Tittle: A Numerical Spray Impingement Model Coupled With A Free Surface Film Model.

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Abstract

A Lagrangian spray wall impingement model is integrated into the Eulerian free surface (Volume of Fluid) module of the multi-physics computational code, CFD-ACE$^+$. The coupling of the two modules enables the modeling of spray impingement and splashing, including the effects of a fluid film on the wall. Results for both microscale and macroscale simulations are presented. The former uses the free surface volume of fluid model to resolve individual droplets with diameters in range of 50-100 microns and evaluate mass, momentum, and energy transfer from the spray droplets to the film as a function of droplet Weber number and dimensionless layer thickness. The macroscale simulations utilize the coupled spray and free surface modules to predict liquid film thickness and transport on the scale of millimeters to centimeters. The predicted results are compared with existing experimental and theoretical results.

Introduction

Liquid spray interaction with solid objects is a fundamental component of a wide range of industrial applications including spray coating, cleaning, combustion, and spray cooling. In the current study, the authors are concerned specifically with spray cooling. For any application, spray-solid interaction is a very complex phenomenon involving the interaction of spray droplets with the surrounding gas flow, solid surfaces, liquid films and, for dense sprays, each other.

Computational modeling can be an effective tool for both spray equipment manufacturers and process engineers. Depending on the application, modeling can also be very complex, requiring accurate physical models for the effects of droplet momentum, layer thickness, gravity, surface tension, surface characteristics and, in the case of spray cooling, phase change. These phenomena must often be simulated over very disparate length scales, for hundreds of thousands of droplets, with diameters that are typically orders of magnitude smaller than the object being impacted.

A combined Lagrangian-Eulerian modeling approach enables the numerical resolution of the multiple scales associated with spray-solid interaction, while keeping the

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computational effort required within practical limits. In this approach, spray droplets are tracked individually, or in representative packets, until such time as they interact with a fluid layer or wall. At that point, mass, momentum and energy are transferred between the droplet and the existing or emerging fluid layer. Any mass gain in the fluid layer is subsequently tracked in an Eulerian reference frame.

An important component of the combined Lagrangian-Eulerian approach is determining the correct amount of mass, momentum and energy to be transferred from one reference frame to the other. As an example, for a given droplet hitting a thin film of liquid of a given thickness, the sub-model must predict the quantity of mass that rebounds or splashes, versus the quantity transferred to the film. Furthermore, it must predict the resulting redistribution of momentum, thermal energy, and droplet sizes for both the liquid film and any rebounding or splashed droplets. Determining appropriate distributions for these quantities has proven to be a non-trivial task. A review of the literature indicates a lack of data and analysis for the range of conditions considered in this study. This lack of data has dictated the need to perform numerical experiments to construct the distributions that are required for the droplet impact model.

In this article, we discuss the current status of both the macroscale Lagrangian-Eulerian spray model and the microscale modeling being performed to develop the detailed transfer models for spray-wall interaction.

Application

The current study is focused on developing simulation tools specifically for spray cooling. As a first step, the flow dynamics of a non-evaporating system are considered. Figure 1 provides an example of this application, where droplets of coolant are sprayed on a heated surface. The expanded view of the spray droplets impinging on the wall highlights the complexity of the problem. At the operating conditions of interest, incident droplet sizes are comparable to the thickness of the liquid film. At the liquid film interface, there are frequent droplet impacts with varying droplet velocity and diameter. In order to predict the effect of spray conditions on the thickness and flow of the resulting liquid film, the mass and momentum transfer resulting from droplet impacts must be addressed. In order to address fluid management for these systems, it is also desirable to describe the resulting liquid film with a numerical formalism that allows thick films to be formed. The liquid films may be several computational grid cells thick, and must correctly affect the system fluid dynamics by modifying the fluid properties in those grid cells.

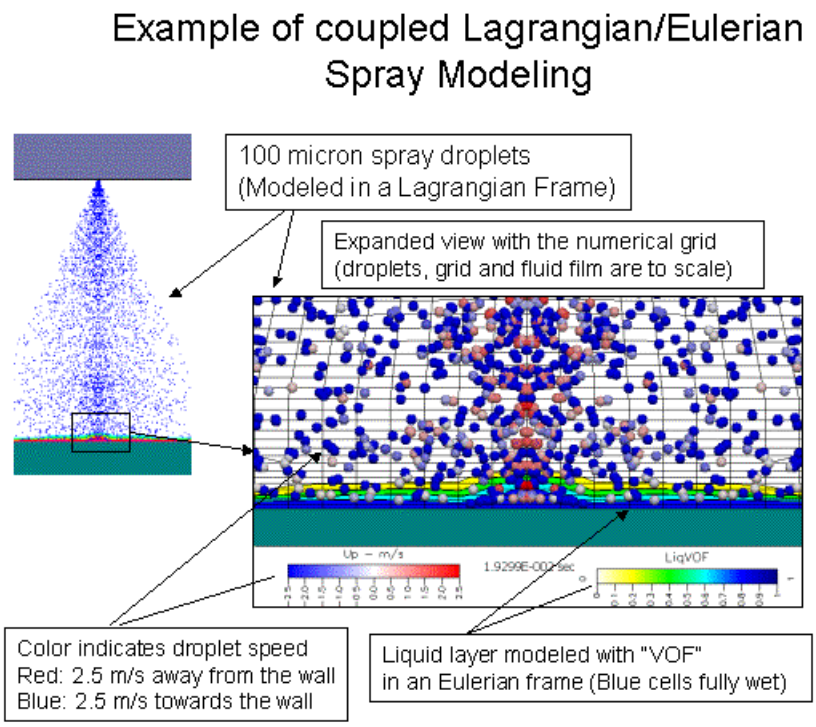


Figure 1. Macroscale model of spray cooling of a heated substrate. The spray is comprised of the fluorinert, FC-72 ™ 3M Company. Spray droplets are modeled in a Lagrangian frame and coupled with an Eulerian (Volume of Fluid) model for the liquid film.

Background

There have been a number of previous efforts to simulate the interaction of a spray with a thin liquid film, primarily by investigators interested in the interactions of fuel sprays with the walls of internal combustion engines[1-7]. For example, Stanton and coworkers developed a wall film model that solves the mass continuity and momentum conservation equations for a two-dimensional film on three-dimensional surfaces[3-5]. This model includes the effects of spray drop impingement and splashing processes, which are addressed by a set of correlations for the distribution of mass and momentum as a function of key dimensionless parameters for the incident droplet. The outcomes of droplet film interactions included four distinct regimes: droplet sticking, bouncing, spreading and splashing. In the stick regime the droplet hits the liquid film and stays on the film. In the bounce regime the droplet bounces off the wall with reduced momentum. Spreading is similar to the stick regime, in that the entire droplet mass is added to the liquid film, but occurs at higher impact energies. In the splashing regime, the incoming droplet produces secondary droplets. Grover and Assanis[7] developed a similar model, with more emphasis on the momentum transfer and viscous dissipation of droplet kinetic energy within the film. For both of these models, the correlations used to determine the

outcome of a particular droplet impact depend on the incident droplet Weber number. Neither incorporates the effect of the thickness of the liquid film, although that has been demonstrated to have an impact on the mass and momentum distribution resulting from a droplet impact.

The studies of droplet wall interactions have included both experimental and numerical investigations over a range of parameters [8-14]. For example, Mundo et al. performed some experimental investigations on liquid droplets impinging on a dry flat wall normally to obtain an empirical model to establish a splashing or depositing limit [9]. These authors defined splashing as occurring when liquid mass was ejected after the drop hit the wall. They derived a criterion, based on the droplet Reynolds and Ohnesorge numbers, which demarcates the onset of splashing. This limit was

$$K = OhRe^{1.25} \geq 57.7 \ ,$$

and when K exceeded 57.7 splashing was observed for both smooth surfaces and surfaces with roughness approximately equal to the impinging droplet diameter. When the value of K was less than 57.7 the liquid drop completely deposited on the surface. The dimensionless parameters characterizing the impinging drop state were the Reynolds (*Re*), Ohnesorge (*Oh*), and implicitly the Weber (*We*) numbers, defined as:

$$Re = \frac{\rho DU}{\mu}$$

$$Oh = \frac{\mu}{\sqrt{\rho \sigma D}} = \frac{\sqrt{We}}{Re}$$

$$We = \frac{\rho DU^2}{\sigma} \ .$$

In these equations D is the diameter of the drop, U is the normal velocity, ρ is the density of the liquid drop, μ is the dynamic viscosity, and σ is the surface tension. Mundo et al. found that the onset of splashing was independent of the impact angle, since the characteristic velocity was defined as the normal component. Correlations were also developed for the size and velocity distributions of the secondary droplets when splashing occurred.

Cossali et al. experimentally investigated the impact of single drop on surfaces containing a pre-existing film[11]. Impingement on a dry surface was also discussed, with the observation that the splashing limit decreases as the surface roughness is increased, meaning that a smooth surface suppresses splashing. The importance of surface roughness on the impingement physics was separated into two regimes depending on the relative length scales of the roughness and the film thickness. When the film thickness was much greater than the surface roughness, the roughness did not influence splashing significantly. However, when the surface roughness was of the same order as the film thickness it had a significant effect on the occurrence of splashing. The following correlation was derived from the experimental data, with a value of Y>1 indicating that the droplet will splash:

$$Y = \frac{WeOh^{-0.4}}{2100 + 5880\delta^{1.44}} \ ,$$

where $\delta = h/D$ and h is the fluid layer height.

A comparison of the division between splashing and sticking regimes developed by Mundo and Cosalli demonstrates that both correlations predict the onset of splashing to scale with the product of the Weber number and the square root of the Reynolds number. As the liquid film thickness increases, Cosalli observed that splashing is more likely for a given droplet state.

The correlations of Mundo and Cossali provide a valuable starting point for the droplet interaction model desired in this work. This model will also need correlations similar to those used by Stanton et al. for the total mass, size distribution, and momentum of secondary droplets produced by splashing events. The regime of interest includes interactions between droplets with *Re* approximately 5000, *Oh* on the order of 0.01, *We* on the order of 1000, and films with thickness similar to the droplet diameter. This regime was determined by considering typical spray velocity and size distributions utilized in spray cooling applications, as well as the effect of employing a cone spray on the distribution of the wall normal velocities. For this regime, we have not found any previous work characterizing the outcome of droplet impacts which produce splashing. Therefore, we have found it necessary to use numerical simulations of droplet impact on a liquid film in order to develop the correlations required for the macroscale model.

Microscale Simulations of Droplet Impact

In order to characterize the outcome of droplet impacts on an existing liquid film, several series of impacts were simulated using the fluid dynamics and free surface capabilities of a research version of the multiphysics computational code, CFD-ACE+ [15]. In these studies, the transient equations for conservation of mass and momentum are solved in conjunction with the evolution of the free surface defining droplet and liquid film boundaries. The free surface evolution is predicted using the Volume of Fluid, VOF, approach[16-19]. In this approach, the continuity equation for a second fluid, in this case liquid, is coupled with the total continuity equation for the liquid and gas. The fraction of liquid in each discrete cell is used to determine the position of the interface and derived quantities such as the average density and curvature of the interface. The simulations include the effects of surface tension as a body force. The primary output of the simulations is the prediction of the mass of fluid ejected or bounced for a given incoming droplet.

The fluid of interest is the Fluorinert liquid FC-72 (3M Company), commonly used for heat transfer applications including spray cooling. The properties of FC-72 were taken at standard atmospheric pressure and are as follows: density 1680 kg/m^3, dynamic viscosity 6.4E-4 kg/m·s, and surface tension 0.01 N/m.

In this work, we will describe the results of droplet impact simulations performed to date, since the complete calibration of splashing behavior for droplets of FC-72 is still in progress. The range of interest spans droplet diameters from 20 to 100 microns, normal velocities from 0 to 15 m/s, and liquid films from 0 to 100 mm thick. In this paper, we

concentrate on the results for 100 μm diameter droplets impinging with a normal speed of 10 m/sec. At these conditions, the droplet Weber number is 1680, and the correlations of Cossali and Mundo both indicate that splashing should occur.

Microscale Simulation Results:

A 2-D axi-symmetric domain, 1100 micron in radius and 450 microns in height, is used for the microscale simulations. The grid cells have a resolution of 5 μm by 5 μm, corresponding to a total grid cell count of 19,800. Variable time steps on the order of 1e-7 seconds were used. The simulation was initialized with a selected layer thickness in the range of 10 to 100 microns and an initial droplet with the desired diameter and a downward velocity of 10 m/s, as shown in Figure 2. A typical simulation requires 12 hours on an AMD Athlon XP 3000 desktop.

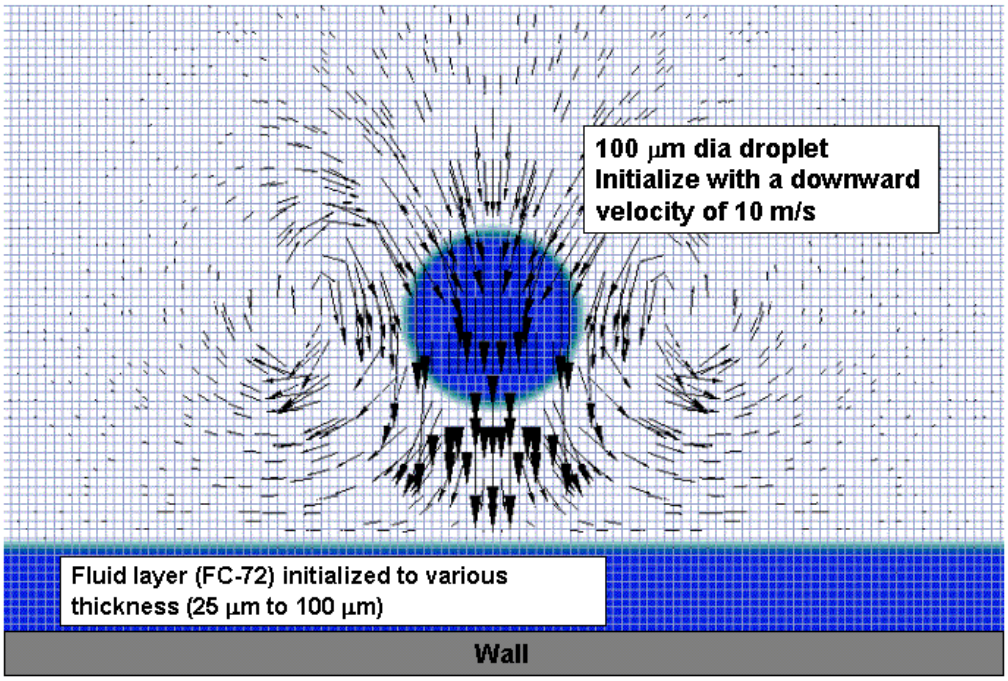
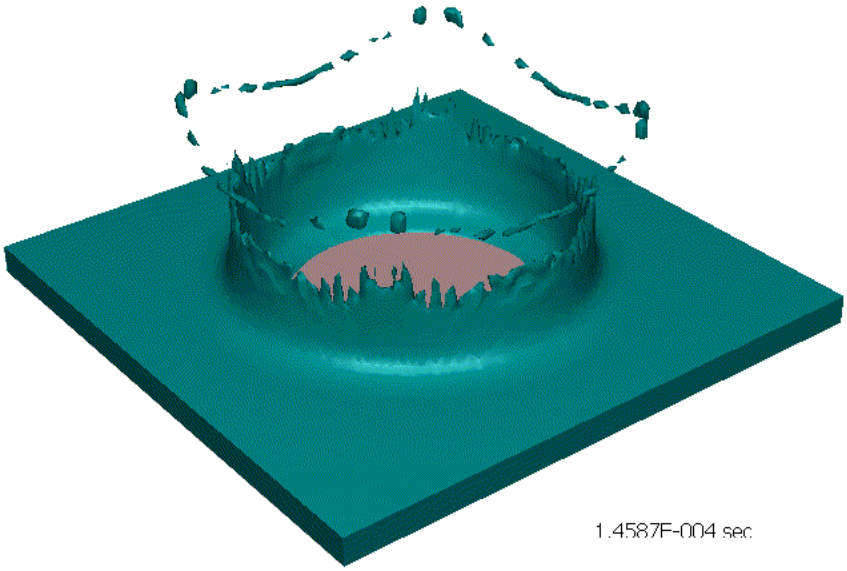
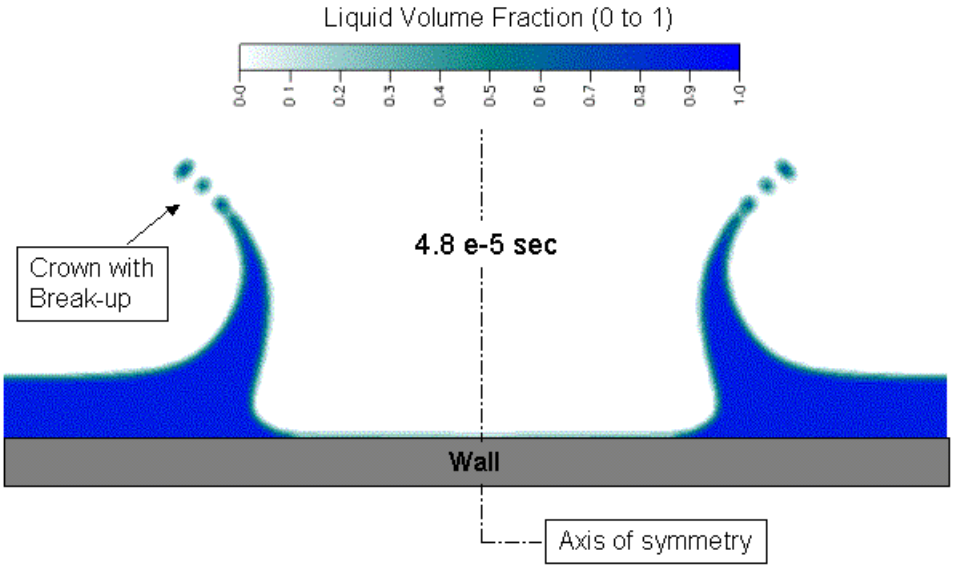


Figure 2. Sample initial condition for Microscale droplet splash simulations.

Upon impact with the layer, an impinging droplet forms a crater in the film layer, creating a crown-like structure. Depending on the initial layer thickness and droplet properties, this crown may break apart and eject liquid, as shown in the 3-D and 2-D simulations in Figure 3.



(a)



(b)

Figure 3. Predicted crowning and liquid expulsion for a 100 μm droplet at 15 m/s impacting a 50 μm layer of FC72. Three-dimensional, (a), and two-dimensional axisymmetric, (b), model results.

Once the crater has grown to its maximum size, it subsequently collapses. Depending on the conditions, this collapse can cause formation of a fountain of liquid and/or ejection of a droplet along the centerline, as shown in Figure 4. Based on preliminary simulations, these two mechanisms of mass ejection appear to be nearly exclusive, as plotted for the baseline case of a 100 μm droplet at 10 m/s in Figure 5. For layers equal to or less than 50

microns, the crown ejects liquid and the subsequent crater collapse lacks the energy to overcome surface tension and eject a droplet. Conversely, for thicker layers, 60 microns or above, the crown lacks the kinetic energy to eject fluid, but the subsequent fountain created by the collapse does. Interestingly, the ratio of total mass ejected to the mass of the impinging droplet does not change significantly in the transition from one ejection mechanism to the other. The result is a relatively linear relationship between the mass ejection ratio and the layer thickness. For thick layers, the mass of the ejected liquid can be an order of magnitude more than the mass of the impinging droplet. Cossali et al. also observed a greater ejected than incident mass for high We droplets incident on a liquid film.

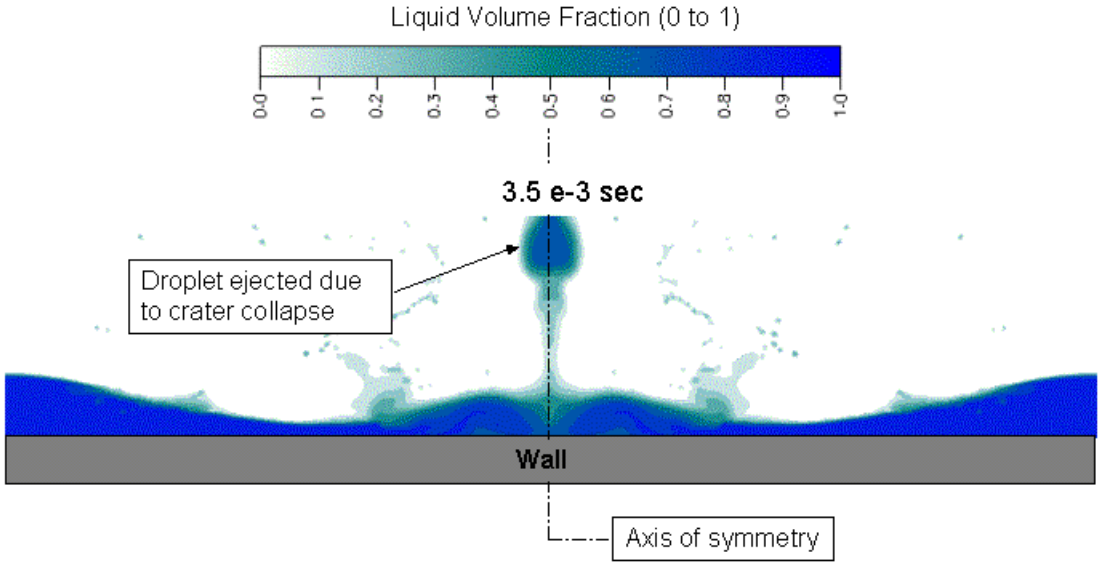


Figure 4. Predicted crater collapse driven liquid expulsion for a 100 μm droplet at 15 m/s impacting an 80 μm layer of FC72.

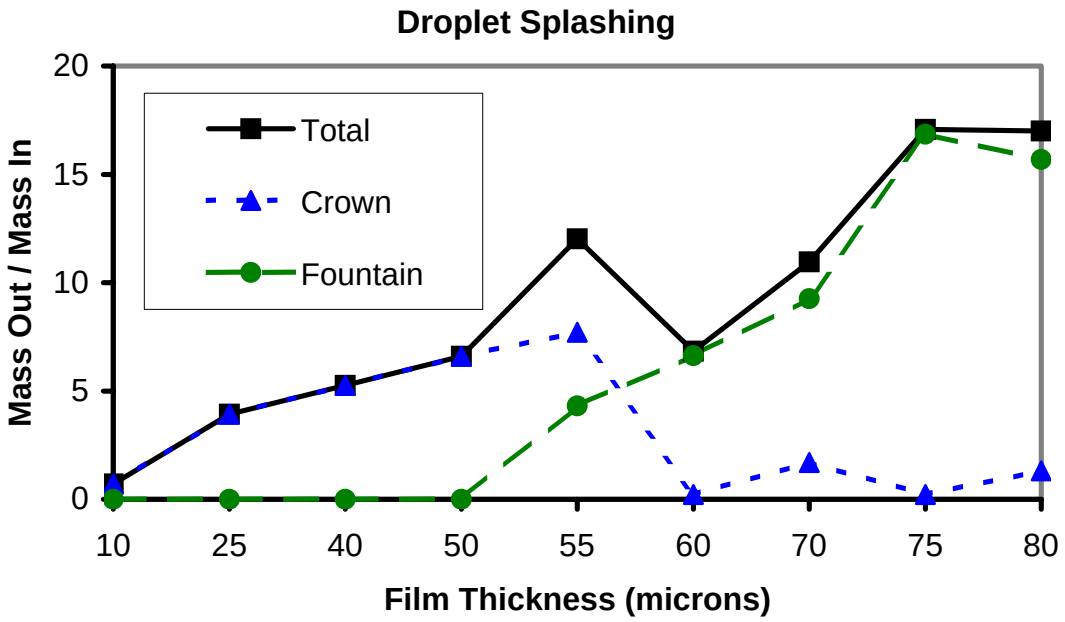


Figure 5. Predicted liquid (FC –72) expulsion (Mass out / Mass in) for a 100 μm droplet at 10 m/s impacting variable thickness layers.

Similar microscale simulations are being run for other droplet sizes and impact velocities in order to produce correlations between droplet Weber number, layer thickness and mass ejected. Simultaneously, momentum and energy balances on the simulation results are providing the information necessary to develop the corresponding energy and momentum transfer correlations. For example, Figure 6 shows the temperature profile for an impact crater approximately 80 microseconds after a 300 K droplet has hit a 329 K fluid layer. These mass, momentum and energy correlations are being incorporated into the macroscale model of spray-wall interaction.

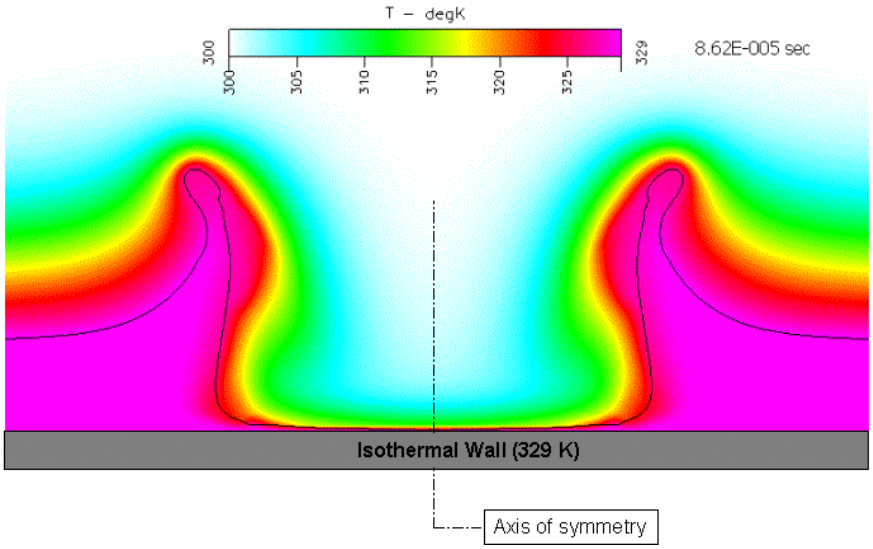


Figure 6. Predicted liquid (FC –72)/air interface shape and temperature distribution for a 300 K, 100 μm droplet at 10 m/s impacting an 80 μm thick layer at 329K. The interface is shown as the black curve. Elapsed time since impact 86.2 microseconds.

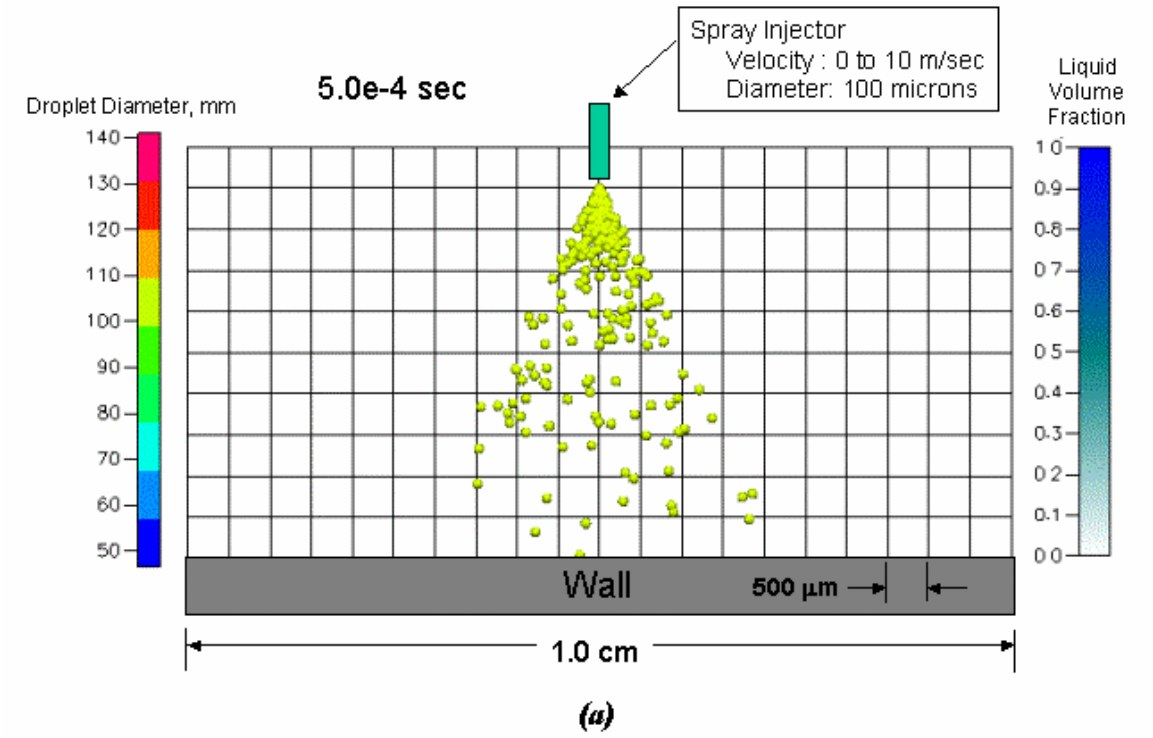
Macroscale Lagrangian-Eulerian Model

In theory, the VOF free surface model used to determine droplet–layer interaction could also be used to model a system of droplets. However, for a high spray rate of fine particles impacting a relatively large surface, as in Figure 1, such an approach is computationally impractical, requiring a prohibitive number of grid cells. A more tractable approach is to model the spray particles individually or in representative parcels using a Lagrangian reference frame, and account for the fluid layer using an Eulerian framework. In this approach, the mass, momentum, and energy of a spray parcel that enters a liquid region (numerical control volume) may be transferred to the liquid in that control volume. The mass, momentum, and energy are subsequently tracked on a control volume basis in the Eulerian framework. Whether the spray parcel is absorbed in the liquid filled cell depends on parameters such as the cell liquid volume fraction and the droplet velocity. If a spray parcel penetrates all the way to a solid wall, its mass, momentum and energy interaction are modeled based on correlations such as discussed in the previous sections. At low Weber numbers, the mass of the droplet will stick to the wall and contribute to any liquid film. At the other extreme, i.e. for higher Weber numbers, the droplet will splash and eject secondary droplets that may have significantly more mass than the original droplet. In the current model implementation, only a single secondary parcel is generated in response to an incident parcel hitting a wall under splashing conditions. The new mass, energy and momentum of that secondary parcel is determined from correlations derived from simulation results such as those in Figure 5. Future implementations will include the possibility of ejecting multiple parcels representing splashed droplets.

Results of a demonstration macroscale simulation using the coupled Lagrangian-Eulerian model to predict the formation and transport of a liquid film are shown in Figure 7. This simulation utilized a simplified implementation of the criteria under development to incorporate Lagrangian spray parcel interactions with the Eulerian model of the liquid film. In particular, the probability of a particular parcel rebounding from the film was a function of only the incident droplet Weber number,

$$We < 80 \qquad P = 0$$
$$80 <= We <= 600 \qquad P = 0.5$$
$$600 < We \qquad P = 0.75$$

where P is the probability. This probability distribution for rebounding was based on the fraction of incident mass splashed used by Grover and Assanis[7]. If the parcel does not rebound from the liquid film, then it may still splash liquid mass up to the sum of the incident mass of the incoming parcel and the mass present in the computational cell within the Eulerian (VOF) model framework. The splashed mass is determined from that constraint and a linear fit of the results shown in Figure 5 above.



(a)

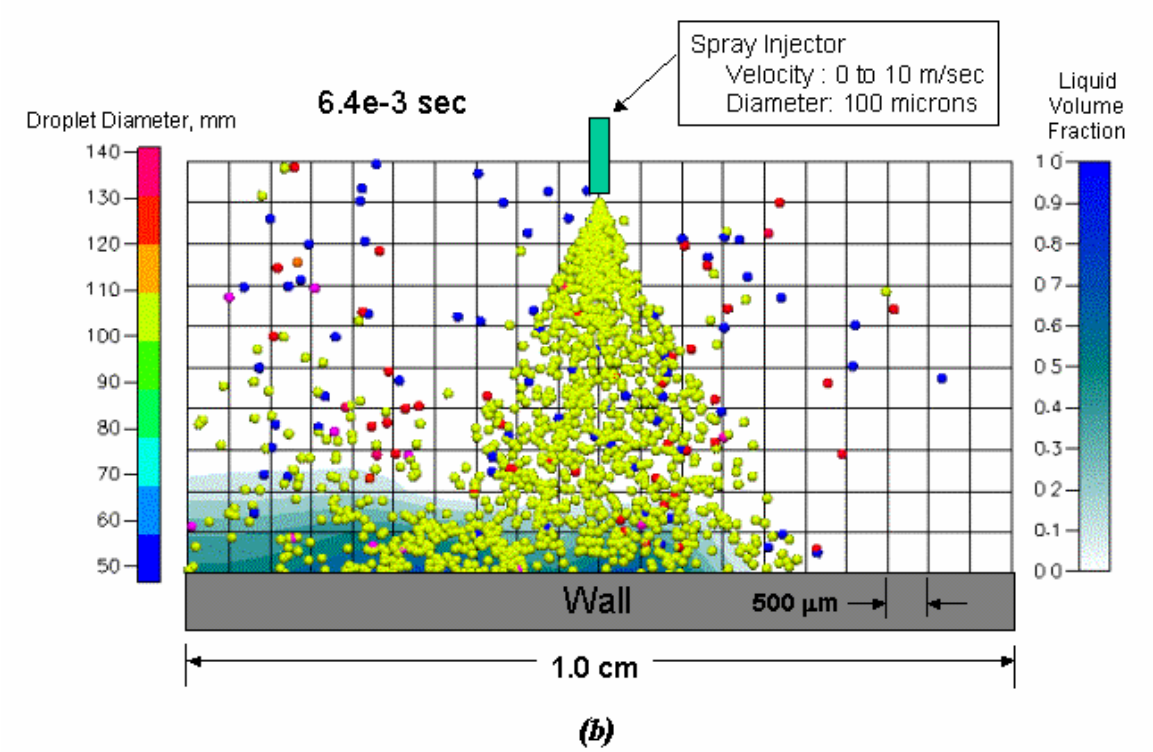


Figure 7. Two-dimensional simulation of Spray – Liquid Layer interaction. (a) Model domain and Lagrangian spray parcel distribution at initial impact with the wall. (b) Injected, splashed, and rebounded Lagrangian spray parcels and the evolving liquid film after 6.4 milliseconds.

The stochastic nature of the model for determining whether parcels rebound or interact with the film resulted in more rapid formation of a liquid film to the left of the spray injector during this demonstration. The velocity fields in both the gas, due to drag and spray-gas interactions, and the liquid film are quickly established and serve to maintain a thicker film on the left of the computational domain. The resulting liquid film inertia causes newly absorbed liquid to flow in that direction. The splashed droplets farther from the developing liquid film tend to have a smaller diameter than the incident droplets, since they were produced before the film was formed or while it was very thin. The majority of the splashed droplets near the wall and liquid film are larger than the incident droplets, reflecting the tendency for splashing from a thicker film to generate droplets with more outgoing than incident mass.

Conclusions

We have demonstrated a functional link between Lagrangian spray transport and Eulerian simulation of fluid dynamics with two distinct fluid phases. This framework will form the basis for simulation of spray-wall and spray-film interactions in a broad set of applications that require the Eulerian approach to efficiently address transport of the liquid film arising from spray sources. Although there have been numerous experimental and theoretical studies of the interaction between impinging liquid sprays and solid

substrates, these have been primarily restricted to situations with no liquid film or a very thin liquid film relative to the impinging droplet diameter. To address the resulting need for greater fundamental understanding of the interaction between impinging spray and liquid films, we have begin employing numerical experiments to develop the required correlations for mass, momentum, and energy transfer from the Lagrangian spray reference frame to the Eulerian fluid reference frame. The initial correlations derived from these microscale simulations were successfully integrated into the coupled model and demonstrated here.

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