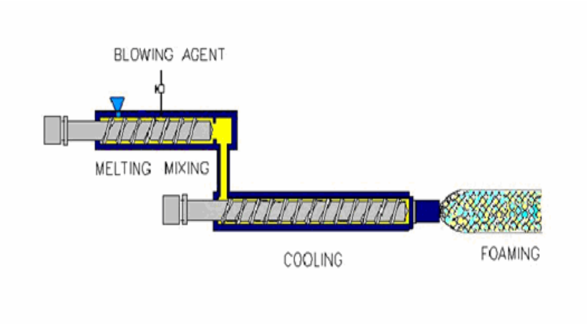
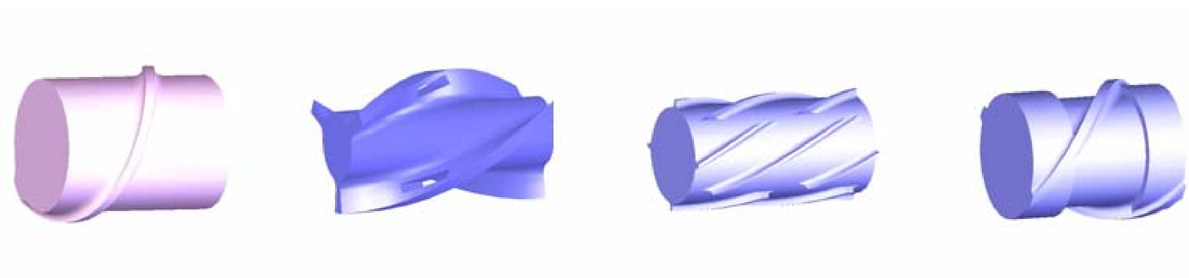


Figure 1: A schematic of a tandem extrusion system

Parameters	Quantity
Screw revolution speed (rpm)	8
Barrel temperature (^{o}C)	19.9
Power-law index	0.4
Reynolds number (Re_n)	1×10^{-4}
Peclet number (Pe)	1×10^{6}
Density(g/ml)	0.910

Table 1: Material data and operating conditions.



(a) Screw 1 (b) Screw 2 (c) Screw 3 (d) Screw 4

Figure 2: Screw elements

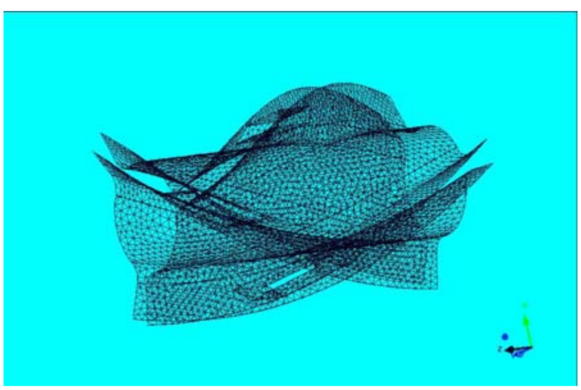


Figure 3: Screw element 2 - mesh

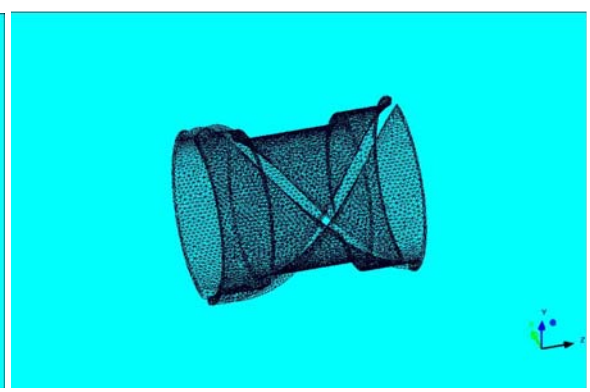


Figure 4: Screw element 4 - mesh

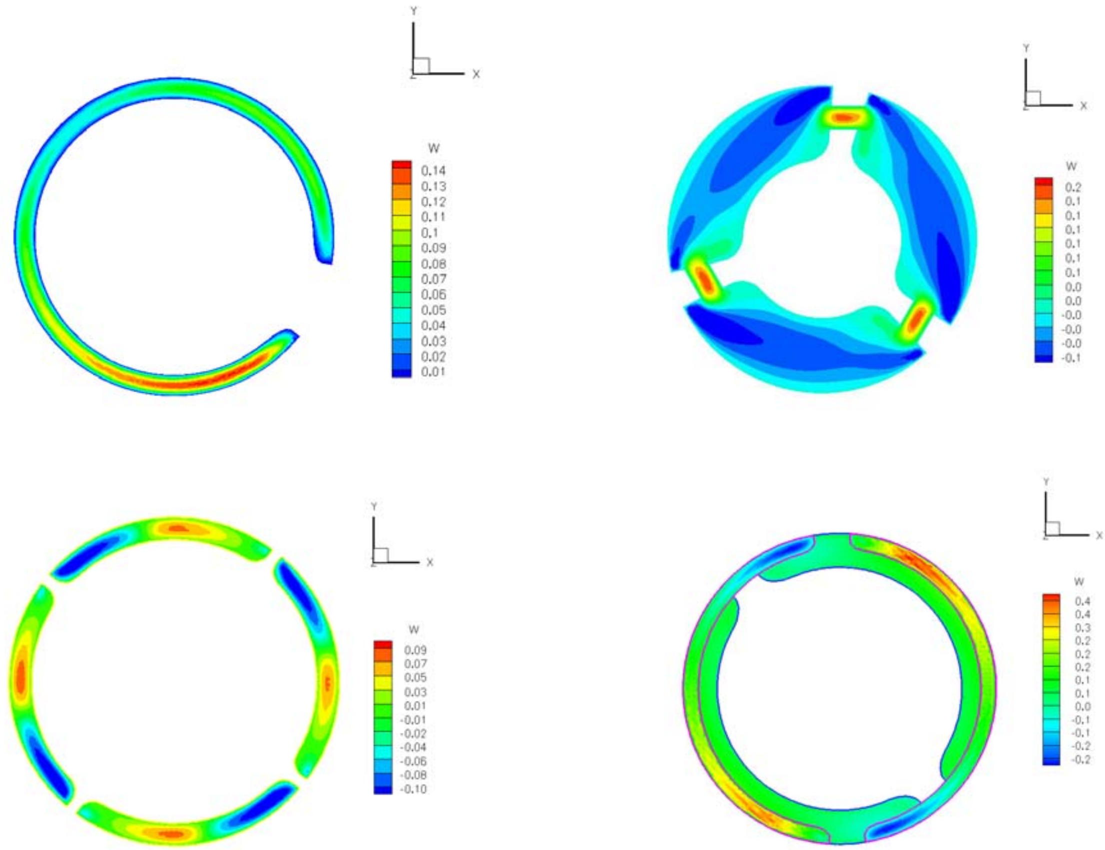


Figure 5: Axial velocity contours

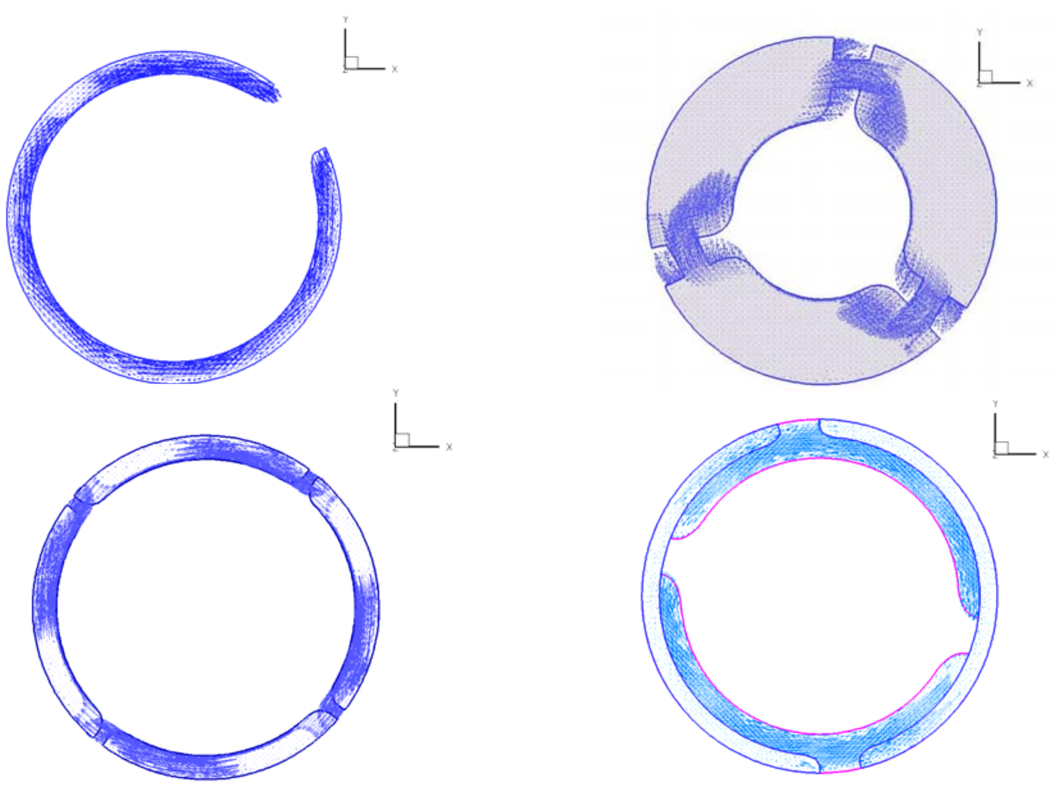


Figure 6: Velocity vectors

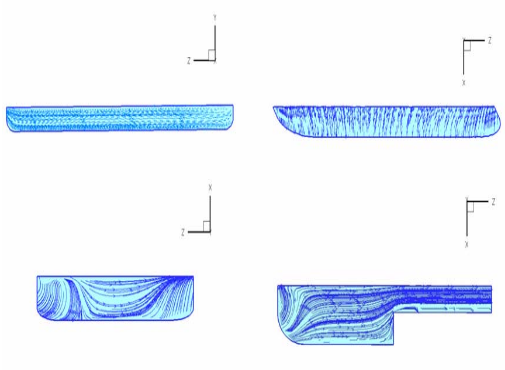


Figure 7: Velocity streamlines

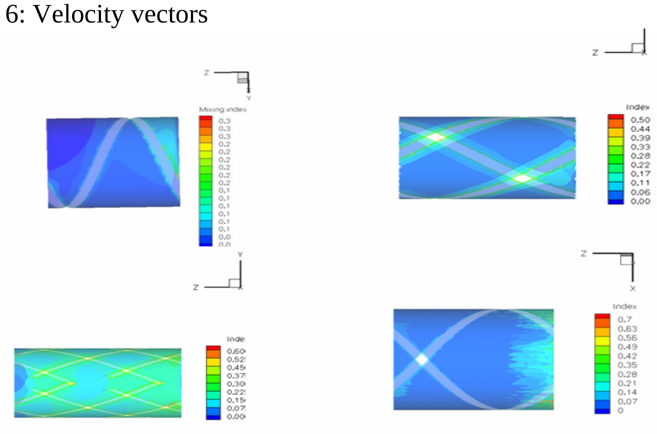


Figure 9: Local mixing index

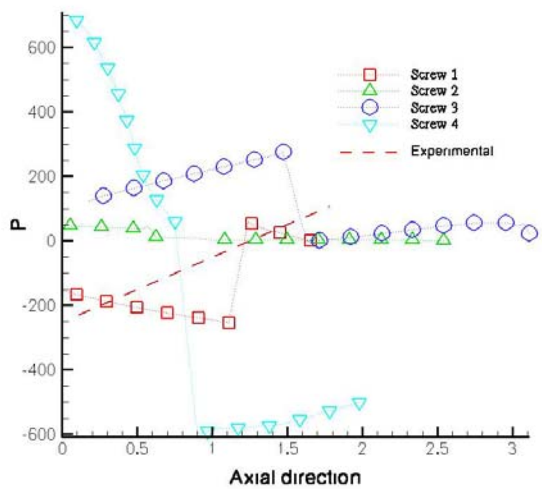


Figure 8: Pressure field

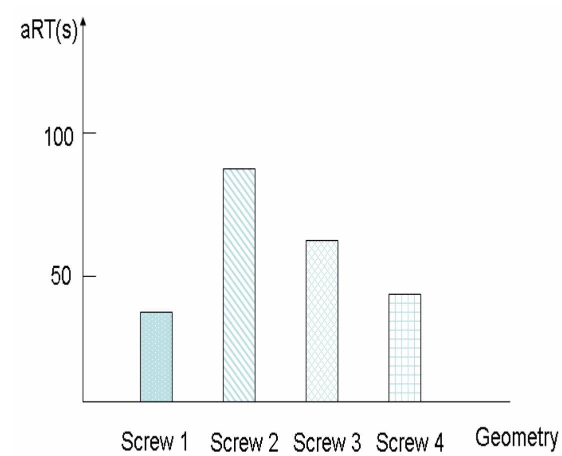


Figure 10: Average residence time

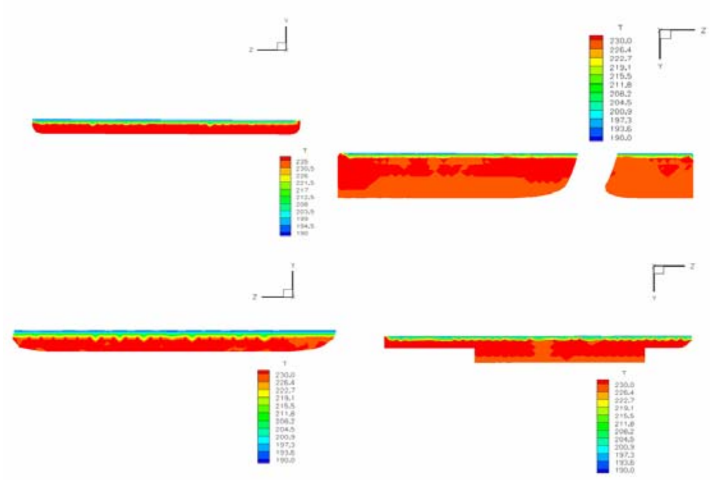


Figure 11: Temperature field