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Improving Freight Fire Safety: Modifying Droplet Behavior to Minimize Ignition

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16. Abstract

Hydrocarbon drops impacting on a flat solid surface were computationally studied to identify the key issues in the dynamics of drop spreading. The experimental data available for diesel, methanol, and glycerin were used, and a general empirical expression (in terms of the Ohnesorge number) was constructed that accurately described the spreading regime. For the simulation part, the drop spreading process was studied numerically with a volume-of-fluid (VOF) approach. Based on these investigations, a new combined static contact angle-dynamic contact angle (SCA-DCA) model was proposed and applied to compute the hydrocarbon drop spreading process. The predicted time-dependent drop shapes agree well, within 5% of both previously published results and the experimental data presented here, while previous models showed at least a 10% deviation from the experiments. This proposed model also avoids the requirement for experimental measurement with specific fluids and only requires the general fluid properties.

In addition to the numerical investigations, a droplet combustion experiment was also carried out. In this experiment, the ignition and combustion of the suspended fuel droplet were recorded using a high speed camera. Image processing techniques were then utilized to measure fuel combustion characteristics such as burning rate and ignition delay.

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Impact speed of the drop (u)

Initial drop diameter (D)

Drop spread diameter at a given time (in spreading simulation) (d)

Droplet diameter at a given time (in combustion experiments) (d_s)

Time measured from the instant of impact (t)

Droplet burnout time (τ_c)

Droplet burning rate (K_c)Viscosity of the liquid (μ)

Density of the liquid (ρ)

Liquid-air surface tension (σ)

Static contact angle (θ_s)

Dynamic contact angle (θ_D)

Spreading velocity (V)

Spread factor (β)

Reynolds number (Re)

Webber number (We)

Ohnesorge number (Oh)

Capillary number (Ca)

static contact angle (SCA)

dynamic contact angle (DCA)

volume of fluid method (VOF)

National Transportation Safety Board (NTSB)

Motor Coach Database (MCF)

Computationa Fluid Dynamics (CFD)

Silicon Carbide (Si-C)

Quadratic Upstream Interpolation for Convective Kinematics (QUICK)

Pressure Implicit with Splitting Operator (PISO)

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Abstract

Hydrocarbon drops impacting on a flat solid surface were computationally studied to identify the key issues in the dynamics of drop spreading. The experimental data available for diesel, methanol, and glycerin were used, and a general empirical expression (in terms of the Ohnesorge number) was constructed that accurately described the spreading regime. For the simulation part, the drop spreading process was studied numerically with a volume-of-fluid (VOF) approach. Based on these investigations, a new combined static contact angle-dynamic contact angle (SCA-DCA) model was proposed and applied to compute the hydrocarbon drop spreading process. The predicted time-dependent drop shapes agree well, within 5% of both previously published results and the experimental data presented here, while previous models showed at least a 10% deviation from the experiments. This proposed model also avoids the requirement for experimental measurement with specific fluids and only requires the general fluid properties.

In addition to the numerical investigations, a droplet combustion experiment was also carried out. In this experiment, the ignition and combustion of the suspended fuel droplet were recorded using a high speed camera. Image processing techniques were then utilized to measure fuel combustion characteristics such as burning rate and ignition delay.

Chapter 1 Introduction

According to recent statistics released by the National Transportation Safety Board (NTSB), 94% of transportation fatalities in 2011 are categorized as highway fatalities with two main sub-categories of passenger cars (35%) and light trucks and vans (27%) [1]. Vehicle crash-induced fires account for over half of the deaths (58%) in transportation accidents. The presence of fire in crash scenarios can increase the severity of the situation, resulting in a severalfold increase in the number of injuries or fatalities which is why 58% of the deaths in transportation accidents are accountable to crash fires [2]. The life threatening danger of fire is not only contained to having contact with the flames, but also from being subjected to its side effects like smoke density, toxicology, and the heat release rate.

The Motor Coach Fire (MCF) database (for the study period of 2004-2006) shows that the two most common origin locations of reported fires were the engine compartment and the wheel wells, with the total contribution of 70% of the fires reported [3]. As soon as fire initiates, it spreads to fuel lines and the engine compartment; fuel lines located near the wheel well fire source or related hot surfaces are often involved in accelerating the fire (fuel lines will spill fuel if there is burn-through). Therefore, a possible way of reducing the likelihood of injury and fatalities in car accidents is to minimize the risk of fuel fire initiation, or enhancing its extinction. The simplest and most direct way to do this is to modify the fuel so that it does not ignite in an accident. One of the ways in which this can be done is through the addition of long chained polymers to the fuel to prevent the break-up of the fuel into a fine mist, as this is typically what gets ignited in crash-induced fires [4]. Previous MTAC-DOT supported work has shown (experimentally) that adding long chained polymers into diesel and its blends imparts non-Newtonian behavior by which mist suppression is enhanced.

The mist-preventing process works by the long-strand polymers inducing a non-Newtonian shear-thickening behavior in the fuel [5]. To evaluate both the shear-thickening effect and regular fuel behavior, both an experimental and computational scenario needs to be employed. There is a wide range of shear stresses in transportation systems from 0.4 Pa in low pressure fuel pumps to 3.87x106 Pa in nozzle of fuel injectors. Therefore, understanding the right shear stress zone for which the modification should be carried out is crucial to enhancing fuel safety while keeping the performance characteristics of fuel unchanged. The scenario utilized in this work uses the experimental data from the impact of hydrocarbon drops on a solid surface (which is a basic component in the liquid fuel breakup process right after fuel spillage, and also its following splatter and moist formation) to develop a simple and clean model to investigate the variable viscosity and shear stress of liquids. The dynamics of hydrocarbon drops (Newtonian liquids) spreading on a flat, smooth surface is studied in this work as a starting point for the non-Newtonian behavior to be investigated in the future.

The second phase of this research would focus on developing a polymer additive that affects the fuel more significantly in the desired shear stress zone, and less in other operating conditions. For this purpose, the shear distribution and its time evolution predicted in phase one will be used. Eventually, this polymer added diesel and its blends will be tested under realistic conditions to make sure its performance characteristics (such as vaporization rate, ignition delay, and burning rate) are not affected. This report presents the first phase of the research (developing a comprehensive model to predict spreading behavior of diesel fuel after impacting a solid surface), and the preliminary steps of the second phase including making the experimental setup and investigating the combustion of an unmodified diesel droplet.

Chapter 2 Dynamic of Drop Impact

The behavior of drops impacting with a solid surface can be characterized into three different modes: bouncing, spreading, or splashing. The mode observed is due to the interactions of initial drop speed, pressure, surface roughness, drop viscosity, and surface tension. The behaviors of water, glycerin, and silicon oil drops impacting with a solid surface have been widely examined through both experimental and numerical studies. These studies produced a consensus that the process of drop spreading on a solid surface experiences four stages [6]: a kinematic regime, a spreading regime, a relaxation regime, and a wetting/equilibrium regime. Figure 1.1 shows the four different stages of a drop impacting with a solid surface in terms of the spread factor, which is defined as the ratio of the spreading diameter to the initial diameter: $\beta = d/D$. For the conditions of interest here (for fuel drops at a moderate speed), the drops reach their maximum diameters on the smooth surface, and the lamellas stop, and the drop is stabilized (as the dot line shown in fig. 2.1). Beyond the spread factor, the contact angle is another important parameter considered in drop impact studies. As the drop spreads, the contact line moves outwards, towards the gas phase with the varying dynamic contact angle (DCA) θ_d. However, since the viscous region in which θ_d is measured is much smaller than both the pixels of experimental images and numerical grid size, the dynamic contact angles are measured at a distance with the macroscopic scale away from the solid surface, and this measured quantity is called the apparent contact angle (θ_d^*). When the contact line reaches the stationary state, the drop stops spreading and is stable with the equilibrium contact angle, called the static contact angle (SCA) θ_e.

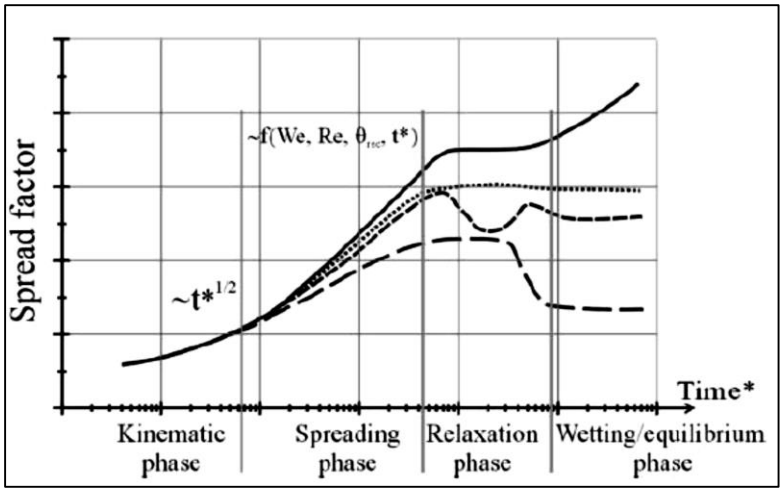


Figure 2.1 Schematic representation of the spread factor with time; the different lines correspond to an arbitrary choice of possible spreading histories, depending on the parameters of the impact [6].

In addition, several non-dimensional parameters are also important: the Reynolds number, the Weber number, the Ohnesorge number, and the Capillary number (Mukherjee & Abraham, 2007). They are defined as:

$$Re = \rho D u/\mu \quad (2.1)$$

$$We = (\rho D u^2)/\sigma \quad (2.2)$$

$$Oh = \mu/\sqrt{\rho\sigma D} \quad (2.3)$$

$$Ca = V\mu\sigma \quad (2.4)$$

Notice that V is the spreading velocity while u is the initial impact velocity.

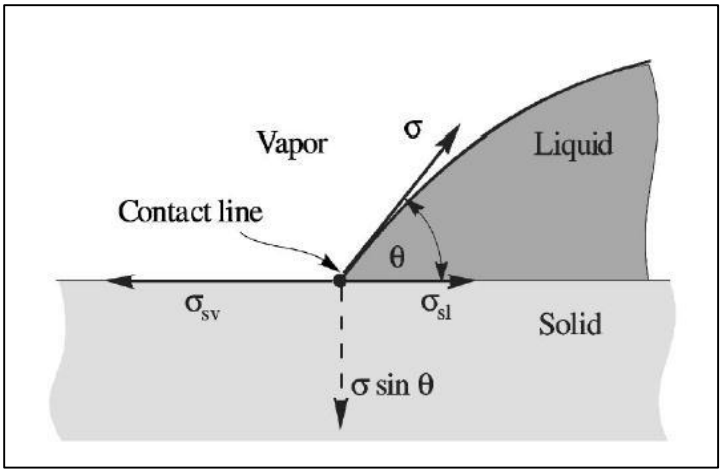


Figure 1.2 Equilibrium wetting line and contact angle

In recent years, computational fluid dynamics (CFD) has been used to understand and predict the complex hydrodynamics of drop impacting with and spreading on a solid surface [7-12]. Both theoretical and empirical models have been developed for numerical analysis. In particular, boundary conditions at the moving contact line of the spreading drop need to be specified in terms of contact angles. According to Young's equation,

$$\sigma cos\theta_e = \sigma_{sv} - \sigma_{sl} \qquad (2.5)$$

static contact angle is ideally a property of the concerned system related to the surface tension of the solid/vapor σ_{sv} and solid/liquid σ_{sl} interfaces [12] (see fig. 2.2). On the contrary, dynamic contact angle θ_d is not a material property, but mostly depends on the capillary numbers Ca. However, the exact expression of dynamic contact angle θ_d in terms of Ca is still unknown. The understanding of variable θ_d has been investigated both theoretically and empirically [8, 11-12]. When these models are applied for numerical analysis, two aspects need to be considered: the precisions of these models compared with the experimental results, and the physical properties and behavior information required by the models for the sake of computational cost.

Since the theoretical expression of θ_d in terms of Ca is still unclear, empirical expressions have been employed in the drop spreading studies [13-16]. Most of the simulations are fairly accurate in predicting the shape of the spreading drop during the kinetic regime where the inertia dominates. However, the prediction of the spreading regime has not been well simulated (with more than 10% error). In addition, the complexity of existing formulas leads to high computational costs while being applied to the 3-D region. Hence, a new generalized contact angle model is needed to serve as the boundary condition in the numerical simulation in order to: (1) improve the accuracy of predicting the drop shape during the spreading regime as compared with existing correlations, (2) reduce the behavior information required as compared with the full DCA model, and (3) extend the materials from water and glycerin to hydrocarbon drops.

The objectives of this work are: (1) study the effect of fluid properties and impact characteristics on dynamic contact angle θ_d, (2) develop a new model of drop behavior for hydrocarbon liquids, (3) the new model should have lower computational and experimental cost, and higher accuracy than those currently available, and (4) examine the applicable range of this new model. The method for achieving these objectives is through high speed imaging of the impact of diesel and methanol drops, followed by experimental analysis and CFD simulations. The volume of fluid (VOF) method [17], which is suited for large topology changes and has a low computational cost, was implemented by using the commercial software Fluent 12.0.16.

Chapter 3 Computation Method

Two different phases are defined in the VOF method, where gas is normally defined as the primary phase whereas liquid is the secondary phase. Each control volume only contains one phase (or the interface between phases). Three different numerical grids are also employed in this work: a three-dimensional (3D) whole domain for the diesel drops, a 3D quarter domain for the methanol drops, and a two-dimensional (2D) domain for the glycerin drops. The main advantage of applying a 1/4 domain is that computational cost could be significantly decreased, compared with the application of a whole domain. However, it is observed that 3D quarter domain shows less accuracy than a whole domain, because the symmetric boundaries in the quarter drop domain restrict the intrinsic instability of drops, inducing an over-predicted spreading velocity [18].

To test our model for glycerin drops and compare the predicted results with Sikalo et al.'s, the same simulation region was employed in this work. A 2D domain is created with the size of 100 × 100 mm in r-z plane and the smallest cell is around 19.5 microns. It is noted that a 2D axisymmetric domain is applicable and shows great accuracy for glycerin drops. Since surface tension of glycerin is much higher than methanol and diesel, fewer oscillations occur during the drop spreading process. Therefore, in the axisymmetric domain, the loss of surface tension energy resulting from the dismissal of non-axisymmetric oscillations could be negligible for glycerin drops.

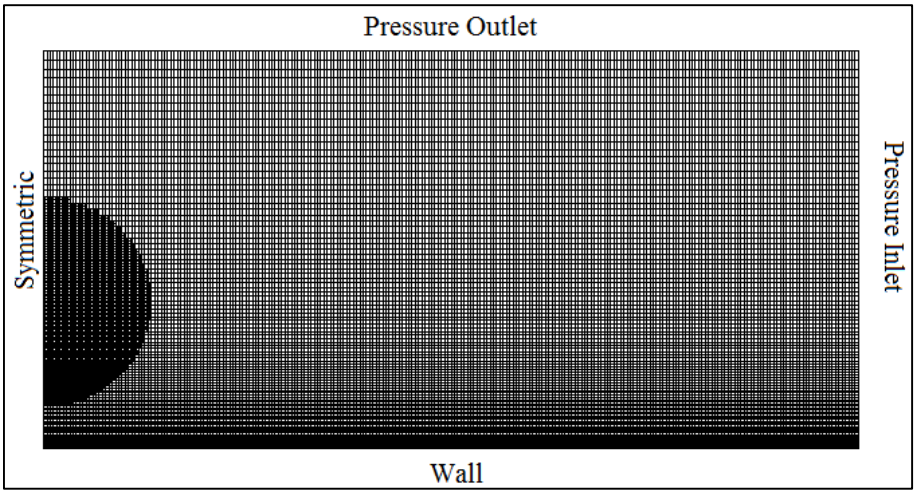


Figure 2.1 A side view of the solution domain (the x-z plane at z = 0) and boundary conditions for the methanol drops; meshes were refined towards the wall.

3.1 Numerical Solution and Boundary Condition

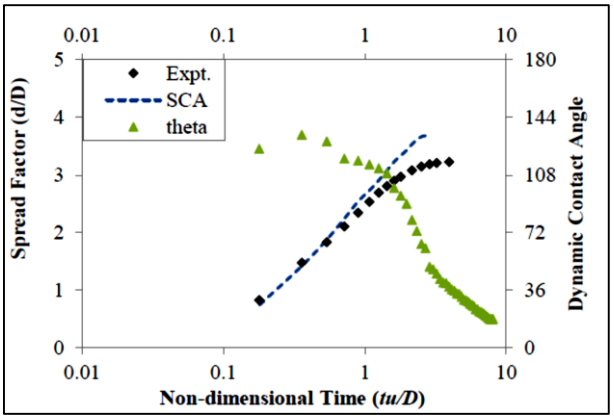
A whole drop is patched in the solution domain with exactly the same diameter and initial velocity as the experimental picture shows (fig. 3.1). The bottom of the solution domain is defined as the wall while the top surface is set as a pressure-outlet, and the side ones are pressure-inlets. No-slip boundary condition is specified at the wall where all the components of velocity are set to be zero. Three different models of contact angles are tested in this work: the SCA model, the combine SCA-DCA model, and the Kistler's correlation [16]. The QUICK scheme is implemented for the mass and momentum equations, and the first-order implicit method is used to discretize the time derivatives. In the momentum equation, pressure and velocity are coupled by the pressure implicit with splitting of operator (PISO) scheme. The applied time step varies in correspondence with the time interval between successive frames of experimental images taken at different camera speeds, ranging from 0.003 ms to 0.0326 ms.

Chapter 4 Numerical Result and Discussion

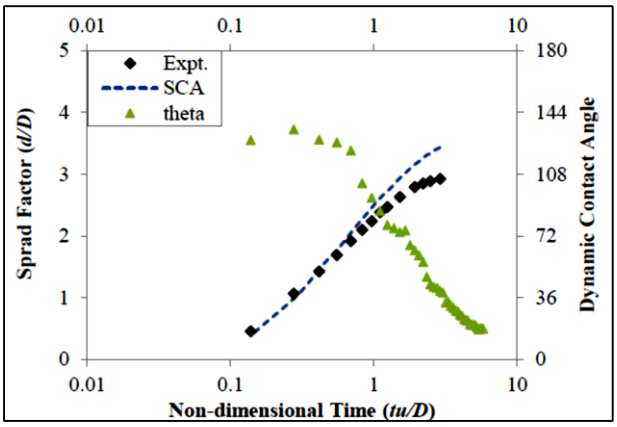
4.1 Drop Impact with SCA Model

A criterion used in this work to compare the experimental and numerical results is a quantifiable comparison of the spread diameter at each time step after drop impacting on the surface.

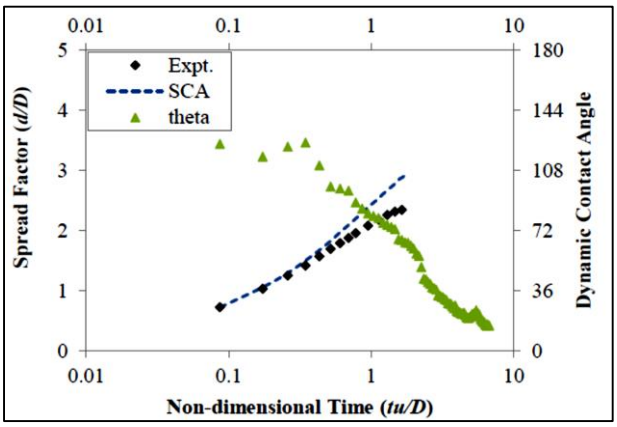
The static contact angle model is tested as the baseline in this work. This model has been widely studied and used in previous studies. In this model, the static contact angle is substituted into the numerical simulation as the boundary condition, assuming that the contact angle is equal to the static contact angle throughout the spreading process, i.e. $\theta_d = \theta_e$. Previous studies have shown that the SCA model lacks accuracy. Again, in this work, by comparing the simulation results of the SCA model with our diesel data, the decrement of the SCA model is shown in figures 4.1 (a) through 4.1 (c) for impact velocities of u = 1.6, 1.2 and 0.7 m/s respectively. At the end of drop spreading, the error of the SCA model is about 16%. Comparing the error of the SCA model with the evolution of contact angles, it could be observed that $tu/D = 0.7$ is the characteristic time when the kinetic regime ends. In other words, the SCA model shows good accuracy in the kinetic regime, and fails in the spreading regime. Hence, this indicates that the SCA model is sufficient to accurately predict the first regime while another model is needed to predict the second regime.



(a)



(b)



(c)

Figure 3.1 Experimental apparent dynamic contact angles and comparisons of the experimental and numerical spread factors with the SCA model of the diesel drop with impact speed (a) u = 1.6 m/s, (b) u = 1.2 m/s, and (c) u = 0.7 m/s.

4.2 Drop Impact with the Combined SCA-DCA Model

The new method to combine both SCA and DCA models comes from the idea of employing the experimental data of apparent contact angle as a boundary condition in spreading regime. To reduce the requirement of experimental data, a general expression for all different materials is preferred here, and this general expression is derived in terms of the Oh number and modified non-dimensional time t^{**} as

$$\theta_d^* \approx \exp[5.70 \times Oh^{0.049} + (-1)^n \times 0.83 \times Oh^{-0.0112} t^{**} + (-1)^{n+1} \times 0.31 \times Oh^{0.56} t^{**2}] \quad (4.1)$$

where $n = 1$ when $Oh < 0.1$, and $n = 0$, when $Oh \geq 0.1$.

Therefore, the SCA model is employed in the first regime while the variable contact angle model with the general expression (eq. 4.1) is applied as the boundary condition in the second regime. This specific model is proposed as the "combined SCA-DCA model". This model was tested for all three materials with different impact speeds. Figure 4.2 shows images of drop deformation obtained from the SCA-DCA model, along with photographs of a diesel drop impacting the surface with u = 1.6 m/s. Predicted spreading diameters were measured from each computed image and compared with the experimental data at the same time (t) after impact.

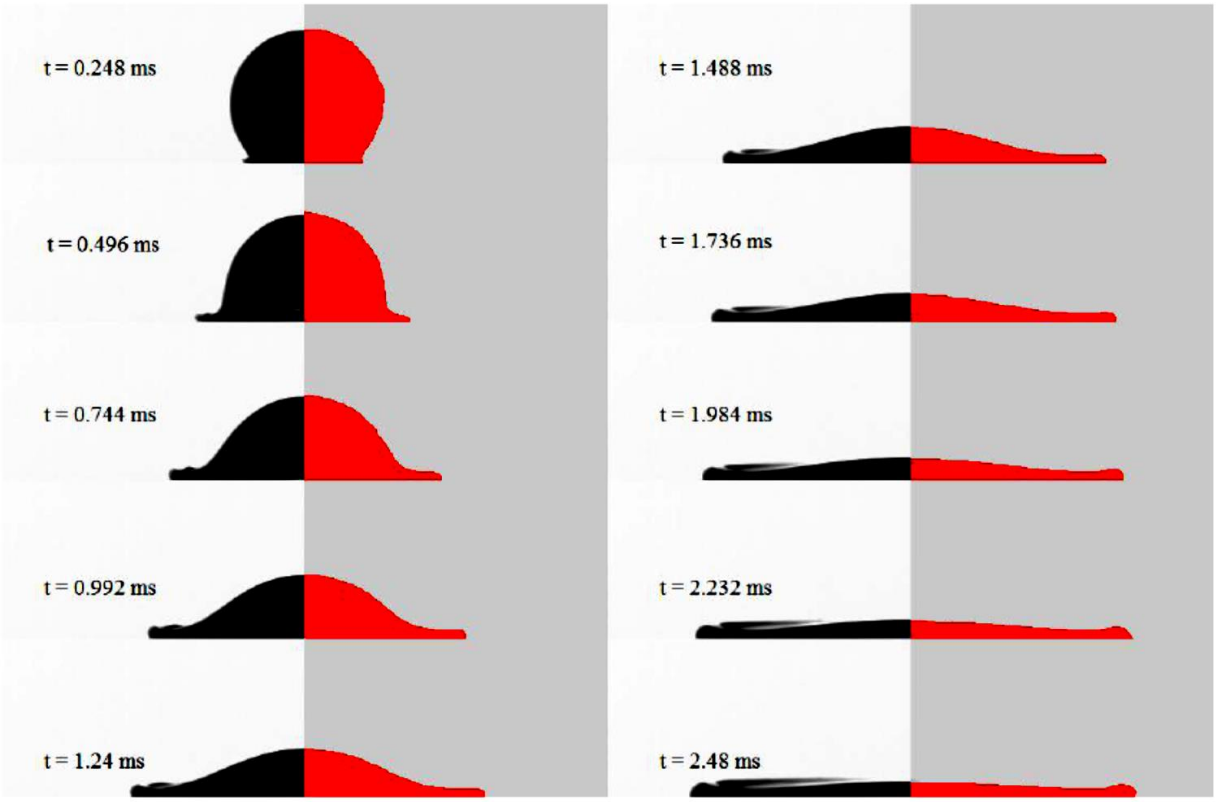


Figure 4.2 Computer generated images (right) compared with photographs of a diesel drop (left) impacting a glass surface with a velocity of 1.6 m/s

Figures 4.3 shows the comparisons of this model with the experimental data for glycerin drop. Table 4.1 shows the errors of predicted spread factors by using SCA-DCA model compared with the experimental data for all the cases. It is clear that the numerical results in most cases have sufficient accuracy within the quality of experiment results, since all experimental uncertainties are reported at a 95% level of confidence.

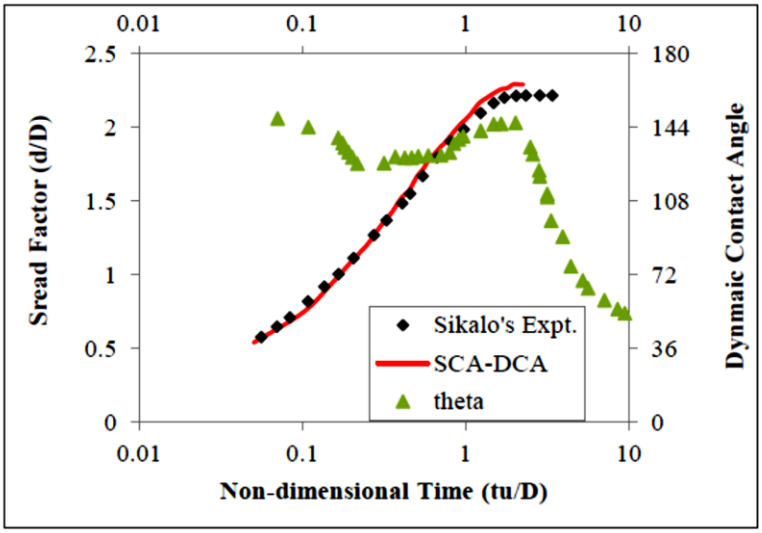


Figure 4.3 Experimental apparent dynamic contact angles and comparison of the experimental and numerical spread factors with the SCA-DCA model of the glycerin drop with impact speed u = 4.1 m/s

Table 4.1 Simulation errors of the SCA-DCA model

Simulation	Liquid	Impact velocity (m/s)	Error
1	Diesel	1.60	4%
2	Diesel	1.21	3.8%
3	Diesel	0.76	0.9%
4	Methanol	2.33	5.2%
5	Methanol	3.05	7.5%
6	Glycerin	1.04	2.5%
7	Glycerin	1.41	1.4%
8	Glycerin	4.1	3.4%

A key benefit of the SCA-DCA model is that it is generated only with the value of static contact angle and a general empirical equation. Hence, in this model, only the values of θ_e and Oh number are needed, both of which are purely based on the properties of the liquid. The requirement of having detailed data (often 50 to 100 points) of the time-varying contact angle that is typically employed in a full DCA model is also avoided. Thus, this model is shown to reduce the experimentally-derived behavior information required as compared with full DCA models. The

second advantage of the SCA-DCA model is that it significantly improves the accuracy over a pure SCA model and other empirical correlations, especially in the spreading regime. Moreover, by employing Oh number instead of Ca number, computational cost is also greatly decreased by using the new model, because Oh is only related to the properties of drops, whereas spreading velocity V in Ca number needs to be updated after each time step, remarkably increasing the computational cost.

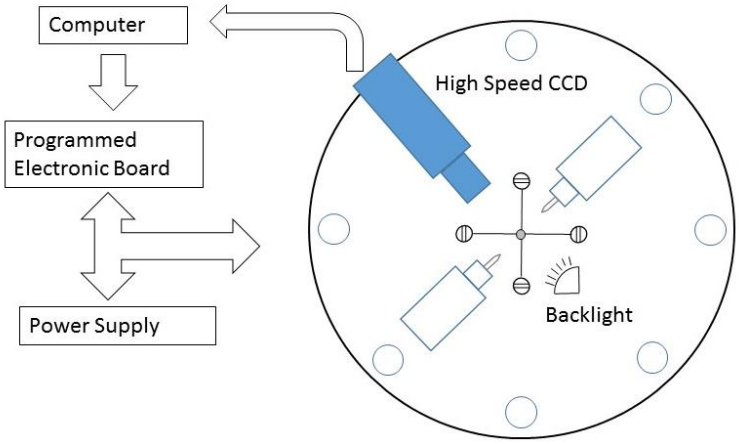
Chapter 5 Experimental Method

Along with the simulation of drop spreading, developing a new experiment was also considered. The main focus of this experiment is to study modified fuel (like polymer added fuels) under combustion scenarios. Previous MATC supported studies proved that adding long chain polymers to diesel would suppress splashing behavior. In a new set of experiments, viscoelastic behavior of these new fuels and their effect on heating, ignition and combustion of a single fuel droplet (which are crucial to trigger fire) are currently being studied. In these experiments, a single droplet of fuel is deployed on a very thin Si-C fiber, and all processes of heating, ignition and combustion are captured with high speed photography for future analysis.

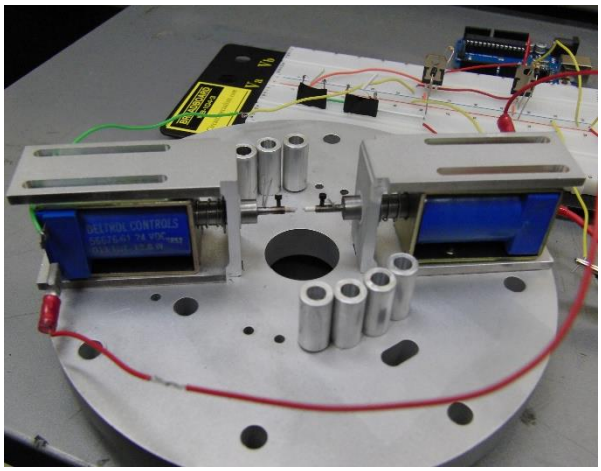
A schematic of the experimental arrangement is shown in figure 5.1. The arrangement mainly consisted of two solenoids, handmade hot wire loops for ignition, and a programmed Arduino board. Since the duration of ignition and combustion of a single droplet is very short, an accurate timing system is required. Therefore, an electronic board was programmed to turn the ignition system right after the camera was triggered. After a pre-specified time for hot wire to be on and very close to the droplet, the electronic board sends two signals to turn the hot wires off and retract them (using the solenoids) away from the combustion zone.

The ignition and combustion processes are captured by a high speed CCD camera, and the recorded images are sent to an image processing software to be analyzed. Base d on d^2 law of droplet combustion, the diameter of the droplet during combustion changes according to the following equation:

$$d_s^2 = d_{s,0}^2 - K_c t \qquad (5.1)$$



(a)



(b)

Figure 5.1 The experimental arrangement: (a) schematic representation and (b) actual set-up

Where d_s^2 and $d_{s,0}^2$ are droplet diameter and initial diameter, respectively, and K_c represents the droplet burning rate constant. Setting $t = \tau_c$ for $d_s = 0$ at complete burnout, we obtain the burning rate as:

$$K_c = \frac{d_{s,0}^2}{\tau_c} \qquad (5.2)$$

Spotlight® software developed by NASA was used to measure the rate of change in the droplet diameter during combustion. By analyzing frame by frame data, the effect of any additive on ignition delay and burning time could be understood. Figure 5.2 shows a series of frames of a burning diesel droplet at different times. The diameters of all droplets at different time steps is then measured by Spotlight and drawn versus combustion time to represent the rate of combustion. Figure 5.3 shows this data for the sample droplet shown before.

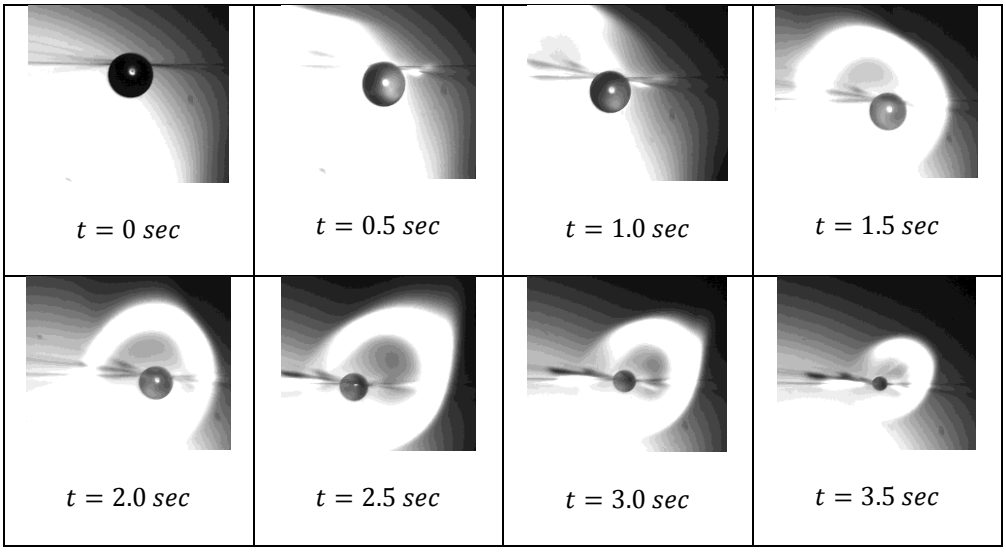


Figure 5.2 Time evolution of a burning diesel droplet on Si-C fiber

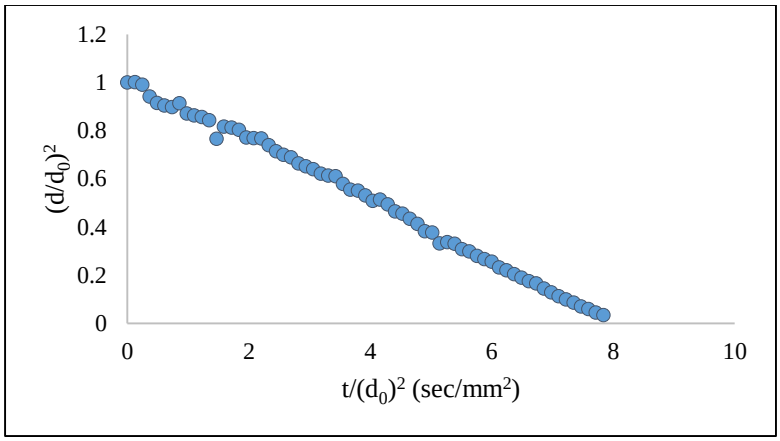


Figure 5.3 Experimental measurements of the droplet for a diesel droplet burning in atmospheric condition

Chapter 6 Conclusion

In this work, the dynamic behavior of impacting drops on a flat, smooth surface were investigated through numerical simulations. Three different hydrocarbon liquids were tested to provide a range of material properties which resulted in a range of observed behaviors. The two-phase spreading phenomena was characterized by the evolutions of the apparent dynamic contact angle and the spread factor. A combined SCA-DCA model was proposed on the basis of the two-phase spreading phenomena, and was employed as the boundary conditions in numerical simulations. In this new model, a general exponential correlation in terms of the Ohnesorge number (Oh) is derived on the basis of experimental results, describing the behavior of the apparent contact angle in the spreading phase. This general expression is employed as the boundary condition in the spreading phase while the SCA model is substituted in the kinetic phase. By comparing the simulation results with the experimental data, this new SCA-DCA model shows better accuracy (error less than 7%), whereas the SCA model and Kistler's correlation [16] have significantly greater error in Phase II.

Along with the simulations, an experiment was designed to evaluate the ignition and burning characteristics of modified fuels. To make sure our experimental procedures and measurements were accurate, the d^2 law of combustion was investigated. Based on this law, the rate of change of the square of the droplet diameter during the combustion process should be constant which was confirmed by results shown in figure 5.3. Further experiments and investigations on modified fuel is considered for the next phases of this research.

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