Chaotic dynamics of inertial particles in three-dimensional rotating flows

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(Dated: March 28, 2005)

Novel methods for determining something in My Dynamical System .... are proposed and implemented.

PACS numbers: 95.10.Fh, 47.11.+j, 47.52.+j, 45.70.Mg, 05.45.-a
Keywords: chaotic advection, Lagrangian particle tracking, two-phase flows

Georgia Tech PHYS 7224:
CHAOS, AND WHAT TO DO ABOUT IT
course project, spring semester 2005
advisor: Dr. Fotis Sotiropoulos

I. INTRODUCTION

Mixing in non-turbulent flows has been the subject of extensive study in recent years, since several geophysical and engineering flows exhibit chaotic dynamics due to stirring produced by continuous stretching and folding of material lines [1]. Chaotic advection theory [2] has been developed to analyze these transport and mixing problems, connecting non-linear dynamics with fluid mechanics, based on the phase-space defined by the Lagrangian representation of fluid particles that show local instability and global mixing of trajectories.

The theoretical framework to describe these flows was first developed to study idealized two and three-dimensional flows, which were specified analitically as solutions of simplified Navier-Stokes equations [3–5]. Several experiments have also been carried out to elucidate the chaotic advection mechanisms driven by vortical structures in the flowfield, which homogenize the concentration of passive scalars [6–8].

Recently, investigations of experimentally realizable three-dimensional flows have given new insights in chaotic mixing of non-diffusive particles. The mechanisms of the rich Lagrangian dynamics of three-dimensional vortex breakdown bubbles in closed cylindrical containers have been studied in numerical and experimental investigations [9, 10], establishing the non-dimensional parameters that determine the Lagrangian characteristics of the flow.

The instability of the flow in a cylindrical container with exactly counter-rotating lids, also called *von Karman swirling flow*, was recently computed and studied in detail [11], identifying the chaotic characteristics of the flow at different Reynolds numbers. Numerical simulations agreed with stability analyses performed previously for this flow [12, 13]. The results [11] also showed how the shear-layer at the center of the container becomes unstable to azimuthal modes and developes radial and axial vortices, determining the onset of three-dimensional chaotic dynamics, while few stable/elliptic periodic orbits remain in islands or within toroidal regions close to the lids. From the flow instability, stationary radial *cat-eye* vortices emerge at the center of the container, in a number equivalent to the most unstable azimuthal wavenumber of the flow depending on the aspect ratio of the container, and the Reynolds number of the flow.

A remarkable finding of this study was the relationship established between the Reynolds number and the intensity of chaotic stirring. As the Reynolds number increases, the mixing increases up to a threshold, after which regions ocuppied by the unmixed islands grow, decreasing the stirring intensity within the flow. This phenomenon was previously studied [14], establishing that for steady and stable, bounded three-dimensional flows, mixing increases as long as viscous terms are important. If the Reynolds number is too large, and the flow remains steady, the chaotic regions and mixing in the flow will decrease.

Despite all this progress in Lagrangian studies of realistic complex three dimensional flows, there have been few investigations relating chaotic mixing of discrete inertial particles.

Particle-laden flows cover a wide range of applications in combustion, sprays, bubbly flows, atmospheric flows, and sediment transport in aquatic enviroments.

Numerical investigations of the Lagrangian properties of inertial particles in these flows have to take into account that solid particles cannot be considered passive scalars, but as a dispersed phase, which is subject to surface and body forces, as well as collisions with solid boundaries or other particles.

Most of the previous studies have been performed in analytical two-dimensional cellular flows or shear-layers. Numerical simulations have found that chaotic behavior of inertial particles depends on the density ratio between the two phases, and on the relative response time of the particles with respect to the time-scale of the vortical structures of the flow [15].

Recently, inertial particles in two-dimensional unsteady flows were analyzed in Hamiltonian systems [16],

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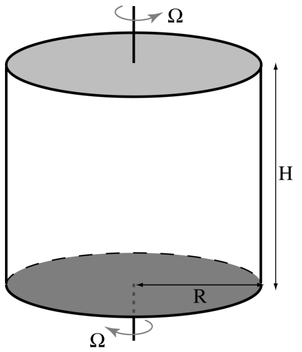

FIG. 1: Flow in a cylidrical container with counter-rotating lids.

using the stream function of Kelvin's cat-eyes vortices, for which chaotic dynamics was only observed in heavy particle systems.

The aim of this research is to investigate numerically the three-dimensional steady flow in a cylindrical container with two exactly counter-rotating lids as shown in Fig. 1, comparing the results obtained in the calculations for passive non-diffusive fluid particles [11].

The simulated particle trajectories will allow us to determine the non-dimensional parameters that characterize the chaotic behavior of the particle system, and the particle dispersion for this particular flow from periodic orbit theory [17].

In sect. II I derive the equations which govern the particle motion, by separating the effects of the different forces acting on the system. Implementation of the model and results are shown in sect. III, and a critical analysis of the results unveiling the effect of inertia is presented in sect. IV

My results are summarized discuss possible improvements of the method in sect. V. Why I failed to .... is explained in appendix A.

II. PROBLEM FORMULATION

The steady incompressible flow in a cylindrical container of radius R and height H, with lids rotating at the same angular velocity magnitude, Ω, but in opposite directions, as shown in Fig. 1, is characterized by two non-dimensional parameters: the Reynolds number, defined as:

$$Re = \frac{\Omega R^2}{\nu} \tag{1}$$

and the aspect ratio of the container:

$$AR = H/R \tag{2}$$

The basic axisymmetric flow is formed by an invariant manifold of two tori where only periodic orbits of fluid particles exist. The upper and lower halves of the cylinder have recirculating patterns due to Ekman pumping, and the radial jet formed at the center of the container creates a shear layer, which is the mechanism responsible for the initiation of chaotic mixing.

Recent studies of this flow for different Reynolds numbers, aspect ratios, and angular velocities of the lids [12, 13, 18, 19], have shown that this azimuthal shear layer becomes unstable, exciting three-dimensional modes that break the symmetry of the flow.

Lackey [11] carried out numerical simulations for $AR = 1$, in a range of Reynolds numbers between 295 and 850, integrating the three-dimensional incompressible Navier-Stokes equations with a second-order accurate scheme, using $81 \times 211 \times 161$ grid nodes. Fig. 2 shows the solution at $Re = 350$, for which the azimuthal mode 3 is excited. The two isosurfaces of radial velocity evidence the three-dimensionality of the flow produced by the radial vortices, whose centers are stable foci on the azimuthal plane. For larger Reynolds numbers, this characteristics of the flow are more evident as it is further discussed in [11].

Fluid particle trajectories from a Lagrangian viewpoint can identify the invariant and chaotic regions within the flow, and we can observe the global stirring effect as a function of the Reynolds number. Through Lagrangian average maps, the simulations showed that new invariant regions appear for $Re > 500$, reducing the size of the mixing area. The stirring intensity was quantified by the variance of concentration, which demonstrated that as long as the flow remains steady, there is a Reynolds number that maximizes stirring. Above this value the mixing declines approximately at $Re^{-1/2}$, confirming the theory developed by Mezić [14].

Here we study numerically the motion of small individual solid particles in this rotating flow, to explore the two-phase dynamics and the particle interaction within the chaotic regions produced by the three-dimensional shear layer instability.

Chaotic motion of inertial non-diffusive particles has been studied mainly for two-dimensional cell flows and ABC flows [15, 16, 23–25]. The chaotic behavior of inertial particles has been related to the ratio between the particle response time, which is a function of the drag force, and the characteristic time of the flow, as well as the density ratio between both phases.

These findings, however, have not been demonstrated experimentally or numerically in realistic three-dimensional flows. In this research we model the particle dynamics for the first time in realizable three-dimensional flows, using the solutions obtained for the cylinder with exactly counter-rotating lids.

To simulate the stirring of inertial dispersed particles that move independently of fluid elements, we need to establish the dynamic equations by modeling the forces acting on each particle. Therefore, the trajectory and momentum can be described by the following system of equations:

$$\frac{dx_{pi}}{dt} = v_{pi} \tag{3}$$

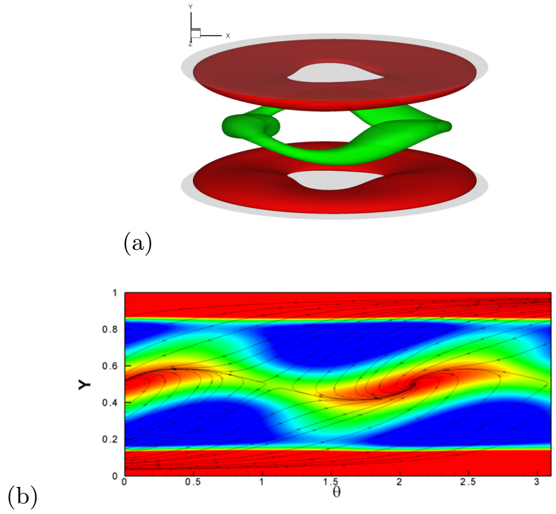

FIG. 2: Fully three-dimensional flowfield at $Re = 350$ and $AR = 1$ [11]. (a) Isosurfaces of radial velocity $u_r = -0.1\Omega R$ and $u_r = 0.065\Omega R$, and (b) Contours of radial vorticity, ω_r, and surface streamlines on the unfolded azimuthal plane $Y-\theta$ at $r = 0.75R$.

$$m\frac{dv_{pi}}{dt} = f_i \tag{4}$$

where v_{pi} and x_{pi} are the velocity and the position of the particle in each coordinate direction respectively, m is the mass, and f_i represents the sum of forces acting over the particle in the i direction.

A. Momentum Equation for an Inertial Particle

The total force acting on the solid particles, f_i in Eq. (4), is composed of three different parts: (1) Gravitational or other body forces; (2) Surface forces exerted by the fluid, such as drag or lift; and (3) Forces due to interaction with other particles and collisions with physical boundaries within the flow.

These forces represent the transfer of momentum between the two phases, which controls the complex real-life motion of fluid and solid particles. Empirical relations of drag, lift, gravity, and added mass effect for spherical particles are considered [20].

The modeled forces are assumed for spherical non-rotating particles, the drag force is obtained from dimensional analysis with a drag coefficient C_D calculated as a function of the particle Reynolds number [21]:

$$C_D = \frac{24}{Re_r}\left(1 + 0.15\ Re_r^{0.687}\right) \tag{5}$$

where the particle Reynolds number, Re_r, is scaled with the diameter and the relative velocity of the particle ($\mathbf{v}_r$):

$$Re_r = \frac{|\mathbf{v}_r|\, d}{\nu} \tag{6}$$

Models for lift and added mass forces in inviscid flows [22], with coefficients C_L and C_m respectively, are employed to derive the non-dimensional momentum equation, which is scaled with the container radius, and the magnitude of the rotational velocity Ω:

$$\begin{aligned}\frac{dv_{pi}}{dt} &= \frac{1}{(SG + C_m)}\left[-\frac{\delta_{i3}}{Fr^2\ \tilde{d}} + \frac{SG}{St}v_{ri}\right.\\ &\left. + C_L(\epsilon_{ijk}v_{rj}\omega_k) + (1 + C_m)\frac{Du_i}{Dt}\right]\end{aligned} \tag{7}$$

where $\tilde{d}$ is the non-dimensional particle diameter, v_{pi} and u_i represent the i component of the particle and flow velocity respectively. The relative velocity is defined as $v_{ri} = u_i - v_{pi}$, and the vorticity of the flow is the curl of the velocity field $\omega_i = \epsilon_{ijk}\frac{\partial u_k}{\partial x_j}$.

Other three dimensionless parameters appear in Eq.(7): The ratio of solid and fluid densities called specific gravity $SG = \rho_s/\rho$, the densimetric Froude number, which relates the inertial and gravity forces:

$$Fr = \frac{\Omega R}{\sqrt{(SG-1)gd}} \tag{8}$$

and the Stokes number, St, used to identify the dynamical relation between the two phases. Since the drag is the dominant force acting on the particles, the Stokes number is defined as the ratio between the particle response time and the characteristic time scale of the flow in the container:

$$St = \frac{\tau_R}{\tau_F} = \frac{4}{3}\frac{d\ SG}{C_D\,|\mathbf{v}_r|}\Omega \tag{9}$$

This parameter reflects the particle behavior due to the flow caracteristics. If the value of $St \ll 1$ a particle has enough time to respond to changes in flow velocity, and it can follow closely the motion of the largest scales of the flow. On the other hand, if $St \gg 1$ the particle velocity is not affected by the flowfield, and trajectories of fluid and solid particles with the same initial conditions diverge very rapidly.

Besides particle rotation, the model given by Eq. (7) also neglects the Basset history force due to the viscous stresses on the particle surface, as well as the Faxén correction on the drag force that accounts for non-uniform flow effects [20].

B. Particle Collision Model

(1) Ho hum
(2) Hee hee

III. ONE-WAY FLOW SIMULATION

The momentum and position equations for the particle, describe the particle with a point-volume representation where all the effects on the particle are concentrated in a point that corresponds to its center of mass, and the continuous background fluid is not affected by the particle motion. These are one-way coupling simulations since the solid phase does not alter the fluid dynamics.

A resolved particle scheme would require a detailed modeling of the particle volume, using boundary interface methods like the scheme developed by

Interaction of particles with the shear layer instability, and Ekman pumping.

A. Numerical implementation

R-K4

B. Flow Topology and Chaotic Dynamics

As is often the case, an understanding of the problem is a prerequisite to successful solution searches. We start by numerical integration of the dynamical system (**??**). Numerical experiments reveal regions where a trajectory

C. Stirring Inertial Particles

Lyapunov exponents, variance of concentration, Particle dispersion: $\langle x^2_{pij} \rangle$.

(Is it possible to do it?)

My system is symmetric under ....

IV. THE HOUR OF TRIUMPH

Nice results

V. DISCUSSION

Ultimate goals of the project was ...

I attained the minimal goal of ...

It was realistic to expect that ...

Then I got incredibly lucky, and....

In order to cope with the difficulty of finding periodic orbits in high-dimensional chaotic flows, we have....

My main result is ....

My method uses information from ... . The method is quite robust in practice.

Acknowledgments

I would like to thank Ernie and Bert for numerous helpful suggestions.

APPENDIX A: PROJECT PLAN

I intend to comment this appendix out when the project is finished - for now it helps Predrag keep track of how far am I along the plan.

Schedule of which part I intend to deliver by which date:

1. **Thu Apr 1:** The governing equations for the particle system will be derived, including the models considered to separate the forces exerted by the fluid and boundaries.
   A particle collision model will be proposed, and the first computations will be performed based on the model.

2. **Thu Apr 8:** Will construct the Poincaré section, and establish the main quantities to be computed: variance of concentration, particle dispersion, Lyapunov exponents, etc.

3. **Thu Apr 15:** Will show the main findings obtained from the simulations, evaluate the validity of the results, and propose new directions for further understanding of the flow.

4. **Thu Apr 22:** Will polish the project to high shine by finishing this report with figures, tables and text.

5. **Thu Apr 29:** Project deadline

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