Turbulent liquid spray mixing and combustion – fundamental simulations

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Abstract. Fundamental simulations are used to investigate the ignition process of turbulent n-heptane liquid fuel spray jets. A DNS quality Eulerian method is used to solve the carrier gas flow field, while a Lagrangian method is used to track the liquid fuel droplets. Two-way coupling between the phases is included through the exchange of mass, momentum and energy. A detailed mechanism with 33 species and 64 reactions is used to describe the chemical reactions. The simulation approach allows studies of larger scale interaction of sprays and turbulence, including evaporation, mixing, and detailed chemical reaction. Both time developing and spatially developing liquid spray jets are studied. The initial carrier gas temperature was 1500 K. Several cases were simulated with different droplet radii (from 10 microns to 30 microns) and two initial velocities (100 m/s and 150 m/s). In the time developing case it was found that evaporative cooling and turbulence mixing play important roles in the ignition process of liquid fuel spray jets. Ignition first occurs at the edges of the jets where the fuel mixture is lean, and the scalar dissipation rate and vorticity magnitude are low. For smaller droplets, ignition occurs later than larger droplets due to increased evaporative cooling. Higher initial droplet velocity enhances turbulence mixing and evaporative cooling. For smaller droplets, higher initial droplet velocity causes the ignition to occur earlier, whereas for larger droplets, higher initial droplet velocity delays the ignition time. In the spatially developing liquid jets, ignition and flame lift-off characteristics similar to diesel sprays are observed. Near the injector, combustion development progresses very rapidly along the stoichiometric surface. In the downstream region of the spray, combustion develops with steep temperature fronts in a flamelet mode.

1. Introduction

Better understanding of liquid fuel spray combustion is critical to improving fuel efficiency and reducing emissions of industrial devices such as gas turbines, diesel engines and direct injection gasoline engines. Liquid fuel spray combustion is a complex phenomenon and a comprehensive understanding is very challenging. To understand the mechanism of spray combustion numerically, direct numerical simulation (DNS) is a useful tool. Recent advances in DNS and related issues can be found in the review article by Vervisch and Poinset [1].

Ignition is a key aspect of liquid fuel spray jets. There have been several previous studies of ignition in gas phase hydrogen and hydrocarbon fueled jets. Two-dimensional simulations of auto-ignition of hydrocarbon fuel vapor in a turbulent mixing layer and a decaying turbulent flow using a simple one-step chemistry mechanism [2-3] have shown that ignition first occurs at locations where
the mixture fraction is very close to the most reactive mixture fraction \( f_{MR} = 0.12 \) and the scalar dissipation rate of mixture fraction \( \chi \) is sufficiently low.

Im et al. [4] investigated the ignition of a hydrogen-air in a turbulent mixing layer using a more detailed chemistry mechanism with nine species and 38 reversible reactions. They found that the ignition kernel tends to be located where the mixing layer is convex towards to the fuel side. They also observed that ignition delay appears to be quite insensitive to the turbulence intensity.

Sreedhara and Lakshmisha [5] performed direct numerical simulations of the auto-ignition of n-heptane fuel vapor in a three-dimensional non-premixed turbulent field using a simple four-step mechanism. They concluded that the topology of auto-ignition spots remains the same irrespective of whether the flow is represented in two or three-dimensions.

Using direct numerical simulation, Viggiano and Magi [6] investigated the auto-ignition in transient jets in a reacting mixing layer between n-heptane fuel vapor and air using the same simple mechanism used by Sreedhara and Lakshmisha [5]. They found that for a lower initial stream temperature, auto-ignition occurs first on the wrinkled interface of the streams of air and fuel. For a higher initial temperature, auto-ignition occurs in both the edges and tip of the jet, where the scalar dissipation rate of mixture fraction has the lowest value.

Since the ignition of n-heptane involves many chemical reactions, single-step or four-step reaction mechanisms probably are not able to describe the reaction paths sufficiently. Therefore, more detailed chemistry mechanisms have been adopted. Wang and Rutland [7] carried out direct numerical simulation of liquid fuel spray ignition using a chemistry mechanism for n-heptane with 44 species and 112 reversible reactions developed by Stanford University and Sandia National Laboratories at Livermore [8]. Effects of initial gas temperature and global equivalence ratio were examined. From the simulations it was found that rapid evaporation of the fuel droplets results in significant cooling and ignition first occurs at a few isolated locations, and with increasing initial gas temperature auto-ignition occurs earlier. However, with increasing initial global equivalence ratio auto-ignition is delayed since increased fuel droplet evaporation decreases the local gas temperature.

In this research we study the ignition process of liquid spray jets using direct numerical simulation. Both temporally and spatially evolving jets are simulated with an n-heptane mechanism consisting of 33 species and 64 chemical reactions. This mechanism was developed by Patel and Reitz [9] and has been validated intensively through the comparison with other mechanisms developed for n-heptane. The mechanism correctly captures both the low and high temperature reaction characteristics of n-heptane fuel, including cool-flame phenomenon. In the current study, we examine the roles of evaporative cooling, turbulent mixing, mixture mass fraction and scalar dissipation in the ignition process. These parameters are correlated with the locations of ignition kernels. In addition, droplet size and initial droplet velocity are varied to examine the effects of evaporation and mixing on ignition. In the spatially evolving spray, the process of ignition and the development of lifted flames and propagating flamelets are described.

2. Governing Equations and Numerical Procedure
The S3D parallel DNS code for turbulent reacting flows was used for the numerical simulations [10-12]. In the simulations, the compressible Navier-Stokes equations are solved using 4th-order explicit Runge-Kutta time integration and 8th-order finite difference schemes. Lagrangian particle tracking and two-way coupling between phases were added to the code [7]. Local gas properties at the droplet locations are obtained by 4th-order Lagrange interpolation. To handle stiff chemical reactions, the implicit VODE solver [13] was used for the gas phase reaction source terms using a time splitting method.

Initially droplets at 300K were distributed in a narrow zone with a width of \( \delta = 0.2 \) mm as shown in Fig. 1. Three initial droplet radii were used: 10 \( \mu \)m, 20 \( \mu \)m and 30 \( \mu \)m. For each droplet size, two
initial droplet velocities were used to examine the effect of mixing. Therefore, in total 6 cases were simulated as shown in Table 1.

**Figure 1.** Schematic diagram for temporally evolving sprays. Domain size: 2.0 cm in x, see Table 1 for y; a uniform grid (Δx=39.1 µm) with periodic boundary conditions in both directions was used.

**Table 1** Initial and ignition parameters: \( r_d \): initial droplet radius; \( u_d \): initial droplet velocity; \( \dot{m} \): initial droplet flow rate; \( L_y \): domain size in the y direction; \( t_f \): droplet lifetime; \( t_{ign} \): ignition delay time; \( Z_{ign} \): mixture fraction at ignition kernels; \( \chi_{ign} \): scalar dissipation rate at ignition kernels; \( \Omega_{ign} \): vorticity magnitude at ignition kernels.

| Case #  | 1    | 2    | 3    | 4    | 5    | 6    |
|---------|------|------|------|------|------|------|
| \( r_d \) (µm) | 10.0 | 20.0 | 30.0 | 10.0 | 20.0 | 30.0 |
| \( u_d \) (m/s) | 100  | 100  | 100  | 150  | 150  | 150  |
| \( \dot{m} \) (g/s) | 0.25 | 0.25 | 0.25 | 0.375| 0.375| 0.375|
| \( L_y \) (cm)  | 1.0  | 1.0  | 1.0  | 2.0  | 2.0  | 2.0  |
| \( t_f \) (ms)  | 0.43 | 1.31 | 2.09 | 0.35 | 1.10 | 2.00 |
| \( t_{ign} \) (ms) | 1.846| 1.394| 1.268| 1.412| 1.608| 1.372|
| \( Z_{ign} \) | 0.025| 0.030| 0.023| 0.022| 0.019| 0.038|
| \( \chi_{ign} \) (s\(^{-1}\)) | 1.25 | 6.64 | 1.10 | 0.88 | 0.33 | 0–7.0|
| \( \Omega_{ign} \) (s\(^{-1}\)) | 1145 | 1128 | 5000 | 1000 | 614  | 0–8000|

2.1. Droplet Governing Equations
The fuel spray droplets are treated in a Lagrangian frame. The drag force is calculated using the Stokesian drag law and evaporation is calculated according to the infinite heat conductivity model inside the fuel droplet [15]. The droplet equations of motion, momentum, mass, and energy can be expressed as:

\[
\frac{dx_{d,i}}{dt} = u_{d,i}
\]  

\[
m_d \frac{du_{d,i}}{dt} = F_{gd,i}
\]
\[
\frac{dm_d}{dt} = -2\pi \rho D_r Sh_d B_M \tag{5}
\]
\[
\frac{dT_d}{dt} = \frac{4\pi r_d^2}{m_d c_{\text{liq}}} \left[ \rho_d \frac{dr_d}{dt} - L_{\text{sup}} + \frac{\lambda_d}{2r_d} \left( T - T_d \right) + Nu_d \right] \tag{6}
\]
where the subscript \(d\) indicates droplet values, \(r_d, u_d, m_d\) and \(T_d\) are the droplet radius, velocity, mass, and temperature, respectively. In Eq. (4) \(F_{gd,i}\) is the drag force exerted by the carrier fluid and is given by:
\[
F_{gd,i} = \frac{1}{2} \rho D_d A_d \left| u_i - u_{d,i} \right| \left( u_i - u_{d,i} \right) \tag{7}
\]
Here \(A_d\) is the frontal area of the droplets, and \(C_D\) is the drag coefficient, which is calculated according to the following expression
\[
C_D = \frac{24}{Re_d} \left( 1 + \frac{1}{6} Re_d^{2/3} \right) \tag{8}
\]
where \(Re_d\) is the droplet Reynolds number, defined as
\[
Re_d = \frac{2\rho |\tilde{u} - \tilde{u}_d| r_d}{\mu} \tag{9}
\]
In Eq. (5) \(Sh_d\) is the Sherwood number, calculated by
\[
Sh_d = \left( 2 + 0.6 Re_d^{1/2} Sc^{1/3} \right) \ln \left( 1 + B_M \right) / B_M \tag{10}
\]
where \(Sc = \mu / \rho D\) is the Schmidt number, \(D\) is the diffusivity of the gas phase fuel in the carrier fluid. Also, \(B_M\) is the mass transfer number defined as
\[
B_M = \frac{Y_{FS} - Y_{FS_s}}{1 - Y_{FS}} \tag{11}
\]
where \(Y_{FS_s}\) is the fuel vapor mass fraction of the fluid, and \(Y_{FS}\) is the fuel vapor mass fraction at the droplet surface, given by
\[
Y_{FS} = \frac{W_{FV}}{W_{FV} + W_{\text{GAS}} (p/p_{st} - 1)} \tag{12}
\]
Here \(W_{FV}\) is the fuel vapor molecular weight; \(W_{\text{GAS}}\) is the molecular weight of the gas mixture; \(p_{st}\) is the saturation pressure for a droplet temperature, \(T_d\); \(c_{\text{liq}}\) and \(L_{\text{sup}}\) are the specific heat and latent heat of the droplets; and \(Nu_d\) is the Nusselt number calculated by
\[
Nu_d = \left( 2 + 0.6 Re_d^{1/2} Pr^{1/3} \right) \ln \left( 1 + B_M \right) / B_M \tag{13}
\]
It should be noted that when the surface temperature of a fuel droplet is required to calculate the gas fluid properties, a weighted averaged temperature is employed: \(T_{\text{AVG}} = \left( T_s + 2T_d \right) / 3\).
3. Results and Discussion

3.1. General Characteristics of Temporally Evolving Sprays

To demonstrate the general characteristics of evaporation and ignition of the liquid fuel spray, we first present the results for Case 1. As the fuel is injected, liquid fuel droplets evaporate and cool the hot carrier gas. The time used for droplet evaporation is designated the droplet lifetime or the evaporation time ($t_f$). As shown in Table 1, with increasing droplet size, evaporation times become longer since the surface area to volume ratio of the droplets decreases. In addition, higher initial velocities increase droplet evaporation through larger relative velocities and increases in the Shorewood and Nusselt numbers.

For Case 1, droplets have evaporated completely by $t = 0.45 \text{ ms}$. Through drag force and evaporation, the momentum of the liquid spray is transferred to the gaseous gas. The momentum transfer causes the gas phase in the narrow zone to move in the positive $x$ direction. The contour plot of the vorticity magnitude at $t = 0.52 \text{ ms}$ is shown in Fig. 2 (left) where it is shown that a number of small vortices have formed along the narrow spray zone in the center of the domain.

Droplet evaporation also reduces the gas temperature. In addition, cold fuel vapor mixes with the hot gas, which further decreases the gas temperature. The temperature distribution at $t = 0.52 \text{ ms}$ is shown in Fig. 3 (right). It is seen that the minimum temperature is around 900 K indicating that evaporative cooling is very significant.

![Figure 2. Case 1, $t = 0.52 \text{ ms}$; left: vorticity magnitude contours (blue=0 s$^{-1}$; red=70000 s$^{-1}$); right: temperature contours (blue=900 K; red=1500 K)](image)

The mixture fraction distribution at $t = 0.52 \text{ ms}$ is shown in Fig. 3 (left), which has the same structure as the temperature distribution since the Lewis number is assumed to be unity. Distribution of the scalar dissipation rate of mixture fraction is shown in Fig. 3 (right), which shows anti-symmetrical fine structures in the $y$ direction.

![Figure 3. Case 1, $t = 0.52 \text{ ms}$; left: mixture fraction contours (blue=0; red=0.28); right: scalar dissipation contours (blue=0 s$^{-1}$; red=300 s$^{-1}$)](image)

As fuel evaporates and mixes with the hot ambient oxidizer, reaction begins to occur. Since n-heptane fuel is characterized by significant low temperature kinetics, this phase of the process is important to the overall ignition characteristics. Eventually, the reactions and heat release reach a sufficient level and we identify ignition kernels of the main combustion process when the local temperature reaches 1700 K. For Case 1 ignition occurs at $t = 1.846 \text{ ms}$ and contours of temperature
and heat release rate are shown in Figs. 4. It is seen that several ignition kernels with significant heat release are developing along the edges of the spray jet. Contours of the mixture fraction are shown in Fig. 5 (left) where mixing has reduced the maximum value from 0.28 in Fig. 3 to 0.13. A scatter plot of temperature and mixture fraction (Fig. 5 - right) shows that the mixture fraction is approximately 0.025 at the ignition kernels indicated by high temperature regions. This corresponds to a lean equivalence ratio of 0.387.

![Figure 4](image1)

**Figure 4.** Case 1 at \( t = 1.846 \) ms; left: temperature contours (blue=1100 K; red=1700 K); right: heat release rate contours (blue=0; red=\(3.47 \times 10^9\) w/m³).

![Figure 5](image2)

**Figure 5.** Case 1 at \( t = 1.846 \) ms; left: mixture fraction contours (blue=0.0; red=0.13); right: scatter plot of temperature and mixture fraction.

Previous studies such as [2,3] found that for non-spray mixing layers of fuel vapor and air, ignition first occurred at very rich locations (e.g. equivalence ratio of 2.34 for methane). However, for the present case with liquid sprays, ignition is unlikely to occur at rich mixtures since these locations have experienced significant evaporative cooling.

Distribution of the scalar dissipation rate of mixture fraction at \( t = 1.846 \) ms is shown in Fig. 6 (left). Again, due to mixing the maximum value of \( \chi \) has significantly reduced to 5.0 s\(^{-1}\) from earlier times (Fig. 3). The scatter plot of temperature and scalar dissipation rate is shown in Fig. 6 (right), from which it is seen that ignition occurs first at locations with very low values of scalar dissipation rate (1.25 s\(^{-1}\)). Scatter plots of vorticity magnitude (not shown) also show ignition occurs in regions of low vorticity.
3.2. Effect of Initial Droplet Size

To examine the effects of initial droplet size we examine Cases 1-3 with initial droplet sizes of 10 µm, 20 µm and 30 µm, respectively (see Table 1). The initial droplet mass flow rate and droplet velocities were the same for all three cases, but the ignition times decreased from 1.846 ms to 1.394 ms to 1.268 ms for Cases 1-3, respectively. As the initial droplet size increased, the evaporation rate is lower and evaporative cooling is less significant. Therefore, the ignition delay time decreases with increasing droplet size.

For Case 2 with an initial droplet radius of 20 µm, the general character of the scatter plots of temperature with mixture fraction and scalar dissipation rate at ignition are similar to those for Case 1. As an example, the scatter plot of temperature with the scalar dissipation rate for Case 2 is shown in Fig. 7. Note that at the ignition kernels, the mixture fraction is 0.03, and the scalar dissipation rate is $6.64 \text{ s}^{-1}$, which are larger than the values in Case 1 due to the shorter ignition delay time (see Table 1). Therefore, similar to Case 1, ignition originates at locations where the fuel mixture is lean, and the scalar dissipation rate and vorticity magnitude are very low for Case 2.

For Case 3 with an initial droplet radius 30 µm, the ignition delay time is 1.268 ms (see Table 1). The ignition delay time is even shorter than Case 2 due to slower evaporative cooling. Similar to Cases 1 and 2, at the ignition kernels the mixture fraction is lean with a value of 0.027, while the scalar dissipation rate and vorticity magnitude are very low compared to the full range of values in the domain. For the variation in droplet sizes in Case 1-3, we can conclude that ignition always occurs at the locations where the mixture fraction is lean, and both the scalar dissipation rate and the vorticity magnitude are very low. With increasing droplet size, ignition delay time decreases because of a slower evaporative cooling.

Figure 6. Case 1 at $t = 1.846 \text{ ms}$; left: scalar dissipation rate contours (blue=0.0 s$^{-1}$; red=5.0 s$^{-1}$); right: scatter plot of temperature and scalar dissipation.

Figure 7. Scatter plot of temperature and scalar dissipation rate at $t = 1.394 \text{ ms}$ for Case 2.
3.3. Effect of Initial Droplet Velocity

Above, we examined the effects of initial droplet size with the same initial velocity 100 m/s. Now, for Cases 4 through 6, the initial droplet velocity is increased to 150 m/s to explore the effect of increased mixing rates. Other initial conditions were kept unchanged. Increase of the initial droplet velocity has several effects: first, a higher initial velocity makes the fuel droplets evaporate faster as shown by $t_f$ in Table 1; second, a higher initial velocity enhances mixing. Figure 8 (left) shows the distribution of the mixture fraction for Case 4 has more structure than that for Case 1 (Fig. 3) at the same time. In addition, at this time the maximum mixture fraction is 0.2 for Case 4 while the maximum mixture fraction is 0.28 for Case 1. Therefore, higher initial droplet velocity enhances mixing.

For Case 4, the ignition delay time is 1.412 ms, which is much shorter than for Case 1 with a lower initial velocity 100 m/s. The Case 4 scatter plots of temperature with the mixture fraction, scalar dissipation rate and vorticity magnitude at ignition ($t = 1.412$ ms) are similar in structure to those in Case 1. For example, compare the temperature-scalar dissipation plot in Fig. 8 (Case 4) with the one in Fig. 6 (Case 1). However, magnitudes are different and Case 4, which has stronger mixing than Case 1, has slightly lower values for mixture fraction, scalar dissipation rate, and vorticity at the ignition kernels (Table 1).

![Figure 8](image)

**Figure 8.** Case 4; left: mixture fraction contours at $t = 0.52$ ms (blue=0.0; red=0.2); right: scatter plot of temperature and scalar dissipation rate at $t = 1.412$ ms

For smaller droplet size cases (Cases 1 and 4), the droplet lifetime is much smaller than the ignition time. Thus, mixing plays a very strong role in the ignition process. Since, the increase of the initial droplet velocity enhances the mixing, the ignition delay time is decreased.

As droplet size increases for the higher initial droplet velocity in Case 5, scatter plots (not shown) are structurally similar to Case 2. Similarly, Cases 2 and 5 have droplet lifetimes that are close to the ignition time (Table 1). This is in contrast to the smaller droplet Cases 1 and 4 which have very short evaporation times. Therefore, evaporation plays a more significant role in the ignition process for Cases 2 and 5. Now, as the initial droplet velocity increases and evaporative cooling is accelerated, the ignition delay time increases from Case 2 to Case 5. This increase occurs despite the fact that Case 5 has higher mixing rates than Case 2 as indicated by lower values for mixture fraction, scalar dissipation rate, and vorticity at the ignition kernels (Table 1).

Comparison of Case 3 and 6 show a similar trend. That is, when droplet lifetimes are significant compared to ignition times, higher initial droplet velocity increases the ignition delay time. In these cases, the droplet lifetimes are actually longer than the ignition delay times. Thus, evaporative cooling has a strong impact on ignition processes and counters the increased mixing that occurs at the higher initial droplet velocity used in this study. The increased mixing in Case 6 is evidenced by the broad range of scalar dissipation rate and vorticity at the high temperature ignition sites (scatter plots not shown). This indicates that the scalar dissipation rate, which is commonly associated with ignition in gaseous systems, may not be a sufficient indicator of ignition in liquid fuel systems.
3.4. Spatially Evolving Sprays

In this section we show the general character of the ignition process in a spatially evolving spray jet. The domain for these simulations is 8 cm long and 2 cm wide with a 39.1 µm uniform grid size and non-reflective outflow boundary conditions in the x direction. Figure 9 shows contours of temperature at the time of ignition. Ignition kernels form on the periphery of the liquid jet consistent with experimental results [14]. Similar to the previous sections, scatter plots (not shown) show that ignition occurs at locations of low scalar dissipation rate, lean mixture fraction, and low vorticity magnitude.

After ignition, the flame kernels spread both upstream and downstream. This ‘spreading’ does not appear to be conventional flame propagation. Instead it may be similar to the spontaneous flame propagation recently studied in simulations [15]. The result is shown in Fig. 10 where nearly stationary lifted flames are established near the injection location, and flamelets propagate downstream following the stoichiometric surface. Lifted flames are commonly seen in visualization experiments of modern, high pressure diesel injection combustion [16]. The downstream flamelets suggest a modification of the diesel combustion schematic suggested by Dec [17]. The original schematic describes quasi-steady flames established along the stoichiometric line. The current results show unsteady flamelets moving through this region. Additional analysis is required to establish the process that is occurring in the downstream, spray plume region.

![Figure 9](image1.png)

**Figure 9**: Temperature contours at the time of ignition for the spatially evolving spray jet. Contour colors indicate temperature and droplet sizes as they are injected at the left boundary. (T\_amb: 1500 K, P\_amb: 1 atm, nozzle diameter 0.2 mm, fuel injection: 100 m/s, 20 µm drop diameter)

![Figure 10](image2.png)

**Figure 10**: Heat release contours after ignition kernels have evolved into lifted flames near the injector and propagating flames in the downstream, spray plume region.
4. Conclusions
This paper investigates the ignition process of liquid fuel spray jets using two-dimensional direct numerical simulations. A chemistry mechanism with 33 species and 64 reactions was adopted for the oxidation of n-heptane fuel. The effects of initial droplet size and droplet velocity were examined through the analysis of the computational results. From the results, it can be concluded that:

- Evaporative cooling and mixing play important roles in the ignition process of liquid fuel spray jets.
- Ignition kernels always occur at locations with lean mixture fraction, lower scalar dissipation rate and lower vorticity magnitude.
- Increase of droplet sizes reduces the ignition delay time due to less significant evaporative cooling.
- For smaller droplets where droplet lifetimes are less than ignition delay times, the ignition process is mixing controlled. Thus, increased droplet velocity reduces the ignition delay time due to a stronger mixing.
- For larger droplets where droplet lifetimes are similar to or longer than ignition delay times, the process is evaporation controlled. Thus, higher initial droplet velocity increase the ignition delay time due to the stronger evaporative cooling effect.
- In spatially evolving sprays, ignition kernels are established near the injector on the spray periphery.
- Ignition kernels propagate upstream to established lifted flames and downstream as flamelet regions following the stoichiometric surface.

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