Chaotic Volumetric Transports in a Single-Screw Extrusion Process

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Volumetric material transports across distinct regions in the Chaos Screw (CS) system were described in terms of the volume-preserving lobe dynamics. Kinematic properties of a spatially periodic Poincaré map were studied first with the volume- and orientation-preserving two-dimensional map, in order to provide mathematical frame works for analyses of manifold structures. The perturbed hyperbolic fixed point and the associated stable and unstable manifolds were obtained numerically. These manifolds form homoclinic tangles, and they divide the cross-sectional area into three distinct regions: left, right, and outer. Six volumetric flow rates between the three regions were described in terms of the associated lobe dynamics. As the perturbation strength increases, representative flow rates between these regions were found to increase linearly as long as the fraction of no-barrier zone is small.

INTRODUCTION

In this paper, we discuss volumetric material transports in the chaotic region of the Chaos Screw (CS) system, one of the successful examples in terms of dynamical systems viewpoint (1–3). The aim is to give an answer to the fundamental question of ‘how much volume of fluids is transported from one region to another due to chaos.’ The question possesses three important implications. The first is about the measure of mixing strength in the three-dimensional volume-preserving chaotic system. The second is about the past and the future of material particles; i.e. where the materials come from and where they go. The third is about the finite-time or finite-period mixing characteristics. The answer to these questions can be found by means of so-called lobe dynamics. Lobe dynamics provides a general theoretical framework based on invariant manifold ideas from dynamical systems theory for describing organized structures in a fluid flow. Lobe dynamics was first introduced by Rom-Kedar and Wiggins (4) and Wiggins (5). Applications of this technique to fluid mixing problems become widespread recently, mostly by Wiggins and his colleagues: e.g. the oscillating vortex pair flow (6), the Rayleigh-Bénard flow (7), etc.

In this study, we apply lobe dynamics to analyze transport problem in the CS system that has practical importance in the polymer mixing industry. This paper is organized as follows: The first section starts with a brief description of the CS system briefly for completeness of the work and introduces a two-dimensional map with its kinematic properties in order to provide mathematical frameworks for analyses of manifold structures. In the second section, we describe the method of finding the fixed point and the associated eigenvectors in the perturbed system and show a three-dimensional manifold structure is obtained from the Poincaré map. In the third section, we first introduce some definitions for studying lobe dynamics and present characteristics of lobe motions in terms of the flow rate conservation and the symmetry. The cross-sectional phase space is divided into three regions, and six different volumetric transports between the three regions are described in terms of lobe dynamics. Finally, the effect of the perturbation strength on the lobe configuration and the material transport is discussed.

SYSTEM AND TWO-DIMENSIONAL DESCRIPTION

System

The unwound geometry of CS is shown in Fig. 1. The coordinate system is also indicated in the figure; x is chosen along the width direction, y along the screw depth, and z along the channel direction from hopper to die. The xy plane is called the cross-sectional plane and the z direction is called the longitudinal direction throughout the study. We denote length of barrier zone by a, the length of no-barrier zone by b, the total length of period by $L (=a + b)$, the height
of barrier by \( h \), the height of flight by \( H \), the width of barrier \( c \) and the width of channel by \( W \).

We regard the periodic removal of barrier as the geometric perturbation so that the fraction of no-barrier zone is much shorter than the fraction of the barrier zone. The strength of perturbation \( \beta \) is defined as the fraction of the no-barrier zone.

\[
\beta = \frac{b}{L} \tag{1}
\]

In this regard, the unperturbed system is full barrier system and its cross-sectional streamlines are presented in Fig. 2. (See the authors' previous works \( (2, 3) \) for detailed description for the unperturbed dynamical system.) Assuming a very long channel with infinite number of periods, the velocity fields are periodic according to the spatial period with the following translational symmetry:

\[
\mathbf{v}(x, y, z) = \mathbf{v}(x, y, z + nL), \quad n = 0, \pm 1, \pm 2, \ldots \tag{2}
\]

The periodic box is a periodic unit of length \( L \) from center of one barrier zone to center of the next barrier zone (Fig. 1). The geometry of the periodic box is fixed as the dimensionless width of channel \( W/H = 4 \), the dimensionless height of barrier \( h/H = 0.66 \), the dimensionless length of period \( \lambda (L/H) = 10 \), and the dimensionless width of barrier \( c/H = 0.1 \). The drag velocity on the top plate is denoted by \( V_d \) in the direction of helix angle \( \alpha = 15 \) (deg.).

To focus our study on the kinematics only, the flow in the CS system is assumed to be the Stokes flow. With the height of flight \( H \) for the characteristic length and with the \( z \) directional component of the drag velocity \( V_d \) for the characteristic velocity, the dimensionless variables can be expressed in the following way:

\[
\mathbf{x}^* = \frac{x}{H}, \quad \mathbf{u}^* = \frac{\mathbf{v}}{V_d}, \quad t^* = \frac{V_d t}{H}, \quad p^* = \frac{1}{\mu} \frac{H}{V_d} p \tag{3}
\]

where \( t \) is time and \( \mu \) is the viscosity. Hereafter, we exclusively use the dimensionless variables, omitting the superscript \(*\). The continuity equation and equations of motions are as follows.

Fig. 1. The unwound screw channel of the chaos screw (CS) and the periodic box.

Fig. 2. Cross-sectional streamlines in the unperturbed system. The dashed line indicates the homoclinic orbit.
\[ \nabla \cdot \mathbf{v} = 0 \quad (4) \]
\[ \nabla \rho = \nabla^2 \mathbf{v} \quad (5) \]

Boundary conditions are also indicated in Fig. 1: drag on the top plate with helix angle and no-slip boundaries prescribed on the screw root, the barrier surface, and the flights. Concerning the inlet and outlet boundaries, it is assumed that the velocity distributions on those surfaces are the same as the unperturbed velocity distribution which depends only on the helix angle. The pressure gradient, usually induced by the die configuration, has been neglected in this study (\( \partial p / \partial z = 0 \)). Before discussing further, it would be worthwhile to mention the explicit assumptions made in this study: (i) The fluid is Newtonian, (ii) the effect of back flow is neglected so that the fluid particles always travel towards the die, (iii) the flow channel is considered full, and (iv) developing flow at the inlet and outlet is negligible.

Since the periodic box has geometric symmetry about the \( yz \) plane and is periodic in \( z \) with period \( \lambda \), symmetry relation will help us understand the global motion of a particle in the CS system. To make use of periodicity in \( z \), it is useful to introduce a periodic phase variable \( \phi \) rather than \( z \) such that
\[ \phi = z/\lambda, \quad \text{mod}(1), \quad \phi \in S \quad (6) \]
where \( S \) is a circle of period 1. The velocity components inside the periodic box have the following identities in \( \mathbb{R}^2 \times S \).

\[
\begin{align*}
  u(x, y, \phi) &= u(-x, y, \phi) = u(x, y, 1 - \phi) = u(-x, y, 1 - \phi) \\
  v(x, y, \phi) &= -v(-x, y, \phi) = v(x, y, 1 - \phi) = -v(-x, y, 1 - \phi) \\
  w(x, y, \phi) &= w(-x, y, \phi) = w(x, y, 1 - \phi) = w(-x, y, 1 - \phi)
\end{align*}
\]

With \( S_{xy} : (x, y, \phi) \mapsto (x, y, 1 - \phi) \) and \( S_{y\phi} : (x, y, \phi) \mapsto (-x, y, \phi) \), which are the reflection symmetries about \( \phi \) and \( y \), respectively, the symmetry in the infinitesimal motion of a particle can be written as
\[ B = S_{y\phi} S_{xy} F S_{xy} S_{y\phi} \quad (\text{or } F = S_{y\phi} S_{xy} B S_{xy} S_{y\phi}) \quad (8) \]
(see Appendix for derivation). The mappings \( F \) and \( B \) indicate infinitesimal forward and backward time integrations such that
\[
\begin{align*}
  Fp &= (x_1 + u_1 \delta t, y_1 + v_1 \delta t, \phi_1 + w_1 \delta t) \\
  Bp &= (x_1 - u_1 \delta t, y_1 - v_1 \delta t, \phi_1 - w_1 \delta t)
\end{align*}
\]
for the material point \( p \) at \((x_1, y_1, \phi_1)\) whose the associated surrounding fluid velocity is \((u_1, v_1, w_1)\). Since the reflection symmetries \( S_{xy} \) and \( S_{y\phi} \) satisfy
\[ S_{xy} S_{xy} = S_{y\phi} S_{y\phi} = I \quad \text{and} \quad S_{xy} S_{y\phi} = S_{y\phi} S_{xy} \quad (10) \]
the time-reversal symmetry in Eq 8 is not restricted to the infinitesimal time step \( \delta t \), yet it can be extended to the finite time step by the successive application.
\[ B_n B_{n-1} \cdots B_2 B_1 = S_{y\phi} S_{xy} F_n F_{n-1} \cdots F_2 F_1 S_{xy} S_{y\phi} \quad (11) \]
for all positive integer \( n \). The symmetry in Eq 11 is described in Fig. 3.

**Description by Two-Dimensional Map**

Dynamical systems of CS are of the following form
\[
\dot{x} = v(x, \beta), \quad x \in \mathbb{R}^3 \quad (\text{or } \mathbb{R}^2 \times S). \quad (12)
\]

Fig. 3. Symmetry within the particle motion in the periodic box (Eq 11). This figure also indicates the symmetry of the two-dimensional map (Eq 18).
and the map \( \mathbf{x}(0) \rightarrow \mathbf{x}(t) \) defines a volume-preserving dynamical system with Eq 4. However, it is desirable to have a simple mapping that describes the system with reduced number of state variables in order to easily visualize the dynamical systems. In this regard, we propose a mapping with respect to the longitudinal coordinate \( z \), not with respect to time.

When the longitudinal component \( w(\mathbf{x}) \) does not change its sign over the cross-sectional domain (in this case \( w(\mathbf{x}) > 0 \)), a continuous map \( \varphi: \Sigma \rightarrow \Sigma \) can be constructed along the flow such that

\[
X(z) = \varphi(z, z_0)X_0,
\]

where \( z > z_0 \) and \( X = (x, y) \in \Sigma \subset \mathbb{R}^2 \). \( \Sigma \) is a cross section identified by the \( z \) coordinate in the CS system and \( X_0 \) is the cross-sectional position \((x_0, y_0)\) of the initial material point located on \( z_0 \). \( \varphi(z, z_0) \) maps the initial cross-sectional position \( X_0 \) on the \( z_0 \) plane into the cross-sectional position \( X \) on the \( z \) plane along the material line. We call the map \( \varphi(z, z_0) \) the two-dimensional map (see Fig. 4). The two-dimensional map in Eq 13 can also be derived directly from the two-dimensional form of Eq 12 by dividing the first two component equations by the third component:

\[
\frac{dx}{dz} = \frac{u(x)}{w(x)} = \bar{u}(x), \quad \frac{dy}{dz} = \frac{v(x)}{w(x)} = \bar{v}(x) \quad (14)
\]

Regarding \( z \) as a role of time variable in unsteady two-dimensional flows, the mapping along the flow with respect to \( z \) would be a natural choice for describing the system. As one can see in Eq 14, the important constraint for the two-dimensional description is the transversal condition, i.e., \( w(\mathbf{x}) \) must not change its sign. The transversal condition seems to be unrealistic in case of the single-screw extrusion process, because there are too many boundaries under the no-slip condition, and, furthermore, a relatively large adverse pressure gradient may cause negative longitudinal components near the screw root. However, if one keeps in mind that there is no parabolic fixed point, a possible dynamics that makes the boundary important, in the CS system, particle motions right at the no-slip boundaries are negligible, since they are not special and cannot be chaotic. And even with the back flow, we found that overall three-dimensional behavior does not change significantly. (See (3), where the authors presented experimental flow-visualization results when the adverse pressure gradient is dominant.)

**Kinematic Properties of Two-Dimensional Map and Poincaré Map**

To provide rigorous mathematical frameworks in using the two-dimensional map, we present four kinematic properties of the map: volume conservation \( (P1) \), orientation preservation \( (P2) \), symmetry \( (P3) \), and commutativity \( (P4) \).

**P1 Volume conservation:** A family of streamlines whose tangent is everywhere parallel to the local velocity vectors can always be defined by the dynamical system. Let us consider a stream tube with two open surfaces, \( A' \) and \( A'' \) whose corresponding velocities and outward normal vectors are \( (\mathbf{v}', \mathbf{n}') \) and \( (\mathbf{v}'', \mathbf{n}'') \), respectively. Then, from the divergence theorem, it can be shown that the inflow rate is the same as the outflow rate (8).

\[
\int \mathbf{v}' \cdot \mathbf{n}' dA' + \int \mathbf{v}'' \cdot \mathbf{n}'' dA'' = \int \nabla \cdot \mathbf{v} dV = 0 \quad (15)
\]

As indicated in Fig. 5, a subdomain \( D \subset \Sigma_{z_0} \) is mapped by the two-dimensional map to give another subdomain \( \varphi(z, z_0)(D) \) on the \( \Sigma_z \) plane. There is no reason that \( D \) and \( \varphi(z, z_0)(D) \) have the same area; that is, the map is not area-preserving. Instead, if one denotes the flow rate through \( D \) by \( F(D) \) and the flow rate through the mapped region \( \varphi(z, z_0)(D) \) by \( F(\varphi(z, z_0)(D)) \), then one can obtain

![Fig. 4. Two-dimensional map, a mapping of cross section into itself along the material line.](image-url)
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$$F(D) = \int_D u(x) \, dA = \int_{\varphi(z, z_0)(D)} u(x) \, dA = F(\varphi(z, z_0)(D)). \tag{16}$$

for all $z$ and for all the choice of $D$, according to the general statement in Eq 20 and we call Eq 16 the volume-conservation property of the two-dimensional map.

**P2 Orientation preservation:** The two-dimensional map also preserves orientation. From the continuity of $dx/dz, dy/dz$, and their partial derivatives with respect to $x$ and $y$, the relative ordering of material points under the map cannot be changed (see Eq 14). Therefore, the deformation processes in the two-dimensional map are sufficiently smooth, as if they were a real two-dimensional flow. This implies that the interior of a closed curve is mapped to the interior of the curve’s image (which is in fact the assumption in deriving the volume conservation of the map). In the mathematical term, the determinant of the two-dimensional map is always positive (orientation preserving) and is not necessarily equal to 1 (non-area preserving).

$$\text{det}(D_\varphi) > 0 \quad \text{and} \quad \text{det}(D_\varphi) \neq 1. \tag{17}$$

**P3 Symmetry:** The time-reversal phase-inversive symmetry in the motion of a particle in Eq 8 can be rewritten in the slightly modified form for the two-dimensional map $\varphi$ as follows:

$$\varphi(-z, -z_0) = S_y \varphi(z, z_0) S_y \tag{18}$$

$S_y$ is the ordinary two-dimensional reflection symmetry about $y$ axis, $S_y: (x, y) \rightarrow (-x, y)$ and $\varphi$ denotes the backward two-dimensional map which satisfies

$$\varphi(t, s) \varphi(s, t) = \varphi(s, t) \varphi(t, s) = id., \quad s > t. \tag{19}$$

As shown in Fig. 3, The material point $(X_0, z_0)$ is mapped to $(X_1, z_1)$ by the forward map $\varphi(z_1, z_0)$, i.e.

$$X_1 = \varphi(z_1, z_0)X_0.$$ 

In the similar way, the point $(S_y X_0, -z_0)$ is mapped by the backward map $\varphi(-z_1, -z_0)$ to the point $(S_y X_1, -z_1)$, where $S_y X_1 = \varphi(-z_1, -z_0) S_y X_0$. Considering $X_1 = \varphi(z_1, z_0) X_0$, the symmetry relation in Eq 18 can be easily checked, since $S_y \varphi(z_1, z_0) = \varphi(-z_1, -z_0) S_y$.

**P4 Commutativity:** The two-dimensional map cannot satisfy the following commutative property.

$$\varphi(s, 0) \varphi(t, 0) \neq \varphi(t, 0) \varphi(s, 0) \neq \varphi(t, s, 0). \tag{20}$$

However, if one introduces the spatial period of the velocity field $\lambda$, one can show that

$$\varphi(\lambda, 0) \varphi(z, 0) = \varphi(\lambda + z, 0) \quad \text{and} \quad \{\varphi(\lambda, 0)\}^n = \varphi(n\lambda, 0) \quad n = \pm 1, \pm 2,... \tag{21}$$

In this kind of mapping, $X_0$ is a fixed point of the mapping $\varphi(n\lambda + z_0, 0)$, if only if the orbit $x(t)$ with the initial condition $x_0 (t) = (X_0, z_0)$ is periodic in $\mathbb{R}^3$, and the fixed point in the two-dimensional map has the same stability type as that of the corresponding orbit in the physical $\mathbb{R}^3$ space.

The Poincaré map can be defined as the commutative two-dimensional map $\varphi(\lambda + \lambda \phi_0, \lambda \phi_0)$ as follows:

$$P_{\phi_0} : \Sigma_{\phi_0} \rightarrow \Sigma_{\phi_0}, \quad P_{\phi_0} = \varphi(\lambda + \lambda \phi_0, \lambda \phi_0) \tag{22}$$

where $\Sigma_{\phi_0} = \{(x, y) \in \mathbb{R}^2 \times S|\phi = \phi_0 \in [0, 1)\}$. The $n$th iterate $P_{\phi_0}^n$ and its inverse are

$$P_{\phi_0}^{-n} = \varphi(-n\lambda + \lambda \phi_0, \lambda \phi_0) \tag{23}$$

where $n$ is a positive integer. Since it is defined as a special case of the two-dimensional map, the Poincaré map satisfies the volume conservation (P1) and orientation preservation (P2) properties as well. The symmetry of the Poincaré map can be derived by the symmetry of the two-dimensional map (Eq 18) and the definition of the Poincaré map (Eqs 22 and 23) and it can be written as follows:
The symmetry in Eq 24 involves the reflection symmetry about the phase variable $\phi$. Only on the $\phi_0 = 1/2$ and on the $\phi_0 = 0$ (or 1) planes, where $1 - \phi_0$ and $\phi_0$ have the same value, the reflection symmetry about $y$ can be achieved between the forward and the backward Poincaré map. These two planes correspond to the center of no-barrier zone and the center of barrier zone, respectively.

**PERTURBED UNSTABLE AND STABLE MANIFOLDS**

*Figure 6* shows continuous cross-sectional deformation patterns in case of $\beta = 0.03$ with respect to the longitudinal coordinate, revealing the fundamental nature of deformations that material near the homoclinic point undergoes. The initial points are arranged on the circle with radius 0.05, which is centered at the hyperbolic fixed point at $z = 0$ (Fig. 6a). We obtained the three-dimensional velocity field and numerical particle trajectories using the same methods as the authors’ previous works (2, 3). The circular area continuously deforms along the (perturbed) unstable manifold and tangles when it approaches to the (perturbed) stable manifold. Both manifolds constitute the homoclinic tangle, a signature of chaos, and the configuration of the manifolds determines the material transports in the chaotic region, which will be discussed throughout this work.

**Finding Fixed Point**

To visualize the perturbed unstable and stable manifolds, one should find the exact location of the perturbed hyperbolic fixed points and the associated directions of eigenvectors. The perturbed hyperbolic fixed point, denoted by $p_\beta$, should satisfy the following condition:

$$p_\beta = P^n_{0\beta}(p_\beta), \text{ for all integer } n. \quad (25)$$

As implied in Eq 25, the location of the fixed point varies not only with the perturbation strength $\beta$ and but also with the phase $\phi_0$ where the Poincaré map is defined, since the perturbed hyperbolic cycle $\gamma_0$ sways periodically along the phase. First one should note that the point $x$, satisfying $\mathbf{v}(x) = \mathbf{0}$, is not the fixed point in the perturbed system $(\mathbf{\bar{v}} = (\mathbf{\bar{u}}, \mathbf{\bar{v}}))$ is the two-dimensional form of the velocity field in Eq 14); the perturbed fixed point should be obtained from the Poincaré map. Since the analytic form of the Poincaré map is not known, we used an iterative graphical method to obtain the exact location of the fixed point and the associated eigenvectors. The rationale behind
this method is that the localized derivative of the Poincaré map, \( DP_0 \), in the neighborhood of the perturbed fixed point \( p_\beta \) is linear and the location of the perturbed fixed point \( p_\beta \) is not much different from the unperturbed fixed point \( p_0 \).

The procedure of the iterative graphical method is as follows: (i) Prepare a rectangular array of points (usually \( 10 \times 10 \)) centered at the location where the fixed point is expected to exist. (The initial guess is \( p_0 \)). (ii) Denoting the arranged points by \( P_i \)'s, evaluate the forward Poincaré map of the points \( p_i \)'s and the backward iterates \( p_i \)'s, i.e., and \( p_i = P_{p_0} (p_i) \), respectively. Then, one can easily identify the neighborhood of the fixed point \( p_0 \), by drawing the arrows from \( p_i \) to \( p_0 \) and from \( p_0 \) to \( p_i \) (Fig. 7). The fixed point \( p_\beta \) must be present in the dotted region so that the region will be the rectangular array for the next trial. By applying the procedure repeatedly, one can obtain the location of the fixed point \( p_\beta \) accurately. From our experience on the CS system, the Poincaré map is found to be linear within the range of around \( p_0 \). Once the fixed point has been obtained, then the direction of the associated eigenvectors can be found easily. Table 1 shows locations of the perturbed fixed points and the associated normalized eigenvectors for various values of the perturbation strength \( \beta \). The eigenvectors 1 and 2 indicate the directions of the unstable and stable manifolds, respectively. Table 1 shows that the value \( y(p_0) \) becomes smaller and the directions of the eigenvectors become stiffer with increment of the perturbation. The absolute values of the calculated \( x(p_0) \)'s have been found less than \( 10^{-5} \) under the single precision calculation, so we put the value of \( x(p_0) \) as zero in Table 1. (The value \( x(p_0) \) must be zero at \( \phi = 0 \) and \( 1/2 \) by the symmetry of the Poincaré map (Eq 24)).

### Three-Dimensional Structures of Perturbed Unstable and Stable Manifolds

Figure 8a and Fig. 8b indicate periodic units of three-dimensional evolution of the perturbed unstable and stable manifolds in case of \( \beta = 0.03 \) in the physical \( \mathbb{R}^3 \) space, respectively. Each of these two manifold structures is composed of 200 Poincaré sections.

It might be of interest to describe how the manifold structures plotted in Fig. 8 are constructed. The initial 3000 points at \( z = 0 \) are arranged along the eigenvector 1 direction at the exponential scale within the distance \( 10^{-3} \) from the perturbed hyperbolic fixed point (Table 1). The range of the initial points should be selected carefully. For two points \( q_0, q_1, \in W^u(p_\beta) \), let us

### Table 1. Locations of the Perturbed Hyperbolic Fixed Point \( p_\beta \) and the Associated Normalized Eigenvectors at \( \phi_0 = 0 \) for Various Values of the Perturbation Strength \( \beta \).

<table>
<thead>
<tr>
<th>( \beta )</th>
<th>( (x(p_0), y(p_0)) )</th>
<th>Eigenvector 1</th>
<th>Eigenvector 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(0.8820116)</td>
<td>(0.9359330, 0.3521782)</td>
<td>(0.9355273, -0.3532544)</td>
</tr>
<tr>
<td>0.01</td>
<td>(0.8816753)</td>
<td>(0.9353046, 0.3538434)</td>
<td>(0.9351235, -0.3543218)</td>
</tr>
<tr>
<td>0.02</td>
<td>(0.8804140)</td>
<td>(0.9342836, 0.3565313)</td>
<td>(0.9344223, -0.3561670)</td>
</tr>
<tr>
<td>0.03</td>
<td>(0.8783667)</td>
<td>(0.9322546, 0.3618029)</td>
<td>(0.9321777, -0.3620004)</td>
</tr>
<tr>
<td>0.04</td>
<td>(0.8758265)</td>
<td>(0.9288073, 0.3705632)</td>
<td>(0.9286921, -0.3708516)</td>
</tr>
<tr>
<td>0.05</td>
<td>(0.8730606)</td>
<td>(0.9248626, 0.3803014)</td>
<td>(0.9244325, -0.3813458)</td>
</tr>
<tr>
<td>0.06</td>
<td>(0.8702478)</td>
<td>(0.9220965, 0.3869838)</td>
<td>(0.9220172, -0.3871487)</td>
</tr>
<tr>
<td>0.07</td>
<td>(0.8675216)</td>
<td>(0.9188362, 0.3946930)</td>
<td>(0.9192060, -0.3937767)</td>
</tr>
<tr>
<td>0.08</td>
<td>(0.8649646)</td>
<td>(0.9151884, 0.4030262)</td>
<td>(0.9158918, -0.4014251)</td>
</tr>
<tr>
<td>0.09</td>
<td>(0.8624303)</td>
<td>(0.9134225, 0.4070126)</td>
<td>(0.9133399, -0.4071980)</td>
</tr>
<tr>
<td>0.1</td>
<td>(0.8600736)</td>
<td>(0.9108143, 0.4128162)</td>
<td>(0.9107667, -0.4129216)</td>
</tr>
</tbody>
</table>
denote \( q_0 \leq u \) \( q_1 \) to indicate that \( q_0 \) is closer to \( p_\beta \) than \( q_1 \) in the sense of arclength along \( W^u(p_\beta) \); and denote the initial points on the eigenvector 1 by \( u_1, u_2, \ldots, u_n \) \((n = 3000) \) such that \( u_i < u_j \) when \( i < j \). Then it is clear that \( P_{q_0}^k (u_i) < u \) \( P_{q_0}^k (u_j) \) for all \( k \) and \( \phi_0 \), since the two-dimensional map (or the Poincaré map) preserves orientation (P2). Since the Poincaré map was found to be linear in the range of \( 10^{-3} \) around \( p_\beta \) in this case, we have chosen \( u_1 \) and \( u_n \) such that \( u_n < u \) \( P_{q_0} (u_1) \) at \( \phi_0 = 0 \), minimizing the distance between \( u_n \) and \( P_{q_0} (u_1) \) at \( \phi_0 = 0 \) and attaining the distance between \( P_{q_0} (u_1) \) at \( \phi_0 = 0 \) and \( p_\beta \) under \( 10^{-3} \). Then 200 Poincaré sections with 200 different \( \phi_0 \) have been evaluated by the 0.05 interval in the \( \phi \) direction during four periods. (During calculation, the points are inserted appropriately if two neighboring points are apart more than 0.01.) The three-dimensional unstable manifolds are obtained by plotting all the Poincaré sections simultaneously. The perturbed stable manifold (Fig. 8b) is obtained from the unstable manifold using the symmetry relation of the Poincaré map (Eq 24).

The unstable and stable manifolds intersect transversely (non-tangentially) and they form enclosed regions surrounded by two manifolds. Such enclosed regions are called lobes. Since the two manifolds are invariant and the Poincaré map preserves orientation, the enclosed region should be mapped another enclosed region infinitely many times along the unstable manifold, as \( t \) \((or \ z) \to \infty \), or, along the stable manifold, as \( t \) \((or \ z) \to \infty \). To preserve the flow rate through the region according to the volume conservation property of the two-dimensional map (Eq 16), the enclosed regions must seriously deform near the perturbed hyperbolic fixed point. As a result, particle motions in the vicinity of the hyperbolic fixed point become very complicated. The Poincaré map near the region produces so called the horseshoe map and it is an evidence of chaos (the Smale-Birkhoff Homoclinic Theorem (10)).

**LOBE DYNAMICS AND VOLUMETRIC TRANSPORTS**

**Definition and Some Remarks**

Lobe dynamics will be first discussed via Fig. 9, showing representative lobes with some notations, based on the Poincaré section with the perturbed unstable and stable manifolds at \( \phi_0 = 0 \), where the reflection symmetry about \( y \) holds. The figure corresponds to the case \( \beta = 0.05 \). The aspect ratio in the figure has been intentionally adjusted to show distinct regions and configuration of lobes more clearly. The thin solid curve and the thin dashed curve indicate the perturbed unstable manifold and the stable manifold, respectively.

Some explanations on the notations and definitions are in order (4). One of the intersection points between the two manifolds is denoted by \( p.i.p. \), the primary intersection point. Bold curves connecting the p.i.p. and the perturbed hyperbolic fixed point \( p_\beta \) along the unstable and the stable manifolds define the boundary between the three distinct regions, \( A_L, A_R \) and \( A_o \). The subscript \( L, R \) and \( O \) indicate the left, right and outer regions, respectively, \( M \) denotes the forward Poincaré map on the manifold, i.e. \( M = P_{q_0} \). For example, the lobe \( D_L \) moves to MD's and the lobe \( E_R \) moves to \( ME_R \) after one period. The lobe denoted by \( E_L \), which initially resides in \( A_O \), enters into \( A_L \) after one period (or, \( E_R \) enters into \( A_R \)). Therefore the lobe \( E \) is called the entrainment. Similarly, the lobe \( D_L \) (or \( D_R \)) is called the detrainment, since the lobe \( D_L \) inside \( A_L \) (or \( D_R \) inside \( A_R \)) enters into \( A_O \) after one period. The two lobes \( D_L \) and \( E_L \) (or \( D_R \) and \( E_R \)) constitute one period. (In general, \( M^k D_L \) and \( M^k E_L \) constitute one period for all integer \( k \).)

Regarding material transports, the amount detrained from the region \( A_L \) (or \( A_R \)) during each cycle is the volumetric flow rate through the lobe \( D_L \) (or \( D_R \)), denoted by \( F(D_L) \) (or \( F(D_R) \)), since the two-dimensional map preserves the volumetric flow rate (Eq 16). Similarly, the amount entrained into the region \( A_L \) (or \( A_R \)) during one period is the volumetric flow rate through \( E_L \) (or \( E_R \)), denoted by \( F(E_L) \) (or \( F(E_R) \)). From
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Fig. 9. Configuration of the perturbed unstable and stable manifolds at \( \phi_0 = 0 \).

...the volume conservation property of the Poincaré map and from the invariance of the manifolds.

\[
F(D_R) = F(M^k D_R), \quad F(E_R) = F(M^k E_R). \tag{26}
\]

for all integers \( k = \pm 1, \pm 2, \ldots \). The same arguments can be applied to the lobes in the left half by the symmetry (Eq 24). In addition, one can obtain the relation between the left half lobe flow rate and right half lobe flow rate by applying the symmetry and Eq 26:

\[
F(M^k D_R) = F(M^l E_L), \quad F(M^k D_L) = F(M^l E_R). \tag{27}
\]

for all integers \( k, l = 0, \pm 1, \pm 2, \ldots \). The numerically calculated flow rates through the lobes and the lobe areas in the right half are listed in Table 2. They have been evaluated by the linear triangular discretization of the lobes. As an example, the triangular discretization for the lobe \( D_R \) is shown in Fig. 10. The flow rate through the region \( D \) is evaluated by the quintic-order Gaussian quadrature integral (11). In Table 2, one can see that the area of the lobe does not preserved, but the flow rate through the lobe is preserved (with some numerical errors due to inaccuracy in the numerical particle tracing and the triangular discretization).

### Volumetric Transports Between Distinct Regions

Transports in this homoclinic tangle are composed of three parts: (i) Transports between \( A_R \) and \( A_O \), (ii) Transports between \( A_L \) and \( A_O \), and (iii) Transports between \( A_R \) and \( A_L \). In this section, these three transports will be discussed in detail. Before doing this, let us consider the Poincaré section in Fig. 11 at the different phase \( \phi_0 = 1/2 \) of the same parametric composition. In fact, the Poincaré section in Fig. 11 is half a period advance of Fig. 9. We also intentionally adjusted the aspect ratio to see detailed structure of lobes. The p.i.p. in each half moves by half a period compared with Fig. 9. Again, the bold curve along the unstable manifold and the bold dashed curve along the stable manifold define the boundaries between \( A_L \) and \( A_O \) and between \( A_R \) and \( A_O \). The Poincaré map at \( \phi_0 = 1/2 \) has the reflection symmetry about \( y \) as well so that lobe motions in the left half can be easily obtained from those in the right half by interchanging \( R \) with \( L \), \( M^k \) with \( M^{-k} \), and \( D \) with \( E \). Figure 12 shows more detailed lobe motions by indicating five iterates for four main lobes: \( D_R, E_R, D_L, \) and \( E_L \). Below we consider volumetric transports between the distinct regions \( A_R, A_L, \) and \( A_O \) in details.

#### Transports Between \( A_R \) and \( A_O \)

For transports between \( A_R \) and \( A_O \), one needs to consider the lobe and \( D_R \) and \( E_R \) their positive and negative iterates. During one period, the only material volume that is transported from \( A_R \) to \( A_O \) is \( F(D_R) \), and the only material volume that is transported from \( A_O \) to \( A_R \) is \( F(E_R) \) (Fig. 11). Denoting these transports by \( F_{R,O} \) and \( F_{O,R} \) respectively, one can obtain

\[
F_{R,O} = F(D_R), \quad F_{O,R} = F(E_R) \tag{28}
\]

However, not all the materials that entrained into \( A_R \) remain in \( A_R \). Let us consider the intersection of the

### Table 2. Flow Rates Through the Lobes and the Lobe Areas on the Right Half in Fig. 9.

<table>
<thead>
<tr>
<th>Lobe</th>
<th>Flow rate through the lobe</th>
<th>Area of the lobe</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_R )</td>
<td>0.0256632</td>
<td>0.0312064</td>
</tr>
<tr>
<td>( E_R )</td>
<td>0.0198248</td>
<td>0.0215880</td>
</tr>
<tr>
<td>( MDR )</td>
<td>0.0255300</td>
<td>0.0783345</td>
</tr>
<tr>
<td>( ME_R )</td>
<td>0.0209457</td>
<td>0.0705066</td>
</tr>
</tbody>
</table>
two lobes $M_{ER}$ and $M^{-1}D_R$, denoted by $M_{ER} \cap M^{-1}D_R$ (Figs. 11 and 12). By taking inverse Poincaré map $M^{-1}$, the intersection is mapped to $E_R \cap M^{-2}D_R$, which is located in $A_O$, and it will enter into $A_R$ on the next iterate, since it is a subset of the lobe $E_R$. On the other hand, taking the forward Poincaré map $M$ on $M_{ER} \cap M^{-1}D_R$, the intersection is mapped to $M^2E_R \cap D_R$, which will enter into $A_O$ on the next iterate. The three regions, in the right half of Fig. 12, represent these intersections. The intersection $E_R \cap M^{-2}D_R$, which will be transported from $A_O$ into $A_R$ on the next period, will return to $A_O$ after three periods. In addition, there must be infinite number of intersections that show the similar behavior, and, in general, they can be written as

$$E_R \cap M^{-k-1}D_R, \ k = 1, 2, 3... \ (29)$$

The intersections in Eq 29 will return to $A_O$ after $(k + 2)$ periods. Two of them are illustrated in Fig. 12. Let us consider the intersections denoted by $M_{ER} \cap M^{-2}D_R$, $M^2E_R \cap M^{-1}D_R$, and $M^2E_R \cap M^{-2}D_R$. The first two intersections are the first and the second iterates of $E_R \cap M^{-3}D_R$; and the last intersection is the second iterate of $E_R \cap M^{-4}D_R$. The volumetric flow rate through the intersections in Eq 29 can represent the escape statistics (6). These flux have been evaluated

and listed in Table 3. We mention two remarks here: (i) There seem to be some numerical errors in evaluating flow rates through lobe intersections, as one can see from the first and the second rows in Table 3. But this kind of error seems inevitable, owing to numerical errors in the finite element method. (ii) There must be intersections that enter into $A_R$ and escape from $A_R$ on some later time (Eq 29) and then enter again into $A_R$ according to the general statement presented by Rom-Kedar and Wiggins (4). Within the limit of the numerical accuracy in this work, such lobes could not be found, even though they must exist.

**Transports Between $A_L$ and $A_O$:** These transports are easily obtained from the symmetry relation (Eq 24). As mentioned earlier, one can obtain the transports by interchanging $R$ with $L$, $M_k$ with $M^{-k}$, and $D$ with $E$. For example, the intersection $M^kD_L \cap M^1E_L$ is symmetric with $M^{-k}E_R \cap M^{-1}D_R$ about $y$ axis. Therefore, one can get the following relations for the material transports:

$$F\left(M^kD_L \cap M^1E_L\right) = F\left(M^{-k}E_R \cap M^{-1}D_R\right) \quad (30)$$

With this in mind, the procedures are pretty much similar to the previous case. During one period, the

![Fig. 11. Configuration of the perturbed unstable and stable manifolds at $\phi_0 = 1/2$.](image-url)
Fig. 12. Detailed lobe transports in Fig. 11.

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only material volume that is transported from \( A_L \) to \( A_O \); i.e., \( F_{L,O} \) is \( D_L \) and the only material volume that is transported from \( A_O \) to \( A_L \), i.e., \( F_{O,L} \) is \( E_L \):

\[
F_{L,O} = F(D_L), \quad F_{O,L} = F(E_L)
\]

(31)

Also, there must be infinite number of intersections that enter into \( A_L \) from \( A_O \) and return to \( A_O \). These intersections can be written as \( E_L \cap M^{-k-1} D_1 \) (\( k = 1, 2, 3, \ldots \)) and they return to \( A_O \) after \( (k + 2) \) periods. In Fig. 12, one can see the six intersections of this kind: \( E_L \cap M^{-1} D_1, M^{-2} E_L \cap D_1, \ldots \). For the first three intersections (in the left half in Fig. 12), \( k = 1 \); for the next two ones, \( k = 2 \); for the last one, \( k = 3 \). Volumetric transports through these lobes are identical to those listed in Table 3 because of the symmetry relation in Eq 30.

Transports Between \( A_L \) and \( A_R \): Transports in this case are more complicated than the previous two cases. We start with the transports from \( A_L \) to \( A_R \) during one period, i.e., \( F_{L,R} \). Let us investigate three consecutive intersections in Fig. 12: \( D_L \cap M^{-1} E_R \) in \( A_L \), \( MD_L \cap M^{-1} E_R \) in \( A_O \) (just above the hyperbolic fixed point), and \( M^2 D_L \cap E_R \). Since the last intersection \( M^2 D_L \cap E_R \) will enter into \( A_R \) on the next period, the first intersection \( D_L \cap M^{-2} E_R \) that resides in \( A_L \) moves to \( A_R \) after three periods. In general, there must be infinite number of intersections that moves from \( A_L \) to \( A_R \); and they can be written as \( D_L \cap M^{-k-1} E_R \) (\( k = 1, 2, 3, \ldots \)). The intersection \( D_L \cap M^{-k-1} E_R \) in \( A_L \) enters into \( A_R \) after \( (k + 2) \) periods. One of these intersections, denoted by \( MD_L \cap M^{-2} E_R \), is indicated in Fig. 12. Since the transport process in the Poincaré section occurs consecutively, all the intersections \( \bigcup_{k=1}^{\infty} [D_L \cap M^{-k-1} E_R] \) can be regarded as material transports during one period. Thus, \( F_{L,R} \) has the following form:

\[
F_{L,R} = \sum_{k=1}^{\infty} F(D_L \cap M^{-k-1} E_R)
\]

(32)

Second, let us consider the transports from \( A_R \) to \( A_L \), i.e., \( F_{R,L} \). Because of lack of symmetry of the CS system.
F_{R,L} is totally different from F_{L,R}. Let us consider the intersection MD_R \cap M^{-2} E_L in the lower side in Figs. 11 and 12. If we take M^{-1}, it moves to D_R \cap M^{-3} E_L that should reside in A_R. Or, if we take M^{2}, then it moves to M^{3}D_R \cap E_L that will be located in A_L after one period. That is, the materials in the intersection D_R \cap M^{-k-2} E_L must be transported from A_R to A_L after four periods. Again there must be an infinite number of intersections; and they can be written as D_R \cap M^{-k-2} E_L (k = 1, 2, 3,...). The intersection D_R \cap M^{-k-2} E_L is transported from A_R to A_L after (k + 3) periods. Moreover, these transports are consecutive so that one can obtain the following material transports from A_R to A_L during one period:

$$F_{R,L} = \sum_{k=1}^{\infty} F(D_R \cap M^{-k-2} E_L).$$

(33)

**Effects of Perturbation Strength**

In this subsection, the effects of the perturbation strength \( \beta \) will be discussed on lobe configurations and related material transports. Figure 13 shows the Poincaré section for five representative \( \beta \) values: (a) \( \beta = 0.02 \), (b) 0.04, (c) 0.06, (d) 0.08, and (e) 0.1. They all evaluated at \( \phi_0 = 1/2 \). Again, the unstable manifolds are indicated by the solid curves and the stable manifolds by the dashed curves. The locations of the intersection points between the two manifolds (transverse homoclinic points) have not been changed a lot; therefore, we used the same labeling policy to indicate the lobes (see Fig. 13d, for example). The first observation is that, as the value of \( \beta \) increases, the homoclinic tangles are more and more distorted from the unperturbed case. As a result, the sizes of the lobes and the sizes of their intersections are increased and one can expect more material transports as \( \beta \) increases. Another observation is the occurrence of the intersection \( M^{-1}E_L \cap MD_R \) that can be found when \( \beta \) is 0.06 or larger (Fig. 13c-e). Even with \( M^{-1}E_L \cap MD_R \) intersection, the material transports in Eqs 28 and 32 are still valid, except for the representation in Eq 33. With the existence of the intersection \( M^{-1}E_L \cap MD_R \), the expression of \( F_{R,L} \) (Eq 33) becomes completely symmetric with \( F_{L,R} \) (Eq 32); i.e.,

$$F_{R,L} = \sum_{k=1}^{\infty} F(D_R \cap M^{-k-1} E_L).$$

(34)

even though the flow rates through the intersections are different.

The flow rate through the four major lobes (hatched regions in Fig. 13d) - \( D_R, E_R, M^{-1}E_R \cap MD_L, M^{-1}E_L \cap MD_R \) - are plotted in Fig. 14. Each of them can be regarded as the approximate value representing \( F_{R,O}, F_{L,O}, F_{L,R}, \) and \( F_{L,L} \). From Fig. 14, one can see that all the four representative volumetric transports increase with \( \beta \) and, moreover, their dependency seems to be almost linear as long as \( \beta \) is small.

In case of \( \beta = 0.1 \), the fraction of \( F(D_R), F(E_R), F(M^{-1}E_R \cap MD_L), F(M^{-1}E_L \cap MD_R) \) to the total flow rate over the cross section are 3.33%, 3.08%, 1.64%, and 1.18%, respectively. Since there are symmetric transports between the left half and the right half, the approximate total volumetric transports during one period is about 15.6% of the total flow rate (15.6% = 2 (3.33% + 2.08%) + 1.64% + 1.18%). Evidently, they are the additional transport due to chaos. If there is no perturbation, these kinds of transports cannot be present. Therefore, one might regard these flow rates through the four major lobes as a scalar measure of mixing in the CS system. Figure 15 shows this scalar measure (the fraction of the approximate total volumetric transport to the total flow rate) in terms of the perturbation strength \( \beta \). The graph indicates that the total volumetric transport is proportional to \( \beta \), as long as the value of \( \beta \) is small (\( \beta \leq 0.1 \)).

**CONCLUSION**

In this study, we discussed volumetric transports in the chaotic region of the CS system in terms of the lobe dynamics. The two-dimensional map was introduced to reduce the number of phase variables and its four kinematic properties (P1-P4) were investigated with those of the Poincaré map; they provided a mathematical framework for analyses of lobe dynamics. The analysis has begun with the description of the method how to find the location of the hyperbolic fixed point and the associated eigenvectors from the Poincaré map in the perturbed system. The graphical method has been used for this purpose. The perturbed unstable and stable manifolds are then obtained numerically. We presented the manifold structures and the associated homoclinic tangle of the perturbed CS system in the three-dimensional physical space. With the appropriate definitions for lobes in the Poincaré section, volume conservation in lobe motion and the associated symmetry have been discussed first. Then, six independent volumetric transports between three distinct regions (\( A_R, A_L \), and \( A_P \)) during one period have been described in detail. In the derivation, the principles we used were the invariance of the manifold, symmetry, the orientation preservation, and the volume conservation properties of the Poincaré map. Finally, the effects of perturbation strength on the lobe configuration and related volumetric transports have been discussed. With increasing strength of perturbation, the flow rate through the lobes increases almost linearly under small values of the perturbation strength. We also found the lobe configurations in case of \( \beta \) greater than 0.6 are different from those of \( \beta \leq 0.5 \).

The importance of this study lies in the three-dimensional nature. This is the first study on lobe dynamics in three-dimensional volume-preserving systems. In terms of the practical importance, lobe dynamics clearly shows how the material volumes are transported between the regions and how much material is transported in the CS system. The flow rate through the lobe across the regions might be used as a scalar measure of mixing in
the chaotic systems. However, two important issues are left untouched in this study, mainly because of the numerical accuracy: (i) Overall material conservation in $A_R$ and $A_L$, and (ii) Transport relations in terms of the period $n$. For the problem (i), one can see that the flow rate through the detrainment is not the same as the flow rate through the entrainment in $A_R$: $F(D_R) > F(E_R)$ (Table 2). (The exactly opposite phenomenon occurs in $A_L$.) Then one might ask a question how the material volume in $A_R$ (or $A_L$) is preserved, since the outgoing volume flow rate of $A_R$ is greater than the incoming flow rate. The answer to this question can be

Fig. 13. Lobe configuration with respect to the strength of perturbation $\beta$. (a) $\beta = 0.02$; (b) 0.04; (c) 0.06; (d) 0.08; (e) 0.1.
found in the nature of the flow, i.e. the absence of symmetry in the CS system. In other words, one can understand that the non-symmetric transports between $A_R$ and $A_L$ in recognition of $F_{L,R} > F_{R,L}$ (see Eqs 32 and 33). This difference might compensate for the difference between $F_{R,O}$ and $F_{L,O}$ in $A_R$ (or between $F_{L,O}$ and $F_{O,L}$ in $A_L$) to preserve overall volume conservation. Unfortunately, however, our numerical computation is not accurate enough to show this fact, since this kind of analysis (very large number of numerical integrations) inevitably suffers from accumulation of numerical errors, especially in the three-dimensional system. The problem (ii) is also closely related to (i): in fact, they are more or less both sides of a coin. Once one has the volume conservation of each region, then the general transports at period $n$ from one region to another are readily achieved. (See the general equations for conservation of areas and conservation of species (4)).

Fig. 14. Volumetric transports through the four major lobes with respect to the strength of perturbation $\beta$.  

Fig. 15. Fractions of approximate total volumetric transport during one period in terms of the perturbation strength $\beta$.  

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APPENDIX

Let us derive Eq 8 from the symmetry of the velocity field (Eq 7). A material point $p^+ = (x_1, y_1, \phi_1)$ moves to

$$ F p^+ = (x_1 + u_1 \delta t, y_1 + v_1 \delta t, \phi_1 + \omega_1 \delta t) $$

(A1)
after the infinitesimal time step $\delta t$. As indicated in Eq 9, $F$ denotes the forward time integration and $(u_1, v_1, \omega_1)$ is the fluid velocity at $p^+$. In the same way, the point before $\delta t$ is

$$ B p^- = (x_1 - u_1 \delta t, y_1 - v_1 \delta t, \phi_1 - \omega_1 \delta t) $$

(A2)

where $B$ denotes the time-reversal mapping. Consider the material point $p^- = (x_1, y_1, 1 - \phi_1)$, which is $S_{xy} S_{y\phi}$ symmetric to the point $p^+$. Let us evaluate the forward and backward time integrations of the point $p^-$. Comparing Eqs A1 with A4 (or Eq A2 with A3), one can find that

$$ B p^- = S_{xy} S_{y\phi} p^+ $$

(A3)

$$ F p^- = F S_{xy} S_{y\phi} p^+ $$

(A4)

Comparing Eqs A1 with A4 (or Eq A2 with A3), one can find that $B p^-$ is $S_{xy} S_{y\phi}$ symmetric to $F p^+$ (or $F p^-$ is $S_{xy} S_{y\phi}$ to $B p^+$), which verifies Eq 8.

ACKNOWLEDGMENT

The authors wish to thank the Korea Research Foundation (1998-018-E00065) and the Ministry of Science and Technology of Korea for the partial support via the National Research Laboratory Program (2000-N-NL-01-C-148).

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