

# A hybrid Eulerian-Lagrangian method for LES of atomising spray

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## Abstract

Our goal in this work is to develop a hybrid Eulerian-Lagrangian technique for simulating the breakup and atomization of liquid jets. The large scales associated with the primary breakup of the liquid jet are captured using an Eulerian surface capturing technique. The present formulation uses the particle level set method of Enright *et al.* [3] implemented on an adaptive Cartesian mesh. The small scales associated with secondary breakup are modeled using a stochastic sub-grid model by tracking the droplets in a Lagrangian framework [1]. The transition from primary (Eulerian) to secondary (Lagrangian) atomization is defined implicitly by the local grid resolution, taking place when the liquid interface can no longer be properly resolved on the grid. The sub-grid droplets thus formed may undergo further breakup according to the secondary breakup model. The formulation is developed and several preliminary cases of drop breakup are performed.

## 1 Introduction

Atomization and breakup of liquid jets in a turbulent flow is fundamental to many combustion and propulsion systems in use, including internal combustion engines, liquid and solid propellant rocket motors, gas-turbine aircraft engines [10]. These applications involve an intricate coupling between the liquid fuel and gaseous oxidizer with dynamically evolving interfacial boundary in the presence of a wide range of length and time scales due to turbulence and chemical reactions. Liquid fuel is usually injected into the combustion chamber through a series of swirl atomizers in the form of conical sheets. In the presence of turbulent shearing flow near the nozzle, the liquid sheets undergo destabilization due to Kelvin-Helmholtz type instabilities. The surface tension acts as a stabilizing force and imposes a lower

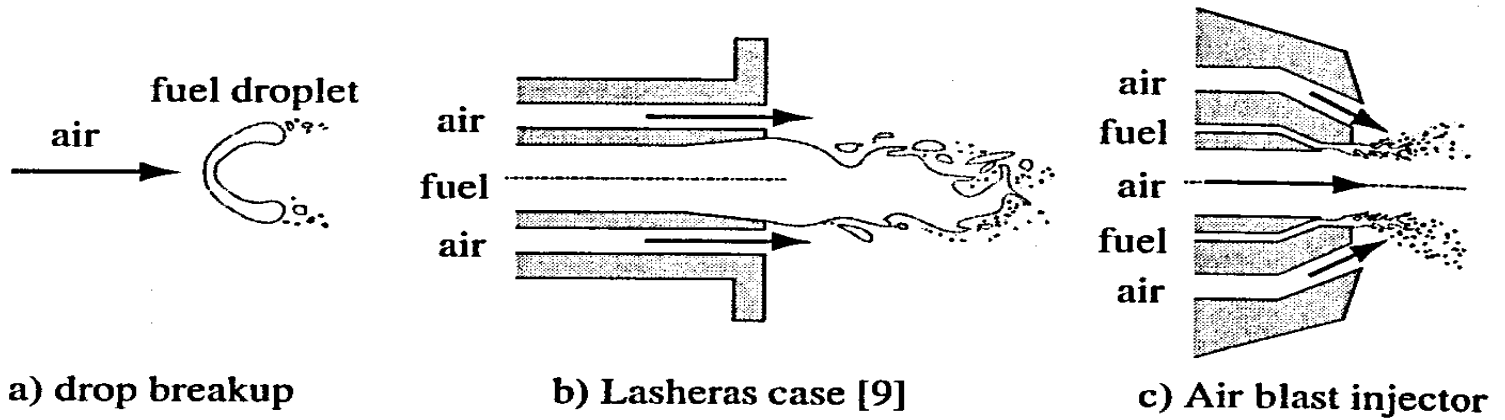


Figure 1: Numerical tools and models are being developed to simulate the above progression of breakup and atomization cases using a hybrid Eulerian-Lagrangian approach for the liquid phase, and large-eddy simulation for the gas phase.

cut-off for the growth of these instability waves. This near-field phenomenon is termed *primary atomization*. The ligaments and liquid lumps stripped off from the central liquid core may still undergo further breakup if the aerodynamic forces exceed the surface tension and viscous forces and is termed *secondary breakup*. These droplets evaporate and the fuel vapor thus formed mixes with the surrounding oxidizer to give spray flames. The liquid atomization process thus plays an extremely important role in efficient functioning of many propulsion devices.

Owing to the complexity of the underlying physical processes involved, the liquid sheet breakup is still poorly understood. In addition, quantitative measurements of the drop size and liquid void fraction are difficult to make and are often subject to large errors [9]. Numerical modeling of primary atomization and sheet breakup are limited to low Reynolds numbers and mainly two-dimensions [20, 18]. The majority of modeling efforts to date have been based upon the secondary breakup, where the liquid sheet is approximated by large droplets of the size of the injector nozzle and the interface dynamics is ignored [12, 14, 17]. These droplets are treated as point-particles, undergo breakup and create new droplets which are tracked using the standard Lagrangian approach. This approach has been successfully coupled with large eddy simulation for the gas phase and used to solve multiphase reacting flows in complex geometry, described elsewhere in this proceedings [2]. While the Lagrangian point-particle approach is well suited to the low liquid volume fractions present in most of the combustor, it is very likely inaccurate near the injector where the liquid volume fraction is much larger, and the relatively simple particle drag laws will be incapable of properly describing the dynamics of the multiphase interaction, even when corrections for deformation are included [5].

This work focuses on developing a new method for simulating atomization of liquid jets by using a hybrid Eulerian-Lagrangian technique for the liquid phase. The primary atomization is captured by the particle level set method of Enright et al. [3] implemented on a Cartesian adaptive grid. Depending on the level of

refinement, this captures the large and intermediate scales of primary atomization. The stripping, breakup of the liquid sheet, collision and coalescence of the liquid lumps is automatically captured by the level set representation. As the liquid sheet gets stretched and deformed the small scales (regions of high curvature) are under-resolved on the grid used. These scales are eliminated from the level set representation and replaced by subgrid droplets of equivalent size to conserve the liquid mass. These droplets now are tracked in the Lagrangian framework and may undergo further breakup according to the secondary breakup model. The details of this model are summarized in brief. It is planned to apply the developed methodology to the series of atomization cases of increasing complexity shown in figure 1. In the present contribution we present some preliminary simulations from the first case of drop breakup.

## 2 Formulation for primary breakup

The liquid/gas interaction and primary breakup is captured using the particle level set method of Enright *et al.* [3] implemented on a Cartesian adaptive grid. Transient refinement and coarsening is used to concentrate the Eulerian resolution near the freesurface and significantly reduce the overall simulation cost. Details of this approach can be found in Young *et al.* [19], and is summarized briefly here.

### 2.1 The level set method

We start with a review of the level set method, and then discuss the particle corrections in a subsequent section. For recent reviews of the level set method and its many applications, the interested reader is referred to Osher and Fedkiw [13] or Sethian [15]. For the present problem, the incompressible, immiscible, two-fluid system is treated as a single fluid with strong variations in density and viscosity in the neighborhood of the interface. The continuity and momentum equations for such a flow can be written in conservative form as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + \sigma \kappa \delta(d) n_i, \quad (2)$$

where  $u_i$  is the fluid velocity,  $\rho$  the fluid density,  $p$  the pressure,  $\tau_{ij}$  the viscous stress tensor,  $g_i$  the acceleration due to gravity,  $\sigma$  the surface tension coefficient,  $\kappa$  the local free surface curvature,  $\delta$  the Dirac delta function evaluated based on  $d$  the normal distance to the surface, and  $n_i$  the unit normal at the free surface.

It is well known that attacking equations 1 and 2 directly in the presence of the discontinuities at the interface will lead to the excessive smearing of the interface over long time integration, and/or numerical “ringing” in the region of the discontinuities due to dispersive errors in the numerical discretization. In the present work,

we capture the interface as the zero-level isosurface of a higher-order function  $\phi$ , the level set function (effectively an additional transported scalar). On either side of the interface, the sign of the level set function can be used to determine which fluid is present. This allows the fluid properties to be written as a function of the level set only, specifically  $\rho = \rho(\phi)$ . The application of chain rule to the continuity equation then yields:

$$\frac{d\rho}{d\phi} \left( \frac{\partial\phi}{\partial t} + u_j \frac{\partial\phi}{\partial x_j} \right) + \rho \frac{\partial u_j}{\partial x_j} = 0 \quad (3)$$

For the case of constant density except in the neighborhood of the zero level set, which represents the fluid interface, the solution of the continuity equation can be decomposed into the solution of the following:

$$\frac{\partial\phi}{\partial t} + u_j \frac{\partial\phi}{\partial x_j} = 0 \Big|_{\phi=0} \quad (4)$$

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (5)$$

Eq. 4 is the standard evolution equation for the level set function, and eq. 5 is the incompressible continuity equation. Note that the level set equation need only be solved near the interface, which we have defined as the zero level set. Away from the interface, it is common to make  $\phi$  equal to a signed distance function.

In a similar way, the application of chain rule to the momentum equation allows the decomposition of the momentum equation into the solution of the level set equation, eq. 4, and the solution of the following momentum equation:

$$\rho \frac{\partial u_i}{\partial t} + \rho \frac{\partial u_j u_i}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + \sigma \kappa \delta(|\phi|) n_i \quad (6)$$

Equations 4 – 6 comprise our governing system for the present work. They are discretized and solved sequentially in each time step as follows. The level set equation is first advanced in time using a 3<sup>rd</sup>-order Runge-Kutta scheme. The spatial derivatives required in the region of the zero level set are approximated by the 5<sup>th</sup>-order WENO scheme of Jiang & Peng [7]. The structured stencil required by this discretization is made available by adapting the Cartesian grids to uniform size in a band about the zero-level set. The same spatial discretization is also used to reinitialize the levelset to a signed distance function. With the level set advanced, the fluid properties (density and viscosity) are recalculated in each control volume, and then the momentum equations are advanced using a standard fractional step method with second-order finite volume discretization of the spatial derivatives.

## 2.2 The particle level set method

Note that the level set formulation results in a system of governing equations that can no longer be written in conservative form. Thus, when the finite volume

method is applied to this system, we cannot expect to achieve discrete conservation of mass and momentum (in the region of the interface). It is the dissipative nature of the level set method that has been its principal criticism. Proper reinitialization of  $\phi$  to a signed distance function after each time step can reduce the error, but mass conservation is not guaranteed. It appears, however, that much of the dissipation can be avoided by using massless Lagrangian particles to correct the zero level set.

In the particle level set method, massless Lagrangian particles are randomly seeded on both sides of the zero level set and used to correct the level set when characteristic information is deleted by the Eulerian WENO scheme. The details of the particle correction algorithm are given in Enright *et al.* [3]. For the present 3d simulations, we used 64 particles per control volume in a band of width three control volumes on either side of the zero level set. The additional computation time for the particles added less than 10% to the overall simulation cost, and significantly improved the conservation properties of the level set method.

### 3 Secondary breakup

A stochastic approach for droplet breakup that takes into account a range of product-droplet sizes is used to model the secondary atomization. Specifically, for a given control volume, the characteristic radius of droplets is assumed to be a time-dependent stochastic variable with a given initial size distribution function. The breakup of parent blobs into secondary droplets is viewed as the temporal and spatial evolution of this distribution function around the parent-droplet size. This distribution function follows a certain long-time behavior, which is characterized by the dominant mechanism of breakup. The size of new droplets is then sampled from the distribution function evaluated at a typical breakup time scale of the parent drop. Kolmogorov (1941) developed a stochastic theory for breakup of solid particles by modeling it as a discrete random process. He assumed that the probability to break each parent particle into a certain number of parts is independent of the parent-particle size. Using central limit theorem, Kolmogorov pointed out that such a general assumption leads to a log-normal distribution of particle size in the long-time limit.

Based on Kolmogorov's hypothesis a numerical scheme for atomization of liquid spray at large Weber numbers is developed by Apte *et al.* [1] The discrete model by Kolmogorov is reformulated in terms of a Fokker-Planck (FP) differential equation for the evolution of the size-distribution function from a parent-blob towards the log-normal law:

$$\frac{\partial T(x, t)}{\partial t} + \nu(\xi) \frac{\partial T(x, t)}{\partial x} = \frac{1}{2} \nu(\xi^2) \frac{\partial^2 T(x, t)}{\partial x^2}. \quad (7)$$

where the breakup frequency ( $\nu$ ) and time ( $t$ ) are introduced. Here,  $T(x, t)$  is the distribution function for  $x = \log(r_j)$ , where  $r_j$  is the droplet radius. Breakup occurs when the Weber number exceeds a critical value and  $t > t_{breakup} = 1/\nu$ . The value of the breakup frequency and the critical radius of breakup are obtained

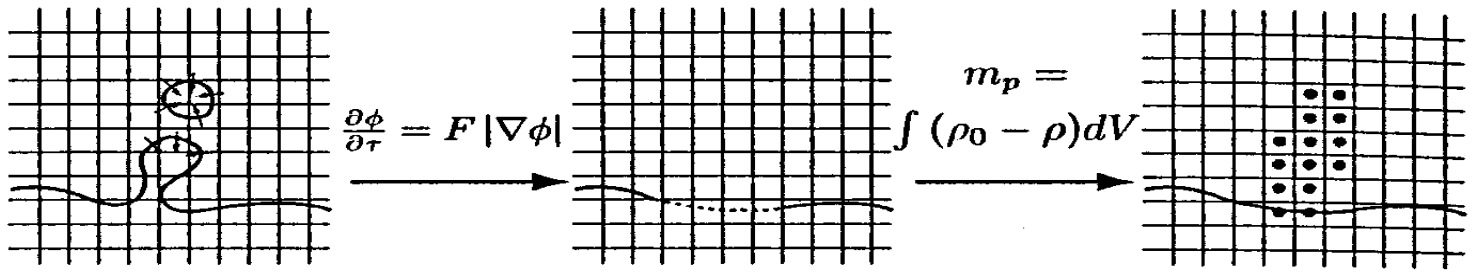


Figure 2: Schematic showing the transition process from Eulerian to Lagrangian description of the liquid phase. Step 1: Small scale structure is removed by solving the curvature-driven flow problem to steady state. Step 2: Lagrangian particles are introduced in control volumes where the fluid density has changed, conserving mass on a per-control-volume basis.

by the balance between the aerodynamic and surface tension forces. The secondary droplets are sampled from the solution of the equation (7) corresponding to the breakup time-scale. The parameters encountered in the FP equation ( $\langle \xi \rangle$  and  $\langle \xi^2 \rangle$ ) are computed by relating them to the local Weber number for the parent blob, thereby accounting for the capillary forces and turbulent properties. The capillary force prescribes a lower bound limit for the produced-droplet size through the local maximum stable (or critical) radius  $r_{cr}$ . As new droplets are formed, parent droplets are destroyed and Lagrangian tracking in the physical space is continued until further breakup events. The evolution of droplet diameter is basically governed by the local relative-velocity fluctuations between the gas and liquid phases. Details of this model can be obtained from Apte et al. [1].

## 4 Transition from Eulerian to Lagrangian

Consistent with the level set method, the transition from the Eulerian to Lagrangian framework was designed to avoid any formal reconstruction of the zero-level set iso-surface, thus avoiding any “emotional involvement” in the breaking and joining of the interface. A level set approach developed to remove noise in image processing is the min/max curvature flow [16]. In the present work, we plan to use a similar technique to remove liquid flow structure with a size near the local grid dimension. The removed Eulerian fluid is then replaced with Lagrangian particles such that mass is conserved. This process is shown schematically in figure 2.

## 5 Preliminary results

At the time of writing, the particle level set method has been implemented on a Cartesian adaptive grid with adaptation performed in a band around the zero level set such that the structured stencils required by the higher-order WENO discretizations are available. The Cartesian adaptive mesh refinement (AMR) method is that

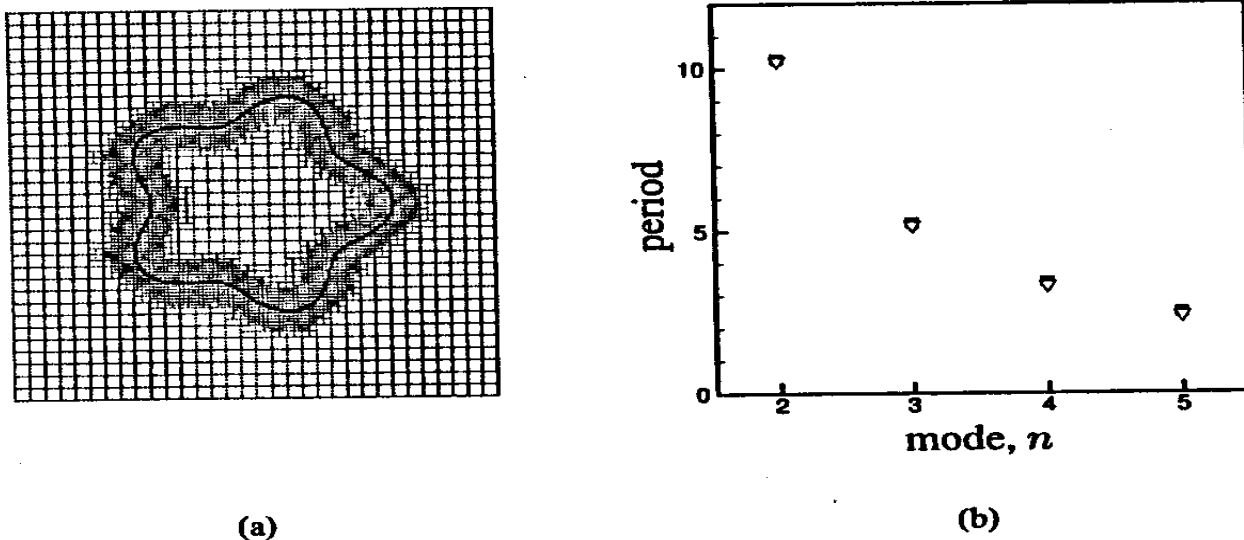


Figure 3: 2d drop oscillation results: a) Adaptive Cartesian grid shown with exaggerated initial amplitude of 15% for the  $n = 5$  mode. b) Comparison of computed results ( $\nabla$ ) to theory of Lamb ( $\blacksquare$ ) [8].

described in Ham *et al.* [4], and allows for arbitrary transient anisotropic refinement and coarsening throughout the domain. In the present simulations we have simply coarsened the grid uniformly by a factor of either 2 or 4 away from the level set band, although flow-based adaptation is planned for future simulations. The method has been validated by solving the standard 2d column and 3d drop oscillation simulations. Some results for the 2d case are presented in figure 3 to clarify how AMR is being used in these simulations.

To test the ability of the code to solve breakup problems we simulated the acceleration and breakup of an initially stationary drop in a uniform velocity field. The 2d breakup problem was investigated numerically at a resolution of  $512 \times 512$  by Zaleski *et al.* [20]. Their results were able to identify different dynamical processes leading to breakup for different sets of simulation parameters. Their initial condition was grid resolution dependent, however, and their simulations were all run with the density ratio  $\rho_l/\rho_g = 10$ . In the present work, a consistent initial condition was used: the flow was accelerated from rest to its characteristic velocity  $U$  in a distance of one drop diameter  $D$ . Figure 4 shows a surface rendering for one of the 3d simulations performed. While some of the qualitative features of the breakup are being captured (e.g. bag formation, ring breakup, and stamen formation) clearly the simulation is contaminated by numerical errors on the underlying Cartesian grid. Additional simulations are being made with higher resolution and with alternative surface tension formulations to quantify these errors.

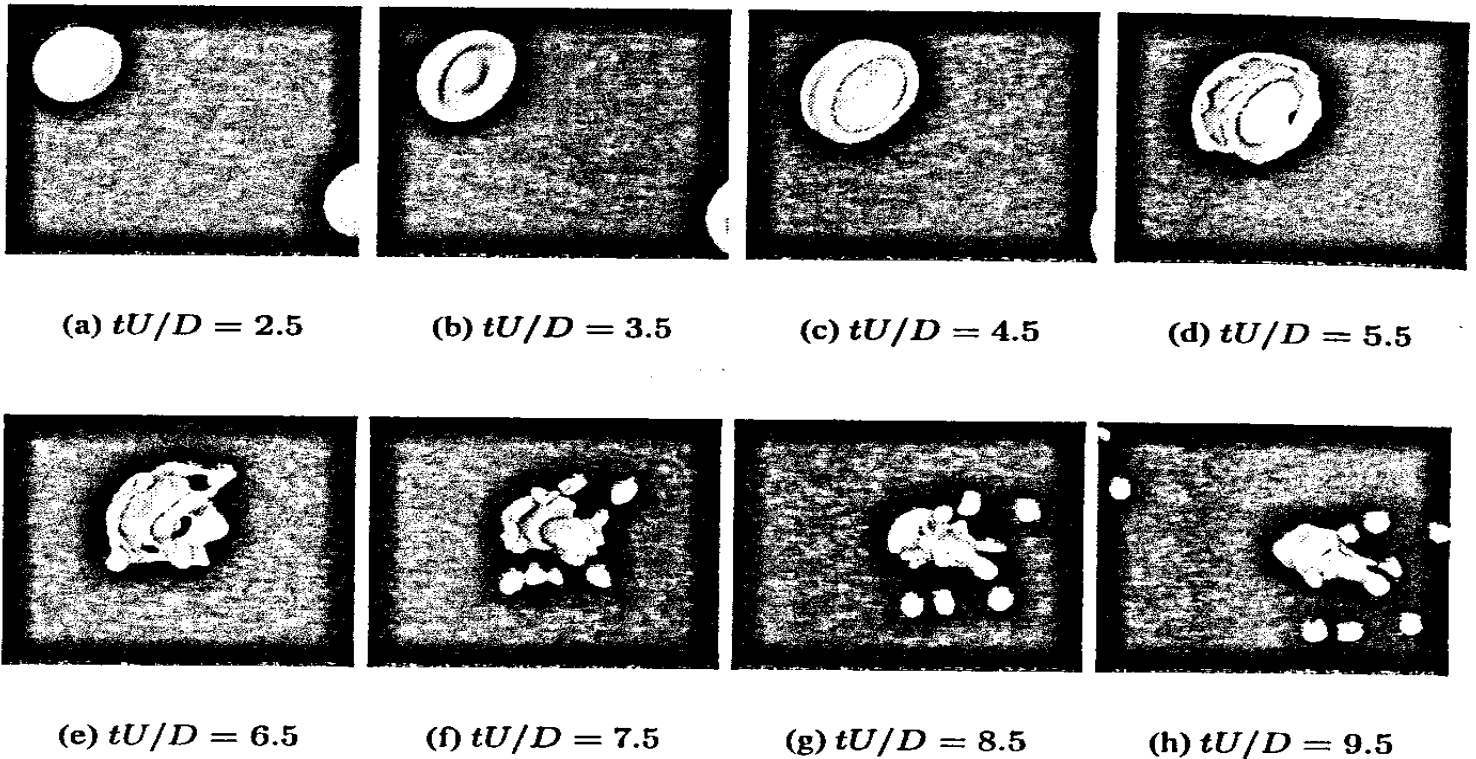


Figure 4: Preliminary results from 3-dimensional drop breakup simulations in uniform flow:  $Re = \rho_g DU / \mu_g = 1000$ ,  $We = \rho_g U^2 D / \sigma = 20$ ,  $Oh = \mu_l / \sqrt{\rho_l \sigma D} = 0.007$ , Domain size =  $5D \times 5D \times 5D$ , equivalent resolution =  $128 \times 128 \times 128$ . Free stream velocity is from top-left to bottom-right.

## 6 Summary

A hybrid Eulerian-Lagrangian method is being developed to simulate the liquid atomization problem. The particle level-set method is used to compute the interface dynamics and primary atomization on a Cartesian adapted grid. Stripping of droplets, collision and coalescence are captured implicitly by this method. This portion of the method has been implemented, and some simulation results for drop breakup presented. As the interface and droplets formed become under-resolved (owing to high curvature and distortion), it is intended to remove small scale structure from the Eulerian field and add an equivalent mass of droplet(s) to the Lagrangian field. These droplets can then be tracked by standard Lagrangian techniques and may undergo further breakup according to a stochastic subgrid model.

A critical limitation of the approach as described in this work is the assumption of a cascade of liquid scales, from the largest resolved scales to smallest droplets. In reality, the atomization problem is characterized by some combination of a scale cascade and the almost immediate production of small scales due to the elongation and stripping of filaments from the main jet. In any simulation at realistic Weber numbers, even with AMR, these small scales will likely be occurring at the



sub-grid level, and will require some sort of sub-grid model to properly include their physical effects. The development of such a model (termed a Large Surface Structure, or LSS model) is being pursued by one of the coauthors [6], and will eventually be included in the present simulation methodology.

## 7 Acknowledgement

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