

Can particle transport coefficients be extracted from symmetry measures?

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Abstract

In a recent investigation of particle transport in numerically computed wavy Taylor vortex flow, Rudman estimated an effective axial transport coefficient, D_{eff} , due to chaotic advection [*AICHE J.* **44** (1998) 1015–1026]. We show that D_{eff} is proportional to symmetry measures averaged over the velocity field. Thus we show that the macroscopic transport behaviour in a flow (a Lagrangian quantity) can be quantified directly in terms of the velocity field and its gradients (Eulerian quantities).

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I. INTRODUCTION

During the past 15 years numerous papers have illustrated the fact that even simple velocity fields can have complicated (i.e., chaotic) particle trajectories [1]. (We assume the particles are passive tracers.) In fact, chaotic particle trajectories arise only when the effective dimensionality of the flow field is greater than two. For example particle trajectories are simple in a steady two-dimensional flow field, but when time-dependent forcing is applied, regions of chaotic trajectories appear. As is well known, the presence of a continuous symmetry and/or constant of the motion reduces the effective dimension of the flow field. This fact is the basis of an Eulerian diagnostic approach that we developed in an earlier paper [2]. In this letter we apply the Eulerian diagnostic methodology to investigate particle transport in velocity fields obtained from numerical solutions of the Navier-Stokes equations for wavy Taylor vortex flow. We show that the Eulerian diagnostic is not only qualitatively correct, but also yields correct information concerning particle transport coefficients.

Mixing by chaotic advection in wavy Taylor-vortex flow, a flow occurring between concentric rotating cylinders (Taylor-Couette system), has been the focus of interest in several recent papers from both the fundamental [3–5,2,6,7] and practical (mixing vessel; dynamic filtration) [6,8–13] points of view. We consider here the case of a Taylor-Couette system with fixed outer cylinder. When the inner cylinder rotation is such that the critical Reynolds number, Re_c , is exceeded only slightly, the resulting flow is a three-dimensional axisymmetric cellular structure known as Taylor vortex flow. The rotational symmetry of this flow ensures that each vortex consists of a set of nested streamtubes (tori) and hence fluid particles are constrained to lie on the surface of tori. Particle transport between tori and between vortices cannot occur.

At larger rotation rates Taylor vortices are unstable to a wavy disturbance which deforms them. This flow is known as wavy Taylor-vortex flow. The wavy perturbation has a two-fold effect on the particle motion. First, the loss of rotational symmetry causes the velocity

field to depend on all three spatial coordinates. General dynamical systems arguments then imply that, under certain conditions, streamtubes (KAM tori) will be destroyed leading to chaotic fluid particle motion and hence to intra-vortex mixing [4,5,14]. Second, the wavy perturbation breaks the invariant surface separating adjacent Taylor vortices, thus creating a complicated pathway enabling fluid particles to wander from vortex to vortex. This gives rise to inter-vortex mixing (axial dispersion) [5,6,15].

Inter-vortex mixing can be quantified by an effective axial diffusion coefficient, D_z [3]. The Reynolds number dependence of D_z for a radius ratio of $\eta = 0.875$ has been investigated in numerical experiments by Rudman over the Reynolds number range $155 \leq \text{Re} \leq 756$ [16]. (Note that $D_{eff} = \nu \text{Re} D_z$, where D_z is the dimensionless and D_{eff} the dimensional effective diffusion constant.) The variation of D_z with Re for a fixed wave state was found to be correlated with V_c , the volume of the 'wavy vortex core' (a region of fluid where particles had long retention times). In Fig. 1 we plot his results for D_z and $V_{out} = V - V_c$ for a flow with six azimuthal waves.

In this letter we reproduce the variation of D_z with Re to well within the error of the numerical particle tracking experiments using the Eulerian diagnostic approach introduced by us in Ref. [2]. The results are shown in the final figure and a possible explanation of the surprising agreement is given at the end of this letter.

FIGURES

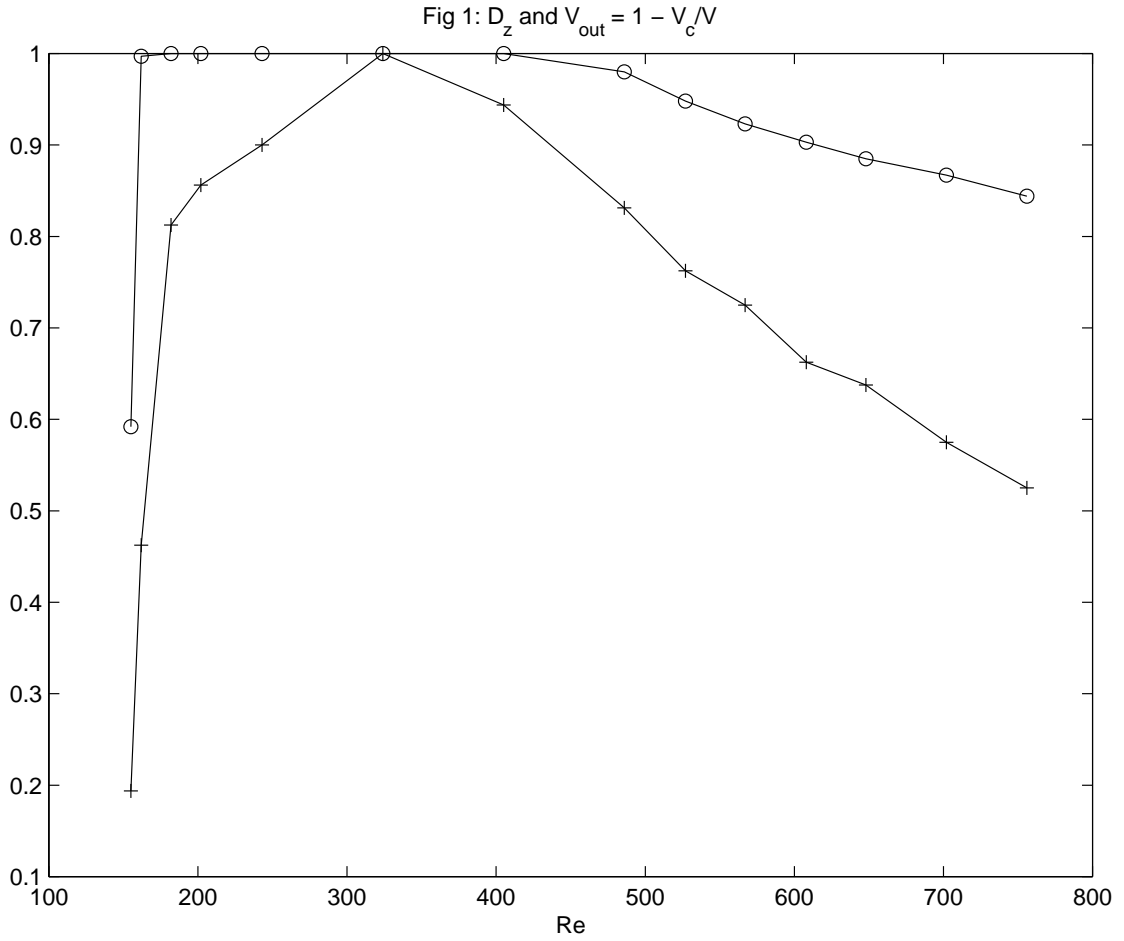


FIG. 1. Results of numerical particle tracking experiments for a wavy Taylor vortex flow with six azimuthal waves and axial wavelength $2.33d$ - taken from Ref. [6]: Reynolds number variation of the effective axial diffusion coefficient, D_z (+), and $V_{out}/V = 1 - V_c/V$ (o) (V_c is the volume of the 'wavy vortex core' where particles had long retention times). D_z is normalized by its value at $Re = 324$; the maximum in D_z corresponds to maximum wave amplitude.

II. METHODOLOGY

A. Numerical method

Our investigation of particle trajectories and particle dispersion in wavy Taylor-vortex flow proceeds in two steps. First, the time-dependent solution of the fluid flow field is obtained in a stationary coordinate frame. Second, the flow solution is used to integrate particle trajectories forward in time in a coordinate frame that rotates about the axis of the cylinders (z -axis) with the azimuthal wave speed. In this frame the flow is steady and an efficient solution of particle trajectories is relatively straightforward.

The flow solution is based on the MAC method of Welch et al. [17] and is a conservative finite difference scheme solved on a staggered mesh. It is second-order accurate in time and space. The initial condition is integrated forward in time until the period of the wave becomes fixed. Particle trajectories are calculated using fourth-order Runge-Kutta integration with a fixed time-step equal to 0.25 times the maximum Courant time-step on the grid. Although a fixed time-step is inefficient, it allows for easier vectorisation and collection of time-history data. Fluid velocities are interpolated to particle positions using quadratic interpolation.

A radius ratio of $\eta = 0.875$ is considered here and corresponds to the geometry used by Coles [18] in his documentation of multistability and hysteresis in wavy vortex flows. The wave state in wavy vortex flow is categorized by the number of azimuthal waves m and the axial wavelength of a vortex pair λ_z .

The computational domain has radial extent d , azimuthal extent $2\pi/m$, and axial extent λ_z . The axial and azimuthal boundaries are periodic, and the domain represents just one oscillation of a wavy vortex in the axial and azimuthal directions in a theoretically infinite Taylor-Couette column. This enforced periodicity admits only those flows in which the phase of the azimuthal wave does not vary axially. The inner radial boundary rotates with a scaled velocity of 1.0 and the outer radial boundary is stationary. The range of Reynolds numbers considered is 155–756. A detailed description of the numerical method and its validation

can be found in [6].

B. Eulerian diagnostic

In Ref. [2] we argued that because integrable behaviour is associated with the presence of a symmetry, chaotic and near-integrable regions of particle paths could be distinguished through a suitable point-wise symmetry test using quantities which are local functions of the velocity and its gradients. It is well known that a symmetry of a vector field can lead to conservation laws which rule out the occurrence of chaotic dynamics. The natural symmetries to consider are geometric ones (rotational, translational), but there are other symmetries which are more subtle. Arnold [19] proved a topological result on integrability of Euler flows, arising from the existence of the so-called Lamb surfaces [20]. The importance of volume-preserving symmetries in this context was recognized in [14,21,22]. We called in [2] a *dynamical* symmetry a symmetry (such as the one in Arnold's theorem) intrinsic to the equations of fluid motion. To explain the dynamical symmetry we consider the Navier-Stokes equations. In a frame rotating with the wave the flow is steady and the incompressible Navier-Stokes equations reduce to

$$\boldsymbol{\omega} \times \mathbf{u} = -\nabla B + \nu \nabla^2 \mathbf{u}, \quad (2.1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2.2)$$

where $\boldsymbol{\omega} = \boldsymbol{\omega}_R + 2\boldsymbol{\Omega}$, $\boldsymbol{\omega}_R$ is the relative vorticity, $\boldsymbol{\Omega}$ is the angular velocity of the azimuthal wave, and $\nu \nabla^2 \mathbf{u}$ is the viscous force. Here B is the Bernoulli function

$$B = \frac{p}{\rho} + \frac{1}{2} \mathbf{u}^2, \quad (2.3)$$

where p is the pressure and ρ is the density. B changes along a particle path according to

$$\frac{dB}{dt} = -\nu (\nabla \times \boldsymbol{\omega}) \cdot \mathbf{u} = \nu (\nabla^2 \mathbf{u}) \cdot \mathbf{u}. \quad (2.4)$$

It is clear that when $\nu = 0$ (i.e., Euler flow), B is a constant of the motion, and this implies integrability unless B is constant throughout space. Chaotic motion may only occur in an

Euler flow when $\mathbf{u} = c\boldsymbol{\omega}$, where c is some constant. This situation is known as Beltrami flow. The action of the symmetry group associated with the existence of B is generated by the vorticity field [22] and we call it the dynamical symmetry.

It was suggested in [2] that the deviation of a velocity field from a geometric or dynamical symmetry could be used as an Eulerian diagnostic for the occurrence of Lagrangian chaos. The Eulerian diagnostic introduced in [2] appropriate to wavy Taylor-vortex flow is

$$\mathcal{D} = \left| \frac{1}{\text{Re}} \nabla^2 \mathbf{u} \right| \left| \frac{\partial \mathbf{u}}{\partial \theta} \right|. \quad (2.5)$$

The quantity $|\partial \mathbf{u} / \partial \theta|$ measures the extent to which \mathbf{u} departs from rotational symmetry, while the magnitude of the viscous force, $|\nabla^2 \mathbf{u}| / \text{Re}$, measures the departure from dynamical symmetry. We take the product of these two quantities, as the existence of any one of these symmetries is enough to produce integrability of the underlying flow. Note that this definition of \mathcal{D} differs from that discussed in [2] because here axial symmetry is not relevant. A contour plot of \mathcal{D} as a function of space highlights regions where \mathcal{D} deviates from zero, and it is in these regions where chaotic streamlines and enhanced mixing are expected.

III. RESULTS

The pointwise diagnostic is illustrated in Fig. 2 where contour plots of $\mathcal{D}(\mathbf{x})$, at a particular phase of the wave in the r, z -plane, are shown. The contour plots are for Reynolds numbers $\text{Re} = 155, 324, 648$. Regions where $\mathcal{D}(\mathbf{x})$ is small (dark) are regions where a remnant of either rotational or dynamical symmetry (or both) persists and consequently the particle trajectories are expected to be close to integrable. Conversely regions where $\mathcal{D}(\mathbf{x})$ is large (light gray) should correspond to strongly chaotic regions. The Poincaré sections (the intersections of particle trajectories with the plane, $\theta = \text{constant}$) superimposed on the contour plots support this argument, even though the agreement is not perfect.

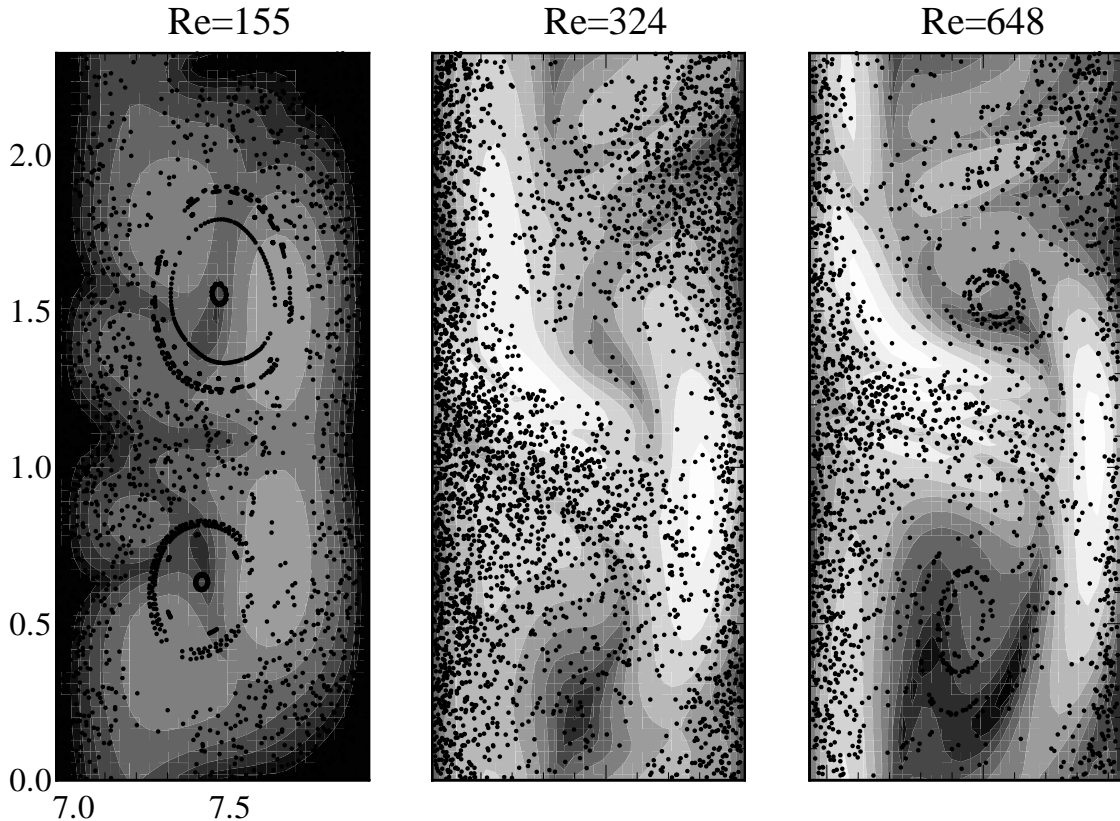


FIG. 2. Poincaré sections of particle orbits superimposed on contour plots of the pointwise diagnostic \mathcal{D} for a counter-rotating pair of wavy Taylor vortices. The results are shown for one phase of the azimuthal wave at $\text{Re} = 155, 324$ and 648 . Note that as the Reynolds number increases, the integrable streamtubes (centered on the vortex cores) in evidence near onset of the waves ($\text{Re} = 155$) disappear ($\text{Re} = 324$) and then reappear ($\text{Re} = 648$).

Contour plots of $\mathcal{D}(\mathbf{x})$ hold a great deal of qualitative information, but yield little on the global nature of the flow, for example, the variation in mixing with Reynolds number. For this reason we introduce volume averaged measures of the geometric and dynamical symmetries, and the diagnostic \mathcal{D} . The average departure from rotational symmetry is defined by

$$\phi_\theta = \frac{1}{V} \int \left| \frac{\partial \mathbf{u}(\mathbf{x})}{\partial \theta} \right| dV, \quad (3.1)$$

and similarly we define ϕ_ν as the averaged departure from dynamical symmetry, and $\phi_{\mathcal{D}}$

as the averaged diagnostic, calculated by averaging the pointwise product of rotational and dynamical symmetries. These averaged measures are shown in Figure 3 for velocity fields computed for the state $(m, \lambda_z) = (6, 2.33d)$ over the range $155 \leq \text{Re} \leq 756$. In Fig. 3c we also plot $\phi_\theta * \phi_\nu$ (the product of the averages). Comparing this quantity with $\phi_{\mathcal{D}}$ (the average of the products), we see that $|\partial \mathbf{u} / \partial \theta|$ and $|\nabla^2 \mathbf{u}| / \text{Re}$ are statistically independent for $\text{Re} < 324$ and weakly dependent for $\text{Re} > 324$. This weak dependence at the larger Re suggests that as the size of the inviscid vortex core increases, it becomes more rotationally symmetric. This is in accord with numerical and experimental observations that the flow becomes more Taylor vortex-like as the Reynolds number gets larger.

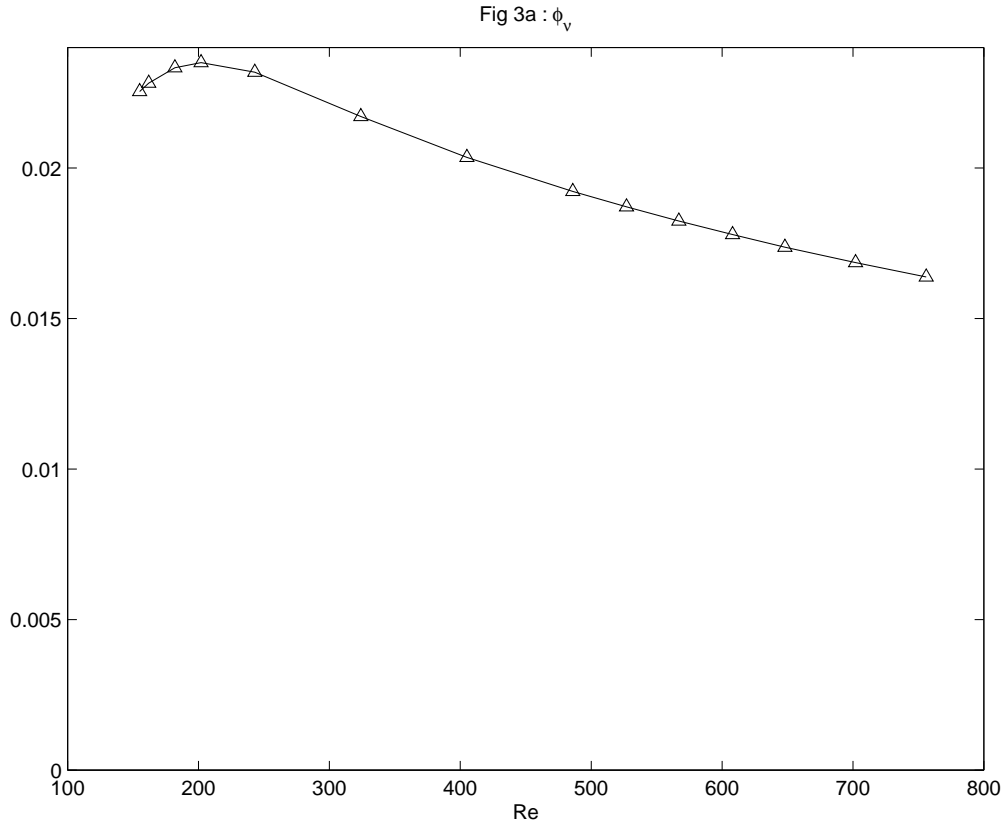


FIG. 3. Reynolds number variation of the volume averaged measures: (a) ϕ_θ ; (b) ϕ_ν ; (c) $\phi_{\mathcal{D}}$ (o) and $\phi_\theta * \phi_\nu$ (Δ) - normalized by their values at $\text{Re} = 324$.

Fig 3b : ϕ_θ

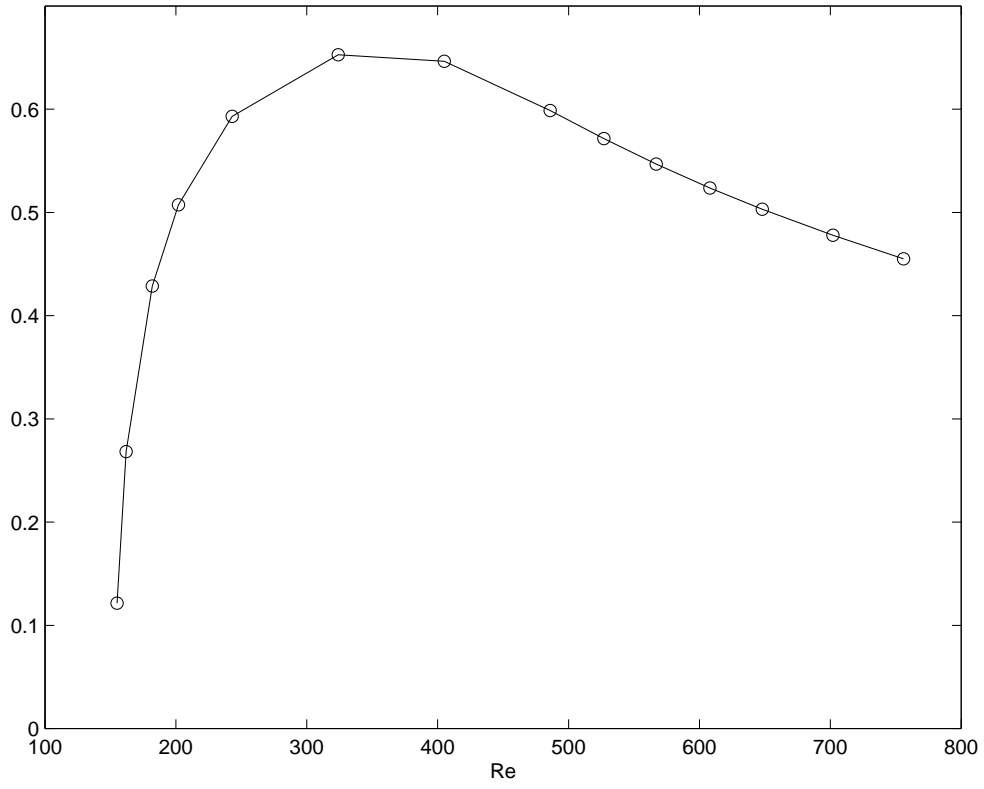
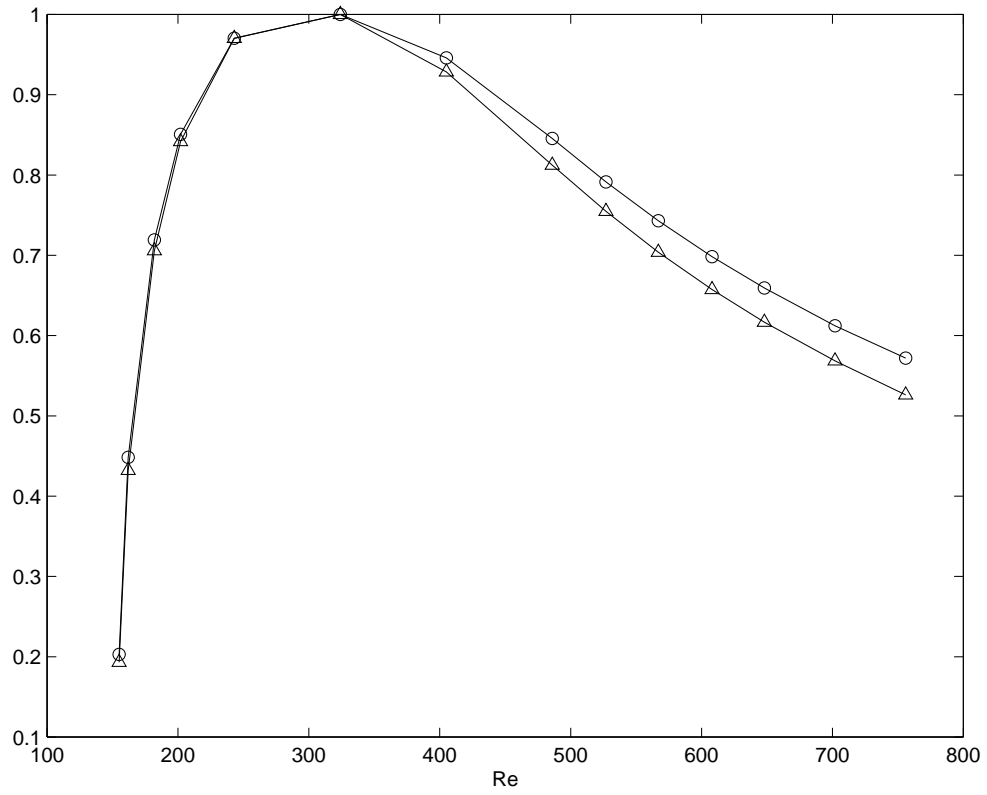


Fig 3c : Comparison of ϕ_D with $\phi_\theta * \phi_v$



We expect these averaged measures to be closely linked with macroscopic quantities, such as the size of the inviscid core and the effective axial diffusion coefficient. In Figs. 4a and 4b we compare the Reynolds number variation of $V_{out} = 1 - V_c/V$ with ϕ_ν and ϕ_θ , respectively. These figures show that for $324 < \text{Re} < 756$, ϕ_ν is proportional to V_{out} and ϕ_θ is proportional to V_{out}^2 . In Fig. 4c we compare D_z with $\phi_\theta * \phi_\nu$. (We compare with $\phi_\theta * \phi_\nu$ rather than ϕ_D because $|\partial \mathbf{u} / \partial \theta|$ and $|\nabla^2 \mathbf{u}|/\text{Re}$ are not statistically independent at large Re .) This figure shows that, except for some minor statistical deviations, D_z is proportional to $\phi_\theta * \phi_\nu$ throughout the entire range $155 < \text{Re} < 756$. Consequently for $\text{Re} > 324$ we find $D_z \propto V_{out}^3$. Furthermore, we find that $V_{out} \propto \text{Re}^{-1/3}$ and thus $D_z \propto \text{Re}^{-1}$ for $\text{Re} > 324$.

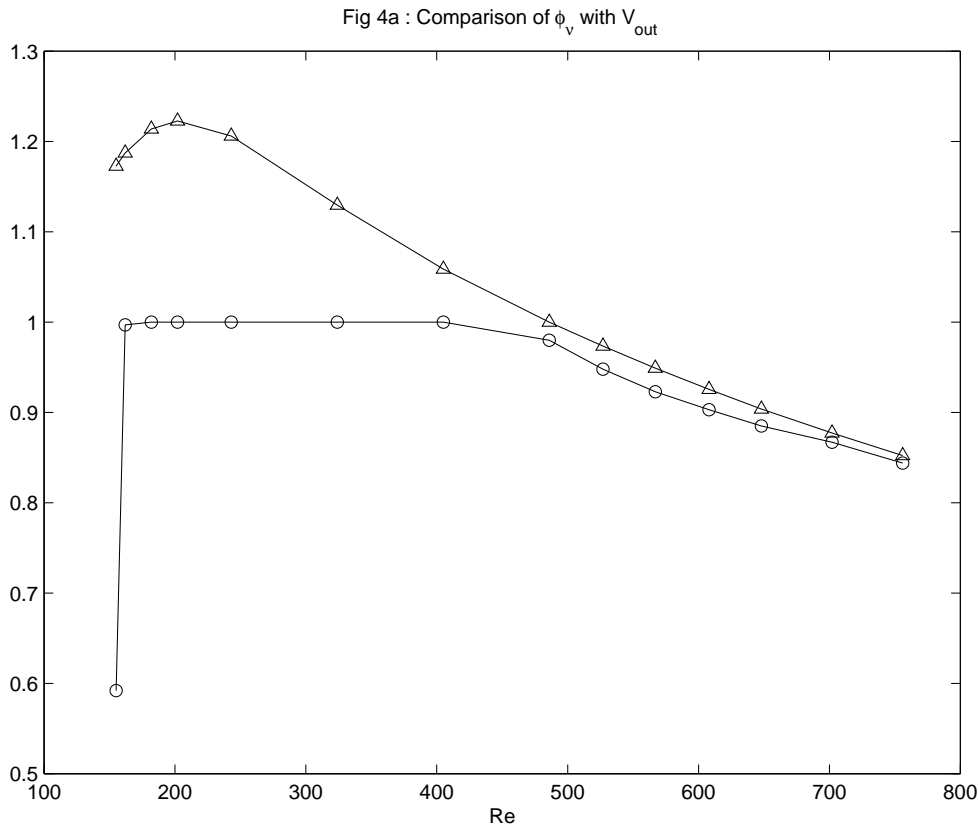


FIG. 4. (a) Comparison of V_{out} (o) with ϕ_ν (Δ). (b) Comparison of V_{out}^2 (o) with ϕ_θ (x). To facilitate comparison ϕ_ν and ϕ_θ have been normalized by their values at $\text{Re} = 486$. (c) Comparison of D_z (+) with the product of the averaged rotational and dynamical symmetries, $\phi_\theta * \phi_\nu$ (Δ). Both quantities have been normalized with their values at $\text{Re} = 324$.

Fig 4b : Comparison of ϕ_θ with V_{out}^2

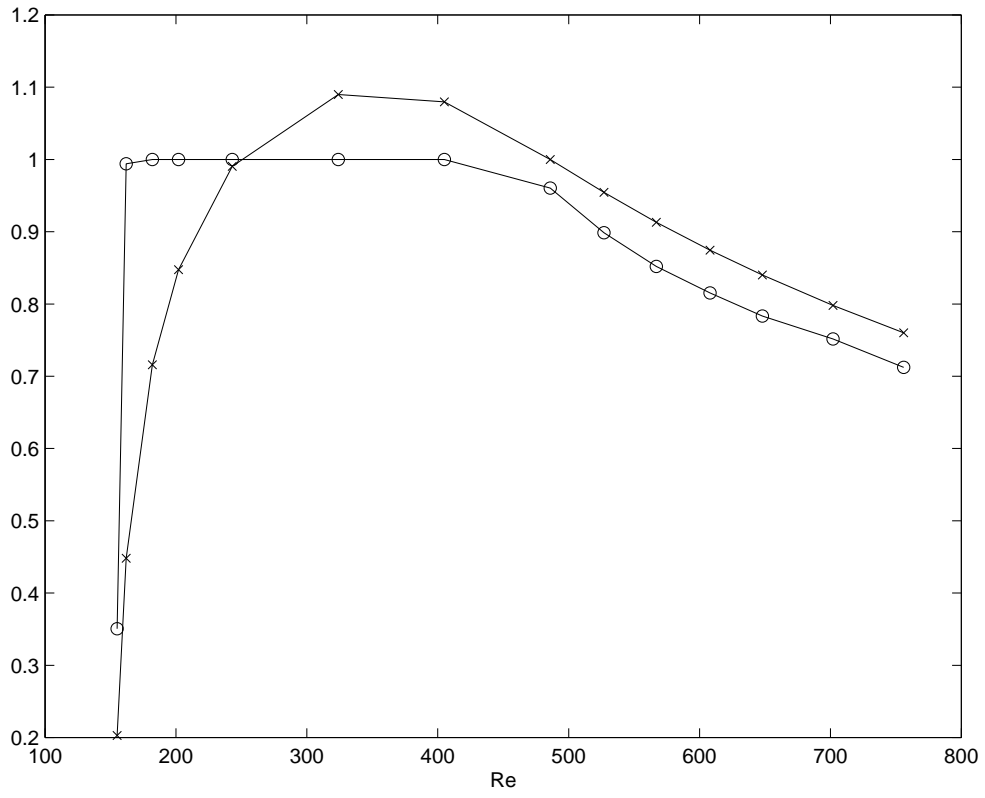
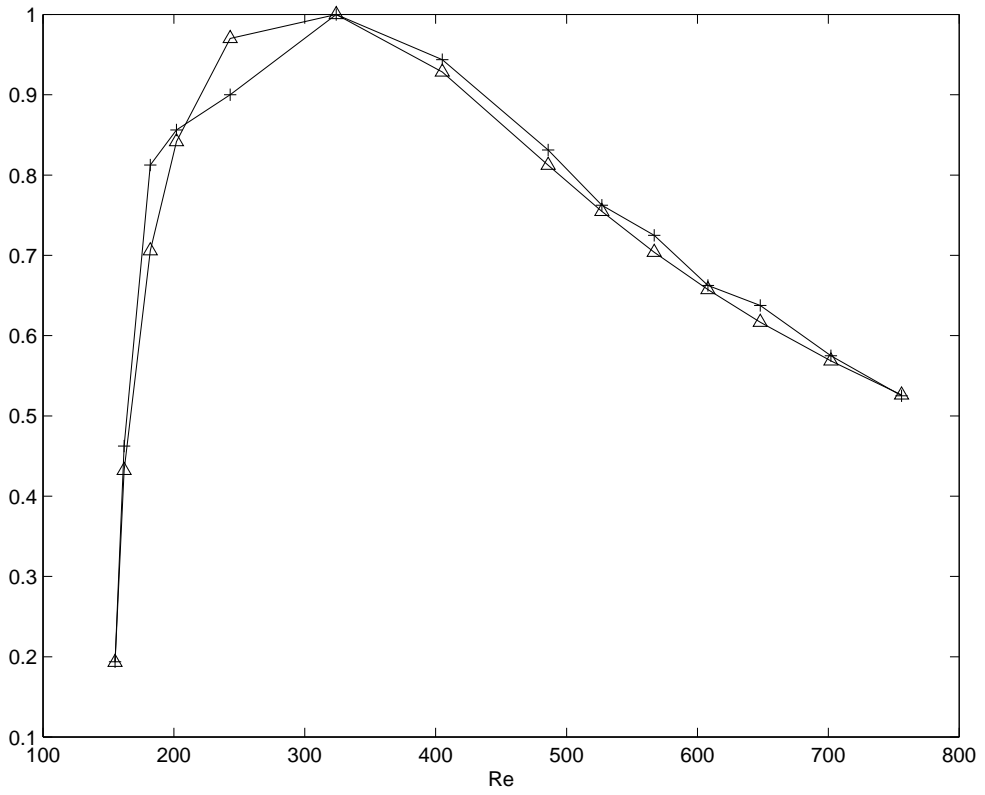


Fig 4c : Comparison of D_z with $\phi_\theta * \phi_v$



IV. DISCUSSION

We now offer a possible explanation for the remarkable agreement between D_z and $\phi_\theta * \phi_\nu$. The effective axial diffusion is related to the transport from vortex to vortex as a result of the wave perturbation. It is known from dynamical systems theory [23], and confirmed by experiment [24], that we can relate the flux of 'material' from vortex to vortex in terms of the volume of the lobe structures defined by the intersections of the stable and the unstable manifolds of the hyperbolic orbits. Therefore it is clear that the larger the volume of these lobes, the more effective the transport from vortex to vortex should be, thus leading to an enhancement of D_z . Up to first order in a perturbation parameter (in the present case, the wave amplitude), the volume of these lobes is related to a Melnikov function (which is a measure of the distance between the stable and unstable manifolds of the hyperbolic orbits). More precisely, a lobe is defined by the intersection of these manifolds, and these are identified with the zeroes of the Melnikov function. The lobe volume (which is proportional to the flux) is equal to the average of the Melnikov function between these intersections. Furthermore in the case where the unperturbed system is an Euler flow, the Melnikov function has been calculated corresponding to the streamlines perturbation due to viscous effects. It is found that the Melnikov function is simply the average of the dissipation of the flow averaged over the unperturbed streamline [25]. This shows that the dynamical symmetry part of our diagnostic is simply the Melnikov function, and from the above reasoning directly related to the inter-vortex particle flux, and hence to D_z . Mezić advanced similar ideas to relate the scaling of D_z with the scaling of boundary layer thickness [15]. However, the Melnikov function involves integration over time along a trajectory lying in the unperturbed separating surface, while our results indicate a connection with an Eulerian quantity integrated over space. This problem is under investigation.

Based on these considerations we expect $\phi_\theta * \phi_\nu$ to be closely related to D_z . This is what is shown in Fig. 4 and to the authors knowledge this is the first time that a close relationship between an essential Eulerian quantity, $\phi_\theta * \phi_\nu$, and an essential Lagrangian quantity, D_z ,

has been identified.

V. CONCLUSIONS

Based on the success of the diagnostic for wavy Taylor-vortex flow, we conjecture that for other flows a suitably defined and averaged diagnostic will be directly related to some type of macroscopic transport coefficient. Then the macroscopic (Lagrangian) behaviour in a flow can be quantified directly in terms of Eulerian quantities such as the flow field and its gradients.

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