Experiments on Chaotic Mixing in a Screw Channel Flow

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Mixing patterns of a passive dye were investigated experimentally in an unwound screw channel flow with periodic barriers that serve to induce a chaotic flow. Continuous cross-sectional and longitudinal mixing patterns were observed as a function of the barrier fraction and were interpreted in terms of dynamical systems theory, along with 3-D numerical simulations. Observations include: periodically invariant cross-sectional mixing patterns due to the resonance bands; pile-up of dye streaks caused by stretching and folding of manifolds near hyperbolic points; unmixed zones due to KAM tori; longitudinal deformation patterns with exit time distributions; and effects of the barrier fraction on the size of unmixed islands, the thickness of the band of dye streaks, and the distribution of exit times.

Introduction

Mixing enhancement in single-screw extruders has been an important research target for many decades, on account of the poor mixing capability caused by regular fluid motions. Since the work of Aref (1984), mixing by chaos has been undoubtedly accepted as the best method for laminar flows under the Stokes regime. The first application of chaotic mixing to the single-screw extrusion process was attempted by Jana et al. (1994). Their analyses and experiments were restricted to 2-D time-periodic flows. However, they indicated that their concept could be extended to 3-D single-screw extruders by introducing spatially periodic changes in the screw geometry. Following this idea, a single screw capable of generating chaotic flow was proposed by Tjahjadi and Foster (1996). Independently, Kim and Kwon (1995, 1996) suggested a new screw design with spatially periodic barriers and named it the chaos screw (CS).

In the language of the dynamical systems, the flow in a single screw with spatially periodic geometrical changes belongs to the regular duct flow class with translational symmetry (Kusch and Ottino, 1992; Mezić and Wiggins, 1994). The flow preserves volume in the 3-D physical space and has an inlet and outlet, while other boundaries remain bounded. Theoretical bases such as the canonical description are rather recent and only a handful of references are available for this class of flows (Bajer, 1994; Mezić and Wiggins, 1994). The first relevant work is the study of the partitioned-pipe mixer (PPM) done by Khakhar et al. (1987). Kusch and Ottino (1992) presented experimental investigations in the PPM, as well as in the eccentric helical annular mixer (EHAM). They indicated that mixing in a regular duct flow could be greatly enhanced either by time-periodic cross-sectional flow (in the case of EHAM) or by spatially periodic cross-sectional flow (in the case of PPM). Jones et al. (1989) studied flows in a twisted pipe by introducing area-preserving Hamiltonian transformation. Fountain et al. (1998) performed detailed experiments for a stirred tank flow, visualizing regular structures such as resonance bands and KAM (Kolmogorov-Arnold-Moser) tori. Recently, using the same apparatus, Fountain et al. (2000) experimentally showed that the frequency ratio determines the configuration of the resonance bands and the KAM tori in the perturbed system. It should be pointed out, however, that this flow does not belong to the regular duct flow class, but that its dynamical system representation is similar to the regular duct flows (Mezić and Wiggins, 1994). Hwang and Kwon (2000) presented a dynamical systems modeling of the CS system and numerically showed that chaotic regions increase with the strength of the perturbation and that the configuration of unmixed islands in the resonance band is determined by the frequency ratio.

The objectives of this study are to visualize the 3-D experimental mixing patterns in the CS screw channel flow and to interpret the underlying mixing mechanisms in terms of the dynamical systems theory along with 3-D numerical simula-

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tions. The CS system and the experimental setup for the CS channel flow is described. Experimental observations are presented such as manifold pile-up around a homoclinic orbit, unmixed island, periodically invariant mixing patterns, and longitudinal mixing patterns, together with their dependencies on the strength of perturbation. An attempt is made to interpret the experimental observations by comparing them with numerical results of the Poincaré sections, deformation patterns, and the exit time distributions.

System

Chaos screw (CS)

The CS is composed of periodic barriers inserted on the metering section of the regular screw. The basic concept behind the CS system is that, by alternating barriers, fluid elements experience a combination of two different flow fields (Kim and Kwon, 1996). Figure 1 shows the unwound screw channel of CS and one of the periodic units. We denote the length of the barrier zone by \(a\), the length of the no-barrier zone by \(b\), the length of the periodic unit \((a + b)\) by \(L\), the height of the flight by \(H\), the height of the barrier by \(h\), the width of the barrier by \(c\), and the width of the channel by \(W\). The drag velocity is denoted by \(V_d\) with the associated helix angle \(\alpha\). The coordinate system is chosen as follows: \(x\) is along the width direction, \(y\) along the screw depth, and \(z\) along the longitudinal direction from hopper to die. The \(xy\) plane is denoted by the cross-sectional plane and the \(z\) axis is along the longitudinal direction throughout this study.

As indicated in the authors’ previous work (Hwang and Kwon 2000), the fraction of the no-barrier zone can be regarded as the geometric perturbation \(\beta\), that is

\[
\beta = \frac{b}{L}
\]  

(1)

which is limited and smaller than the fraction of the barrier zone \(a/L\), \(\beta \leq 0.4\) throughout the study. In this setting, the unperturbed system \((\beta = 0)\) is the full barrier system. The unperturbed velocity field is independent of the longitudinal coordinate \(z\) and the cross-sectional streamlines corresponding to this case are presented in Figure 2. The shape of streamlines resembles the phase portrait of the well-known Duffing equation with no damping and with the negative elastic stiffness (Guckenheimer and Holmes, 1983). There are two homoclinic orbits intersecting at the hyperbolic fixed point and two symmetric families of nonlinear elliptic rotations around the elliptic fixed point. (The dashed curve in Figure 2 indicates the homoclinic orbit.) Therefore, one might expect the dynamics of the perturbed CS system to follow the well-known routes to chaos, such as perturbation of the ho-
moclinic orbit, and creation/destruction of resonant and invariant orbits.

**Experimental setup**

The experimental apparatus was designed and built in order to visualize 3-D mixing patterns in the CS channel flow. Figure 3 shows the experimental setup. The apparatus is composed of three major parts: (a) a transparent grooved channel with core barrier parts and a motor-driven oblique slider; (b) two fluid reservoirs, a valve and a drain system; and (c) two CCD cameras and an image grabbing system. Below, we describe each component in detail.

**Transparent Grooved Channel with Core Barrier Parts and Motor-Driven Oblique Slider.** The unwound CS channel (Figure 1) is made of transparent acrylic plate, and it has a long slot in the longitudinal direction. The slot is for installation of the core barrier part which contains the barrier configuration. The \( \beta \) values used in this experiment are 0 (unperturbed), 0.1, 0.15, 0.2, 0.3, 0.4, and 1 (the conventional screw case). In all cases, each core barrier part has 30 periodic units. The geometrical dimensions of the channel and the barrier are listed in Table 1. The ratio of the channel width to the longitudinal period \( W/L \) is selected to attain many periods in the limited length of this apparatus. The channel is inverted upside down and tightly fastened on the rubber pad to minimize leakage flows from the gap between the flight and the moving slider. The slider is driven by an AC motor with a velocity control unit. The drag velocity was \( 7.365 \times 10^{-2} \) m/s and the helix angle was selected as \( \theta = 69^\circ \) to have sufficient helical turns in the limited length.

**Reservoirs, Drain, and Valve System.** It is essential to keep the flow rate constant during the experiment to achieve steady velocity fields. For this reason, we adopted a system composed of two reservoirs (denoted by 1 and 2), a drain and a valve, as indicated in Figure 3. The valve controls the flow rate between the two reservoirs. The drain in the reservoir 2 keeps the pressure head at the inlet constant.

**CCD Cameras and Image Grabbing System.** To observe 3-D mixing patterns, two CCD cameras have been fitted up. CCD1 is for observing the cross-sectional mixing patterns, and CCD2 is for the longitudinal patterns. A camera lane for the CCD2 has been arranged right above the channel. The experimental images were captured by the image grabber (SASEM Co., Korea) at the rate of 15 frames per second and stored as 640×480 pixel digital images.

Silicone oil (Shinetsu Co., Japan), a highly viscous Newtonian fluid, was used for the working fluid. The viscosity \( \mu \) and the density \( \rho \) are 0.974 (Pa·s) and 0.967×10^{-3} (kg/m^3), respectively. The dye material is the blue-colored 1,000cs silicone oil (KE BL70) of the same company. The size of the

**Table 1. Channel Dimensions in the Experimental Apparatus \((\times 10^{-2} \text{ m})\)**

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height of flight, ( H )</td>
<td>2</td>
</tr>
<tr>
<td>Height of barrier, ( h )</td>
<td>1.36</td>
</tr>
<tr>
<td>Length of period, ( L )</td>
<td>4</td>
</tr>
<tr>
<td>Total length of channel</td>
<td>150</td>
</tr>
<tr>
<td>Width of channel, ( W )</td>
<td>8</td>
</tr>
<tr>
<td>Width of barrier, ( c )</td>
<td>0.2</td>
</tr>
</tbody>
</table>

**Figure 3. Experimental apparatus.**
colored powder (CoAlO₃) is approximately 20 μm; the diffusion coefficient $D$ is estimated as $1.1 \times 10^{-17}$ (m²/sec). The density of the dye material is considered to be the same as the working fluid; the diluted dye immersed in the beaker of the silicone oil neither sinks nor rises within an hour. The dilute dye fluid is injected with a syringe needle through a small hole, which is located near the center of the channel in the longitudinal direction (Figure 3) and is filled with an elastic silicone sealant to close the hole automatically right after removal of the needle.

With the characteristic velocity $V_d$ and the characteristic length scale $H$, the Peclet number and the Reynolds number in the experiment can be evaluated as follows

$$Pe = \frac{V_d H}{D} = 1.3 \times 10^{14}, \quad Re = \frac{\rho V_d H}{\mu} = 1.462 \quad (2)$$

The quite large value of the Peclet number guarantees the insignificant effect of dye diffusion in this experiment. A Reynolds number of $O(1)$ has come to be known as the best compromise between minimizing dye diffusion in the time scale of the experiment (short experiment preferable) and minimizing inertial effects (long time scale preferred) (Chien et al., 1986; Leong and Ottino, 1989).

It is important to mention a limitation of the experimental device. The most significant difficulty is leakage between channel and slider. Since the long channel is inverted upside down and the bottom part of it contacts with the moving slider, some amount of leakage is inevitable. We lined the slider on rubber pads and tightened up the channel on the frame. However, we have observed that, in case of the unperturbed channel (the worst case), the experimentally obtained velocity at the center of the rotation can be reduced by 8% during dye fluids’ forward movement of the two longitudinal periods (for 11 s in time). This leakage indicates that care should be exercised in comparing the experimental results to the numerical analyses.

**Experimental Results**

**Mixing patterns**

Experimental mixing patterns are presented for three representative cases: regular screw channel flow, unperturbed CS channel flow ($\beta = 0$), and perturbed CS channel flow with $\beta = 0.1$.

The cross-sectional and longitudinal mixing patterns in the regular screw channel flow are presented in Figure 4. The initial dye configuration, shown in Figure 4a, is approximately the same for all experiments in this study. (Therefore, we will not indicate the initial dye configuration for the remaining cases.) The bold arrows indicate the drag directions. The cross-sectional mixing patterns after 20 s (Figure 4b) and after 40 s (Figure 4c) reveal the lamellar structure bounded by the stream surfaces. From dynamical systems viewpoint, this is an integrable system and each stream surface plays a role of constant of the motion in order that a material point initially located on a stream surface always resides on the surface. As a result, the mixing performance of this case is poor. The corresponding longitudinal mixing patterns are also regular; particles in the inner region move faster than those in the outer region. The exit time of a particle is completely determined by the initial stream surface. In practical terms this may cause thermal degradation of polymeric materials in real single-screw extruders.

The mixing patterns after 20 s and after 40 s in the unperturbed CS channel flow ($\beta = 0$) are presented in Figures 5a and 5b, respectively. As mentioned previously, the motion of a particle in this case is also regular and integrable. There are one hyperbolic and two elliptic points in the cross-sectional streamline (Figure 2), rather than just one elliptic fixed point as in the case of the regular channel flow. The cross-sectional mixing patterns in both figures clearly show the eyeball-type structure presented in Figure 2. A small portion of the dye that is initially located outside the homoclinic surface can travel between the right half and the left half. However, a majority of the dye initially located inside the homoclinic surface in the left half simply rotates, centered at the elliptic fixed point. In this regard, the boundary between the empty...
region and the thin dye streak in the right half of the cross section may be considered to represent the homoclinic orbit. The longitudinal mixing patterns, though they look quite complicated, can be explained in the same way. The regular cluster in the right half indicates the collection of dye materials initially located inside the homoclinic surface; it cannot escape from inside. Many thin dye streaks over the whole longitudinal section represent the deformation patterns of the dye materials that were initially located outside the homoclinic surface.

Figures 6a and 6b indicate the mixing patterns in the perturbed CS channel flow with $\beta = 0.1$ after 20 s and after 40 s, respectively. According to the authors’ previous work (Hwang and Kwon, 2000), the region around the homoclinic orbit becomes chaotic and the elliptically rotating region becomes either resonance bands or KAM tori, depending upon frequency ratios. From the cross-sectional mixing patterns in Figure 6, one can find that the band of dye streaks around the homoclinic orbit is thicker than that in the unperturbed case, resulting in a smaller empty region in the right half. The thick band of dye streaks is the consequence of the stretching and folding of the unstable manifolds around the homoclinic orbit, which is a typical characteristic of chaos. The associated mechanism will be presented in the next section. The empty region in the right half is formed either by the existence of KAM tori or of resonance bands. With these short-time experimental mixing patterns, one cannot distinguish one from the other, because the resonance band may play a role of complete barrier for the material transport as well. (From now on, we call this region the unmixed island) In addition, by symmetry, an unmixed island must be present in the left half of the channel. One can observe that some portion of the dye materials initially located at the left half is trapped in this unmixed zone. In the longitudinal mixing patterns, dye materials are more evenly distributed than those in the unperturbed case, but the existing unmixed island still forms a cluster in the right half.

Periodic structure

The resonance band is a representative periodic structure and forms a banded region in the cross section (an annulus in 3-D). In a finite-time finite-period experiment, most of the orbits in this structure might be considered to have the same time (and spatial) period. Therefore, one may expect to observe periodic mixing patterns near the resonance band. This is exactly what we were able to observe experimentally as described below.

Figure 7 shows the ten cross-sectional mixing patterns for the case of $\beta = 0.025$. Each pattern was captured at the time when some portion of the mixing pattern around the elliptically rotating region becomes almost identical. Figure 8 shows the time interval between each frame of those similar patterns and one can recognize that the mixing patterns in Fig-
Figure 9. Consecutive cross-sectional mixing patterns in the unperturbed CS channel flow. They indicate a typical nonlinear rotation (a) \( t = 19 + 1/15 \) s; (b) \( 23 + 12/15 \) s; (c) \( 28 + 8/15 \) s; (d) \( 33 + 5/15 \) s.

Figure 10. Consecutive longitudinal mixing patterns corresponding to the case \( \beta = 0.025 \). (a) \( t = 19 + 1/15 \) s; (b) \( 21 + 6/15 \) s; (c) \( 23 + 12/15 \) s.

Figure 11. Cross-sectional mixing patterns for various values of the perturbation \( \beta \) (t = 30 s). (a) \( \beta = 0 \) (unperturbed); (b) 0.1; (c) 0.15; (d) 0.2; (e) 0.3; (f) 0.4.

Figure 12. Longitudinal mixing patterns for various values of the perturbation \( \beta \) (t = 30 s). (a) \( \beta = 0 \) (unperturbed); (b) 0.1; (c) 0.15; (d) 0.2; (e) 0.3; (f) 0.4.

The average distance traveled during one period was found to be \( 2 \times 10^{-2} \) m, that is, the periodic structure rotates twice during one longitudinal period \( L \) \( (4 \times 10^{-2} \) m). The corresponding resonance band would be period 1/2 and the corresponding frequency ratio would be 2.

**Effects of perturbation strength**

One can expect that the larger the \( \beta \) value is, the larger the chaotic region and the smaller the unmixed zone will be. Cross-sectional and longitudinal mixing patterns after 30 s for six different \( \beta \) values are presented in Figures 11 and 12, respectively. It may be noted that a portion of the dye materials initially located at the left half is trapped in the unmixed zone on the left half and that the rest of them spread over the chaotic region. They are prevented from penetrating the unmixed zone in the right half. Therefore, the size of the
unmixed zone in the right half may roughly represent the size of either the KAM or the resonance band.

The observations as \( \beta \) increases are summarized as follows:

(a) The maximum height \( h_y \) (Figure 11c), representing the size of the unmixed zone, is plotted as a function of \( \beta \) in Figure 13. Obviously the size of the unmixed zone decreases.

(b) The band of dye streaks around the homoclinic orbit, representing the chaotic region, becomes thicker as shown in Figure 11. The relative thickness of the chaotic region can be estimated by \((1 - h_y/H)\) as a function of \( \beta \) from Figure 13.

(c) The longitudinal distribution of mixing patterns becomes random (Figure 12). The motion of a particle in the chaotic region is essentially random in nature. Particles in this region wander around inside the region, experiencing a random exposure to the longitudinal velocity. As a result, while the chaotic region becomes wider in the cross-sectional mixing patterns, material points cover a larger area in the longitudinal mixing pattern as well.

**Numerical Study and Discussion**

Numerical simulations have been carried out using 3-D finite-element analysis of the Stokes flow and the particle tracing technique. As mentioned earlier, the experimental apparatus suffers from inevitable leaking, so the experimental flow rate cannot be used with full confidence to determine the pressure gradient in the \( z \) direction \((\partial p/\partial z)\). We assume that \( \partial p/\partial z \) is zero so that the numerical results are used only in qualitative comparisons. (Our experience reveals that overall dynamic behaviors do not change significantly by varying \( \partial p/\partial z \) (Hwang, 2001).) The boundary conditions, the material properties, and the channel dimensions correspond to those in the experimental study.

A full 3-D finite-element analysis is used to solve the velocity field (Gupta and Kwon, 1990; Hwang and Kwon, 2000). Since it is difficult to solve the velocity field with multiple barriers, the analysis has been done with only one periodic unit, from the center of one barrier zone to the center of the next one (Figure 1). The inlet and outlet boundary conditions are specified by the unperturbed channel flow solution. Therefore, our numerical results are restricted to small \( \beta \) values cases (less than 0.2). In solving the unperturbed velocity field, the \( x \)- and \( z \)-directional drag flows are evaluated separately and then the solutions are superposed using the helix angle \( \alpha \). An example of the finite-element mesh is shown in Figure 14.

Figure 15a shows the distribution of frequency ratios with respect to \( y \) at \( x = x_c \) in the unperturbed channel flow case \((x_c = 2.0635 \times 10^{-2} \text{ m}, \text{ the } x \text{ value of the elliptic fixed point in the right half})\). The frequency ratio is the number of the cross-sectional rotations during one longitudinal period traveled by an orbit, and it is a function of the stream surface (Dombre et al., 1986; Hwang and Kwon, 2000; Fountain et al., 2000). The ratios become zero around \( y = 0.5 \) and \( y = 1.9 \) where the homoclinic orbit coincides (that is, the period of the cross-sectional rotation is infinity). The ratio inside the homoclinic orbit varies continuously from 0.8 to 1.1, indicating the nonlinear elliptic rotation inside the homoclinic orbit. The continuously varying time-period distribution of the cross-sectional rotations inside the homoclinic orbit is also indicated in Figure 15b. Within the nonlinear rotation in the unperturbed case, one shall not observe the periodically invariant patterns, as mentioned earlier.

Figure 16 shows cross-sectional mixing patterns corresponding to the case \( \beta = 0.025 \). The initial points (Figure 16a) were arranged to resemble the initial dye configuration in the experiment. The numerical integration was performed with increments \( \Delta z = 0.1 \), using the fourth-order Runge-Kutta method. During integration, the intermediate points are inserted as needed to obtain smooth mixing patterns. The material lines in the elliptic rotation region rotate and deform slightly, as mentioned in the experimental section. On the other hand, the initial points located near the homoclinic orbit deform significantly and make a tangled structure. The deformed patterns in this region represent the perturbed unstable manifold associated with the perturbed homoclinic orbit. Figure 17 shows a magnified region of the square in Figure 16d and demonstrates the manifold pile-up near the hyperbolic cycle, caused by stretching and folding of the unstab-
ble manifold. The experimentally observed “thick” band of dye streaks around the homoclinic orbit is formed in this manner. The tangled structure is a typical signature of chaos (Wiggins, 1990). It is evident that, as $\beta$ increases, the tangled region becomes larger due to the larger stretching and folding of the unstable manifold (Refer to Hwang (2001) for the configuration of unstable manifolds with increasing $\beta$.) As a result, the thickness of dye streaks in the experimental observation (Figure 11) increases also with $\beta$. For the cases of $\beta$ larger than 0.1, material points occasionally pass through the small nonbarrier zone between two adjacent barriers, causing numerical troubles in obtaining smooth mixing patterns.

Three consecutive cross-sectional deformation patterns at $z = 0.02$ m (dotted), 0.06 m (solid), and 0.1 m (dashed), all at the center of the no-barrier zones, are presented in Figure 18 together with the corresponding Poincaré section evaluating at the center of the no-barrier zone. The Poincaré section was obtained by integrating 72 equally distributed initial points for 150 periods. There are resonance bands of period-1 (outside the largest KAM torus) and of period-10 (inside the largest KAM torus) in the Poincaré section, as expected from the distribution of frequency ratios (Figure 15a). In the right half of Figure 18, the three deformation patterns intersect one another at the period-1 resonance band. (These common areas are denoted A and B.) This illustrates how the periodically invariant patterns in Figure 7 are formed. In the period-10 resonance band, one can observe that the deformation patterns jump from one elliptic point to the neighboring one in the counterclockwise direction, since the associated frequency ratio is 9/10.
The Poincaré sections at the center of the barrier zone are shown in Figure 19 for $\beta = 0.1$ and 0.2. (We present only the right half due to symmetry.) The chaotic region is found to increase with $\beta$, whereas the regular regions, such as resonance bands and KAM tori, shrink. Figures 20a and 20b roughly show the distributions of the exit time after 15 periods for those two cases corresponding to Figures 19a and 19b, respectively. The exit time was indicated at the initial cross-sectional location of the point. Comparing Figures 19 and 20, it is apparent that the exit times in the chaotic region are quite random, because the material point wanders over the chaotic region, experiencing random longitudinal velocities. On the other hand, one can observe that the neighboring region of the KAM torus and the resonance band shows nearly the regular exit time distribution. From these numerical observations, one can easily expect to have a larger spread in the longitudinal mixing patterns with larger $\beta$, which is confirmed by the experimental observations in Figure 12.

Conclusion

An experimental apparatus has been built to observe both continuous cross-sectional and longitudinal mixing patterns in a modified extruder flow capable of generating chaotic mixing. Experimental mixing patterns have been compared with numerical simulations. Experimental observations, interpreted in the context of dynamical systems, are summarized as follows: (a) Periodically invariant mixing patterns were observed and, with the aid of numerical Poincaré sections and deformation patterns, were found to be related to the existence of resonance bands. (b) The thickness of the band of dye streaks around the homoclinic orbit—the results of the manifold pile-up as observed in the numerical deformation patterns—was observed to increase with the geometric perturbation $\beta$ and it corresponds to the chaotic region. (c) Un-
mixed zones, due to the existence of KAM tori or resonance bands, were identified either by empty zones or by material trapping. The size of the regions was found experimentally to decrease with $\beta$, and was also confirmed by numerical Poincaré sections. (d) Longitudinal distributions of experimental deformation patterns were found to be closely related to the cross-sectional dynamical structures. The unmixed zone and the chaotic zone in the cross-sectional patterns correspond to the regular cluster and the randomly distributed particles in the longitudinal mixing patterns, respectively, which was confirmed by numerically obtained Poincaré sections and the exit time distributions.

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Literature Cited