Steps for the Optimization of Pipe and Tubing Extrusion Dies

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Abstract: The extrusion of polyolefin pipes suffers degradation due to mechanical design problems of the extrusion die that is commonly used. This study uses numerical and computational approaches to detect problematic areas in the die geometry. Simulations show that in the conventional die there are areas of stagnation and recirculation of the melt flow, resulting in greater residence times, one of the main causes of degradation. This study introduces the use of novel profiles, which reduce stagnant regions, recirculation events, and can optimize the pipe extrusion process. Additionally, this study illustrates a methodology based on residence time distribution (RTD), a parameter that can be applied in extrusion and injection molding optimization of the tooling and equipment.

Keywords: Degradation, crosslinking, Residence Time Distribution (RTD), Cumulative Residence Time Distribution (CRTD), Poincaré sections, lattice basket die.

1. Introduction

Degradation is a significant obstacle that harms both the extrusion and injection molding processing and recycling of plastics. This chemical reaction adversely affects the flow and mechanical properties of the material and the surface finish of the products. Factors such as temperature, shear, and residence time history contribute to this negative effect and need further study [1, 2, 3]. One application that is susceptible to this problem is the extrusion of polyethylene pipes. During the processing of polyethylene pipes, the resin experiences exceedingly high residence times and small blemishes, referred to as gels, appear in extruded products [1].

The aim of this study is to simulate the tooling used in the polyolefin pipes industry, and to analyze how the mechanical design of the extrusion die contributes to degradation in the final products. To that end, this study used a methodology traditionally applied in mixing [1]. This methodology consisted of the following steps: the simulation model was described first, and the residence time distribution (RTD) chosen as the target quantity. Physical and material properties and the mathematical model were obtained using the transport phenomena method [4]. Through numerical techniques, the velocity, velocity gradients, streamlines, viscosity, and pressure profiles were calculated. In a second simulation, the RTD, tracer curves, and Poincaré sections were calculated. Based on the RTD results, problem areas in the proprietary die design were identified. The same methodology was then applied to develop an optimized die model. Finally, the optimal model was adapted to a profile that can be manufactured.

2. Degradation in Extrusion and Injection Molding Processes

The processing and reprocessing of plastics has an effect on the flow and mechanical properties of the material, as the molecular weight changes each time the material is heated and sheared during the pelletizing and manufacturing process. The reduction in molecular weight is reflected by increases in the melt flow index (MFI) [1]. A common technique used to detect degradation, is to evaluate changes in the MFI. Figures 1.a and 1.b present the change in the MFI of various polymers for extrusion and injection molding processes, respectively [5]. Here we see that PE-LD and PMMA actually experience an increase in molecular weight (decrease in MFI), which indicates crosslinking during processing. This is commonly observed with polyethylenes, when the material experiences exceedingly high residence times, and small blemishes, referred to as gels, appear in extruded products [1].

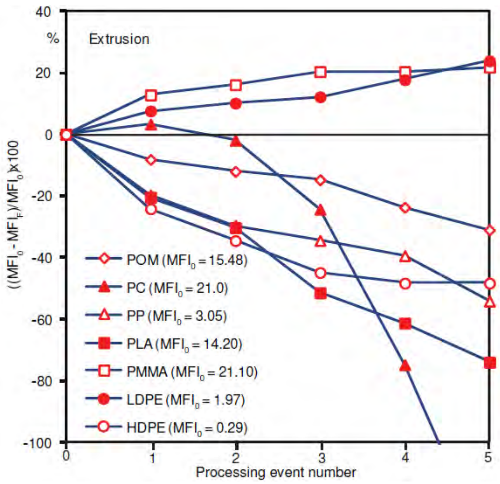

Figure 1.a Change in MFI as a function of number of extrusion processing events [1].

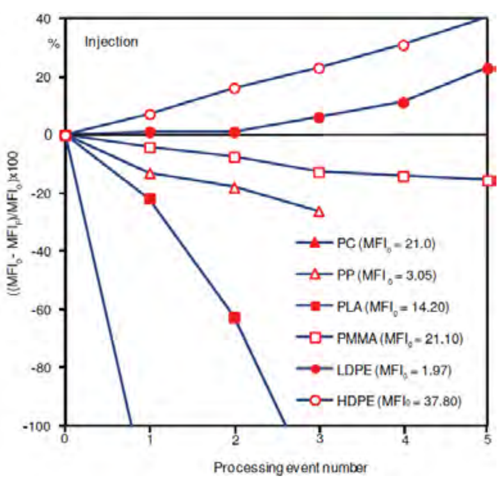

Figure 1.b Change in MFI as a function of number of injection molding processing events [1]

3. Methodology

Case study: Understanding degradation in the production of polyolefin pipes.

3.1 Model: Lattice Basket Die[1]

Numerical and computational approaches were utilized to find the particle trajectories and residence times in a customary pipe extrusion die (lattice basket die, *LB die*). This die is adopted in the tubing extrusion of polyolefins by virtue of its capacity to produce a high quality surface appearance as well as increased mechanical strength. These advantages are due to a borehole pattern which materializes several weld lines around the surface instead of one weld line in the middle of the pipe [6]. Figure 2.a shows a slice of the melt flow profile inside the LB die (18^o radially, of the 3D profile).

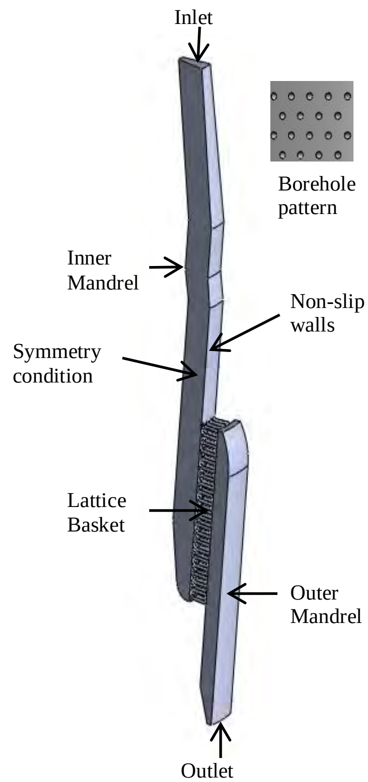

Figure 2.a 18° radial slice of the melt flow profile inside the lattice basket (LB) die.

The die receives the melt axially from the extruder in an annular cavity. The cavity results from the assembly of the conical shaped inner mandrel and the LB [6]. Thereafter, the single melt stream is divided into several streams when crossing radially through the borehole pattern of the LB, which is composed of thousands of small holes (diameter 1 to 2.5 mm) [6]. At the exit of the LB, another annular cavity receives the streams and redirects them axially. The second annular cavity is the pocket between the LB and

[1] Customary die adopted in the industry in pipe and tubing extrusion applications.

the external mandrel. The melt streams are pushed through the die ring zone and the relaxation zone. These two zones help the melt streams merge with multiple non-visible weld lines. The relaxation zone shapes the melt to the desired dimensions and eliminates part of the stresses imposed on the material during the extrusion process [6]. Figure 2.a does not include the melt flow profile in the die ring zone and relaxation zone.

3.2 Target Quantity: Residence Time Distribution (RTD)

In this methodology, the RTD was determined first. In mixing applications, The RTD is a parameter used to assess the mixing quality of a continuous flowing system. The residence time distribution is a measure of how much time the melt spends inside a continuous mixing device [7]**.** In this study, the RTD is a measure of the time it takes for particles entering at one plane to exit at another plane depending on the trajectory that they follow [7]. However, it is more common to assess mixing using the cumulative residence time distribution (CRTD). For the purpose of this study, the CRTD is the normalization of the RTD over the time (t) that takes the first melt particle to appear at the exit of the die [7]**.**

3.3 Physical and Material Properties

The operation conditions, including physical and material properties were identified. The polyolefin used in the study was a high-density polyethylene (HDPE), with a melt index (MI) of 0.35 g/10 min (190^{o}C, 2.16 kg). This resin had a solid density of 0.952 g/cm^3, and based on the pvT diagram [8], had a melt density of 0.766 g/cm^3, under the operation temperature of 183^{o}C. The mass flow rate of the extruder was 450 lb/h (204 kg/h). The pressure drop measured at the exit by means of a pressure transducer, was 1925 psi (13.72 MPa).

3.4 Mathematical Model: Application of the Transport Phenomena Method

The conservation laws and the constitutive equations were considered and simplified using the transport phenomena method [9] as follows: Since the borehole pattern was not axisymmetric, the fluid was modeled in 3D, which greatly increased the computational cost. To decrease the computational cost only five percent (18^{o}, radially) of the total LB was considered. A schematic of the melt flow profile is depicted in Figure 2.a. The slice shown in Figure 2.a is representative of a radial symmetry. The model was considered in steady state neglecting the startup of the equipment. Creeping flow, characteristic in polymeric melts was considered, with the understanding that the effect of the inertia is negligible in comparison with the viscous effects (Reynolds number Re <<1)**.** Gravity forces are smaller in comparison with viscous forces (Poisseuille number Ps<<1), and therefore neglected. The fluid was considered in an isothermal stage where the density and viscosity are independent of the temperature. The melt was assumed incompressible. The Bird-Carreau constitutive model [10] counted for the non-Newtonian behavior of the HDPE. The equation of continuity (Eq.1), the equation of motion (Eq.2), the shear stress tensor (Eq.3 and Eq.4) and the constitutive equation (Bird-Carreau model) for non-Newtonian fluids (Eq.5 and Eq.6) follow using Bird notation [9]**:**

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

$$0 = -\nabla p - [\nabla \cdot \boldsymbol{\tau}] \tag{2}$$

$$\boldsymbol{\tau} = \eta \dot{\boldsymbol{\gamma}} \tag{3}$$

$$\dot{\boldsymbol{\gamma}} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^t) \tag{4}$$

$$\frac{\eta - \eta_o}{\eta - \eta_\infty} = [1 + (\lambda \cdot \dot{\gamma})^2]^{\frac{(n-1)}{2}} \tag{5}$$

$$\dot{\gamma} = \sqrt{\frac{1}{2}(\dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\gamma}})} \tag{6}$$

Table 1. Parameters Bird-Carreau constitutive model.

Parameters	***Symbol***	***Range***	***Units***
Rate of deformation tensor	$\dot{\gamma}$	10-14000	s^{-1}
Dimensionless parameter	n	0.3	*Dim.*
Time constant	λ	0.0259	s
Zero shear rate viscosity	η_0	5600	$\frac{N \cdot s}{m^2}$
Infinite shear rate viscosity	η_∞	0	$\frac{N \cdot s}{m^2}$

With **u** the velocity vector, p the pressure, $\boldsymbol{\tau}$ the shear stress tensor, $\dot{\boldsymbol{\gamma}}$ the rate of strain tensor, $\dot{\gamma}$ the magnitude of the rate of strain tensor, η the viscosity for a non-Newtonian case, n a dimensionless parameter, and λ a time constant. The Bird-Carreau model parameters used in this study [10] appear in table 1.

The boundary conditions consisted of the following assumptions (Figure 1.a): a constant mass flow rate at the inlet of the die, a pressure difference equal to zero at the outlet of the die, and non-slip walls (the phenomenon of wall slip presented in high molecular weight polyethylene [6, 11] was neglected). The cuts on the sides of the die walls were considered as symmetry conditions.

3.5 Solution: Implications of the Lattice Basket and Mandrel surfaces.

The solution of the mathematical model was computed, and to that end, the Finite Elements Method (FEM) was implemented since the equations did not have an analytical solution. COMSOL Multiphysics version 4.2a was used to solve for the velocity, velocity gradients, and pressure profiles. These parameters were reused in a second simulation to solve for the RTD, tracer curves, and Poincaré sections.

The results of the numerical model for the velocity and velocity gradients showed the absence of a streamline pattern (zones A and B) in the solid walls of the borehole arrangement, as shown in Figure 2.b. These zones represent problematic locations with low or zero velocity. Seeking further insight into flow channel surfaces and edges, the Poincaré sections and tracer curves were modeled. The Poincaré sections show the trajectory of several particles during the extrusion process as they travel through the die. Tracer curves represent the preferable paths in which the particles flow from the inlet to the outlet of the die. Zones without particles (zones A and B in Figure 2.c) represent low velocity regions that lead to stagnation locations and/or recirculation regions, that are reflected in empty zones without tracer curves in Figure 2.d (Zones A and B).

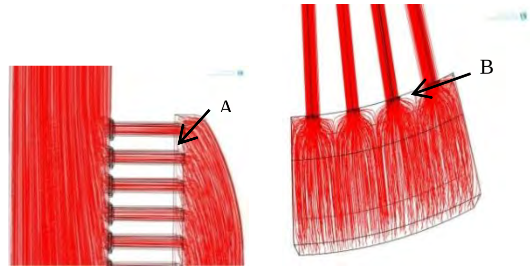

Figure 2.b Streamline pattern in the LB die. Corners of the mandrels with the borehole arrangement.

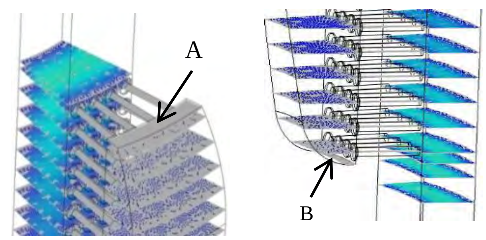

Figure 2.c Particle tracking in the LB die. From left to right: top corner of the outer mandrel and bottom corner of the inner mandrel.

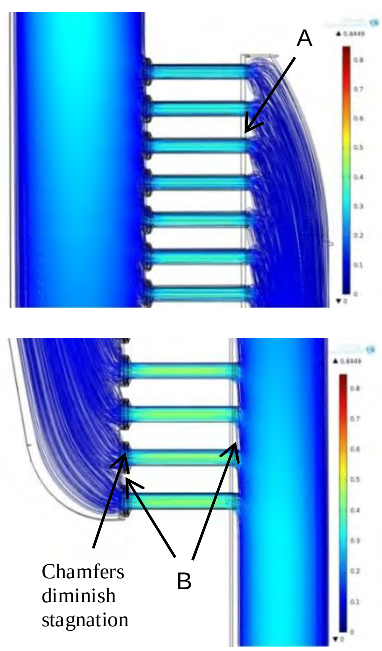

Figure 2.d Tracer curves of the particles trajectory in the LB die.

The presence of stagnation regions and recirculation zones in the LB die leads to detrimental effects in the mechanical strength and the surface appearance of the pipe. This problem is a consequence of longer residence times. The simulation indicated that the surfaces around the boreholes on both the inner and outer walls of the LB were rheologically inadequate. These unwanted regions are the result of the borehole pattern and the inner and outer corners of the basket-mandrel assembly (Figure 2.a). Based on the results of the numerical model, approximately 9% of the polyolefin circulates and experiences limited flow in the problematic regions. The prolonged permanency of the resin in these zero velocity locations leads to manifested degradation of the material. After several hours of continuous production, the polymer chains of HDPE suffer crosslinking, which produces gelation, degredation events [2]. It is necessary to correct the stagnation areas found in the flow channel design. Another aspect of these results reveal that chamfers in the inner wall of the basket can have a positive effect, and diminish stagnation. Chamfers are used in the novel die design presented in this work (Figure 2.d).

To determine an ideal RTD a second simulation with the LB removed was conducted, and by applying the previous method, the velocity gradients, streamline pattern, Poincaré sections, and tracer curves were calculated. The results illustrate recirculation of material in the corners of the mandrels, as shown in Figure 3. In the new model, the inner and outer mandrel profiles were modified (see section 4).

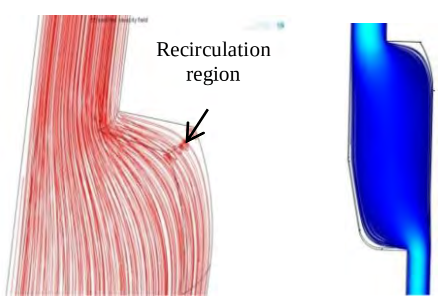

Figure 3 Streamline pattern and traces curves of the die having removed the LB.

The profile shown in Figure 4 is the ideal model and was used as the reference for the analysis of the RTD. The inner and outer corners of the mandrel were rounded based on the tracer curves profile of the die that excludes the LB (Figure 3). The modifications made on the model eliminated the recirculation zone, as depicted in Figure 4.

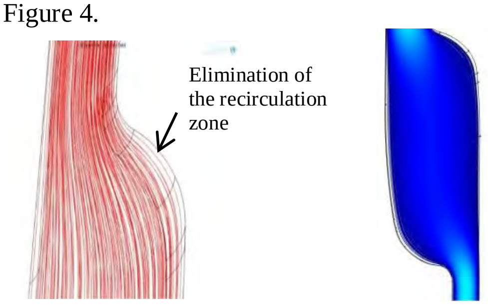

Figure 4 Streamline pattern and traces curves of the ideal model.

4. Novel flow channel profiles.

In the novel design, the borehole pattern was replaced with horizontal slots. The flat surfaces were replaced with chamfers in the inner and outer walls of the basket (Figure 5). This eliminated the non-flow areas and decreased stagnation. With these cavities, recirculation was reduced by 50% using horizontal slots, and 75% using vertical slots (Figure 6 and 7).

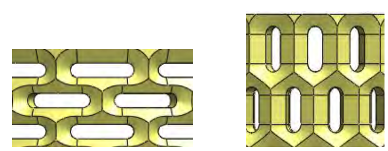

Figure 5 The borehole pattern has been replaced by slots in a horizontal and vertical fashion.

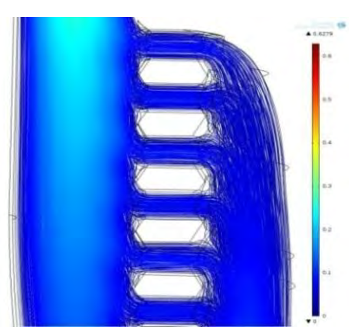

Figure 6 Top section of the tracer curves of the horizontal slots die.

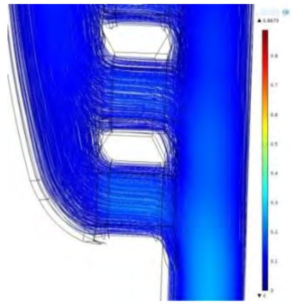

Figure 7 Bottom section of the tracer curves of the vertical slots die.

5. Discussion and Conclusions

Analysis of the results revealed that a lattice basket with a borehole pattern suffers from stagnation and recirculation regions that produce degradation of the resin because of longer residence times. Novel geometry profiles were simulated while seeking substitutes for the boreholes in the lattice basket that would not drastically alter the mechanical design of the die. These substitute boreholes would instead reduce the residence time. After modeling several profiles, a simple yet elegant solution was found. This study introduces the use of vertical and horizontal slots as a suitable, light, and easily machineable geometrical profile that can replace the original borehole.

Figure 8.a and 8.b and Table 2 (see Appendix 1) show the results of the particle tracking analysis and the CRTD for the different models. The horizontal slots model halves the RTD and the vertical slots model shows a reduction of 75% in the RTD of the trapped particles in comparison with the LB. Additionally, the horizontal slots retain 60% less material and the vertical slots retain three times less material than the proprietary boreholes model. Smaller total pressure losses, higher volumetric flow rates, and lower power uses under the same operation conditions are benefits achieved with these reshaped cavity profiles. The simulation allows the analysis of several models without having to cut metal, saving time, resources, and cost consumption.

This research still has room for improvement. The inferior chamfer of the inner wall and the superior chamfer of the outer wall still lack polymer flow (see Figure 6 and 7). However, the profile of the chamfer is based on a real manufacturing process and no perfect profile can be achieved due to technological limitations. Further investigations would improve the shape of the chamfers possibly by using fillets or other reliable geometries, or by considering alternative, non-mechanized manufacturing processes.

Further studies would explore the effect on the surface finish of the pipe due to the reduction of the number of cavities in the novel design (by 16 times in the case of the horizontal slots, and by 4 times in the case of the vertical slots. See Table 3). Additionally, the effect of the increase in the area of the cavities on the surface finish is still poorly understood. The new die and LB must be manufactured in order to evaluate the effect of the design change on the surface finish of the pipe.

One of the limitations of the proposed method is the isothermal assumption. Therefore, the Brinkman number Br, a dimensionless parameter used in polymer processing which relates heat conduction to viscous dissipation can be used. For smaller Br numbers, heat conduction dominates and the model can be considered in an isothermal stage. On the other hand, for larger Br numbers, viscous dissipation dominates and the fluid mechanics model has to be coupled with a heat transfer model. Characteristic values of every model simulated will be evaluated with the Brinkman number to determine whether it is necessary to implement the energy equation in the current simulation.

Current studies include a more rigorous optimization of the vertical slots profile by simulating different size distributions (Figure 9). Additionally, the spiral mandrel die is considered. The spiral mandrel die is conventionally used in the tubing and pipe extrusion of PVC. Early reports for the most basic geometry of the spiral mandrel indicate it is less effective than the vertical and horizontal slots model (Figure 10). However, this does not necessarily exclude the spiral mandrel as a replacement for the old LB model. In order to thoroughly compare the performance of the model proposed in this study with the spiral mandrel model, more simulation profiles for the spiral mandrel model must be generated.

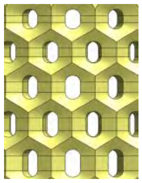

Figure 9 Area of the vertical slots increases as the melt flow goes down.

6. Acknowledgements

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7. References

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9. Appendix

Table 2. Analysis of number of particles released.

$$Transmision\ Probability = \frac{number\ of\ particles\ \ which\ reach\ the\ outlet}{number\ of\ particles\ released}$$

Model	Number of particles released	Particles that reached the outlet	Transmission Probability	Retained particles
Lattice basket die	2000	1852	0.91	148
Die without lattice basket	2000	1929	0.9645	71
Ideal model	2000	1939	0.9695	61
Slots in a horizontal fashion	2000	1911	0.9555	89
Slots in a vertical fashion	2000	1941	0.9705	59
Spiral Mandrel	2000	1543	0.7715	457

Table 3. Ratio of the cavities and surface area.

Geometry	Number of cavities	Total area [mm^2]	Ratio of the cavities	Ratio of areas
Lattice basket	2100	3.00	1.00	1.00
Vertical slots	550	59.63	3.82	19.85
Horizontal slots	126	108.63	16.67	36.16
Spiral mandrel manifold	4	127.68	525.00	42.50

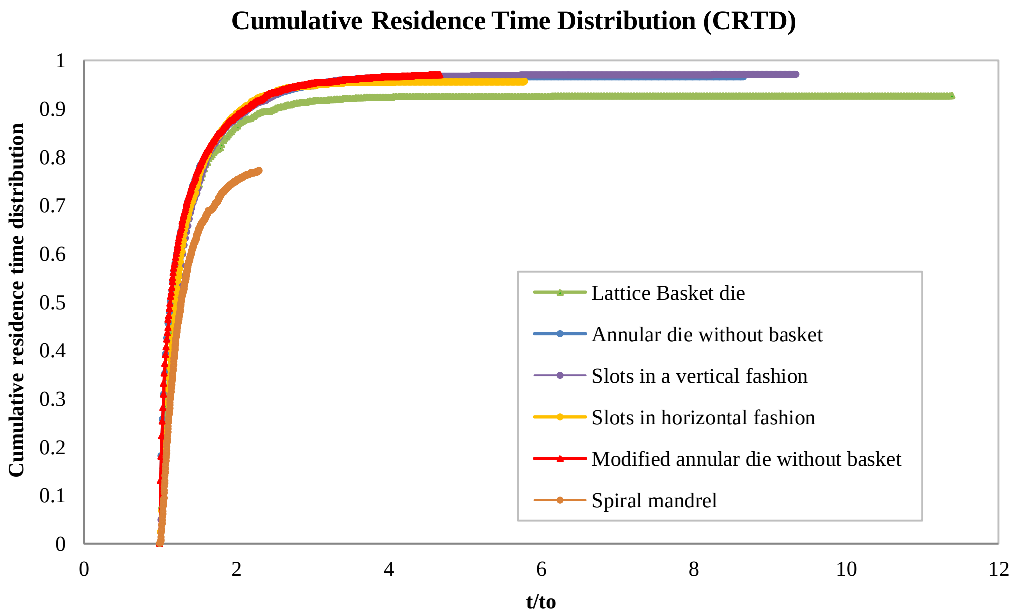

Figure 8.a Cumulative residence time distribution (CRTD).

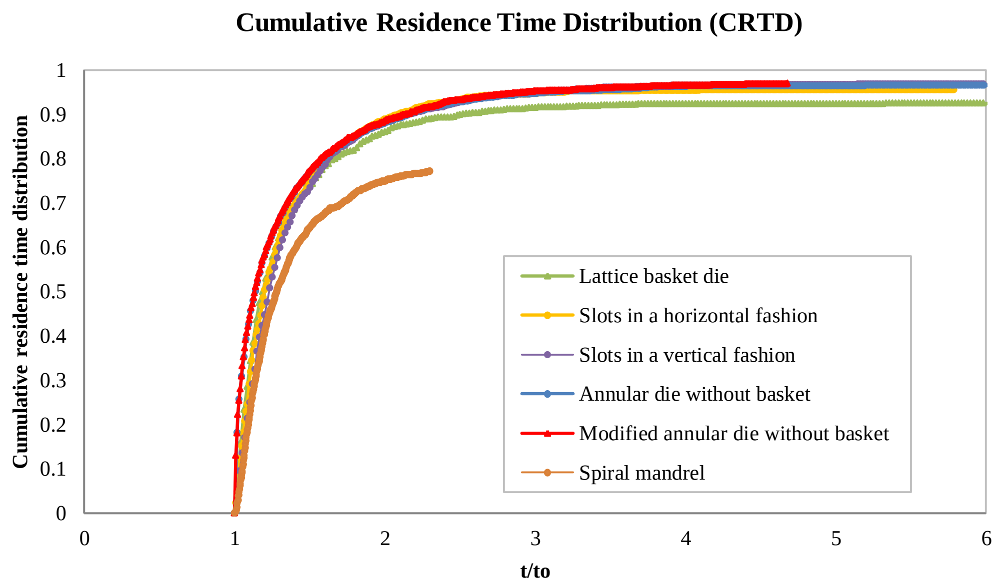

Figure 8.b Cumulative residence time distribution (CRTD).

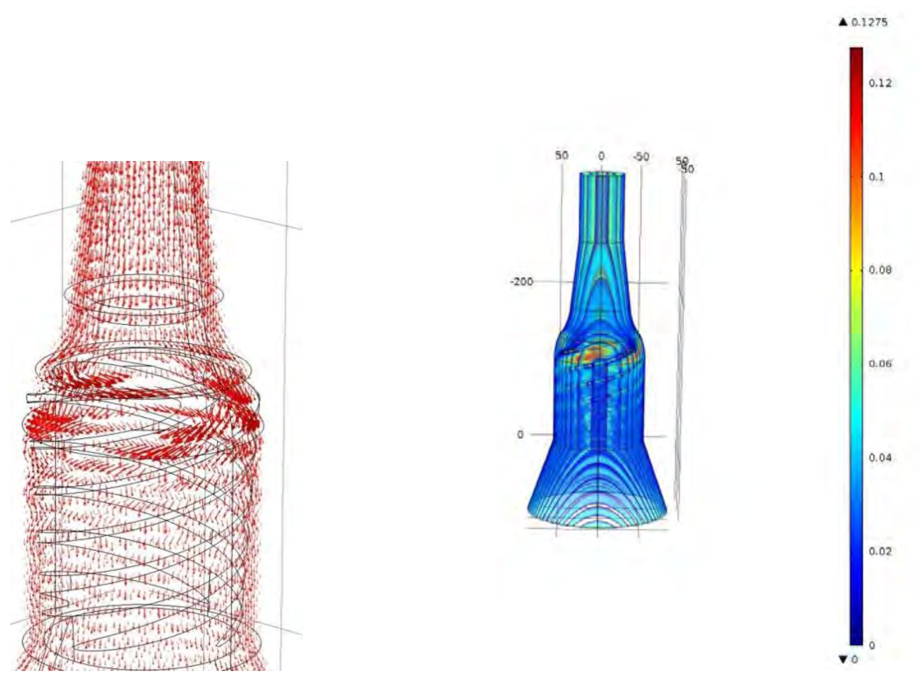

Figure 10. Velocity vectors and tracer curves of the spiral mandrel die with 4 channels. Radial spiral distributors [6]