Resonant chaotic mixing in a cellular flow

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This letter presents a quantitative theory of resonant mixing in time-dependent volume-preserving $3D$ flows using a model cellular flow introduced in [T. Solomon and I. Mezic, *Nature* **425**, 376 (2003)] as an example. Specifically, we show that chaotic advection is dramatically enhanced by a time-dependent perturbation for certain resonant frequencies. We compute the fraction of the mixed volume as a function of the frequency of the perturbation and show that, at resonance, essentially complete mixing in $3D$ can be achieved.

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In recent years, a number of studies of mixing via chaotic advection in time-dependent flows found the mixing efficiency to exhibit a pronounced resonant dependence on the frequency of the time-periodic component of the flow. Qualitatively similar results were obtained in the numerical and experimental studies in the presence of molecular diffusion [1–3] as well as without it [4–6], suggesting that molecular diffusion likely does not play a significant role in this phenomenon. The importance of resonance phenomena in chaotic advection was recognized in [7] and later considered in [6, 8], however no quantitative theory of the process was constructed.

In the present letter we develop such a quantitative theory capable of describing both how quick and how thorough the mixing via chaotic advection is, using the $3D$ time-dependent volume-preserving flow

$$\begin{aligned}\dot{x} &= -\cos(\pi x)\sin(\pi y) + \varepsilon \sin(2\pi x)\sin(\pi z)\\ &+ \pi b \sin(\pi x)\sin(\pi y)\sin\omega t,\\ \dot{y} &= \sin(\pi x)\cos(\pi y) + \varepsilon \sin(2\pi y)\sin(\pi z)\\ &+ \pi b \cos(\pi x)\cos(\pi y)\sin\omega t,\\ \dot{z} &= 2\varepsilon\cos(\pi z)\left[\cos(2\pi x)+\cos(2\pi y)\right].\end{aligned} \tag{1}$$

System (1) is a linearization of the flow introduced in [4] as a qualitative model of Lorenz-force driven cellular flow in a channel of rectangular cross-section ($-0.5 < y, z < 0.5$). The solutions (or streamlines) represent the trajectories of passive tracers (e.g., dye particles) carried by the flow. The terms proportional to ε describe a weak correction to the main flow (Eckman pumping). The time-dependence of the flow represents an external perturbation describing the shift, with amplitude b, of the boundaries between the cells (planes $x = n + 1/2$, $n \in Z$). Since the dynamics in all cells is identical, we will consider only the cell with $-0.5 < x < 0.5$.

Following [4], we consider the limit $0 \le \varepsilon, b \ll 1$. The unperturbed system ($\varepsilon = b = 0$) possesses two integrals of motion:

$$z = \text{const}, \quad \Psi \equiv \cos(\pi x)\cos(\pi y) = \text{const},$$

where Ψ is proportional to the streamfunction of the unperturbed flow in the (x, y) plane. All the streamlines

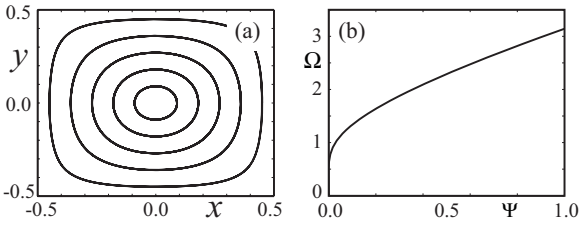

FIG. 1: Unperturbed system: (a) typical streamlines in the $z = \text{const}$ plane and (b) the frequency $\Omega(\Psi)$.

$\Gamma_{z,\Psi}$ of the unperturbed flow are closed (see Fig. 1(a)), with the period of motion

$$T(\Psi) = 2\int_{x_{min}}^{x_{max}} \frac{1}{\dot{x}}\,\mathrm{d}x = 4\int_0^{x_{max}} \frac{dx}{\sqrt{\cos^2(\pi x) - \Psi^2}},$$

where $x_{min} = -x_{max} = (1/\pi)\cos^{-1}\Psi$. The corresponding frequency $\Omega = 2\pi/T$ is shown in Fig. 1(b) and ranges between $\Omega = 0$ at the boundaries of the cell and $\Omega = \pi$ in the center. On every $\Gamma_{z,\Psi}$ we can introduce a uniform phase χ mod(2π) such that $\chi = 0$ on the positive x-axis and $\dot{\chi} = \Omega$. Every interior point of the cell can be specified by the coordinates Ψ, z, and χ.

Next, consider the effect of the Eckman pumping ($\varepsilon > 0$), ignoring the time-dependent shift for the moment ($b = 0$). In this limit, flow (1) is steady but conserves neither z, nor Ψ. The dynamics is characterized by two different time scales: the variable χ (and hence x and y) is fast (changes on $O(1)$ time scale), while the variables z and Ψ are slow (change on $O(1/\varepsilon)$ time scale) and can be described by the averaged equations (see [9])

$$\dot{\Psi} = -\varepsilon \frac{\pi}{T(\Psi)}\frac{\partial \Phi}{\partial z}, \quad \dot{z} = \varepsilon \frac{\pi}{T(\Psi)}\frac{\partial \Phi}{\partial \Psi}. \tag{2}$$

In (2),

$$\Phi = \frac{16}{\pi}\cos(\pi z)\int_0^{x_{max}} \frac{\Psi}{\cos(\pi x)}\sqrt{1 - \frac{\Psi^2}{\cos^2(\pi x)}}\,dx \tag{3}$$

is the flux of the perturbation (ε-dependent terms in (1)) through a surface bounded by a streamline $\Gamma_{z,\Psi}$. It fol-

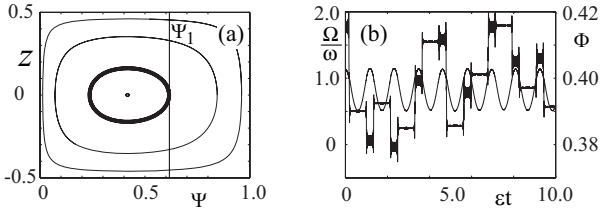

FIG. 2: (a) Projection of averaged streamlines on the (Ψ, z) plane. The vertical line is the $1:1$ resonance and the bold curve is Γ_{Φ^*}. (b) Plots of Ω/ω (dashed line) and Φ (solid line) *vs.* time for complete flow (1) with $\varepsilon = b = 10^{-4}$ and $\omega = 2.5$.

lows from (2) that Φ is an invariant of the averaged system and, hence, is an adiabatic invariant (AI) of the exact system: away from the cell boundaries, where $\Omega(\Psi) = 0$, the value of Φ oscillates with an $O(\varepsilon)$ amplitude [10].

Trajectories with $b = 0$ lie on nested tori τ_Φ defined as the level sets of the AI. The (quasi-periodic) motion along these tori corresponds to motion (with slow period $T_\varepsilon(\Phi)$) of averaged system (2) along closed curves Γ_Φ on the (Ψ, z) plane (see Fig. 2(a)). The AI reaches its maximum value $\Phi_c \approx 0.7845$ on a closed curve that resides in the center of the nested tori and is given by

$$z = z_c = 0, \quad \Psi = \Psi_c \approx 0.418. \tag{4}$$

The minimal value $\Phi = 0$ is reached at the cell boundary.

Addition of the time-dependent perturbation can make the structure of the flow much more complex. Numerical simulations show that the limit $0 < b \ll \varepsilon$ is qualitatively similar to the case with $b = 0$ and $\varepsilon > 0$. The limit $0 < \varepsilon \ll b$ is qualitatively similar to the case with $\varepsilon = 0$ and $b > 0$, where the flow is effectively 2-dimensional and a narrow chaotic domain of $O(b)$ width appears near the cell boundaries. The case where b and ε are of the same order is of the most interest. Hence, in what follows, we assume $\beta \equiv b/\varepsilon = O(1)$. Furthermore, since we are interested in resonant dependence of mixing on the frequency ω of the perturbation, we will take $\omega = O(\Omega) = O(1)$.

The exact equations for the slow variables are

$$\begin{aligned} \dot\Psi &= -\varepsilon\pi \sin(\pi z)\Psi\,(2 - \cos(2\pi x) - \cos(2\pi y)) \\ &- \frac{1}{2}\varepsilon\pi^2\beta \sin(2\pi y)\sin(\omega t), \\ \dot z &= 2\varepsilon\cos(\pi z)\,(\cos(2\pi x) + \cos(2\pi y))\,, \end{aligned} \tag{5}$$

If Ω and ω are incommensurate, then averaging over Ω and over ω can be performed independently (see, e.g., [10]). In this case, the time-dependent terms in the expression for $\dot\Psi$ average out, so we would expect AI (3) to be conserved as before. Results of numerical integration of (1) over the time period of order $1/\varepsilon$ are presented in Fig. 2(b). The AI remains essentially constant except for short periods of time when $\Omega(\Psi(t)) \approx \omega$. This fact indicates that the breakdown of adiabatic invariance is a consequence of resonant processes. A quantitative description of these processes can be constructed based on the theory of resonance phenomena in multiple-frequency systems developed recently by Neishtadt [10].

As the value of Ψ slowly drifts, so does $\Omega(\Psi)$. Hence, at certain values of Ψ, a resonance condition

$$n\Omega(\Psi) - \omega = 0 \tag{6}$$

will be satisfied for some non-zero integer n. Since Ω is independent of z, the resonance surfaces R_n defined by (6) are vertical cylinders in the physical space or straight lines $\Psi = \Psi_n(\omega) = \text{const}$ in the slow plane (see Fig. 2(b)).

Near R_n we can expect neither the averaged system to adequately describe the exact dynamics, nor the value of Φ to be conserved. Hence, we must consider the dynamics near resonances separately. Introduce a pair of new phase variables:

$$\gamma = n\chi - \omega t, \quad \varphi = \chi, \tag{7}$$

such that (1) can be rewritten as

$$\begin{aligned} \gamma' &= \frac{1}{\sqrt{\varepsilon}}\,(n\Omega - \omega)\,, \\ \Omega' &= \sqrt{\varepsilon}\,\frac{\partial\Omega}{\partial\Psi}\,\frac{\dot\Psi}{\varepsilon}, \quad z' = \sqrt{\varepsilon}\,\frac{\dot z}{\varepsilon}. \end{aligned} \tag{8}$$

In (8), the prime denotes the derivative with respect to the rescaled time $\overline{t} = \sqrt{\varepsilon}\,t$ and $\dot\Psi$, $\dot z$ were defined in (5). Of the new phases, γ is slow and φ is fast. Thus, we can average equations of motion over φ (so-called *partial averaging*).

For most of the initial conditions, tracers pass through the vicinity of resonance in a relatively short time and the value of Φ undergoes a relatively small jump. In the first approximation, we can fix the slow variables (Ψ, Ω and z) at their resonant values, which yields a forced pendulum-like equation for γ:

$$\gamma'' = \frac{1}{\sqrt{\varepsilon}}\,n\Omega' = a_n + b_n\cos\gamma. \tag{9}$$

In (9), a_n and b_n are the averages of the first and the second terms defining $\dot\Psi$ in (5) over the fast period $T_n = T(\Psi_n)$, respectively:

$$\begin{aligned} a_n &= -\frac{\omega}{2}\Psi\sin(\pi z)\frac{\partial\Omega}{\partial\Psi}\int_{T_n}(2 - \cos(2\pi x) - \cos(2\pi y))\,\mathrm{d}t, \\ b_n &= \frac{\pi}{4}\omega\beta\frac{\partial\Omega}{\partial\Psi}\int_{T_n}\sin(2\pi y)\sin(\omega t)\,\mathrm{d}t. \end{aligned}$$

In the definition of a_n, b_n (and c_n below), $x = x(t)$, $y = y(t)$ is a solution of the unperturbed system for $\Psi = \Psi_n$ such that $\chi = 0$ at $t = 0$. Note that a_n, b_n, and c_n are functions of ω only. Similarly, the average of $\dot\Phi$ over T_n can be computed using (2) and (5), yielding

$$\begin{aligned} \langle\dot\Phi\rangle &= \left\langle\frac{\partial\Phi}{\partial\Psi}\frac{\mathrm{d}\Psi}{\mathrm{d}t} + \frac{\partial\Phi}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t}\right\rangle = -\varepsilon\frac{\pi^2}{2}\beta\langle\dot z\sin(2\pi y)\sin(\omega t)\rangle \\ &= \varepsilon\pi\beta\,c_n\cos(\pi z)\cos\gamma, \end{aligned} \tag{10}$$

where the coefficient c_n is given by

$$c_n = -\int_{T_n} (\cos(2\pi x) + \cos(2\pi y)) \sin(2\pi y) \sin(\omega t)\, \mathrm{d}t.$$

Finally, the jump of the AI on crossing the resonance can be computed as a change in Φ over a time interval (t_1, t_2) during which the resonance is crossed once, at time t_*, and such that $|t_{1,2} - t_*| \sim 1/\varepsilon$:

$$\Delta\Phi = \int_{t_1}^{t_2} \dot{\Phi}\, \mathrm{d}t \approx \int_{t_1}^{t_2} \langle\dot{\Phi}\rangle\, \mathrm{d}t = \\ = -2\pi s\sqrt{\varepsilon}\, \beta\, c_n \cos(\pi z) \int_{s\infty}^{\gamma(t_*)} \frac{\cos\gamma}{\sqrt{2\,(h - V)}}\, \mathrm{d}\gamma, \quad (11)$$

where $V = -a_n\gamma - b_n \sin\gamma$, $h = V(\gamma(t_*))$, and $s = \mathrm{sign}(a_n)$. The dependence of $\Delta\Phi$ on the order of resonance is determined by the fact that a_n, b_n, and c_n are Fourier coefficients of smooth functions, and, hence, decay exponentially. Thus, only low-order resonances play important role in the dynamics:

$$\Delta\Phi \sim \sqrt{\varepsilon}\, e^{-\alpha n}, \quad (12)$$

where α is some constant. The value of $\Delta\Phi$ can be calculated exactly for any initial condition. However, a small change of order ε in the initial conditions produces, in general, a large change in $\Delta\Phi$. Hence, for small ε it is possible to treat ξ as a random variable uniformly distributed on the unit interval [10].

Generally, a non-zero ensemble average of $\Delta\Phi$ results in the drift of Φ. However, in the current problem, two successive crossings occur at almost opposite values of z. Thus, it can be shown that they cancel each other *on average*, and the aggregate change of Φ on one period of the slow motion has zero mean. Individually, the jumps on two successive crossings can be considered to be statistically independent random processes [11].

It should be mentioned that few tracers may follow trajectories near the resonance surface (*capture into resonance*), qualitatively different from the ones considered above (*scattering on resonance*). It was shown in [10] that capture can be considered a probabilistic process, too: for a ball of initial conditions, only a tiny fraction, of order $\sqrt{\varepsilon}$, is captured. Captured tracers move near the cylinder $\Psi = \Psi_n(\omega)$ and, due to the symmetry $z \to -z$ of (3), are released from resonance at the value of z opposite to that at which the capture occurred. It follows from (3) that (in the first approximation) the values of Φ before the capture and after the release are the same. Thus, capture does not contribute to the change in the AI and hence to the mixing process. Capture into resonance will be discussed in detail in a subsequent publication.

It was shown before that the accumulation of jumps of an adiabatic invariant after many resonance crossings leads to the diffusion of the AI, chaotic advection, and mixing [6]. Two useful metrics that describe the efficiency of chaotic advection are the size of the chaotic domain and the characteristic rate of mixing inside the chaotic domain. We start by describing the size (and shape) of the chaotic domain.

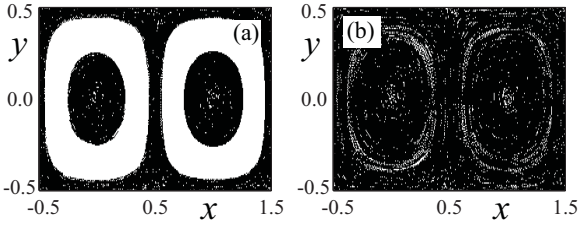

FIG. 3: Partial and complete mixing at $\varepsilon = b = 0.05$. $z = 0$ Poincaré section of the flow: (a) $\omega = 4.0$, (b) $\omega = 2.5$.

On every period $T_\varepsilon(\Phi)$ of the slow motion along a given trajectory (see Fig. 2(a)), the value of Ψ changes between Ψ_{min} and Ψ_{max}. If no (low-order) resonance Ψ_n falls between Ψ_{min} and Ψ_{max}, then that trajectory (and all trajectories inside of it) remains regular. If, on the other hand, the trajectory crosses a resonant surface, the AI experiences jumps and the motion becomes chaotic.

In the $\varepsilon \to 0$ limit, the boundary between the chaotic and the regular domains is, thus, given by the trajectory Γ_{Φ^*} that (i) touches a resonance surface and (ii) has the largest value Φ among all such trajectories on the (Ψ, z) plane. (Condition (ii) is necessary when multiple resonances are considered). In the physical space the boundary is formed by the corresponding torus τ_{Φ^*}. The corresponding value of the AI is given by (3) with $z = 0$ and $\Psi = \Psi_n$ (see Fig. 2(a)). The Poincaré section of the complete flow (with periodic boundary conditions at $x = -0.5$ and $x = 1.5$) by the plane $z = 0$ (see Fig. 3(a)) confirms that the space inside the torus τ_{Φ^*} corresponds to the regular domain discovered in [4], while the rest of the physical space belongs to the chaotic domain. Moving the frequency ω closer to resonance completely wipes out the regular domain (see Fig. 3(b)).

The width d of the regular domain can be computed for any value of ω (see Fig. 4). For $0 < \omega \ll 1$, all the resonances are located near $\Psi = 0$. As ω is increased, the first, $1:1$, resonance penetrates deeper into the cell. For $0 < \omega \leq \pi$, Γ_{Φ^*} is tangent to the resonance $\Psi = \Psi_1$. As ω approaches π, the $1:1$ resonance moves out of the cell and the $1:3$ resonance becomes dominant for $\pi < \omega \lesssim 3\pi$ (it can be shown that even resonances do not lead to jumps in Φ and can be disregarded). Then the process repeats itself: as ω is increased further, higher and higher resonances become dominant. Finally, as $\omega \to \infty$, there are infinitely many resonances and they cover all the domain in Ψ. However, the impact of the high resonances is negligible ($\Delta\Phi \sim e^{-\alpha n}$).

Complete mixing can be achieved by eliminating the domain of regular dynamics. This can be accomplished

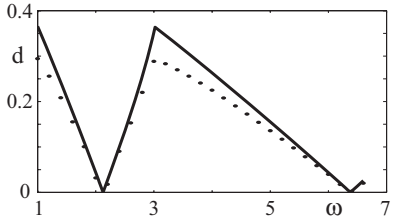

FIG. 4: The width d of the regular domain (along the x-axis) as a function of the perturbation frequency, ω: solid line – theoretical prediction, dots – numerical simulations. Other parameters are $\varepsilon = b = 10^{-4}$.

by setting the frequency ω of the perturbation such that $\Psi_n(\omega) = \Psi_c$ for some n. More precisely, the resonance must be within the distance $|\Psi_n - \Psi_c| \sim \sqrt{\varepsilon}$, as the chaotic domain penetrates inside Γ_{Φ^*} by an $O(\sqrt{\varepsilon})$ distance [12]. This property, negligible in most similar problems, is important here as the magnitude of the jumps vanishes at Ψ_c. Indeed, $\dot{\Phi} \sim \dot{z}$ according to (10), so $\Delta\Phi = 0$ at $\Psi = \Psi_c$, as $\dot{z} = 0$ there. Since the width of the regular domain $d \sim |\Psi_n(\omega) - \Psi_c|$, we find the width of the resonant peaks (where $d \approx 0$) to scale as $\Delta\omega \sim \sqrt{\varepsilon}$ (see Fig. 2f of Ref. [4]). The finite penetration depth also explains why the theory overestimates the width of the regular domain for finite ε (see Fig. 4).

In defining the regular and chaotic domains, we assumed that the system evolves over an infinite time. However, for a finite time interval that is characteristic of a given experiment, the dynamics may be quite different. While the evolution inside the regular domain remains qualitatively the same, the thoroughness of mixing in the chaotic domain (as well as the mixed volume fraction) depends on the time interval of observation.

A characteristic time of mixing can be defined as the time needed for a localized distribution of initial conditions to diffuse over the entire chaotic domain. For small times t, the width of the distribution inside the chaotic domain (and hence the mixed volume fraction) grows as $\sigma(\Phi)N^{1/2}$, where $N = 2t/T_\varepsilon(\Phi)$ is the number of resonance crossings, $\sigma(\Phi) \sim \sqrt{\varepsilon}\, e^{-\alpha n}$ is the dispersion of $\Delta\Phi$ over one slow period $T_\varepsilon(\Phi) \sim 1/\varepsilon$, and n is the order of the dominant resonance. It takes $N \sim \bar{\sigma}^{-2}$ resonance crossings for the distribution to diffuse over the entire chaotic domain, where $\bar{\sigma}$ is a weighted average of $\sigma(\Phi)$ which can be computed analytically (to be discussed in more detail in a subsequent publication). Therefore, the characteristic time of mixing is

$$T_M \sim T_\varepsilon\, N \sim e^{2\alpha n}/\varepsilon^2. \qquad (13)$$

A more accurate estimate can be obtained by including the contributions to the dispersion from all the resonances that a given trajectory crosses. As only the low-order resonances are important and they are far apart, their effect may be considered independently. However, the weight of different resonances can be quite different, depending both on the resonance order (e.g., only odd resonances contribute) and on the value of Ψ_n (e.g., the jumps near $\Psi_n = \Psi_c$ are strongly suppressed).

Summing up, we have shown that the mixing in the periodically driven cellular flow considered here is due to the changes the adiabatic invariant experiences when the streamlines cross the surfaces on which the perturbation frequency is in resonance with the natural frequency of the base flow. The resonant dependence of the mixed volume on the frequency of the perturbation was traced to the position of the resonant surfaces. In particular, we have shown that resonances of different order (e.g., $1:1$ or $1:3$) can be used to achieve essentially complete mixing inside the cell, albeit after a relatively long time.

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[1] C. Christov and G. Homsy, submitted to Phys. Fluids (2006).
[2] T. Ward and G. Homsy, Phys. Fluids **15**, 2987 (2003).
[3] A. Rodrigo *et al.*, AIChE Journal **49**, 2749 (2003).
[4] T. Solomon and I. Mezic, Nature **425**, 376 (2003).
[5] B. Noack, I. Mezic, G. Tadmor, and A. Banaszuk, Phys. Fluids **16**, 867 (2004).
[6] D. Vainchtein, A. Neishtadt, and I. Mezic, Chaos **16**, 043123 (2006).
[7] M. Feingold, L. Kadanoff, and O. Piro, J. of Statistical Physics **50**, 529 (1988).
[8] I. Mezic, Physica D **154**, 51 (2001).
[9] D. Vainshtein, A. Vasiliev, and A. Neishtadt, Chaos **6**, 67 (1996).
[10] A. Neishtadt, Proc. of the Steklov Institute of Mathematics **250**, 183 (2005).
[11] D. Dolgopyat, preprint of U. Maryland (unpublished).
[12] D. Vainshtein, A. Vasiliev, and A. Neishtadt, Chaos **6**, 514 (1996).