1 INTRODUCTION

Mixing enhancement has a major influence on the chemical or mechanical properties and the integrity of plastic products. It is more crucial to the single-screw extrusion process, since its lack of mixing performance compared with the twin-screw extruder impedes widespread applications regardless of the single-screw process’s superiority in power consumption, cost, maintenance, etc. Therefore, many researchers have tried to improve the mixing capability of the single-screw extrusion process in many ways—cavity transfer mixer (CTM), Twente mixing ring (TMR), pin-barrel extruder and a number of different types of pin mixers, for example (1).

From the mid-1980s, however, a new science has explored dynamics and kinematics of mixing. This is chaos. There is only one possible mode of fluid flow in the polymeric flows—laminar flows, which will not lead to the intriguing random motions of turbulence. The only way to make the polymeric flows random is to give rise to chaos in the system. Aref (2), Wiggins (3), Ottino (4), and other pioneers have discovered these chaotic transport problems. They presented a large number of examples and investigated nonlinear dynamics and chaos in the systems—flow in two eccentric cylinders, two-dimensional time periodic cavity flow, pulsatile flow in a wavy channel, flow in a partitioned pipe mixer, etc. (4)

In 1994, Kim and Kwon found that mixing in a single-screw extrusion process can be enhanced by inserting periodic barriers in the screw channel and named it Chaos Screw (CS). They carried out numerical and experimental studies, and showed the amazing mixing enhancement performances (5, 6). The recent investigation also shows that the domain-averaged Liapunov exponent in CS is positive, indicating the flow in CS is chaotic [Lee and Kwon (7)]. Furthermore, remarkable features of CS are the simple geometry and the facility in machining, installation and maintenance compared with the previously suggested screws. However, their understanding of the chaotic mixing mechanism in CS was not complete in the sense that the route to chaos was not fully exploited. Rigorous understanding of the chaotic mixing mechanism could be a milestone in designing more efficient CS. Anyway, CS is regarded as the first practical application of chaotic mixing to the single-screw extrusion process (8).

In this study, we describe the dynamical modeling of CS in the context of nonlinear dynamics and chaos. We first construct the unperturbed system, which is an only-barrier screw system. Then, we introduce the...
periodic no-barrier zone as a perturbation. The perturbed system shows the universal features of chaotic transport phenomena such as the resonance bands, homoclinic tangles, KAM tori, etc. From the full three-dimensional numerical simulation of non-Newtonian fluid flows, we will explain the route to chaos in CS and discuss the universal phenomena of chaos accompanied to CS.

2 BASIC CONCEPTS OF CHAOS SCREW

In this section, we briefly introduce the basic concepts of CS (5, 6). Figure 1 shows the schematic diagram of an unwound channel of CS along the flow direction with periodic insertions of barriers. Suppose we imagine that the screw channel is composed of an only-no-barrier zone like a conventional screw, then a fluid particle moves on a closed streamline in the xy plane (two-dimensional manifold in the xyz space) as shown in Fig. 2(a). On the other hand, if the screw channel consists of only-barrier zones, then the fluid particles will move along different patterns of the streamlines as shown in Fig. 2(b). Neither of the two cases is expected to improve mixing performance, since the existing closed curves prevent transports between the neighboring regions. If the two modules are present in turn, however, the trajectories will be very complicated, and hence, we expect a drastic enhancement of the mixing performance. This is the basic concept of CS (5). The apparent geometric design variables are the length of barrier zone (A zone) a, the length of no-barrier zone (B zone) b, the total length L (= a + b), the height of barrier h, the height of flight H, the helical angle α and the parameters for the flow conditions are the drag velocity (screw rotation speed) Vd and the adverse pressure gradient dp/dz, etc.

3 PHYSICAL MODELING

The flow domain and the boundary conditions are shown in Fig. 3. We restrict our analysis to the metering section of the single-screw extruder. Ignoring the inertial and the gravitational forces, the system can be considered as the incompressible isothermal flow of non-Newtonian fluids. The continuity and the momentum equations are

\[
\nabla \cdot \mathbf{v} = 0 \tag{1}
\]

\[
\nabla \cdot \sigma = 0 \tag{2}
\]

The constitutive equation adopted in the present study is the generalized Newtonian fluid model.

\[
\sigma = 2\mu \varepsilon - p\mathbf{I} \tag{3}
\]

Then, the momentum equation becomes

\[
\nabla \cdot (2\mu \varepsilon) - \nabla p = 0 \tag{4}
\]
where the velocity \( \mathbf{v}(u,v,w) \in \mathbb{R}^3 \), the rate of deformation tensor \( \varepsilon = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T) \), the kinematic viscosity \( \mu = \mu(\dot{\gamma}) \) with the effective shear rate \( \dot{\gamma} = \sqrt{2\varepsilon : \varepsilon} \).

For later usage in the analysis of the unperturbed system, we consider a special case where further simplification is possible with the constant cross section along the down-channel direction (z-direction). In this case, the \( xy \)-plane cross-sectional motions can be decoupled with the z-directional motions except for the shear rate effect on the viscosity. This is very important, since these simplifications enable us to construct the integrable structure in the dynamical modeling as will be described in the next section. The continuity and the momentum equations for the \( xy \)-plane motions are

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{5}
\]

\[
\frac{\partial p}{\partial x} = 2 \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \tag{6}
\]

\[
\frac{\partial p}{\partial y} = \frac{\partial}{\partial x} \left( \mu \frac{\partial v}{\partial y} \right) \right] + 2 \frac{\partial}{\partial y} \left( \mu \frac{\partial v}{\partial y} \right) \tag{7}
\]

and for the z-directional motions,

\[
\frac{\partial w}{\partial z} = 0 \tag{8}
\]

\[
\frac{\partial p}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial w}{\partial y} \right) \tag{9}
\]

Note that the above decoupled sets of equations are for the flow in the uniform cross section along the z direction, that is, for either the only-no-barrier or the only-barrier screw channels. We have special interest in the only-barrier case, since it constitutes the unperturbed system for the dynamical modeling of CS.

**4 DYNAMICAL MODELING**

We start from the construction of the unperturbed system. The unperturbed system is the only-barrier case. If the CS system consists of the infinite number of A zones (barrier zone) successively, i.e. periodically, the distributive mixing characteristics of the passive

---

**Fig. 2.** The streamlines in \( xy \) plane. (a) when the CS consists of successive non-barrier zones (B zones); (b) when the CS consists of successive barrier zones (A zones).

**Fig. 3.** The flow domain of interest and the boundary conditions of CS.
Scalars in the CS can be described by integrating the following evolution equation with an initial condition $x_0$ (3).

$$\dot{x} = v(x; y)$$  \hspace{1cm} (10)

where $x(xyz) \in R^3$. We denote the solution of Eqs 5–9 by $v$ in Eq 10. We call the above system the unperturbed (or integrable) system. The $xy$ cross-sectional view of the solution of Eq 10 has already been shown in Fig. 2(b).

Before discussing the details of the dynamical modeling of CS system further, it would be nice to check the analogy of the unperturbed system to the Hamiltonian system. Since the system is autonomous, there exists a stream function that satisfies the following relationships.

$$u(x,y) = \frac{\partial \Psi(x,y)}{\partial y}$$  \hspace{1cm} (11)

$$v(x,y) = -\frac{\partial \Psi(x,y)}{\partial x}$$  \hspace{1cm} (12)

The stream function $\Psi$ has the same mathematical structure as the Hamiltonian $H$. Therefore, the unperturbed system is Hamiltonian. A one-dimensional Hamiltonian system is integrable, that is, the motion with a given initial condition satisfies a constant of motion—the stream function $\Psi$ (3).

The periodically inserted B zone (no-barrier zone) is regarded as the periodic perturbation in our modeling. In this case, we have the evolution equation with a parameter $\beta$ as follows.

$$\dot{x} = v(x; \beta)$$  \hspace{1cm} (13)

Note that the solution of the above evolution equation is not only the function of cross-sectional location $(x,y)$, but also the function of the channel direction $z$. $\beta$ appears as a control parameter, representing the strength of perturbation. Since we regard B zone as the perturbation, it is natural to define $\beta$ as the dimensionless length of B zone to the total length $L$.

$$\beta = \frac{b}{L} = \frac{b}{a + b}$$  \hspace{1cm} (14)

In the next step, we define a new spatially periodic phase space variable $\phi$ of modulo 1.

$$\phi = \frac{z}{L} \mod(1), \quad \phi \in S$$  \hspace{1cm} (15)

where $S$ is a circle of period 1. The reason why we define the new state variable $\phi$ instead of $z$ will be apparent in the next section. The spatially periodic return map describing the perturbed system is the Poincaré map defined as follows.

$$p^{\phi_0} : \Sigma^{\phi_0} \rightarrow \Sigma^{\phi_0},$$

where $\Sigma^{\phi_0} = \{(x,y,\phi) \in R^2 \times S | \phi = \phi_0 \in [0,1)\}$  \hspace{1cm} (16)

5 GEOMETRICAL ASPECTS AND CHAOS

5.1 The Unperturbed System

As noted in the previous section, the unperturbed (integrable) system is the solution of the evolution equation Eq 10 in case of the only-barrier screw channel, that is, which consists of the infinite number of A zone. Figures 4 and 5 are schematics of the integrable system in $xyz$ state space and in $xy\phi$ state space, respectively.

Now, we investigate the integrable structure shown in Fig. 5 in detail. There are two homoclinic connections intersecting at a hyperbolic (saddle) cycle, and the hyperbolic cycle intersect the Poincaré section to give rise to a saddle point $p_0$. The homoclinic orbits $\Gamma_{p_0}$ is defined as

$$\Gamma_{p_0} = W^s(p_0) \cap W^u(p_0)$$  \hspace{1cm} (17)

where $W^s(p_0)$ and $W^u(p_0)$ are the stable and the unstable manifolds, respectively.

---

**Fig. 4. Structure of the integrable system in the $xyz$ state space.**
Let us focus on the two nested sets of tori in the $xy$ state space. There are two competing frequencies in each $\Psi$ torus. $f_1$ is the frequency associated with the motion of the trajectories around the large circumference of the torus and $f_2$ is associated with the motion around the small cross-section of the torus in the $xy$ plane (Fig. 5). The frequency ratio $\Omega$ is usually defined as follows:

$$\Omega = \frac{f_2}{f_1}, \mod (1)$$

(18)

Note that $\Omega$ is a function of $(x,y)$ and this implies non-linear rotation.

If the frequency ratio is rational, we have the two smallest integers $m, n$ satisfying $\Omega = f_2/f_1 = m/n$.

Then, the Poincaré section will consist of $n$ points on the orbit and the points skip over $m - 1$ points after each mapping. The orbits of the irrational frequency ratio are dense. In that case, the point never returns to its own original position (9).

5.2 The Perturbed System

We introduce the B zone periodically as the perturbation. As we increase the strength of perturbation $\beta$ from zero, the chaos will happen. A schematic view of this situation in the $xyz$ state space is shown in Fig. 6.

There are two routes to chaos in CS system. One is related to the homoclinic tangles with sufficient perturbation, and they lead to the Smale horseshoe map.

Fig. 5. Structure of the integrable system in the $xy\Phi$ state space.

Fig. 6. A schematic structure of the perturbed system with homoclinic tangles and resonance in the $xyz$ state space.
around the hyperbolic point, which is the very complicated Cantor set with the infinite number of periodic points and much larger (uncountable infinite) number of aperiodic points. It is a kind of the global bifurcation phenomena and the Smale-Birkhoff Homoclinic Theorem guarantees the existence of such map in CS (10). The neighboring region of the homoclinic tangle is transformed into the stochastic (chaotic) region.

The remaining regular regions of nonlinear rotations surrounded by the homoclinic tangle are of our interest with regard to the mixing enhancement, since those regions cannot be affected by the homoclinic tangle. Hence, the more important transition to chaos in terms of the mixing performance is due to the nonlinear oscillations of the nested tori surrounded by the homoclinic tangle. If a torus (or an orbit) with the rational frequency ratio $\Omega = m/n$ is slightly perturbed, the regions in the vicinity of the $\Omega = m/n$ orbit will be resonant at the same frequency ratio so that the resonance band of period $n$ is formed. The resonance band is the banded region associated with the same rational winding number $\omega$ that is the frequency ratio of the perturbed system. Therefore, the resonance band that stems from the frequency ratio $\Omega = m/n$ has the winding number $\omega = m/n$ near the unperturbed $\Omega = m/n$ orbit.

From the subharmonic Melnikov method (10, 11), the resonance band of $\omega = m/n$ has $2n$ fixed points. The stability types of fixed points will change in turns; $n$ points are saddle, and the remaining $n$ points are elliptic. The resonance band constitutes local barriers to transport, since the neighboring region of elliptic fixed points form the islands of stability (dead spots) and the flux between inside and outside the resonance band is restricted by the lobe dynamics of the corresponding heteroclinic orbits (3). There are a lot of examples showing the similar dynamics. Some famous examples are the standard map and the Henon map (12). As the perturbation increases, the size of the dead spots gets smaller and finally disappears [Moser Twist Theorem (3)]. Therefore, the stochastic region in which the random motions take place becomes larger.

6 NUMERICAL STUDIES

The numerical study for the CS system is based on the analysis of the Poincaré map as defined in Eq 16. We first solve the governing equation Eq 4, to obtain the velocity fields, and then integrate the velocity fields with initial conditions to get the particle trajectories and the Poincaré map in the end. We used multivariate finite element method (FEM) developed by Gupta and Kwon (13, 14) to get the velocity fields, and the 4th order Runge-Kutta method is applied to integrate the velocity fields.

6.1 The Finite Element Formulation

The weak form of incompressible fluid flows defined Eq 1–4 over the domain $D$ with the domain boundary $\partial D$ is expressed as follows (13, 14).

Find $(u, p) \in V_u \times Q$ such that

$$
\int_D 2\mu \epsilon(u) : \epsilon(v) \, dD - \int_D p(\nabla \cdot v) \, dD = \int_{\partial D} \mathbf{T} \cdot v \, d\Gamma, \quad \forall v \in V_0 \quad (19)
$$

$$
\int_D (\nabla \cdot u) q \, dD = 0, \quad \forall q \in Q \quad (20)
$$

where the solution space of pressure $Q$ is square-integrable, $V$ is the Sobolev space of square-integrable up to the first order derivatives, the solution space of velocity is $V_u = \{v \in V, v_i = \dot{u}_i \text{ on } \partial D_u\}$, the test function space is $V_0 = \{v \in V, v_i = 0 \text{ on } \partial D_u\}$, $\partial D_u$ is the boundary on which the $i$-directional velocity $\dot{u}_i$ is specified, and $\mathbf{T}$ is the traction force specified on the boundary.

Introducing the interpolation functions $N_u$ and $N_p$ for the velocity and the pressure, respectively,

$$
\{u\} = [N_u](u), \quad \{p\} = [N_p](p) \quad (21)
$$

and, substituting Eq 21 into Eq 19 and Eq 20, we will get the nonlinear system of equations for non-Newtonian fluid flows.

The velocity-pressure formulation of incompressible fluid flows may have oscillating pressure solutions due to the spurious pressure mode, unless proper interpolation functions are selected for the velocity and the pressure. The mathematical criteria for the choice of the interpolation function in the finite element is the Babuška-Brezzi condition (15). The spurious pressure mode causes more critical problems for the three-dimensional element than two-dimensional one. Ordinary 8-node cubic element with tri-linear velocity and constant pressure suffers from the spurious pressure mode for the nontrivial boundary conditions often encountered in the single-screw extrusion. In this respect, Gupta and Kwon developed the $Q1^+P0$ element, which has the bilinear tangential velocity and the bi-quadratic normal velocity on the element faces. The $Q1^+P0$ element satisfies the Babuška-Brezzi condition with the additional degree of freedom and successfully describes incompressible characters like vorticity (13, 14). In the present study, $Q1^+P0$ element has been used for the finite element analysis.

6.2 Velocity Fields

Boundary conditions for the finite element analysis are described in Fig. 3. The two side walls, the bottom of the channel and the barrier surfaces have the no-slip condition, whereas the top surface is dragged obliquely with the helix angle $\alpha$ and the drag velocity $V_d$, and there is an adverse pressure gradient $d\rho/dz$ (> 0) along the z direction as is often the case of the single-screw extrusion process. To assign the boundary conditions at the inlet and the outlet surfaces, we assume that the velocity fields at the inlet and the outlet are identified by the velocity of the only-barrier case which can be solved by Eqs 5–9 with the
Quasi-3D model (6). However, there are some technical problems in doing this. Although we apply the boundary conditions described above even to the only-barrier case in the full three-dimensional simulation, we may not have the developed velocity fields along the channel direction such that $\partial v/\partial z = 0$. This is because the interpolation scheme of the Quasi-3D simulation is different from that of Q1P0 element. We carried out iterations, until $\partial u/\partial z = 0$ is obtained near the inlet and the outlet. As a result, we obtained steady and periodic boundary conditions for the full three-dimensional finite element simulation at the inlet and the outlet surfaces.

We performed numerical analyses for four cases by changing the strength of perturbation $\beta$: $\beta = 0$ (unperturbed), $\beta = 0.1$, $\beta = 0.2$, $\beta = 0.3$. The values of geometry variables are $W = 15.75 \times 10^{-3}$ m, $H = 3.5 \times 10^{-3}$ m, $h = 2.0 \times 10^{-3}$ m, $w = 0.4 \times 10^{-3}$ m, $L = 35.0 \times 10^{-3}$ m. The flow conditions such as the drag velocity, the helix angle, the pressure gradient and the material characterizations are the same as those of Quasi-3D simulations presented in Kim and Kwon (6). Finite element meshes are shown in Fig. 7(a)–(d).

Figure 8(a) and 8(b) are the cross-sectional velocity fields at the center in the $z$ direction ($\phi = 0.5$) for the $\beta = 0$ and $\beta = 0.1$ cases, respectively. The unperturbed case ($\beta = 0$) has been used not only to assign the boundary conditions at the inlet and the outlet surfaces to the perturbed system as explained above, but also to calculate the frequency ratio plot, which will be discussed in Sec. 6.5. Since the no-barrier zone (B zone) is located at $\phi = 0.5$ for the unperturbed case [Fig. 7(b)], one can expect the velocity fields in the B zone of the perturbed system will not be the same as that of the only-no-barrier case. Figure 8(b) shows the velocity fields for small perturbation ($\beta = 0.1$) is similar to the only-barrier case. In other words, there are
two elliptic points and one hyperbolic point even in the B zone of the perturbed system. Moreover, there are cross-sectional accelerations and decelerations near the center \((x = 0)\) in Fig. 8(b).

6.3 Particle Tracing

Integrating the velocity field obtained from the finite element analysis with initial conditions, one can obtain the particle trajectories and finally the Poincaré maps. As a numerical integration method, the 4th order Runge-Kutta method has been employed. For a given initial condition \(x_0\) and integration time step \(\delta t\), the next point \(x\) is calculated as follows.

\[
\begin{align*}
\mathbf{k}_1 &= \delta t \mathbf{v}(x_0) \\
\mathbf{k}_2 &= \delta t \mathbf{v}\left(x_0 + \frac{\mathbf{k}_1}{2}\right) \\
\mathbf{k}_3 &= \delta t \mathbf{v}\left(x_0 + \frac{\mathbf{k}_2}{2}\right) \\
\mathbf{k}_4 &= \delta t \mathbf{v}(x_0 + \mathbf{k}_3) \\
x &= x_0 + \frac{\mathbf{k}_1}{6} + \frac{\mathbf{k}_2}{3} + \frac{\mathbf{k}_3}{3} + \frac{\mathbf{k}_4}{6} + O(\delta t^5)
\end{align*}
\]

where \(\mathbf{k}_i = (k_{1i}, k_{2i}, k_{3i}) \in \mathbb{R}^3\) \((i = 1, 2, 3, 4)\) and the time step \(\delta t\) is obtained from \(\delta t = S/|\mathbf{v}_{pre}|\) with the previous velocity \(\mathbf{v}_{pre}\) and a predetermined constant \(S = 0.05\). The unperturbed streamline indicated in Fig. 2(b) is the result of the numerical integration for the \(\beta = 0\) case.

6.4 The Frequency-Ratio Distribution for the Unperturbed System

The characteristics of elliptic nonlinear rotations inside the homoclinic orbit in the unperturbed system are essential to understand underlying phenomena such as the resonance bands and KAM tori which appear in the perturbed Hamiltonian system. The characteristics of the elliptic rotation can be represented by the distribution of the frequency ratio \(\Omega\). The index of each orbit (or torus in the \(xy\) space) can be distinguished by the coordinate \(\zeta\) which is a coordinate in the negative \(y\) direction from the center of elliptic rotation \((x_c, y_c)\) (Fig. 9). \(\Omega\) is a function of \(\zeta\) and can be calculated for each torus by the following formula:

\[
\Omega(\zeta) = \frac{f_2(\zeta)}{f_1(\zeta)} = \frac{1}{n_1(\zeta)} = \frac{L}{\int \omega \frac{dl}{\sqrt{u^2 + v^2}}}
\]

where \(n_1\) is the number of rotation of the large circumference during one period of the small cross-sectional rotation. Note that \(n_1\) is not integer but real in general. The distribution of the frequency ratio is shown in Fig. 10. This plot has very important implications. The first observation is that \(\Omega\) is not constant which means the associated set of the elliptic rotations is nonlinear. The second is that the value of \(\Omega\) vanishes very rapidly near \(\zeta = 1.4\) at which the homoclinic orbit of the infinite period exists. The more interesting point is the fact that the dominant rational value of
the frequency ratio is 1/3 around $\zeta \approx 0.5$. Since the distribution of the winding number $\omega$ of the small perturbed system is slightly different from the frequency-ratio distribution $\Omega$ of unperturbed system, one can expect the perturbed system to have a resonance band of period three and the Poincaré sections will indicate three islands of stability (unmixed zones, or dead spots) near the $\Omega = 1/3$ orbit.

6.5 The Poincaré Sections

The Poincaré sections for the three cases are shown in Fig. 11, 13 and 14. We have obtained the Poincaré sections by integrating the velocity fields for 100 periods with the equally-spaced 41 initial points.

We first investigate the small perturbed case of $\beta = 0.1$ in Fig. 11. We varied the cross-section $\Sigma^{b_0}$
from $\phi = 0$ to $0.8$ with increment of 0.2. These are denoted by (a)-(e). Varying cross section on which the Poincaré section is defined corresponds to shifting the phase of the periodic orbits (11). By doing this, we reconstruct the dynamical structure in $x,y$ state space.

Fig. 11. Poincaré sections for $\beta = 0.1$ case: (a) $\phi = 0$, (b) $\phi = 0.2$, (c) $\phi = 0.4$, (d) $\phi = 0.6$, (e) $\phi = 0.8$.

Apparently, there are three islands of stability rotating in each side of barrier in Fig. 11(a)-(e). These islands constitute the resonance band of period three. Compared with the frequency-ratio plot in Fig. 10, the winding number associated with the resonance band
will be $\omega = m/n$ with $m = 1$ and $n = 3$. Each dead spot constituting the resonance band is mapped into the adjacent dead spot after one period (counterclockwise). This phenomenon is exactly what we predicted in the previous section.

Schematic descriptions of this phenomenon are indicated in Fig. 12. Figure 12(a) shows how the subharmonic orbit (the resonance band) of period three is constructed by the periodic perturbation, when the frequency-ratio distribution is nonlinear. As depicted in Fig. 10, the derivative of frequency ratio $\Omega$ with respect to $\xi$ is positive in the vicinity of the $\Omega = 1/3$ orbit ($d\Omega/d\xi > 0$). When the periodic perturbation is imposed, the orbit outside the winding number $\omega = 1/3$ orbit is relatively faster compared with the winding number $\omega = 1/3$ orbit, whereas the inner orbit is relatively slower. The subharmonic Melnikov method assures that there are six fixed points in the perturbed Poincaré map (S. Wiggins (1990) (11), Sec. 1.2, p. 135). Three fixed points are the elliptic and the remaining three are hyperbolic as discussed in Sec. 5.2.

The resulting schematic diagram of the Poincaré section is indicated in Fig. 12(b). Compare this Figure to Fig. 11(a)–(e).

Concerning the mixing performance, this is not such a good case. The inner island of stability (the large KAM) surrounded by the resonance band is very large and three small KAM tori constituting the resonance band are also relatively large. It might be reminded that the resonance bands and KAM tori are the regular structures where random particle motions cannot take place.

An interesting point is unsymmetry in the Poincaré section. In the left side, there are a lot of points inside the KAM, whereas there is no point at the same location in the right side. Once points are present inside the KAM, then they never escape from the KAM. In the same way, once points are present outside the KAM, they never penetrate into the KAM. In spite of this fact, the mixing performance of this case is much better than that of the conventional screw (only-no-barrier case) or the only-barrier screw, since the perturbed homoclinic tangle gives birth to the chaotic region nearby the homoclinic orbit and the resonance band works as a partial barrier, as explained in Sec. 5.2.

Now, we proceed to the next case, $\beta = 0.2$. The Poincaré section at $\phi = 0$ is presented in Fig. 13, which shows the wider stochastic (chaotic) region in the vicinity of the homoclinic orbit than the $\beta = 0.1$ case. The resonance band of period three has vanished and the smaller KAM torus is present. A careful observer would find the small resonance band outside the KAM torus. The corresponding rational number is not clarified. From the distribution of frequency ratio (Fig. 10), however, we may estimate its possible range as $0.3 \sim 1/3$ (0.3 is the frequency ratio of center of rotation (extrapolated) and 1/3 is the frequency ratio of the vanished resonance band of period 3).

The last case is the most perturbed case, $\beta = 0.3$, in our study. The Poincaré section at $\phi = 0$, shown in Fig. 14, does not seem to be different from the $\beta = 0.2$ case, except for the absence of the higher order resonance band which is present in the $\beta = 0.2$ case. There is a large chaotic region near the homoclinic orbit and the smaller KAM torus is located at the center of rotation.

7 CONCLUSION

We have presented the dynamical modeling for the CS developed for the mixing enhancement of the single-screw extrusion process and found the route to chaos in CS. Also, we have carried out full three-
Dynamical Modeling of Chaos Single-Screw

The only-barrier channel is described as the unperturbed system and periodically inserted no-barrier zone is regarded as the perturbation. The unperturbed system has a homoclinic orbit and nested (nonlinearly) oscillating elliptic tori.

If the strength of perturbation is small, the homoclinic orbit is changed into the homoclinic tangle and the nearby region becomes chaotic. Simultaneously, oscillating tori inside the homoclinic orbit are changed into either the partial barrier (the resonance band) or the complete barrier (KAM torus) for transports, depending on the commensurability of the frequency ratio of the orbit. As the strength of perturbation increases, the regular structures, such as resonance bands or KAM tori, have been vanished gradually and the stochastic regions become larger.

To check the dynamical modeling via numerical simulations, we obtained velocity fields by the full three-dimensional finite element method using multivariable elements and performed particle tracing by the 4th order Runge-Kutta method.

From the small perturbation case ($\beta = 0.1$), we found period three resonance band and KAM torus. The resonance band corresponding to the $\Omega = 1/3$ orbit is composed of three islands of stability of period three, which shows good agreement with our prediction based on the dynamical modeling. As the strength of perturbation increases, the stochastic regions become larger and the regular region smaller.

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**NOMENCLATURE**

- $a$: length of barrier zone
- $b$: length of non-barrier zone
- $D$: flow domain
- $\partial D$: domain boundary
- $f_1$: frequency of the motion around the large circumference of the torus
- $f_2$: frequency of the motion around the small cross section of the torus
- $h$: height of barrier
- $H$: height of flight
- $k_i$: $i$-th integration variable in 4th order Runge-Kutta method
- $L$: total length of periodic module ($a + b$)
- $N_v, N_p$: shape functions for velocity and pressure
- $V_d$: drag velocity with its components ($V_{dx}, V_{dz}$)
- $p$: pressure
- $P$: Poincaré map
- $S$: weight determining time step in the 4th order Runge-Kutta methods
- $v$: velocity with its components ($u, v, w$)
- $V$: Sobolev space
- $V_0$: test function space
- $V_u$: trial function space
- $w$: width of barrier
- $W^s, W^u$: stable and unstable manifolds
- $x$: position in state space with its components ($x, y, z$)

**Fig. 13.** Poincaré sections for $\beta = 0.2$ at $\phi = 0$.

**Fig. 14.** Poincaré sections for $\beta = 0.3$ at $\phi = 0$. 

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Greek Letters

- \( \alpha \) helix angle
- \( \beta \) dimensionless length of no-barrier zone
- \( \epsilon \) shear rate
- \( \dot{\gamma} \) effective shear rate
- \( \Gamma \) homoclinic orbit
- \( \mu \) kinematic viscosity
- \( \omega \) rotation number
- \( \Omega \) frequency ratio
- \( \phi \) periodic state variable
- \( \Psi \) streamfunction
- \( \sigma \) stress
- \( \zeta \) coordinate from the center of elliptic rotation

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