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Numerical simulation of spray coalescence in an Eulerian framework: Direct quadrature method of moments and multi-fluid method

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Abstract

The scope of the present study is Eulerian modeling and simulation of polydisperse liquid sprays undergoing droplet coalescence and evaporation. The fundamental mathematical description is the Williams spray equation governing the joint number density function $f(v, \mathbf{u}; \mathbf{x}, t)$ of droplet volume and velocity. Eulerian multi-fluid models have already been rigorously derived from this equation in Laurent et al. [F. Laurent, M. Massot, P. Villedieu, Eulerian multi-fluid modeling for the numerical simulation of coalescence in polydisperse dense liquid sprays, J. Comput. Phys. 194 (2004) 505–543]. The first key feature of the paper is the application of direct quadrature method of moments (DQMOM) introduced by Marchisio and Fox [D.L. Marchisio, R.O. Fox, Solution of population balance equations using the direct quadrature method of moments, J. Aerosol Sci. 36 (2005) 43–73] to the Williams spray equation. Both the multi-fluid method and DQMOM yield systems of Eulerian conservation equations with complicated interaction terms representing coalescence. In order to focus on the difficulties associated with treating size-dependent coalescence and to avoid numerical uncertainty issues associated with two-way coupling, only one-way coupling between the droplets and a given gas velocity field is considered. In order to validate and compare these approaches, the chosen configuration is a self-similar 2D axisymmetrical decelerating nozzle with sprays having various size distributions, ranging from smooth ones up to Dirac delta functions. The second key feature of the paper is a thorough comparison of the two approaches for various test-cases to a reference solution obtained through a classical stochastic Lagrangian solver. Both Eulerian models prove to describe adequately spray coalescence and yield a very interesting alternative to the Lagrangian solver. The third key point of the study is a detailed description of the limitations associated with each method, thus giving criteria for their use as well as for their respective efficiency.

Keywords: Liquid sprays; Coalescence; Direct quadrature method of moments; Multi-fluid model; Spray equation; Number density function

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1. Introduction

In many industrial combustion applications such as Diesel engines, fuel is stocked in condensed form and burned as a dispersed liquid phase carried by a gaseous flow. Two phase effects as well as the polydisperse character of the droplet size distribution (since the droplets dynamics depend on their inertia and are conditioned by size) can significantly influence flame structure. Size distribution effects are also encountered in a crucial way in solid propellant rocket boosters, where the cloud of alumina particles experiences coalescence and become polydisperse in size, thus determining their global dynamical behavior [17,18]. The coupling of dynamics, conditioned on particle size, with coalescence or aggregation as well as with evaporation can also be found in the study of fluidized beds [36] and planet formation in solar nebulae [5,6]. Consequently, it is important to have reliable models and numerical methods in order to be able to describe precisely the physics of two-phase flows where the dispersed phase is constituted of a cloud of particles of various sizes that can evaporate, coalesce or aggregate and also have their own inertia and size-conditioned dynamics. Since our main area of interest is combustion, we will work with sprays throughout this paper, keeping in mind the broad application fields related to this study.

Generally speaking, two approaches for treating liquid sprays corresponding to two levels of description can be distinguished. The first, associated with a full direct numerical simulation of the process, provides a model for the dynamics of the interface between the gas and liquid, as well as the exchanges of heat and mass between the two phases using various techniques such as the volume of fluids (VOF) or level set methods [3,15,19,35]. This "microscopic" point of view is very rich in information on the detailed properties at a more local level concerning, for example, the resulting drag exerted on one droplet depending on its surroundings. The second approach, based on a more global point of view, describes the droplets as a cloud of point particles for which the exchanges of mass, momentum and heat are described globally, using eventually correlations, and the details of the interface behavior, angular momentum of droplets, detailed internal temperature distribution inside the droplet, etc., are not predicted. Instead, a finite set of global properties such as mass, momentum, temperature are modeled. Because it is the only one for which numerical simulations at the scale of a combustion chamber or in a free jet can be conducted, this "mesoscopic" point of view will be adopted in the present paper.

Furthermore, we are interested in sprays where droplet interactions (e.g., coalescence) have to be taken into account, which corresponds to liquid volume fractions between 0.1% and 1%. O'Rourke [30] classified the various regimes from the "very thin spray", which are transported by the gaseous carrier phase without influencing the gaseous phase, through the "thin spray" regime, for which there is two-way coupling through the momentum equation between the two phases, up to the "thick spray" regime for which the volume fraction of liquid is high enough so that droplet–droplet interactions have to be taken into account, but is still low enough so that the liquid volume fraction is negligible as compared to the gaseous one. Because our primary focus is on the ability of Eulerian methods to capture droplet coalescence, our study is limited here to the "thick spray" regime. By restricting our attention to one-way coupling, we can avoid difficulties (e.g., grid convergence) associated with using Lagrangian methods with two-way coupling, and it will thus be possible to make detailed comparisons between Eulerian and Lagrangian simulation results.

In the mesoscopic framework, there exists considerable interest in the development of numerical methods for simulating sprays [18,17,27,28,22,32]. The principal physical processes that must be accounted for are (1) transport in real space, (2) droplet evaporation, (3) acceleration of droplets due to drag, and (4) coalescence of droplets leading to polydispersity. The major challenge in numerical simulations is to account for the strong coupling between these processes. Williams [37] proposed a relatively simple transport equation based on kinetic theory that has proven to be a useful starting point for testing novel numerical methods for treating coalescing liquid sprays. In the context of one-way coupling, the Lagrangian Monte-Carlo approach [9], called Direct Simulation Monte-Carlo method (DSMC) by Bird [4], is generally considered to be more accurate than Eulerian methods for solving Williams equation. However, its computational cost is high, especially in unsteady configurations. Moreover, in applications with two-way coupling, Lagrangian methods are difficult to couple accurately with Eulerian descriptions of the gas phase. There is thus considerable impetus to develop Eulerian methods for describing sprays. In this paper, we limit our attention to one-way coupling with a given