Influence of initial conditions on distributive mixing in a twin flight single screw extruder

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Running Head: Chaos and Distributive Mixing

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Abstract

Passive advection of light particles carried by a high viscosity fluid in polymer processing equipment exhibits complex behavior due in part to the non-linearity of the equation of motion. The particles motion also exhibits sensitivity to the initial positions. A fundamental understanding of the influence of initial positions of particles on the quality and rate of distributive mixing is essential for the optimization and design of processing equipment.

In this work we analyze a twin-flight single screw extruder. Based on a detailed knowledge of the flow patterns, obtained through 3-D FEM numerical simulations, we study particle motion and implicitly mixing in the extruder. In our model particles are massless points that do not affect the flow field or the motion of other particles.

We visualize the complexity of the advection by using two-dimensional Poincaré-like sections. We then examine quantitatively distributive mixing for different initial locations of the light particles. Renyi entropies for different values of the parameter $\beta$ were calculated and related to the various distributive-mixing characteristics they reveal.

1. Background

Mixing is an important component of most polymer processing operations. Due to the high viscosity of the polymer melt, flows in such systems are characterized by low Reynolds numbers and lack of turbulence. However, as first pointed out by Aref [1, and references therein] advection of light particles in laminar flows can exhibit chaotic features, due to the geometric and operational complexity present in some systems. Advection in polymer processing equipment provides an important example of such a system. Analysis of the chaotic features and their relevance to mixing is needed for a better understanding of how to improve mixing in processing equipment.

Numerical simulations of polymer processing equipment provide an effective means of analyzing the capability of a given machine. There are two types of mixing associated with polymer processing equipment: dispersive mixing and distributive mixing. We restrict this study to distributive mixing. In distributive mixing repeated rearrangement of the minor component enhances system homogeneity by reducing the scale and intensity of segregation of the system.

Chaos exhibits itself through sensitivity to initial conditions [2]. Thus initial positions of the tracers should have a profound effect on distributive mixing that warrants study. We use Poincaré-like sections to identify chaotic flow features in a twin-flight single screw extruder and focus on these regions to analyze the influence of initial conditions on the minor component distribution in the system. We quantify distributive mixing by means of Renyi entropies [3, 4].

2. Procedures and Results

2.1. Numerical simulations:

In this project, we first looked at the flow patterns in a twin-flight, single screw extruder [5]. Three dimensional, isothermal Newtonian flow simulations were performed using FIDAP, a commercial computational fluid dynamics package from Fluent Inc. The physical parameters of the extruder are given in consistent dimensionless length units. The radius of the
barrel was 4.009623, and the radius of the screw was 3.534884, the flight clearance was 0.0096, and the flights were 0.44 thick. The extruder is square pitched, so one pitch corresponds to approximately eight length units. The finite element mesh shown in Figure 1 contains 16200 8-node brick fluid elements, and 8340 4-node quadrilateral boundary elements, for a total of 20535 nodes. At the operating conditions used in the flow simulations (1 revolution of the screw per unit time and a throttle ratio of –1/2), the Reynolds number is less than 1/2. After checking that the inertial terms in the Navier-Stokes equation can be safely neglected at this low Reynolds number, the results presented in this paper were obtained by neglecting the inertial terms, which is equivalent to a zero Reynolds number.

In work previously done by our group[6, 7], an algorithm was developed for tracking massless points that affect neither the flow field nor other particles. We use a coordinate system that rotates with the same angular velocity as the screw, so that one finite element model could be used for all the calculations. We also use a periodic boundary condition to simulate an extruder longer than the finite element model. Due to the no-slip boundary conditions, a particle, which runs into, or overshoots a wall, is considered stuck there and no longer moves.

2.2. Surface sections:

Chaotic features of flow can be qualitatively examined via Poincaré-like surface sections. By converting the 3-D flow field into a 2-D cross-sectional map, the complexity of the system is reduced. In our case we use an axial cross section at the end of each pitch. From the particle tracking algorithm results, the intersection of the particle paths and the selected cross-sections are plotted. The resultant map can be visually inspected for regions of good mixing and poor mixing.

As in our previous work [8], in this project ten identical clusters of 547 particles each were evenly distributed at the entrance cross section of the extruder. They were tracked for sixty revolutions. The intersection between the particle paths and 12 axial cross-sections taken from the end of each of the first twelve pitches is shown in Figure 2. We assume that we continuously inject particles at their initial positions and that the cross-sections are taken from a system at steady-state. Due to symmetry only the top half of the cross sections is shown. There is evidence of a strong attractor at the position indicated by the arrow and the close up view of the region. There is also a weak attractor, which appears to be larger in area because it is slower in condensing the particle concentration within its region of influence. The close up of the weak attractor shows a small void region in the center. There is also a large void region pointed out in the figure, indicative of a repellor. Though we call this regions attractor/repellor because particles are attracted/repelled towards these regions, we do not imply that they are equivalent to strange attractors present in dissipative systems.

These features are discussed in more detail in Ref [8].

2.3. Distributive mixing analysis:

We have demonstrated [3,4] that the Renyi entropies are rigorous and efficient measures of distributive mixing [7]:

$$S(\beta) = \frac{1}{1-\beta} \ln \left( \sum_{j=1}^{M} p_j^\beta \right)$$  

where $p_j$ is the relative frequency of outcome #j with a set of $M$ possible outcomes. The Renyi entropy is a generalization of the Shannon information entropy:

$$S = -\sum_{j=1}^{M} p_j \ln p_j$$  

Equation (1) reduces to Equation (2) in the limit $\beta \rightarrow 1$. For high values of $\beta$, the higher concentrations bins contribute more heavily to the entropy, Equation (1), than the low concentration bins. The parameter $\beta$ signifies the weighting given to the concentration of the minor component in small, localized regions. When $\beta \rightarrow 0$ the Renyi entropy is determined by the distribution of empty bins or void spaces. When $\beta \rightarrow \infty$, the sum in Equation (1) is dominated by the largest probability, thus the entropy in this case is heavily weighting the regions of largest concentration of the minor component in the system. By using different values of the parameter $\beta$, different aspects of mixing quality can be probed.

To normalize the absolute entropy to values between 0 and 1, we use the relative Renyi entropy:

$$S_{\text{relative}}(\beta) = S(\beta)/\ln(M)$$  

The best distributive mixing is achieved when the relative entropy is unity and the worst mixing is achieved when the relative entropy is zero.
To examine the influence of initial positions on distributive mixing we divide each half of the axial cross section into 21 zones, three in the radial direction and 7 in the angular direction. The zones are illustrated in Figure 3. In each zone, we randomly place 4000 particles. These 84,000 particles are tracked for 25 revolutions. Particles are continuously injected into the system at their initial positions and the spatial distributions obtained at the exit of the 3rd pitch are at steady state. In this work we concentrate on the nine zones that cover a chaotic feature.

The relative Renyi entropies are used to analyze the spatial distributions of the particles from each zone. Figure 4 shows the relative Renyi entropies for Renyi parameter values from zero to ten for the nine zones closest to the chaotic features of flow. It is immediately obvious that the relative Renyi entropy for high values of $\beta$ indicates that mixing is worst for zones 5 and 6 (zones nearest the strong attractor). Particles that start near the attractor usually experience very small changes in their relative positions in a 2D cross section, thus inhibiting improvement in their distribution.

It is also interesting to note that the particles from the repellor region (zones 17 and 18) are also poorly distributed after 3 pitches. This suggests that particles from these zones end up mostly in the region of the strong attractor, as also confirmed by the analysis of the spatial distributions.

The zones exhibiting the best distributive mixing are those near the screw (zones 4, 10, and 16), as well as those near the weak attractor (zones 11 and 12). These are the particles that move slower and are in a region that have the greatest circulatory flow. Also particles starting in these zones are less likely to be drawn into the attractor and therefore exhibit the best distributive mixing.

These particular features of particle motion are also observed when we examine the dynamics of distributive mixing using a pulse feed of the particles rather than the steady-state assumption of continuous feeding. In this case we continuously introduce the particles for only 12 revolutions, and then look at the relative Renyi entropy of the spatial distributions after the 3rd pitch, at each time step. 1125 bins are used to calculate the Renyi entropy: 5 bins in the radial direction and 225 bins in the angular direction. Figure 5 shows the evolution of the relative Renyi entropy and the particle count for that axial cross section. Also shown is the ideal relative Renyi entropy as determined from a random distribution of 5470 particles in the axial cross-section.

Prior to the 12th revolution none of the particles have reached yet the end of the 3rd pitch. The system approaches the steady state values for the Renyi entropies around the 23rd-25th revolution. After the 25th revolution the particles begin to leave the cross section, and the relative Renyi entropies for $\beta = 1, 2, 10$ exhibit a jump, whose magnitude increases with $\beta$. This gives a very good indication with regards to the type of particles that leave the cross section first. Since the higher values of the Renyi parameter give more weight to the bins with higher concentrations, the particles that travel the fastest are the ones that are most clustered together. We know from examining the surface section that the region of highest concentration is the attractor. Thus, particles from the attractor leave the cross-section first, improving the overall particle distribution.

This result prompted us to study the rate of distributive mixing in a quantitative manner. We first determined the time evolution of the 3D Renyi entropies for each of the zones. This allows us to examine the dependence of the rate of mixing on initial position. For this analysis 11520 bins were used to calculate the Renyi entropy: 2 bins in the radial direction, 90 bins in the angular direction and 64 bins in the axial direction. To calculate the 3D Renyi entropies, 16000 particles were randomly distributed in each of the 21 zones and tracked for 8 revolutions. The evolution of the 3-D Renyi entropy in two pitches of the extruder for each of the initial zones was followed.

Figure 6 shows the evolution of the Renyi entropy for $\beta=1$ in selected zones. We have demonstrated [8] that the time evolution of the entropy is well described as a logarithmic dependence:

$$S = a \ln(t) + b$$

(4)
The logarithmic coefficient $a$ measures the rate of mixing $a = \frac{dS}{dt}$. We apply the logarithmic fit to these curves. Particles from the repellor region (zones 16,17 and 18) show the best rate of mixing (i.e. largest $a$), while the particles from the strong attractor show the worst rate of mixing (i.e. lowest $a$).

3. Conclusions

Through the use of Poincaré-like surface sections we have identified chaotic features of flow in a twin-flight single screw extruder. We focused on these regions to determine the influence of initial conditions on distributive mixing. The ability of the Renyi entropies to focus on different aspects of distributive mixing allowed for a better understanding of the minor component behavior at different times and spatial positions.
In correlating the chaotic features of flow with the distributive mixing characteristics, it appears that proximity to such features does not necessarily improve mixing. We see this reflected by the jump in the 2D pulse Renyi entropies when the fastest, most clustered particles are not included. The particles starting in the strong attractor region showed a slow rate of mixing and were poorly distributed. The repellor shows the best rate of mixing, but particles starting in the repellor region, have a great chance to be drawn into the strong attractor, resulting in poor distributive mixing. On the other hand, the weak attractor and regions near a strong chaotic feature but not directly on the feature lead to the best distributive mixing in the extruder.

This type of analysis can be performed in order to determine the importance of initial positions on the rate of distributive mixing as well as the final state of distributive mixing. Being able to quantify this influence will help optimize design and operating specifications in single screw extruders. Moreover this work can be extended to other polymer processing equipment.

4. Acknowledgments

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5. References

Figure 1: Finite element model for a twin-flight single screw extruder
Figure 2: Surface section of 65640 points from the axial cross-sections at the end of the first 12 pitches with close-ups of attractors. Shown is only the top half of the surface section.
Figure 3: Location of the 21 Zones
Figure 4: Influence of initial particle positions on distributive mixing characteristics; lines are color-coded based on the initial zone as shown in Figure 3.
Figure 5: Relative Renyi entropies after 3 pitches for 5470 particles with a pulse-feeding period of 12.
Figure 6: Evolution of Shannon entropy for the 16000 tracers per zone for each of the nine zones closest to the chaotic features of flow; the data is color-coded based on the initial zones as shown in Figure 3.

\[ f(4) = 0.4746 \ln(t) + 4.3189 \quad R^2 = 0.7940 \]
\[ f(5) = 0.3261 \ln(t) + 3.4108 \quad R^2 = 0.7490 \]
\[ f(6) = 0.4180 \ln(t) + 3.9906 \quad R^2 = 0.9109 \]
\[ f(10) = 0.5846 \ln(t) + 4.3045 \quad R^2 = 0.9011 \]
\[ f(11) = 0.5981 \ln(t) + 3.8349 \quad R^2 = 0.9087 \]
\[ f(12) = 0.7224 \ln(t) + 4.1313 \quad R^2 = 0.9517 \]
\[ f(16) = 0.7202 \ln(t) + 4.3066 \quad R^2 = 0.9421 \]
\[ f(17) = 0.7247 \ln(t) + 4.1366 \quad R^2 = 0.9620 \]
\[ f(18) = 0.8853 \ln(t) + 4.2986 \quad R^2 = 0.9820 \]