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Numerical and experimental investigation of induced flow and droplet–droplet interactions in a liquid spray



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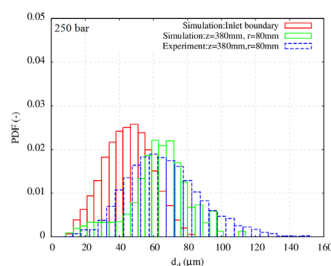
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HIGHLIGHT

- An Euler–Lagrange model for isothermal sprays is presented.
- Droplet collisions are detected using a novel Direct Simulation Monte Carlo method.
- The model is validated against phase Doppler interferometry experiments on water.
- The spatial evolution of droplet size distribution is predicted semi-quantitatively.

GRAPHICAL ABSTRACT



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ABSTRACT

An Euler–Lagrange model is presented that describes the dynamics of liquid droplets emerging from a high-pressure spray nozzle in a relatively large volume (of the order of almost a cubic meter). In the model, the gas phase is treated as continuum, solved on an Eulerian grid, and the liquid phase is treated as a dispersed phase, solved in a Lagrangian fashion, with interphase coupling through state-of-the-art drag relations obtained from direct numerical simulations. The droplets are introduced into the system at high velocities, leading to a turbulent self-induced gas flow which is solved using large eddy simulation. Despite the relatively low liquid volume fraction in the spray, the number density of droplets at the nozzle is still more than 10^{10} m^{-3} , which is why we employ a highly efficient stochastic Direct Simulation Monte Carlo approach to track collisions between droplets. The droplet collision frequency is calculated on the basis of local droplet number density, droplet size and relative velocities of neighbouring droplets within a dynamically adapting searching scope, as described in Pawar et al. (2014. Chem. Eng. Sci. 105, 132–142). We use known correlations from literature to determine the outcome of a binary droplet collision, which depending on characteristic dimensionless numbers can be coalescence, bouncing or, for high velocity impacts, stretching or reflexive separation leading to formation of satellite droplets. Our simulation model is compared with droplet velocities and size distributions obtained from phase Doppler interferometry experiments on an industrial scale hollow-cone pressure swirl nozzle spray. We find semi-quantitative agreement for spray characteristics such as the axial and radial spray velocity, spray jet width, and the dependence of the droplet size distribution on position within the spray. The simulation model enables us to study the relative importance of different droplet collision events occurring in the spray volume.

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1. Introduction

Atomization of a liquid is an important step in spray drying, air conditioning, spraying pesticides in agriculture, liquid fuel-combustion in gas turbines, oil furnaces, rocket engines, and in many other engineering areas (Nasr et al., 2002; Marchione et al., 2007; Tratnig et al., 2009; De Luca et al., 2009). Pressure swirl nozzles are often used to generate a spray of droplets. The operating principle of a pressure swirl nozzle relies on the conversion of pressure into kinetic energy to achieve a high relative velocity of the liquid with respect to surrounding gas. The swirling part of the nozzle gives a swirling motion to the liquid. The centrifugal forces acting on the liquid lead to a conical liquid sheet leaving the nozzle orifice. This liquid sheet becomes unstable and breaks up into small droplets. This initial droplet size distribution subsequently evolves to other distributions due to a multitude of droplet coalescence and collision-induced breakup events occurring continually inside the spray.

In this paper we describe a simulation model that can predict the evolution of a liquid spray beyond the initial atomization stage. Our work combines and builds on methods and insights generated by previous experimental and simulation studies of initial spray formation and subsequent spray evolution, which we will now shortly review.

Many experimental studies have been carried out focusing on the initial liquid sheet break-up and initial droplets emerging from a pressure swirl nozzle using different experimental techniques, such as high-speed photography, phase Doppler anemometry, particle image velocimetry, planar laser-induced fluorescence (Dombrowski and Fraser, 1954; Lozano et al., 2001), ballistic imaging (Paciaroni and Linne, 2004; Linne et al., 2006), structured laser illumination planar imaging (Berrocal et al., 2005, 2007–2009), X-ray radiography (Powell et al., 2000), and high-resolution shadowgraphy (Crua et al., 2012). Linne (2013) provides a detailed overview of the different experimental imaging techniques for dense spray analysis. As a result of these studies, many features of the liquid sheet breakup and initial droplet size distribution are understood reasonably well.

Other experimental studies focus on the spray evolution beyond the initial atomization stage. Often phase Doppler interferometry (PDI, sometimes also referred to as phase Doppler anemometry, PDA) is used to investigate spray properties such as the droplet size distribution and mean droplet velocity at various radial and axial locations for different liquid injection velocities (Sommerfeld, 1998; Ghorbanian et al., 2003; Wigley et al., 2004; Li and Shen, 1999). A disadvantage of PDI measurements is that they are intrinsically point measurements. To alleviate this limitation, Berrocal et al. (2005, 2007–2009) and Mishra et al. (2014) have extended SLIPI with LIF/Mie radio technique to extract a two-dimensional mapping of the droplets sauter mean diameter (SMD) throughout the spray in a single experiment. The average (SMD) values of droplet diameters agree well with PDI measurements. Berrocal et al. (2005, 2008, 2009) combined the light scattering experiments with Monte Carlo simulations of light propagation in the spray using assumed droplet size distributions. With this method, the inverse problem of predicting the droplet size distribution from the light scattering phase function could be solved. Note that this experimental method can be used both in the dense and in more dilute regions of a spray.

Despite the above experimental developments, accurate measurements of the droplet size distribution, droplet velocity, as well as coalescence and break-up events are difficult to perform close to the nozzle exit and deep inside the spray because the spray is usually optically very dense. Therefore, there is a growing interest to use computational fluid dynamics (CFD) for the investigation of

sprays. Just as with the experiments described above, it is important to distinguish between CFD studies focusing on the initial spray formation and CFD studies focusing on large scale evolution of the spray. For the former, fully resolved gas–liquid flow simulations are necessary (Menard et al., 2007). Such simulations are still difficult and computationally very expensive. They usually concern a few cases, representative of what can be encountered during an atomization process (Hirth and Nichols, 1981; Chang et al., 1993; Preussner et al., 1998; Nonnenmacher and Piesche, 2000; Iyer and Abraham, 2003; Renze et al., 2011).

Other CFD studies, including the one described in this work, focus on the evolution of the spray beyond the initial atomization step (O'Rourke and Bracco, 1980; Pinsky et al., 1999; Ruger et al., 2000; Vallet et al., 2001; Sommerfeld, 2001; Blei et al., 2002; Lebas et al., 2009; Luret et al., 2008). In particular, Sommerfeld (2001) and Blei et al. (2002) have carried out numerical simulations in which droplets are traced in a Lagrangian fashion to obtain droplet collision rates. They introduced a stochastic collision model based on an Euler–Lagrange approach where fictitious collision partners are generated; this approach is very economic with regards to computer time, because it does not require a search for a possible collision partner in the vicinity of the considered particle. However, for the generation of the velocity of the fictitious particle, assumptions about the velocity fluctuations need to be made. Such assumptions need not be made when collision partners are also explicitly tracked. An important development in this direction is the Direct Simulation Monte Carlo (DSMC) method, first proposed by Bird (1976). In DSMC, collisions between pairs of particles are detected stochastically instead of deterministically. The method is very popular for the investigation of large numbers of particles, because real particles can be represented by a lower number of representative particles, and the trajectories of only these representative particles are calculated. For CFD studies of this type, it is important to have an accurate model for the outcome of a binary droplet collision. Usually correlations, obtained from detailed experiments on single droplet collisions, are used (Ashgriz and Poo, 1990; Jiang et al., 1992; Qian and Law, 1997; Brenn et al., 2001; Ko and Ryou, 2005; Kuschel and Sommerfeld, 2013). Such detailed experiments show that collisions may lead to bouncing, coalescence or breakup of droplets, depending on the impact velocity and angle.

The objective of the present work is to introduce and validate a simulation model that can predict the temporal and spatial evolution of the droplet size distribution in a spray beyond the initial atomization step. We focus on isothermal sprays where droplet evaporation can be neglected. The model uses an Eulerian simulation method to capture the effect of induced air flow and a Lagrangian simulation method for the droplet phase. The Lagrangian method is a novel version of Direct Simulation Monte Carlo (DSMC) which we recently developed (Pawar et al., 2014). We will show that the predictions of our model compare favourably with experimental measurements in an isothermal water spray obtained from Phase Doppler Interferometry (PDI) experiments, focusing on the droplet velocity field, the droplet size distribution, and its spatial evolution characterized by the Sauter mean diameter.

In future work we will study the droplet–droplet interactions under non-isothermal conditions, and extend the collision model to include dried particles, all of which are relevant to the case of spray dryers. See e.g. Mezhericher et al. (2015) for recent work along these lines.

This paper is organized as follows. In Section 2 details are given of the numerical model for the gas phase and the discrete droplet phase, including a summary of the Direct Simulation Monte Carlo model for detection of droplet collisions, and the model to determine the outcome of such collision events. Details and parameters of the test geometry are given in Section 3. Section 4

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