## Report on the PhD thesis presented by Sofía Allende Contador

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The PhD thesis presented by Sofía Allende Contador with title "Dynamics and statistics of elongated and flexible particles in turbulent flows" is focused on the dynamics of small objects, with complex shape and structure, immersed on a turbulent environment. In particular, Sofía presents the results of numerical simulations of inertial spheroids and flexible fibers transported by homogeneous isotropic turbulence at high Reynolds number. The thesis is divided in 6 chapters.

In chapter 1, Sofía presents an introduction to the problem of transport of particles in fluids, providing examples of its fundamental relevance for biology, geophysics, epidemiology and industrial applications. She introduces the notion of complex particles, describing the features which determine their degree of complexity. Then she focuses on the two classes of particles considered in her thesis: Heavy, elongated particles, which are modeled by inertial spheroids, and flexible inextensible fibers. Finally, she presents the problem of modeling fragmentation processes of fibers transported by turbulent flows. The scope and the layout of the thesis are clearly presented at the end of this chapter.

In chapter 2, Sofía presents a review of the phenomenology of turbulent flows. After introducing the Navier-Stokes equations, she summarizes the theory of fully developed turbulence derived by Kolmogorov in 1941, presenting the main properties of turbulence in spectral and physical spaces. Then she discusses the phenomenon of intermittency, which leads to Kolmogorov 62 theory based on the concept of the refined self-similarity hypothesis, and its connection with the local structures of the dissipation field. In the end, she presents the Lagrangian description of turbulence, highlighting the long correlations which are observed along the fluid trajectories. In this chapter, she also discusses the use of numerical simulations to solve the Navier-Stokes equations in spectral space, presenting the specific numerical solver used in her study.

In chapter 3, Sofía reports the results of her study on the statistics of small inertial spheroids in turbulent flows. First, she introduces the description of the shape of the ellipsoids in terms of the aspect ratio and the parametrization of their orientation and rotation in terms of the Euler parameters. Then she discusses the equations which describe their translational and rotational dynamics. The equations used here are valid in the limit of small, heavy particles, with a density much larger than that of the fluid, such they are surrounded by a Stokes flow. Further, the particles are assumed to be very diluted, which allows describe their interaction with the flow by one-way coupling and to neglect the hydrodynamic interactions between them. The rest of the chapter contains the original results obtained from the numerical simulations. Sofía shows that the translational motion of the particles is almost independent on their orientation. In particular, the statistics of the rms velocity and acceleration of particles with different shape displays a universal behavior which solely depends on the dimensionless harmonic Stokes number of the particles. She also reports the presence of weak correlations between the translational motion and the orientation of the particles, which are observed for the autocorrelation of the velocity and the acceleration along the axis of symmetry of the particles. Then she reports the results on the rotational motions. The statistics of the orientation is found to be correlated over long timescales, and it cannot be reduced to that of a sphere with equivalent harmonic Stokes number. The rotation rates of particles are shown to be non-universal as well. Sofía explains the rapid decay of the rotation rates as a consequence of the ejection of the particles from regions of high vorticity. In the last part of chapter 3 she reports the results on the fractal clustering of the particles, which is quantified in terms of the correlation dimension. In view of future studies, I suggest that she investigates as well the preferential concentration in the elliptic and hyperbolic regions of the flow, which are introduced in Sect.2.4.4. This could give quantitative support to the argument of the vortical ejection discussed in the previous section 3.3.2.

In chapter 4, Sofía reports the results of her study of inextensible flexible fibers, passively transported by homogeneous, isotropic, turbulent flows. In the first part of the chapter, she discusses the mechanical properties of an inextensible, flexible cylindrical rod. Then she derives the local slender body theory, that provides a suitable model to describe the dynamics of small fibers immersed in a fluid in the turbulent regime. She discusses the assumptions which are required for the validity of the model. The fiber must be very small, such that the flow around the fiber can be approximated by a Stokes flow. It must be very thin, such that it can be modeled as a continuous line of punctual forces. Moreover, the inertia of the fiber is supposed to be negligible. Then Sofía focuses on the case of inextensible fibers, whose dynamics depends only on their flexibility. After discussing the numerical method for the integration of the dynamics of the fibers, she presents the results obtained. First, she introduces the buckling instability, and she discusses two alternative methods to identify the buckling events, based on the bending energy and on the end-to-end length. Then she shows that the statistics of the buckling events resembles that of an activation process in which the flexibility plays the role of temperature. She shows that the buckling rates follow an anomalous Arrhenius law. She also investigates the statistics of alignments of the fibers, introducing the notion of super-buckling events, corresponding to maximum misalignment of the fiber with respect to the direction of a rigid rod. She shows that the super-buckling rates follow again an Arrhenius law. In the last part of the chapter 4 she discusses the perspective and the ongoing works on the dynamics of fibers.

In chapter 5, Sofía reports her study on the modeling of fragmentation processes of brittle fibers. She recalls the definition of brittle materials, describing the two mechanisms which causes the breaking of brittle fibers. The first is the tensile failure, which occurs when the fiber is subject to strong stretching forces such that the internal tension exceeds a critical threshold. The second is the flexural failure, which occurs when the compression of the fiber causes a bucking event during which the local curvature becomes too high. Then she discusses how these mechanisms are implemented in the numerical simulations. In the ideal case of a fiber without defects, the tensile failure causes the breaking of the fiber in two identical parts. This process can occur recursively for the daughter fragments, resulting in a sequence of equal pieces whose final number is a power of two. Then Sofía presents a model which estimates the statistics of the pieces produced by a flexural failure. Finally, the statistics of individual failure events is used to derive a stochastic Lagrangian population model for the fragmentation of fibers. A key ingredient of the model is the statistics of waiting times between two buckling events. Sofía shows that it can be approximated by a Weibull distribution. In the end of the chapter 5, she discusses the limitations and shortcomings of the model presented. She also proposes a series of improvements of the model, e.g., the inclusion of a random distribution of defects within the fiber, the relative dispersion between the daughter fragments, and the inertia of the fragments.

In chapter 6, Sofía summarizes in a clear way the results reported in the previous chapters, and she discusses the perspectives for future studies, aimed to extend the results presented in this thesis to a broader class of particles and flow configurations.

The thesis includes also six appendices, which contain: A) The details of the equations for a particle with ellipsoidal shape; B) The derivation of the flexural forces; C) The numerical scheme to integrate the local slender body model; D) An introduction to activated processes; E) The definition of the Weibull distribution; F) The derivation of a kinetic equation for the fragmentation of fibers.

My overall impression on the thesis presented by Sofía is very positive. The subject of the thesis is of noticeable scientific interest. The high level of the research presented is attested by the publication of the results in international journals. The thesis is written in a clear way. The scope of the study is clearly stated both in the abstract and in the introduction. The pertinent literature has been properly reviewed at the beginning of each chapter. The original contributions of Sofía are presented in a well-organized structure.

For this reason, I express a very favourable opinion for Sofía Allende Contador to defend her PhD in front of the Committee.

Torino 11/02/2021

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