International Journal of Multiphase Flow 000 (2018) 1–25

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmulflow

Modelling of the evolution of a droplet cloud in a turbulent flow

Andreas Papoutsakis[a,*], Oyuna D. Rybdylova[a], Timur S. Zaripov[a,b], Luminita Danaila[c], Alexander N. Osiptsov[d], Sergei S. Sazhin[a]

[a] Sir Harry Ricardo Laboratories, Advanced Engineering Centre, School of Computing, Engineering and Mathematics, University of Brighton, Brighton, BN2 4GJ, UK
[b] High Performance Distributed Computing Laboratory, Kazan Federal University, Kazan, 420097, Russia
[c] CORIA, UMR 6614, Université de Rouen, Avenue de l'Université, BP 12, Saint Etienne du Rouvray 76801, France
[d] Institute of Mechanics, Lomonosov Moscow State University, Michurinskii 1, Moscow, 119899, Russia

A R T I C L E I N F O

Article history:
Received 9 February 2017
Revised 13 February 2018
Accepted 14 February 2018
Available online xxx

Keywords:
Fully Lagrangian approach
Turbulent diffusion
Droplet mixing
Second order structure
Caustics

A B S T R A C T

The effects of droplet inertia and turbulent mixing on the droplet number density distribution in a turbulent flow field are studied. A formulation of the turbulent convective diffusion equation for the droplet number density, based on the modified Fully Lagrangian Approach, is proposed. The Fully Lagrangian Approach for the dispersed phase is extended to account for the Hessian of transformation from Eulerian to Lagrangian variables. Droplets with moderate inertia are assumed to be transported and dispersed by large scale structures of a filtered field in the Large Eddy Simulation (LES) framework. Turbulent fluctuations, not visible in the filtered solution for the droplet velocity field, induce an additional diffusion mass flux and hence additional dispersion of the droplets. The Lagrangian formulation of the transport equation for the droplet number density and the modified Fully Lagrangian Approach (FLA) make it possible to resolve the flow regions with intersecting droplet trajectories in the filtered flow field. Thus, we can cope successfully with the problems of multivalued filtered droplet velocity regions and caustic formation. The spatial derivatives for the droplet number density are calculated by projecting the FLA solution on the Eulerian mesh, resulting in a hybrid Lagrangian–Eulerian approach to the problem. The main approximations for the method are supported by the calculation of droplet mixing in an unsteady one-dimensional flow field formed by large-scale oscillations with an imposed small-scale modulation. The results of the calculations for droplet mixing in decaying homogeneous and isotropic turbulence are validated by the results of Direct Numerical Simulations (DNS) for several values of the Stokes number.

1. Introduction

The analysis of droplet dynamics and their spatial distribution in turbulent flows is important for various engineering applications, ranging from fuel injection in internal combustion engines to droplet dispersion in environmental flows (e.g. Sazhin (2014)). Inertial droplets suspended in turbulent flow fields undulate under the influence of flow fluctuations along their trajectories. The droplet velocities are controlled by both the history of the droplet motion and the spatially correlated structures of the turbulent flow field. A variety of characteristic responses of the discrete phase to the turbulent fluctuations of the carrier phase have been identified. These responses include the macroscopic scale turbulent mixing (Fung et al., 2003), de-mixing or un-mixing of particles (Fessler et al., 1994; Reeks, 2014), Random Uncorrelated Motion (RUM) (Meneguz and Reeks, 2011) and increasing settling velocity (Wang and Maxey, 1993; Maxey, 1987). In large-scale engineering and environmental applications, the behaviour of sufficiently low-inertia droplets/particles, characterised by small values of the Stokes number (the ratio of the droplet velocity relaxation time to the macro time scale) in turbulent flows, has been successfully described by the convective diffusion equation with different models for the turbulent diffusion coefficient (Fuchs, 1964; Berlyand, 1974).

Two approaches are commonly used for the analysis of turbulent droplet/particle laden flows: Eulerian–Eulerian and Eulerian–Lagrangian (see Marchioli, 2017; Simonin et al., 1993). The Eulerian–Eulerian approach gives satisfactory results for describing large-scale structures and some integral parameters of turbulent gas-particle flows in channels, jets, and boundary layers. In this approach, uniqueness of all parameters of the particulate continuum is assumed. However, the mesoscale flow regions with possible formation of local droplet accumulation zones are asso-

* Corresponding author.
E-mail addresses: a.papoutsakis@brighton.ac.uk (A. Papoutsakis), s.sazhing@brighton.ac.uk (S.S. Sazhin).

https://doi.org/10.1016/j.ijmultiphaseflow.2018.02.014
0301-9322/© 2018 Published by Elsevier Ltd.

ciated with intersecting droplet trajectories and caustics in the dispersed-phase velocity field. The appearance of local regions of intersecting droplet trajectories with singularities in the droplet number density on the edges of these regions (caustics), and the types of these singularities in non-uniform and unsteady flows with inertial droplets, were described by Osiptsov (1984). Further investigations can also be found in Falkovich et al. (2002) and Wilkinson et al. (2006). Classes of two-particle models that allow for singularities in the phase space and intersecting trajectories (see Zaichik and Alipchenkov, 2007; Zaichik and Alipchenkov, 2009; Chun et al., 2005; Gustavsson and Mehlig, 2011a; Pan and Padoan, 2010), are presented in Bragg and Collins (2014b,a). Also, Eulerian models for the particulate continuum inferred from the kinetic equations for particles or from the equations for the probability density functions (PDF) of particles are presented by Zaichik et al. (2008) and by Shrimpton et al. (2014). In the Eulerian–Eulerian approach several versions of the two-fluid $k-\varepsilon$ model have been used (Pakhomov and Terekhov, 2013). In engineering publications on turbulent gas-droplet flows, the carrier flow field has been described on the filtered scale, with the system of droplets described in the framework of the continuum approximation (e.g. Volkov and Emelianov (2008)).

In many engineering applications (e.g. fuel spray injection and mixing, two-phase flows in combustion chambers), it is important to have information about the structure of local particle/droplet accumulation zones to estimate the rates of possible droplet collisions and the effect of droplet accumulation on heating and evaporation of droplets and combustion of fuel vapour/air mixtures (Sazhin, 2014). This information can be inferred only from Lagrangian tracking of the dispersed phase. In the standard Eulerian–Lagrangian approach for gas-particle/droplet flow modelling (e.g. Crowe et al., 1977; Sazhin, 2014), the carrier-phase flow parameters are calculated on a fixed Eulerian mesh and the particles/droplets are tracked along chosen Lagrangian trajectories. Direct modelling of individual droplet trajectories in the carrier phase leads to satisfactory results for the droplet velocity field (e.g. Sazhina et al., 2000). However, the correct calculation of the droplet number density field presents serious difficulties. This was instructively demonstrated by Healy and Young (2005), who showed that to reach a satisfactory accuracy in the calculation of the droplet number density in a laminar flow it is necessary to have about 10^3 Lagrangian droplet trajectories per Eulerian cell.

An approach that incorporates the solution of the droplet number conservation equation in Lagrangian form is the Fully Lagrangian Approach (FLA). In the paper by Healy and Young (2005) it was demonstrated for laminar flows that the number density of non-colliding particles along a chosen particle trajectory, and the trajectory itself, can be much more efficiently calculated based on the Fully Lagrangian Approach (FLA) proposed by Osiptsov (1984) (see also Osiptsov, 2000). FLA is based on the Lagrangian form of the continuity equation for the particulate phase, treated as a continuum, and the additional equations for the components of the Jacobi matrix of transformation from the Eulerian to the Lagrangian coordinates. This is essentially a method of characteristics for the solution of the continuity equation on the Lagrangian trajectories. This approach can deal with such complex cases as the regions of intersecting droplet trajectories and caustics. In Ijzermans et al. (2009), the efficiency of the FLA for the calculation of the droplet number density and its modelling capability in identifying the spatial structure of caustics was demonstrated.

The introduction of the FLA into the study of turbulent flows (see Picciotto et al., 2005) resulted in the identification and analysis of spatial structures of the dispersed phase distribution using the moments of concentration. The analysis by Meneguz and Reeks (2011) showed that the distribution of the particle concentration in the long term is log normal. This is consistent with the analysis by Monchaux et al. (2012) where, using Voronoï tessellation, the authors observed the same log normal distribution. Also, FLA studies on DNS of homogeneous and isotropic turbulence led to identification of the mechanisms involved in the segregation process (Meneguz and Reeks (2011); Reeks (2014)). The introduction of the FLA in the study of turbulent flows resulted in the quantification of the singularities related to trajectory intersections and the establishment of a relation between the frequency of their occurrence and the Stokes number.

The application of FLA in the Eulerian–Lagrangian context for gas-droplet flows, makes it possible to drastically reduce the number of calculated droplet trajectories, since in this case it is sufficient to have only one Lagrangian trajectory per Eulerian cell (or fold in an Eulerian cell) to ensure the required level of accuracy in the calculation of droplet concentration. This method has been successfully used for calculations concerning particle/droplet concentration fields in various flows (e.g. Tsirkunov et al. (2002); Golubkina et al. (2011); Govindarajan et al. (2013); Wang et al. (2006); Lebedeva and Osiptsov (2009); Ravichandran and Govindarajan (2015)).

Lebedeva et al. (2013) proposed a method based on a combination of the Lagrangian viscous-vortex method for the carrier phase and the Fully Lagrangian Approach for the dispersed phase. This is the fully meshless approach which makes it possible to avoid a cumbersome procedure of remeshing the dispersed phase parameters from the Eulerian to Lagrangian grids, which is typical for standard Eulerian–Lagrangian approaches.

In some publications (e.g. Picciotto et al., 2005; Meneguz and Reeks, 2011; Reeks, 2014), the Fully Lagrangian Approach for the dispersed phase was used alongside the DNS calculations of the carrier phase flow fields in a turbulent channel flow and in forced homogeneous turbulence simulations. These authors identified the formation of multiple singularities in the particle concentration fields.

Note that the carrier-phase velocity fluctuations lead to increased dispersion of suspended particles/droplets (hereafter referred to as droplets) which can be identified as turbulent mixing (see Reeks, 1977). Analogies between the mixing of droplets in turbulent flows and Brownian diffusion have been drawn by Xia et al. (2013) and Fung et al. (2003). This allows one to assume that the interaction between discrete phase and small scale turbulent fluctuations can be regarded as a Fickian diffusion process. Also, it has been observed that coherent turbulent structures of the carrier phase induce segregation of droplets at least at the level of the integral length scale of the flow field (Fessler et al., 1994), and the formation of patterns as described by Wood et al. (2005), and by Soldati and Marchioli (2009).

Droplet dispersion in turbulent droplet laden flows has been found to be far more sophisticated than the scalar mixing of a contaminant in a turbulent flow field (see Reeks, 1977; Fessler et al., 1994). It was shown that the turbulence of the carrier phase is responsible not only for droplet turbulent mixing (Fickian diffusion) (see Phythian, 1972), but also for the un-mixing of droplets to form coherent structures controlled by the integral length scale of the turbulent flow field (see Fessler et al., 1994; Ijzermans et al., 2010) and their accumulation in caustic formations. Thus, mixing and unmixing processes in this case can co-exist (Xia et al., 2013).

In addition to mixing, dispersed flows exhibit a wide range of responses to the fluctuation of the carrier phase flow field. With increasing droplet inertia (Stokes number), the effects of memory on the droplet motion become more pronounced. Direct numerical simulation of the behaviour of inertial droplets in forced isotropic turbulence shows that, as a rule, the distribution of inertial droplets in a turbulent velocity field is markedly non-uniform. Maxey (1987) identified the segregation of