Large eddy simulation of turbulent spray with a filtered density function

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Abstract
Liquid atomization is a fundamental process found in inhalation aerosols, fuel injectors, and agricultural sprays, yet our methods for predicting the process are underdeveloped. Current state-of-the-art computational methods either prescribe primary atomization or are prohibitively expensive. We present a novel filtered density function (FDF) method for the large eddy simulation (LES) of primary atomization. A single fluid formulation is considered, such that the Eulerian governing equations are solved throughout the domain for both phases, while a set of phase-identifying Lagrangian/stochastic particles define the local volume of fluid. A Lagrangian volume of fluid provides conservation and, when coupled to a FDF, sub-grid-scale phase resolution. We consider both smoothed particle hydrodynamics and the finite particle method for construction of the particle-based interface geometry, as well as the pairwise force and curvature-based methods for determination of the surface tension term. These different particle approaches are compared with respect to geometric convergence and dynamic performance. This serves as a significant step in the development of a LES methodology for simulating turbulent sprays.
Introduction

Successful use and control of sprays requires a thorough understanding of primary atomization, but spray dynamics in general and primary atomization in particular are still not fully understood due to the complexity of the underlying processes. Experimental and physical techniques have difficulty exploring the dense, three-dimensional, highly turbulent zone where primary atomization occurs. Numerical simulation offers the ability to provide insights in underlying processes [1, 2].

Large eddy simulation (LES) – which resolves the large-scales and models the small-scales or sub-grid scale (SGS) effects – has achieved great success in the single phase flow modeling through years of developments [3]. For multiphase interfacial flows however, the situation is more involved. In recent applications, LES has been coupled with the VOF method to simulate atomization processes [4, 5]. In these studies, the surface tension force and SGS scalar flux are both neglected with the assumption that the Weber number is large and the effects of these terms can be small compared to inertial forces. However, these terms can play a significant role at the small scales, since curvature increases with decreasing length scale [2]. Thus, at small scale, the SGS interfacial forces can be as important as the resolved forces and should not be neglected for the correct prediction of the small droplet formation. In the filtered Navier-Stokes equation for the multiphase flows, the SGS surface tension is a nonlinear term which can be difficult to close. This is especially so given that droplet formation during atomization is not a cascade process as the dynamics in the single phase turbulence in the momentum equation [7, 8, 5], but at present we focus on developing a modeling context for the filtered surface tension term. A separate phase-identifying function is introduced in Eulerian formulations called the volume of fluid, \( \phi \), (VOF) for tracking the location of each phase. The function assumes a value of \( \phi = 1 \) in one phase and \( \phi = 0 \) in the other phase. The VOF transport equation is given by

\[
\frac{\partial \phi}{\partial t} + \frac{\partial u_j \phi}{\partial x_j} = 0, \tag{1}
\]

and in filtered form by

\[
\frac{\partial \langle \phi \rangle_L}{\partial t} + \frac{\partial (u_j) \langle \phi \rangle_L}{\partial x_j} = -\frac{\partial \Theta_j}{\partial x_j}, \tag{2}
\]

where \( \Theta_j = \langle \phi u_j \rangle_L - \langle \phi \rangle_L (u_j) \) is the SGS VOF flux representing the unresolved VOF interactions. The SGS VOF term, in addition to the momentum terms, requires modeling.

Closure strategy

The SGS stress, \( \tau_{ij} \), may be modeled with a variety of closures, including eddy viscosity models [9, 3], and is not the focus of this work. The modeling challenge of interest is rather closure of \( \langle F_i^s \rangle_L \) and \( \Theta_j \). We propose a new framework for closure based on the filtered density function method.

Probability-based methods have been used in the modeling of chemically-reacting flows and may be useful in effectively representing the filtered surface force term \( \langle F_i^s \rangle_L \). The value of PDF methods is that nonlinear source terms appear in closed form. Givi and co-workers extended the probability transport approach to LES – the filtered density function (FDF) – and have used it to model and simulate a variety of turbulent reacting flows [10, 11]. Solution of FDF transport equation is accomplished through Lagrangian Monte Carlo simulation, where the stochastic elements are the fine-grained densities of the VOF [10]. The Monte Carlo solution is equivalent to solving Eq. 2 with an assumption of gradient diffusion. The real benefit is that the filtered surface tension term can be closed by the Monte Carlo simulation.

Lagrangian volume of fluid

The Monte Carlo solution requires multiple phase-identifying particles carrying the local VOF \( \phi \) to be seeded in each Eulerian grid cell. In the liquid phase \( \phi = 1 \) and in the gas phase \( \phi = 0 \). This field of particles allows for the construction of

Methodology

Governing equations

The flows are governed by the filtered mass and momentum equations for an incompressible, immiscible multiphase system. The filtered momentum equations contain two sub-grid-scale terms to be closed - the SGS stress and the filtered surface tension. The latter includes contributions from both the resolved-scale and SGS surface tension. Generalized multiphase flows (those with variable density and viscosity) include multiple additional terms in the momentum equation [7, 8, 5], but at present we focus on developing a modeling context for the filtered surface tension term.
an implicit interface, composed of a color function $c$, normal vectors $n$, and curvature $κ$. Each particle in the neighborhood of the interface carries these interfacial geometry terms from which the surface tension on each interfacial particle $i$ can be computed. The accuracy of the resultant filtered surface tension term depends on the accuracy of the particle method used to develop the implicit interface.

In general, SPH uses kernel approximations to construct functions and derivatives by sampling nearby particles with a weight function $W$ that has a particular set of properties [13]. This formulation formally has second order accuracy and first order consistency for uniformly distributed particles, but falls below zeroth order consistency when the particles become disorganized. Although this formulation has been successfully implemented in the context of fully Lagrangian simulations and may be satisfactory for well-behaved particle fields, the requirement may be restrictive in the context of the LVOF and turbulent flows. An alternative is the finite particle method, which is a generalization of corrective smoothed particle hydrodynamics (CSPH).

The FPM produces the solution with a selected order of accuracy and retains first order consistency for irregular particle distributions [13]. As it is derived from Taylor series, the FPM must operate on a smooth field. For this purpose a preliminary color function is constructed through a CSPH expression. Solution of the FPM is achieved by considering as many weight functions as unknowns (the selected weights must produce a unique solution), and solving the associated linear system produces the implicit interface. In this case, the solution has third order accuracy because derivatives through second order have been retained. The resulting FPM formulation has first order consistency for the color function and all of its derivatives for both regular and irregular particle distributions. This is a significant improvement over previous CSPH approaches.

Preliminary Results

We use the particle methods in the previous section to compute the particle surface tension, and then compute the Eulerian surface tension term according to the CSPH and FPM approaches. The particle positions are evolved according to

$$\frac{dx_i}{dt} = \mathbf{u}_i^p, \quad (3)$$

where $\mathbf{u}_i^p$ denotes the velocity vector of particle $i$ obtained from a first order interpolation of the Eulerian velocity. In the cases that follow we do not present all of the numerical parameters, because actual validation is reserved for future work. Here we present results to demonstrate capability.

First we consider the simulation of two-dimensional temporal mixing layers. At sufficiently high Reynolds numbers, mixing layers undergo transition due to Kelvin-Helmholtz instability. Surface tension at the interface of multiphase mixing layers can modify and even completely damp the transition. Researchers have extensively explored this phenomena both analytically and computationally [14]. We test the ability of the proposed LVOF method to produce a surface tension to dampen instability development at the interface of two immiscible fluids of equal density and viscosity.

The pertinent weber number for this configuration is defined as

$$We = \frac{\rho \lambda \gamma^2}{\sigma}, \quad (4)$$

where $\rho$ is the fluid density, $\lambda$ is the wavelength of the interface instability (here taken to be the span of the domain), $\gamma$ is the mean shear rate defined as $\gamma = -2V_\infty$ where $V_\infty$ is the far field velocity, and $\sigma$ is the surface tension coefficient. For an inviscid flow (here we consider $Re = 400$), there are no unstable modes for $We < 4\pi$ [14]. We therefore consider a variety of Weber numbers in this neighborhood to determine if the LVOF method for surface tension can damp the surface instability in the proper neighborhood of $We$.

For perspective, we provide a temporal evolution of a mixing layer with $We = \infty$ in Fig. 1 to demonstrate the undamped development of the interface. The dark fluid is one phase and the light fluid is a different phase, but both phases have the same density and viscosity. The mesh resolution is $128^2$, and 16 LVOF particles are initialized in each Eulerian cell. The weight function has an influence radius of $2\Delta$. The dimensionless time $t^*$ is defined as $t^* = tV_\infty/(2\pi)$. At time $t^* = 0$ the fluid at the top of the domain moves to the right and the fluid at the bottom of the domain moves to the left. The interface becomes unstable near time $t^* = 4.8$ and begins to roll up, as shown at $t^* = 8.0$.

We consider the interfacial development at three different Weber numbers, as demonstrated in Fig. 2. These computations were performed with the FPM formulation of the LVOF. The first Weber number is $We = 15.7 > 4\pi$, meaning the mixing layer should be unstable, and indeed this case has demonstrated instability (the wave is not smooth and periodic). The second case, $We = 7.9 < 4\pi$, is within 40% of the critical Weber number, but does not demonstrate instability. Lastly, the third case...
has a Weber number well below the critical value $We = 3.14 \ll 4\pi$, and presents a low amplitude surface oscillation. These results suggest the FPM-LVOF method for computing surface tension has successfully described the transition from unstable to stable mixing layer dynamics near the critical Weber number. This problem was also tested on a $32^2$ mesh with similar results.

References


Figure 1. Development of a temporal mixing layer with no surface tension ($We = \infty$): (a) $t^* = 0$; (b) $t^* = 4.8$; (c) $t^* = 8.0$. 

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Figure 2. Temporal mixing layers with various Weber numbers at $t^* = 8.0$: (a) $We = 15.7$; (b) $We = 7.9$; (c) $We = 3.14$. 