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High-fidelity simulation of drop collision and vapor–liquid equilibrium of van der Waals fluids

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Abstract

The availability of a method to accurately predict the interaction of fuel drops and vapor–liquid equilibrium is crucial to the development of a predictive spray combustion model. The objective of this paper is to present such a method. A numerical method, based on the smoothed particle hydrodynamics (SPH), was coupled with a cubic equation of state for simulating the fuel drop dynamics and liquid–vapor distributions at various temperatures in the present study. SPH is a Lagrangian particle-based method, which is useful to simulate the dynamics of fluids with large deformations without the need for a transport equation to track the interface. The present study, furthermore, coupled SPH with van der Waals equation of state to simulate the phenomena of liquid oscillation, drop collisions at high velocity and characteristics of vapor–liquid equilibrium. This approach was found to offer the convenience of using a single set of equations, without the need for submodels, to predict drop breakup or vaporization. A hyperbolic spline kernel function was employed to eliminate the tensile instability that often has been reported in the literature. The numerical method presented here was found to successfully model the merging, stretching separation, fragmentation, and generation of secondary droplets in high-velocity collisions. In predicting vapor–liquid equilibrium, a variable-smoothing-length function was implemented to better facilitate the evaluation of vapor density at low temperatures. Finally, the results of this study indicate that, as the critical temperature was approached, no clear distinction was observed between the liquid and gas phases.

Keywords: Drop collision; Van der Waals fluid; Smoothed particle hydrodynamics; Vapor–liquid equilibrium

1. Introduction

The hydrodynamics and vaporization of liquid fuel drops play an important role in the combustion process. The interactions of high-velocity fuel drops affect the distribution of combustible mixtures and, consequently, the combustor

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performance. These phenomena are often simulated using criteria that predict the outcomes, based on the use of non-dimensional parameters. High-fidelity simulations of fuel drop dynamics can provide useful insight into the fundamental physics of such processes.

In this context, the smoothed particle hydrodynamics (SPH) method has the potential to simulate such phenomena in detail. SPH is a Lagrangian particle-based method, which uses kernel interpolation to evaluate fluid properties at any location. SPH was initially developed for astrophysics simulation [1,2]. Additionally, SPH has been successfully utilized to solve other fluid dynamics problems, such as shock, ocean wave formation and breakup, and solid mechanics phenomena, such as fracture and fragmentation [3,4]. Use of the SPH formulation in solving these types of fluid dynamics problems is particularly effective because it does not require an explicit definition of the free surface location, and thereby allows large deformations to be simulated in greater detail.

Furthermore, the SPH formulation can incorporate the equation of state to describe the vapor–liquid equilibrium [5]. This is useful, particularly, because it does not necessitate separate sets of equations to model the liquid and vapor phases. The cohesive term of the pressure equation manifests itself in the form of surface tension at the liquid–vapor interface, and generates phase boundaries without the explicit description of their location or curvature [5]. It was observed that particle rings were formed in the liquid phase at low temperature conditions, a phenomenon attributed to the SPH tensile instability [6]. Tensile instability has been shown to occur when the product of the second-order derivative of the kernel function and the principal stress is positive [6]. This instability causes particles to agglomerate or disperse away during simulation. A previous study has demonstrated that such instability can be reduced by adding an artificial pressure term in the momentum equation when the local pressure was negative [3]. This same methodology was applied to simulate the bending of solid beams [4] and the motion of van der Waals (vdW) fluids [7,8]. It was also suggested that a kernel function with only positive second-order derivatives (e.g., hyperbolic spline) can ensure that the simulation is stable in compression [6,9].

In predicting vapor–liquid equilibrium, deviations in saturated vapor densities at low temperatures can occur when the kernel smoothing length is a fixed value [5]. In a sparse medium, particles tend to have very little, or no, interaction with neighboring particles, because the latter are located beyond the compact support of the smoothing kernel. Previous studies predicted the spinodal decomposition of non-equilibrium square drops into two stable phases by use of a Korteweg stress tensor, a form of a body force generated by density gradients [10,11]. A variable smoothing length for better kernel evaluation was used in the vapor phase to obtain equilibrium conditions, closely matching those of the binodal curve. In a study, binary collisions of two infinitely long cylindrical vdW liquids were simulated using SPH, but the collisions were limited to small impact energy with $23 < Re < 68$ and $1 < We < 10$ [12]. It is apparent that new formulations, based on SPH, are required to accurately predict the outcomes of drop collisions and vapor–liquid equilibrium for combustion application.

In this paper, a numerical method based on SPH, coupled with cubic equations of state, was developed and applied to simulate the dynamics of a vdW drop at high Reynolds number (Re) and Weber number (We). One of the novelties of this work was the implementation of a hyperbolic kernel function combined with a variable smoothing length to eliminate the tensile instability that was reported in the literature [13,14]. The numerical simulations included the collision and vaporization of droplets. These two phenomena are critical to the mixture distribution, which in turn determines ignition and the quality of combustion. The vdW equation of state was integrated into the SPH formulation to predict the vapor–liquid equilibrium at high temperatures, and the numerical results were quantitatively compared with analytical data. Stable simulations of head-on and off-center binary collisions were achieved for high-velocity drops at $16.9 < Re < 132.5$ and $1.62 < We < 104$, an achievement not previously reported in the literature. This work lays the foundation for high-fidelity simulation of drop–drop and drop–wall collisions at high-temperature and high-pressure combustor conditions.

2. SPH formulation of van der Waals fluid

In the SPH methodology [1,2,15], every field variable (scalar or vector) can be evaluated according to Eq. (1), which is a finite kernel approximation of the true smoothed estimate given by Eq. (2). Here N is the number of particles within the support domain. The value of the kernel interpolation approaches the true estimate as N becomes very large [1,2]. $W(r\text{-}r', h)$ is the smoothing kernel used for the interpolation summation. r is the position vector of the particle, at which the variable is evaluated. r' is the position vector of the neighboring particle. h is the smoothing length, or resolution scale, which determines the support of the kernel function. In this paper, the hyperbolic kernel function was used (Eqs. (3) and (4)). Here, α_d has the values of $1/(7\,h)$, $1/(3\pi h^2)$ and $15/(62\pi h^3)$ in one-, two- and three-dimensions, respectively.

$$F(r) = \sum_{b=1}^{N} \frac{m_b}{\rho_b} F(r_b) W(r - r_b, h) \tag{1}$$