Chaotic Advection in Thin Films?

Jean-Luc Thiffeault and Khalid Kamhawi

Department of Mathematics
Imperial College London

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A thin layer of fluid flowing down an inclined substrate. Reduce to two-dimensional problem by asymptotic expansion: PDE for the height field. But the velocity field is still three-dimensional, with a nontrivial vertical component. Steady three-dimensional flows can exhibit chaotic trajectories. This leads to fluid particles rapidly decorrelating: good for mixing. Can suitable substrate shapes lead to good horizontal mixing?
Strategy

- Thin-layer expansion in the direction normal to the substrate.
- For simplicity, assume steady flow.
- Use non-orthogonal coordinates, since globally orthogonal coordinates do not usually exist.
- Correct velocity field to satisfy kinematic constraints — this is crucial for particle advection.
- Integrate trajectories and make Poincaré sections in a spatially periodic domain.
Aside: Inviscid Theory

Inertia is great for chaos...

...but particle trajectories (characteristics) cross all over the place. Fix as Sam Howison did yesterday?
Coordinate System

Surface \( y = \eta(x^1, x^2) \)

Substrate \( y = 0 \) at position \( X(x^1, x^2) \)

\[
\mathbf{r}(x^1, x^2, y) = \mathbf{X}(x^1, x^2) + y \mathbf{\hat{e}}_3(x^1, x^2)
\]

\[
\mathbf{e}_\alpha = \frac{\partial \mathbf{X}}{\partial x^\alpha} = \partial_\alpha \mathbf{X} ; \quad \mathbf{\hat{e}}_3 = (\mathbf{e}_1 \times \mathbf{e}_2) / \| \mathbf{e}_1 \times \mathbf{e}_2 \| 
\]
Coordinate Vectors in the Bulk

Vectors corresponding to coordinates in the fluid:

\[ \tilde{\mathbf{e}}_\alpha = \partial_\alpha \mathbf{r} = \mathbf{e}_\alpha - y \ K^\beta_\alpha \mathbf{e}_\beta, \quad \tilde{\mathbf{e}}_3 = \mathbf{e}_3 = \hat{\mathbf{e}}_3 = \frac{\partial \mathbf{r}}{\partial y}, \]

- Summation of repeated indices;
- Greek indices always take the value 1 or 2 (never 3);
- Roman indices always take the value 1, 2, or 3;
- Tilde quantities are evaluated in the ‘bulk’ (away from the substrate), and thus depend on \( y \).

Curvature tensor \( K^\beta_\alpha \) defined by

\[ \partial_\alpha \hat{\mathbf{e}}_3 = -K^\beta_\alpha \mathbf{e}_\beta, \]

Note that the \( \mathbf{e}_\alpha \) are not necessarily orthogonal or normalised.
Metric Tensor

To express the length of vectors in the \((x^1, x^2, y)\) coordinates, we need the metric tensor \(\tilde{g}_{\alpha\beta}\)

\[
\tilde{g}_{ij} = \tilde{e}_i \cdot \tilde{e}_j = \begin{pmatrix} \tilde{G}_{\alpha\beta} & 0 \\ 0 & 1 \end{pmatrix}
\]

where

\[
\tilde{G}_{\alpha\beta} := \tilde{e}_\alpha \cdot \tilde{e}_\beta = G_{\alpha\beta} - 2yK_{\alpha\beta} + y^2 K_{\alpha\gamma}K_{\gamma\beta},
\]

\[
G_{\alpha\beta} := e_\alpha \cdot e_\beta.
\]

The full metric \(\tilde{g}_{ij}\) is block-diagonal. The \(2 \times 2\) metric \(G_{\alpha\beta}\) is the surface metric, and \(\tilde{G}_{\alpha\beta}\) is its extension into the bulk of the fluid. We have used the surface metric to lower an index on \(K\):

\[
K_{\alpha\beta} = G_{\alpha\gamma}K_{\beta\gamma}
\]
The Dilatation of the Coordinates

A crucial quantity is the determinant of the metric,

\[ \tilde{\omega} = (\det \tilde{G}_{\alpha\beta})^{1/2} = \tilde{\omega} w, \quad w = (\det G_{\alpha\beta})^{1/2}, \]

where

\[ \tilde{\omega} = 1 - \kappa y + \mathcal{G} y^2, \]

and

\[ \kappa = K_\alpha^\alpha \text{ mean curvature;} \]
\[ \mathcal{G} = \det K_\alpha^\beta \text{ Gaussian curvature.} \]

The volume element is given by by \( \tilde{\omega} w \, dx^1 \, dx^2 \, dy \).

If \( \tilde{\omega} \) becomes negative, then substrate normals cross within the fluid and the coordinate system becomes invalid. OK as long as

\[ 0 \leq y < \left\{ \max(k_1, k_2, 0^+) \right\}^{-1}, \quad k_{1,2} := \frac{1}{2} \left( \kappa \pm \sqrt{\kappa^2 - 4\mathcal{G}} \right), \]

where \( k_1 \) and \( k_2 \) are the principal curvatures.
There are three types of quantities in our development:

1. Quantities with a \textit{tilde} (e.g., $\tilde{\epsilon}_\alpha$ and $\tilde{w}$) are evaluated between the substrate and the free surface and are functions of $(x^1, x^2, y)$.

2. Quantities with an \textit{overbar} (e.g., $\bar{\epsilon}_\alpha$ and $\bar{w}$) are evaluated on the free surface $y = \eta(x^1, x^2)$ and are functions of $(x^1, x^2)$.

3. \textit{‘Bare-headed’} quantities (e.g., $e_\alpha$ and $w$) are evaluated on the substrate $y = 0$ and are functions of $(x^1, x^2)$, or they are quantities that do not depend on $y$ at all (e.g., $\hat{e}_3$).
Mass Conservation

We introduce a steady velocity field

\[ \mathbf{u} = \tilde{u}^\alpha \hat{e}_\alpha + \tilde{v} \hat{e}_3. \]

Mass conservation is imposed via the divergence-free condition, \( \nabla \cdot \mathbf{u} = 0 \); in terms of our coordinates,

\[ \partial_\alpha (\tilde{w} \tilde{u}^\alpha) + \frac{\partial}{\partial y} (\tilde{w} \tilde{v}) = 0. \]

We integrate this from 0 to \( \eta \) and use the no-throughflow condition \( \tilde{v}(x^1, x^2) = 0 \) to get

\[ \tilde{w} \tilde{v} = - \int_0^\eta \partial_\alpha (\tilde{w} \tilde{u}^\alpha) \, dy = \tilde{w} \tilde{u}^\alpha \partial_\alpha \eta - \partial_\alpha \int_0^\eta (\tilde{w} \tilde{u}^\alpha) \, dy. \]
Mass Conservation (cont’d)

Now we use the kinematic boundary condition at the top surface,

\[ \bar{u}^\alpha \partial_\alpha \eta = \bar{v}, \]

to find

\[ \partial_\alpha \left( w \bar{q}^\alpha \right) = 0, \]

where the flux vector is

\[ \tilde{q}^\alpha(x^1, x^2, y) := \int_0^y \tilde{\omega} \tilde{u}^\alpha dy, \quad \bar{q}^\alpha(x^1, x^2) = \tilde{q}^\alpha(x^1, x^2, \eta). \]

If we divide through by \( w \), we recognise the covariant divergence,

\[ \nabla_\alpha \bar{q}^\alpha = 0. \]

Note that there are no assumptions on the thinness of the layer: everything is exact.
Dynamical Equations

We now assume $u$ satisfies the Stokes equation,

$$\Delta u = \nabla p - \hat{g},$$

where $p$ is the pressure and $\hat{g}$ is a unit vector in the direction of gravity. The velocity satisfies the boundary conditions

- $u = 0$ at $y = 0$ no-slip at substrate
- $t_\alpha \cdot \tau \cdot \hat{n} = 0$ at $y = \eta$ tangential stresses at free surface
- $-p + \hat{n} \cdot \tau \cdot \hat{n} = \sigma \kappa_{surf}$ at $y = \eta$ normal stress at free surface

where

$$\tau := \nabla u + (\nabla u)^T$$

is the deviatoric stress, $\hat{n}$ is the unit normal to the surface, $t_\alpha$ are tangents to the surface, and $\kappa_{surf}$ is the mean curvature of the surface. All quantities are dimensionless.
Small-parameter Rescaling

The time has come to make the layer thin: we do this by assuming that horizontal scales vary slowly:

\[ x^\alpha = \varepsilon^{-1} x^\alpha^*, \quad \tilde{v} = \varepsilon \tilde{v}^*, \quad p = \varepsilon^{-1} p^*, \quad \sigma = \varepsilon^{-2} \sigma^*. \]

Everything else is of order unity, including vertical scales. We immediately drop the * superscripts, and expand the fields as

\[ \tilde{u}^\alpha = \tilde{u}^\alpha_{(0)} + \varepsilon \tilde{u}^\alpha_{(1)} + \ldots, \]
\[ \tilde{p} = \tilde{p}_{(0)} + \varepsilon \tilde{p}_{(1)} + \ldots. \]

Note that we leave \( \tilde{v} \) unexpanded (more on this later).
Order $\varepsilon^0$

At order $\varepsilon^0$, the velocity field and pressure satisfy

$$\frac{\partial^2 \tilde{u}^\alpha_{(0)}}{\partial y^2} = \partial^\alpha \tilde{p}_{(0)} - \hat{g}_s^\alpha,$$

$$\frac{\partial \tilde{p}_{(0)}}{\partial y} = 0,$$

where $\partial^\alpha = G^{\alpha\beta} \partial_\beta$. These are readily integrated to give

$$\tilde{u}^\alpha_{(0)} = -\frac{1}{2} \left( \hat{g}_s^\alpha + \sigma \partial^\alpha \kappa \right) y(y - 2\eta),$$

$$\tilde{p}_{(0)} = -\sigma \kappa,$$

where the boundary conditions have been applied.
Order $\varepsilon^1$

At order $\varepsilon$,

\[
\frac{\partial^2 \tilde{u}_{\alpha}^{(1)}}{\partial y^2} = (\kappa \delta_{\beta}^{\alpha} + 2 K_{\beta}^{\alpha}) \frac{\partial \tilde{u}_{\beta}^{(0)}}{\partial y} + \partial_{\alpha} \tilde{p}_{(1)} + 2y K_{\beta}^{\alpha} \partial_{\beta} \tilde{p}_{(0)} - y \hat{g}^{\beta}_{s} K_{\beta}^{\alpha},
\]

with solution

\[
\tilde{u}_{\alpha}^{(1)} = A_{\alpha}^{1} y (y - 2\eta) + B_{\alpha}^{1} y (y^2 - 3\eta^2)
\]

where the coefficients $A_{\alpha}^{1}$ and $B_{\alpha}^{1}$ involve the substrate curvature tensor and gradients of the mean curvature.

In fact, the $\varepsilon^0$ solution can be incorporated to the coefficient $A$, to give

\[
\tilde{u}_{\alpha} = A^{\alpha} y (y - 2\eta) + B^{\alpha} y (y^2 - 3\eta^2).
\]
The Mass Flux

The horizontal velocity field is sufficient to find the mass flux,

\[ \bar{q}^\alpha = \int_0^\eta \tilde{\omega} \tilde{u}^\alpha dy = \int_0^\eta (1 - \varepsilon \kappa y)\tilde{u}^\alpha dy + \mathcal{O}(\varepsilon^2), \]

\[ = \bar{q}_{\text{grav}}^\alpha + \bar{q}_{\text{surf}}^\alpha, \]

\[ \bar{q}_{\text{grav}}^\alpha = \frac{1}{3} \eta^3 \left\{ \hat{g}_s^\alpha - \varepsilon \hat{g}_s^\beta (\kappa \delta_\beta^\alpha + \frac{1}{2} K_\beta^\alpha) \eta + \varepsilon \hat{g}_y \partial^\alpha \eta \right\} \]
\[ + \varepsilon^2 \frac{1}{120} \eta^4 \kappa \left\{ \eta \hat{g}_s^\beta (9 \kappa \delta_\beta^\alpha + 11 K_\beta^\alpha) - 25 \hat{g}_y \partial^\alpha \eta \right\} + \mathcal{O}(\varepsilon^2), \]

\[ \bar{q}_{\text{surf}}^\alpha = \frac{1}{3} \sigma \eta^3 \left\{ \partial^\alpha \kappa_{\text{surf}} - \varepsilon \eta \kappa \partial^\alpha \kappa + \frac{1}{2} \varepsilon \eta K_\beta^\alpha \partial^\beta \kappa \right\} \]
\[ + \varepsilon^2 \frac{1}{120} \sigma \eta^4 \kappa \left\{ 9 \eta \kappa \partial^\alpha \kappa - 14 \eta K_\beta^\alpha \partial^\beta \kappa - 25 \partial^\alpha (\kappa_2 \eta + \Delta \eta) \right\} + \mathcal{O}(\varepsilon^2), \]

Note that we’ve kept some second-order terms but not others. The above fluxes are only asymptotic to order \( \varepsilon^1 \), but they preserve the free-surface kinematic BC to all orders...
The Vertical Velocity

The vertical velocity is obtained from mass conservation:

$$\tilde{v} = -\frac{1}{1 - \varepsilon \kappa y} \int_0^y \partial_\alpha ((1 - \varepsilon \kappa y) \tilde{u}^\alpha) \, dy,$$

not expanded in $\varepsilon$.

Mass conservation follows from using this form for $\tilde{v}$, and the free-surface kinematic boundary condition is satisfied exactly if the second-order terms are included in the flux.

The exact kinematic constraints are crucial for particle advection:

- Mass preservation prevents the existence of attractors in the flow where particles bunch up.
- The kinematic boundary condition prevents particles escaping from the top surface of the flow.

These are only exact to the extent that $\nabla_\alpha \bar{q}^\alpha = 0$ is satisfied numerically, but this is a much smaller error than $\varepsilon^2$. 
The Shape of the Substrate

The shape of the bottom substrate is given by the vector $\mathbf{X}(x^1, x^2)$. The generality of the formulation allows us to choose $(x^1, x^2)$ as cylindrical (or any other) coordinates, which could be used to describe a ‘bumpy fibre.’ However, we stick to Cartesian and write

$$\mathbf{X}(x^1, x^2) = (x^1, x^2, f(x^1, x^2))^T,$$

which rules out a multivalued substrate (no overhangs). $f(x^1, x^2)$ gives the vertical height of the substrate at $(x^1, x^2)$. We assume the substrate is periodic in both directions. The flow is driven by the tilt $\theta$ of the gravity vector with respect to the substrate:

$$\hat{\mathbf{g}} = (\sin \theta \cos \phi \quad \sin \theta \sin \phi \quad - \cos \theta)^T$$
Numerical Solution

We now solve $\nabla_{\alpha} \bar{q}^\alpha = 0$ for the height field $\eta(x^1, x^2)$. The pictures below are for

$$f(x^1, x^2) = f_0 \sin(2\pi x^1) \sin(2\pi x^2).$$

Parameters: $f_0 = 0.05$, $\varepsilon = 0.06$, $\theta = 0.1$, $\phi = 0$, $\sigma = 0$. 
Numerical Error in Kinematic BC

For a numerical resolution of $100 \times 100$,

<table>
<thead>
<tr>
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<th>Uncorrected</th>
<th>Corrected</th>
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</thead>
<tbody>
<tr>
<td>Kinematic BC error</td>
<td>$4 \times 10^{-4}$</td>
<td>$2 \times 10^{-9}$</td>
</tr>
<tr>
<td>Incompressibility error</td>
<td>$4 \times 10^{-3}$</td>
<td>$9 \times 10^{-7}$</td>
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The factor of $10^4$–$10^5$ improvement makes a huge difference when doing particle advection: it means that particles can skirt the surface without escaping.
• The particle explores the top and bottom of the layer.
• It is confined in a narrow region in $x_2$. 
**Poincaré Section**

![Poincaré Section Diagram]

x1=0

- **Axes:**
  - x1: 0 to 1
  - y: 0 to 0.07
  - x2: 0 to 1

- **Trajectories:**
  - Blue line
  - Red dots

- **Grid:**
  - Gridlines are present at intervals of 0.2 for x1 and x2, and 0.01 for y.

**Key Points:**
- The diagram illustrates a Poincaré section for a dynamical system.
- The section is taken at x1=0, showing the system's behavior at that point.
- The blue line represents the trajectory of the system, while red dots indicate specific points of interest.

**Conclusion:**
- Analysis of the Poincaré section can provide insights into the system's stability and periodicity.

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**References:**
- [Dynamical Systems Theory](https://www.jstor.org/stable/10.1007/978-3-030-50737-6)
Breaking the Symmetry

\[ f(x^1, x^2) = f_0 \left\{ \sin(2\pi x^1) \sin(2\pi x^2) + \delta \sin(4\pi x^2) \right\}, \quad \delta = 0.2 \]

- Two types of trajectories: straight and diagonal.
- Explore a wide range in \( x^2 \).
- The diagonal trajectories are chaotic: ‘jump’ between channels.
Chaotic Poincaré Section

The mixed regular–chaotic phase space is evident in the section:
Conclusions

- Relate substrate properties (curvature tensor) to chaotic features.
- Applications? Coating flows?
- Experiments
- Time-dependence: induce chaotic mixing by vibrating the substrate or sending waves through it.
- Effect of surfactants, surface tension, Marangoni stresses...