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TITLE TRANSPORT OF A PASSIVE TRACER IN TIME-DEPENDENT
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Transport of a passive tracer in time-dependent Rayleigh-Bénard convection

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Abstract

The transport of a passive tracer in a Rayleigh-Bénard cell is considered, when the convection rolls are subject to oscillatory instability. We propose a mechanism for the roll to roll transport and introduce formulae for quantifying the spreading of the tracer, which are valid for as long as the molecular diffusivity can be neglected. A criterion for weighing the effects of diffusivity is discussed, and we provide some example by numerically simulating the flow in presence of molecular diffusivity.

1 Introduction

In the past few years an interesting framework for the application of the dynamical systems point of view to problems in fluid mechanics has arisen. Suppose $v(x, t)$, $x \in R^n$, $n = 2$ or 3 , is a solution of the Navier-Stokes equations, i.e., a velocity field for a fluid flow. Then if one is interested in the dynamics of fluid particle trajectories, the stretching of material interfaces, or a variety of other questions concerning fluid particle kinematics the information is contained in the following dynamical system

$$\dot{x} = v(x, t) , \tag{1}$$

which are simply the equations of motion for fluid particle trajectories in the absence of molecular diffusion. The phase space of this dynamical system is actually the physical space in which the flow occurs.

A more traditional and direct connection can be made with much previous work in dynamical systems theory if the flow is incompressible, two-dimensional, and time

periodic. In this case the velocity field can be derived from a stream function and it takes the form

$$\begin{aligned} \dot{x}_1 &= \frac{\partial \psi}{\partial x_2}(x_1, x_2, t) \\ \dot{x}_2 &= - \frac{\partial \psi}{\partial x_1}(x_1, x_2, t), \quad (x_1, x_2) \in \mathbf{R}^2. \end{aligned} \quad (2)$$

Someone familiar with classical mechanics will recognize (1) as a $1\frac{1}{2}$ degree-of-freedom Hamiltonian system where the stream function, ψ , plays the role of the Hamiltonian. Thus the most natural way to analyze (2) is to consider the associated two-dimensional area-preserving Poincaré map. In this context one can consider KAM tori, cantori, or Smale horseshoes arising which must have an effect on the dynamics of fluid particle trajectories. However, relating these dynamical systems structures to the physics of fluids is not straightforward. Indeed, most of the previous work along these lines has been a classification of fluid mechanical structures via dynamical systems terminology (phenomenology). Part of the problem stems from the fact that a successful analysis of such flows requires more than an application of existing dynamical systems methods. Indeed, it requires the creation of new methods. This is because the goals of dynamical systems theory are very different from those of the theory of convective mixing and transport processes in fluid mechanics. Dynamical systems theory can be described as a study of the asymptotic behavior of a dynamical system and most of the important issues arising in the study of convection and transport involve finite time dynamics. Nevertheless, a variety of new techniques have been developed over the past few years and we want to describe some of them by considering their application to a specific example - a two-dimensional, time periodic cellular flow.

2 The flow

The physical setting is as follows. We consider a convection cell whose horizontal length is much larger than its height and where the convection rolls are aligned along the y -axis. In this situation the flow is essentially two-dimensional and, assuming stress-free boundary conditions and single-mode convection, an explicit form for the velocity field is given by (see Chandrasekhar [3])

$$\begin{aligned}\dot{x} &= \frac{-A\pi}{k} \cos \pi z \sin kx \equiv -\frac{\partial \psi_0(x, z)}{\partial z} \\ \dot{z} &= A \sin \pi z \cos kx \equiv \frac{\partial \psi_0(x, z)}{\partial x}\end{aligned}\tag{3}$$

with

$$\psi_0(x, z) = \frac{A}{k} \sin kx \sin \pi z\tag{4}$$

where A is the maximum vertical velocity, $k = \frac{2\pi}{\lambda}$, and the length measures have been nondimensionalized with respect to the distance between the top ($z = 1$) and bottom ($z = 0$) of the surfaces.

2.1 The Experiments of Solomon and Gollub

If the temperature difference between the top and bottom of the convection cell is increased an additional time-periodic instability occurs resulting in a time-periodic velocity field (see Clever and Busse [4] and Bolton et al. [1]) Solomon and Gollub [7] studied the transport of a **passive scalar** in this situation experimentally. They observed the following

1. There **was a dramatic** enhancement in the enhanced diffusivity as compared to the case of steady convection.
2. Molecular diffusion appeared to play no role in the transport.

3. The flux per period across the roll boundaries depended linearly on the amplitude of the oscillatory instability and was independent of the wavelength of the roll pattern, λ .

It should be evident that the transport of a passive scalar is radically different in the unsteady case as compared to the steady case. In order to understand these differences Solomon and Gollub introduced the following model of the even oscillatory roll instability

$$\begin{aligned}\dot{x} &= -\frac{A\pi}{k} \cos \pi z [\sin kx + \varepsilon k f(t) \cos kx] \equiv -\frac{\partial \psi}{\partial z}(x, z, t) \\ \dot{z} &= A \sin \pi z [\cos kx - \varepsilon k f(t) \sin kx] \equiv \frac{\partial \psi}{\partial x}(x, z, t)\end{aligned}\tag{5}$$

where

$$\begin{aligned}\psi(x, z, t) &= \psi_0(x, z) + \varepsilon \psi_1(x, z, t) \\ &= \frac{A}{k} \sin kx \sin \pi z + \varepsilon A f(t) \cos kx \sin \pi z\end{aligned}\tag{6}$$

and $f(t)$ is a periodic function which we will take as $f(t) = \cos \omega t$. The small parameter ε is proportional to $(R - R_c)^{1/2}$ where R is the Rayleigh number and R_c is the critical Rayleigh number at which the time-periodic instability occurs (see Gollub and Solomon [5] for details). This model has several deficiencies which are discussed in detail [7]. The main two deficiencies are the neglect of higher order modes and a weak three-dimensional component. However, the three-dimensional component is essentially parallel to the roll boundaries and we expect it to play virtually no role in the roll-to-roll transport. In any case, we expect that for ε small (5) accurately models the mechanisms and the physics of roll-to-roll transport. This is born out by the experiments of Solomon and Gollub and the agreement of our analytical predictions with their experiments.

The starting point of our analysis will be the model (5). Motivated by the experimental results of Solomon and Gollub [7] we will specifically address the following four questions:

1. What is the mechanism for roll-to-roll transport?
2. Can we quantify the spreading of a passive scalar from roll to roll?
3. Can we predict the number of rolls invaded by the passive scalar as a function of time?
4. What would be the effects of the addition of a small amount of molecular diffusion?

We begin the analysis with a preliminary remark. As mentioned earlier, we will study the kinematics of the flow by analyzing the Poincaré map is constructed as follows; let $(x(t), z(t))$ be a solution of (5), then the Poincaré map is

$$F_{t_0} \begin{pmatrix} x(t_0) \\ z(t_0) \end{pmatrix} \equiv \begin{pmatrix} x(t_0 + T) \\ z(t_0 + T) \end{pmatrix} \quad (7)$$

where $T = \frac{2\pi}{\omega}$ is the period of the velocity field and $t_0 \in [0, T]$ represents the “initial phase” of the fluid particle trajectory, or, equivalently, the cross-section on which the Poincaré map is defined. It is important to note that the curves that we will be showing in the Poincaré sections to come are *not* fluid particle trajectories, but, rather, invariant surfaces or manifolds in the flow formed by families of fluid particle trajectories that conspire together to form a surface. These invariant manifolds form a “template” in the flow which govern the mixing and convection properties of interest.

3 The Mechanism for Roll-to-Roll Transport

The Poincaré map for (5) appears as in Fig. 1. That is, for stress-free boundary conditions, the stagnation points on the wall become hyperbolic fixed points with their stable and unstable manifolds intersecting transversely to form the heteroclinic tangles as shown in the figure. This heteroclinic tangle lies at the heart of the roll-to-roll transport.

In justifying this statement the first question that should be addressed is “what is the roll” since, as we see from Fig. 1, the boundaries have been so radically deformed under the time-periodic perturbation.

We define the rolls in the time-dependent case by using pieces of stable and unstable manifolds emanating from the hyperbolic stagnation points on the boundaries and ending at heteroclinic points as shown in Fig. 2. As shown in the figure, these distinguished heteroclinic points are chosen to lie on $z = \frac{1}{2}$ (the existence of such points can be easily proven) and are denoted by c_j ; the remainder of the heteroclinic tangle is not shown in order to enhance visual clarity.

Once the roll boundaries are defined we can then address the question of flux across the boundary. We refer the reader to Fig. 3. The heteroclinic point c_0 is used to define the boundary between the rolls labeled R_0 and R_1 . Now the segments of the stable and unstable manifolds between c_0 and $F^{-1}(c_0) \equiv q_0$ form two “lobes” labelled $L_{0,1}$ and $L_{1,0}$ where $L_{0,1}$ enters R_1 under an iterate of F and $L_{1,0}$ enters R_0 under an iterate of F as shown in the figure (hence, the meaning of the subscripts on the notation for lobes should be clear). This is the mechanism for flux. The lobes $L_{1,0}$ and $L_{0,1}$ are referred to as a “turnstile” and they entirely control the transport between R_0 and R_1 . Indeed, it is not hard to prove that a point that enters R_1 from R_0 on the n -th iterate of F must be in $L_{0,1}$ on the $(n - 1)$ -iterate and a point that enters R_0 from R_1 on the n th iterate of F must be in $L_{1,0}$ on the $(n - 1)$ -iterate. Thus the complicated geometry associated with the heteroclinic tangle is a consequence of the dynamics of the two turnstile lobes; a fact that we will exploit more fully shortly. From this discussion it follows that the amount of fluid moving from R_0 (resp. R_1) into R_1 (resp. R_0) during one period, i.e. the flux, is given by $\mu(L_{0,1})$ (resp. $\mu(L_{1,0})$) where $\mu(L_{0,1})$ (resp. $\mu(L_{1,0})$) denotes the area of the lobe $L_{0,1}$ (resp. $L_{1,0}$). Since the fluid is incompressible we have $\mu(L_{1,0}) = \mu(L_{0,1})$. It is

possible to derive an analytical approximation for the lobe area. A Taylor series in ε for the distance between the stable and unstable manifolds is given by

$$d(\tau, \varepsilon) = \varepsilon \frac{M(\tau)}{\|\nabla \psi_0(x(-\tau), z(-\tau))\|} + O(\varepsilon^2) \quad (8)$$

where

$$M(\tau) = \int_{-\infty}^{\infty} \left[\frac{\partial \psi_0}{\partial x} \frac{\partial \psi_1}{\partial z} - \frac{\partial \psi_0}{\partial z} \frac{\partial \psi_1}{\partial x} \right] (x(t-\tau), z(t-\tau), t) dt \quad (9)$$

is the Melnikov function,

$$\begin{aligned} x(t-\tau) &= 0 \\ z(t-\tau) &= \frac{1}{\pi} \sin^{-1}(\operatorname{sech} \pi A(t-\tau)) \end{aligned} \quad (10)$$

is the unperturbed heteroclinic orbit, ψ_0 and ψ_1 can be found from (6), and τ can be viewed as parametrically representing the distance along the unperturbed heteroclinic orbit. Since $\|\nabla \psi_0(x(-\tau), z(-\tau))\|$ is only zero on the unperturbed hyperbolic fixed points, zeros of $M(\tau)$ imply that $d(\tau, \varepsilon) = O(\varepsilon^2)$. If these zeros are nondegenerate, then the implicit function theorem can be used to show that nearby there is a zero of $d(\tau, \varepsilon)$. Hence, nondegenerate zeros of the Melnikov function imply the existence of intersection points of the stable and unstable manifolds. Furthermore, it can be shown that

$$\mu(L_{1,0}) = \mu(L_{0,1}) = \varepsilon \left| \int_{\tau_0}^{\tau_1} M(\tau) d\tau \right| + O(\varepsilon^2) . \quad (11)$$

where τ_0 and τ_1 represent adjacent zeros of the Melnikov function. An exposition of the Melnikov theory along these lines can be found in Wiggins [8].

Using (9) and (10) we find that

$$M(\tau) = \omega \operatorname{sech} \frac{\pi \omega}{A} \sin \omega \tau . \quad (12)$$

Substituting this expression into (11) gives

$$\mu(L_{1,0}) = \mu(L_{0,1}) = 2\varepsilon \operatorname{sech} \frac{\pi \omega}{A} + O(\varepsilon^2) . \quad (13)$$

Hence we have an analytical expression for the flux that is independent of the wavelength of the roll pattern, λ , and is linear in ε . This agrees with the experimental findings of Solomon and Gollub.

4 The Spreading of a Passive Scalar

The problem that we wish to address is the following: Suppose the roll R_1 is uniformly filled with a passive scalar (species S_1) at $t = 0$. How much of species S_1 is contained in roll R_j at any $t > 0$? First, we establish some notation. Let $T_{1,j}(n)$ denote the total amount of species S_1 contained in roll R_j immediately after the n th iterate. Let $a_{1,j}(n)$ denote the flux of species S_1 into R_j on the n th iterate. Note that by incompressibility we have $a_{1,j}(n) = T_{1,j}(n) - T_{1,j}(n-1)$.

Recall our earlier discussion; associated with R_j are two turnstiles, one for each vertical boundary, formed by the lobes $L_{j,j+1}, L_{j+1,j}$ and $L_{j,j-1}, L_{j-1,j}$, respectively. Similarly, associated with R_1 are two turnstiles, one for each vertical boundary, formed by the lobes $L_{1,0}, L_{0,1}$ and $L_{1,2}, L_{2,1}$, respectively. Now transport out of R_1 and into R_j is completely governed by these eight lobes; so it seems reasonable that an expression for $a_{1,j}(n)$ can be given solely in terms of these lobes. Recently, a general theory for such situations, referred to as “lobe dynamics,” has been developed by Rom-Kedar and Wiggins [6]. Using this theory, the expression for $a_{1,j}(n)$ is given by

$$\begin{aligned} a_{1,j}(n) = & \delta_{j,2}\mu(L_{1,2}) + \delta_{j,0}\mu(L_{1,0}) + \\ & \sum_{k=1}^{n-1} \left\{ \sum_{r,s=0,2} [\mu(L_{j-1+r,j} \cap F^k L_{1,s}) - \mu(L_{j-1+r,j} \cap F^k L_{s,1})] \right. \\ & \left. - \sum_{r,s=0,2} [\mu(L_{j,j-1+r} \cap F^k L_{1,s}) - \mu(L_{j,j-1+r} \cap F^k L_{s,1})] \right\} \quad (14) \end{aligned}$$

where $\delta_{j,2}$ and $\delta_{j,0}$ denote the usual Kronecker delta. Using various symmetries of the Poincaré map (see Camassa and Wiggins [1990] for the details) this expression can be

further simplified to

$$\begin{aligned}
T_j(n) - T_j(n-1) &= \\
&= (\delta_{j,2} + \delta_{j,0}) \mu(L_{1,0}) + \\
&\quad \sum_{k=1}^{n-1} \left\{ 2\mu(L_{j-1,j} \cap F^k L_{1,0}) - 2\mu(L_{-j+2,-j} \cap F^k L_{1,0}) \right. \\
&\quad - 2\mu(L_{j,j-1} \cap F^k L_{1,0}) + 2\mu(L_{j-1,j} \cap F^{k-1} L_{1,0}) \\
&\quad + \mu(L_{j+1,j} \cap F^k L_{1,0}) - \mu(L_{j,j+1} \cap F^{k-1} L_{1,0}) \\
&\quad - \mu(L_{j,j+1} \cap F^k L_{1,0}) + \mu(L_{-j+1,-j} \cap F^k L_{1,0}) \\
&\quad + \mu(L_{-j+2,-j+1} \cap F^k L_{1,0}) - \mu(L_{j-2,j-1} \cap F^k L_{1,0}) \\
&\quad \left. - \mu(L_{j-2,j-1} \cap F^{k-1} L_{1,0}) + \mu(L_{j-1,j-2} \cap F^k L_{1,0}) \right\}. \quad (15)
\end{aligned}$$

Thus to compute $a_{1,j}(n)$ one merely locates the lobes indicated in (15), iterates $L_{1,0}$ (i.e. a grid of points covering $L_{1,0}$), determines the area of intersection of the appropriate iterates of $L_{1,0}$ with the other lobes in (15), and adds up the result according to the recipe provided by (15). Numerically, this procedure is extremely efficient affording tremendous savings in CPU time over standard “brute force” methods, details are discussed in Camassa and Wiggins [2].

5 The Number of Rolls Invaded by a Passive Scalar as a Function of Time

Using lobe dynamics type arguments, invariance of the manifolds as well as translation and reflection symmetries, an upper and lower bound can be placed on the time that a passive scalar initially in R_1 first invades R_j . These bounds are expressed in terms of two integers, denoted $\bar{m}$ and $\bar{m}'$, that we refer to as the “signatures” of the manifolds. The signatures are defined as follows; $\bar{m}$ is the smallest integer such that $f^{\bar{m}} L_{1,0} \cap L_{0,-1} \neq \emptyset$ and

$\bar{m}'$ is the smallest integer such that the boundary of $f^{\bar{m}+\bar{m}'}L_{1,0}$ intersects the boundary of $L_{-1,-2}$ in 4 distinct points. If we denote the first time that a passive scalar uniformly filling R_1 initially invades R_{-j} , $j > 0$, by t_I^j , $j \geq 2$, we can show

$$(j\bar{m} + 1)T \leq t_I^j \leq [(j - 1)\bar{m} + \bar{m}' + 1]T . \quad (16)$$

We refer the reader to Fig. 4 for an illustration of the geometry associated with the signatures for $\bar{m} = 1$, $\bar{m}' = 2$.

Numerical Simulations reveal that for $A = 0.1$, $\varepsilon = 0.1$ and $\omega = 0.6$ we have $\bar{m} = \bar{m}' = 3$ indicating that 1 roll is invaded every 3 periods, for $A = 0.1$, $\varepsilon = 0.1$, and $\omega = 0.24$ we have $\bar{m} = \bar{m}' = 1$ indicating that 1 roll is invaded every period, and for $A = 0.1$, $\varepsilon = 0.01$, and $\omega = 0.6$ we have $\bar{m} = \bar{m}' = 4$ indicating that 1 roll is invaded every 4 periods. Thus the number of invaded rolls grows linearly in time if we neglect the effect of molecular diffusion.

6 Relative Time-Scales of Lobe Transport Versus Transport by Molecular Diffusion

All of our fluid transport results thus far have completely neglected molecular diffusion. This could be justified in several ways. One way would be to say that we are only interested in the transport and mixing properties for “short times.” This is in marked contrast to standard perturbation approaches to molecular diffusion problems which are typically valid in the limit $t \rightarrow +\infty$. Indeed, in many technological applications where fluid transport and mixing problems are an issue the goal is often to move and/or mix the fluid(s) in as short a time as possible with the least amount of energy expenditure. Nevertheless, what constitutes a “short time” depends on the application. If the molecular diffusion coefficient of the passive scalar were “small” this might provide an alternate justification

for the neglect of molecular diffusion. However, what “small” means is related to what “short time” means above. If the molecular diffusion coefficient is small we would expect that neglecting diffusion of the passive scalar would be valid on some time scale. Yet no matter how small the molecular diffusion coefficient of the passive scalar, in the limit $t \rightarrow +\infty$ diffusion will have an impact on the transport and mixing properties. We must therefore devise a criterion which takes into account the molecular diffusion coefficient of the passive scalar and allows us to determine a time scale on which molecular diffusion has a negligible impact on the transport and mixing properties of interest.

In this example the transport of a passive scalar, in the absence of molecular diffusion, along a row of convection rolls has been determined entirely in terms of the dynamics of the turnstiles associated with the roll boundaries. The following criterion therefore seems reasonable: transport via lobes will dominate over molecular diffusion provided that the time scale for a passive scalar to diffuse across a distance of the order of a turnstile width, T_d , is long compared to the time for the turnstile to be mapped across the roll boundary, i.e., T . We can obtain a very accurate estimate for T_d . Let

$$\bar{d}(\varepsilon) = \max_{\tau \in [0, T]} d(\tau, \varepsilon) \quad (17)$$

where $d(\tau, \varepsilon)$ is given by (8), then T_d is given by

$$T_d = \frac{(\bar{d}(\varepsilon))^2}{D} \quad (18)$$

where D is the molecular diffusion coefficient of the passive scalar. Using (6), (8), and (12) (and neglecting the $O(\varepsilon^2)$ terms), we obtain

$$\frac{T_d}{T} = \frac{[\varepsilon \frac{\omega}{A} \operatorname{sech} \frac{\omega}{2A} \cosh \frac{\pi^2 A}{2\omega}]^2}{TD} \quad (19)$$

Thus, in terms of (19), our criterion for lobe transport to dominate over molecular diffu-

sion would be expressed by requiring

$$\frac{T_d}{T} \gg 1. \quad (20)$$

One could view (19) as a type of “chaotic Peclet number.”

Now we want to check the validity of our criterion. For this we will take $D = 5.0 \times 10^{-6} \text{ cm}^2/\text{s}$ since this is very close to the molecular diffusion coefficient of methylene blue which was used as a passive scalar by Solomon and Gollub in their experiments. For $A = 0.1, \varepsilon = 0.1, \omega = 0.6$

$$T_d \approx 200T \quad (21)$$

and for $A = 0.1, \varepsilon = 0.01, \omega = 0.6$ we have

$$T_d \approx 2T. \quad (22)$$

Thus in the first case we would expect lobe transport to dominant molecular diffusion for about 200 periods and in the second case only for about 2 periods.

We will check this by adding diffusion to the equations for fluid particle paths as follows

$$\begin{aligned} \dot{x} &= -\frac{\partial \psi}{\partial z}(x, z, t) + \xi(t) \\ \dot{z} &= \frac{\partial \psi}{\partial x}(x, z, t) + \zeta(t), \end{aligned} \quad (23)$$

where $\zeta(t)$ and $\xi(t)$ are random variables with a Gaussian probability distribution such that their correlations satisfy

$$\begin{aligned} \langle \xi(t)\xi(t') \rangle &= \langle \zeta(t)\zeta(t') \rangle = 2D\delta(t - t') \\ \langle \xi(t)\zeta(t') \rangle &= 0. \end{aligned} \quad (24)$$

In Figs. 5 and 6 we show numerical simulations of the spreading of a passive scalar for the two cases. The solid lines are the results using lobe dynamics (i.e., neglecting

diffusion) and the dashed lines are the results obtained by numerically integrating (23) (which requires vastly more CPU time). These results indicate that our criteria works quite well.

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Figure captions

Figure 1. The tangle of the stable (solid) and unstable (dashed) manifold of, respectively, the hyperbolic points close to the line $x = 0$, for the Poincaré section $t_0 = 0$.

Figure 2. The definition of the time dependent analogue of the roll regions R_j .

Figure 3. The turnstile lobes between region R_1 and R_0 .

Figure 4. The stretching of $L_{1,0}$ for $\bar{m} = 1, \bar{m}' = 2$.

Figure 5. Comparison between the exact results (solid) and the ones simulating numerical diffusivity (dashed) for the j -th roll content of R_1 -species vs. time, $j = 0, \dots, -4$, with $\epsilon = 0.1$, $\omega = 0.6$ and $A = 0.1$.

Figure 6. Comparison between the exact results (solid) and the ones simulating numerical diffusivity (dashed) for the j -th roll content of R_1 -species vs. time, $j = 0, \dots, -4$, with $\epsilon = 0.01$, $\omega = 0.6$ and $A = 0.1$.

fig. 1

fig. 2

fig. 3

fig. 4

fig. 5

fig. 6