

Ignition Delay and Flame Radius for Single Particle Combustion in High-Temperature Flammable Gas/Air Mixtures

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1 Introduction

It has long been known that the explosion severity of a combustible dust/air mixture can be increased from the addition of a flammable gas. These so-called “hybrid mixtures” may arise as industrial process hazards and are relevant to mining (e.g., coal/methane [1]), pharmaceutical (e.g., lactose/vaporized solvents such as methanol [2]), and manufacturing industries (e.g., nylon fibres/combustible fumes [3]). Although a phenomenological understanding of dust and hybrid dust/flammable gas explosion has been achieved through experimental testing, the small scale details during combustion are not well established and linking these details to industrial situations remains to be completed.

In the current investigation transient, spherically symmetric, numerical simulations are performed for combustion of isolated *n*-octadecane ($C_{18}H_{38}$) and 1-octadecanol ($C_{18}H_{38}O$) particles with a focus on ignition delay and flame radius. Comparison is made to combustion of isolated *n*-heptane droplets (C_7H_{16}) in hot environments containing air only and containing flammable gas/air mixtures. The size of the condensed fuel is varied from 50–1000 μm , which encompasses the larger diameters typically studied for droplet combustion, as well as the smaller sizes required for dust explosion.

2 Numerical Model

The numerical model used in the current investigation was based on the methods developed by Marchese et al. [4] and Basevich et al. [5] for droplet combustion. The computational domain is broken into condensed fuel and gas regions separated by an interface. The transient, one-dimensional, spherically symmetric, governing equations for multicomponent conservation of mass and energy are solved for initially quiescent and isobaric conditions at one atmosphere (e.g., see [4]). Whereas the above mentioned references include adaptive meshing to capture surface regression, the interface location is held constant in the current work. In this simpler approach the condensed phase density decreases in response to surface gasification. Gasification is controlled by equilibrium of partial pressures between the fuel vapour and surroundings.

The internal boundary condition ($r = 0$ mm) assumes zero temperature gradient at the centre of the condensed fuel. The external boundary condition also assumes zero gradient in temperature, specie mass fractions, and density, but allows mass inflow/outflow during the simulation. This approach represents isolated particle combustion and the domain is kept large enough that gradients near the external boundary are small.

The governing equations and boundary conditions provide $2 + N_s$ relations for $3 + N_s$ unknowns, where N_s is the number of gas phase species in the simulation, and enthalpy, density and gas velocity are the remaining unknowns. The equations are also non-linear including variable transport coefficients and thermophysical parameters.

A semi-implicit, iterative procedure is used to find a converged solution at each simulation timestep. The previous timestep is taken as a guess of the density, mass fraction, and temperature fields, and used to predict the transport and thermophysical coefficients. An updated solution is achieved by solving the governing equations for temperature and mass fraction. An updated density field is calculated using the ideal gas law for closure and is used to find an updated velocity field. With the updated velocity and density, the temperature and mass fraction equations are no longer satisfied, and the solution procedure is iterated until convergence is achieved. The fluid velocity magnitude remained small during the simulation with a maximum observed value of 5 cm/s during ignition of large droplets, but more often magnitudes less than 1 cm/s.

3 Thermophysical and Reaction Modeling

Temperature and composition dependent models were used for gas and condensed phase thermal conductivity, latent heat of vaporization, and specific heat capacity. Mixed gas phase thermal conductivity was calculated using the Wassiljewa relation with the Mason and Saxena modification, as reported in Poling, Prausnitz, and O'Connell [6]. Component thermal conductivities were calculated using the Chapman-Enskog formulation [6], with an empirical collision integral expression, and Lennard-Jones parameters estimated from critical pressure and temperature data. Liquid thermal conductivity was calculated using the Sastri method with group contribution parameters as reported in Poling, Prausnitz, and O'Connell [6]. Solid thermal conductivity was computed using the empirical relation of Graves et al. [7] for octadecane and used for both octadecane and octadecanol in this work.

Variable latent heat of vaporization was computed with the empirical model of Pitzer as reported by Poling, Prausnitz, and O'Connell [6], using the condensed fuel critical temperature and acentric factor data reported in their text. Latent heat of melting was assumed constant at 244 kJ/kg and 257 kJ/kg for octadecane and octadecanol, respectively.

Specific heat at constant pressure was computed for O_2 , N_2 , CO_2 , and H_2O species with seven term equation fits. The remaining gas species for heptane, octadecane, and octadecanol were fit to Benson group contribution data [6]. Liquid specific heat was computed using the empirical relation of Ruzicka and Domalski, again with group contribution parameters [6]. The solid phase specific heat was treated in a simplified manner and taken as constant at 1911 J/kg-K and 2100 J/kg-K for octadecane and octadecanol, respectively.

A global single-step reaction mechanism was used in the current work. Kinetic parameters for heptane [8] were used for all three fuels, with the molar concentrations raised to a power of unity as used by Botros, Law, and Sirignano [9]. Using the same reaction parameters for all fuels allows the impact of heating, melting, and gasification to be investigated more directly. For hybrid simulations the flammable gas added to the ambient atmosphere is the same as the condensed fuel. For simplicity a constant diffusivity coefficient was assumed for all species using a representative value for heptane in air ($26 \text{ mm}^2/\text{s}$), unless otherwise noted.

4 Liquid Droplet Results

Simulation results for heptane combustion are presented in this section and compared to experimental and numerical results from the literature. Typical gas temperature and specie profiles are given in Figure 1 for ignition of a spherical droplet instantaneously immersed in air at 1100 K. Three distinct stages are shown: droplet heating and vapour accumulation, flame ignition at some distance from the surface followed by premixed burning towards the surface, and lastly, diffusion-limited with the flame moving away from the surface with time. These features are commonly found in single droplet combustion [4, 5, 10].

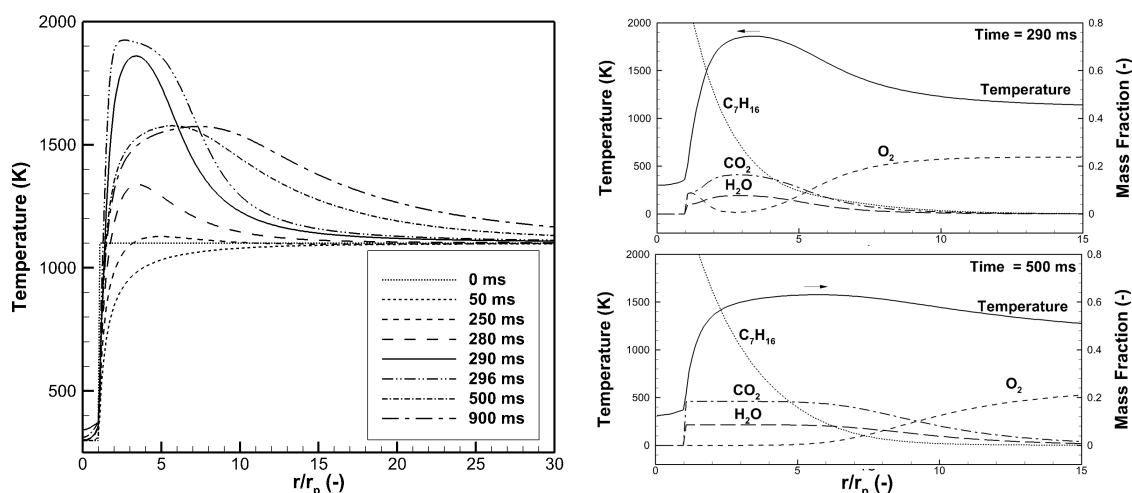


Figure 1: Gas temperature and specie profiles during ignition of 1.3 mm *n*-heptane droplets in 1100 K air. The arrows in the right figure indicate direction of flame movement.

Ignition delay for the condensed phase is important to consider for hybrid interaction. Furthermore, for dust flame propagation the fuel concentration is often many times stoichiometric, suggesting that the ignition process may be more important than the later time particle burning characteristics (e.g., most of the fuel remains unburned and the flame may travel from particle to particle based on ignition). Ignition delay time is given for 1.3 mm heptane droplets in the right side of Figure 2, and is compared to previous experimental results [11] and detailed numerical modeling [4]. The maximum gas temperature as a function of time for the current model is also given in the left side of Figure 2. The ignition delay time is taken as the point where the temperature first increases above the ambient value. In subsequent analysis the flame radius is taken as the location of this temperature increase in space.

The sensitivity of the simulation to the choice of diffusion coefficient was investigated (see Figure 2) and showed a moderate impact on ignition delay time. This suggests that the differences between the detailed modeling of Marchese et al. [4] and the more simplified modeling completed here are due to the global reaction mechanism instead of transport phenomena. The agreement between experimental data and the current model at lower ambient temperatures is encouraging in lieu of the simplified methods used. A constant value of 26 mm²/s was used as the diffusion coefficient for the remainder of simulations in this work.

5 Solid Particle and Hybrid Results

One of the significant differences between isolated combustion of liquid droplets and solid particles is the increased heating requirements associated with melting and gasification. The left side of Figure 3

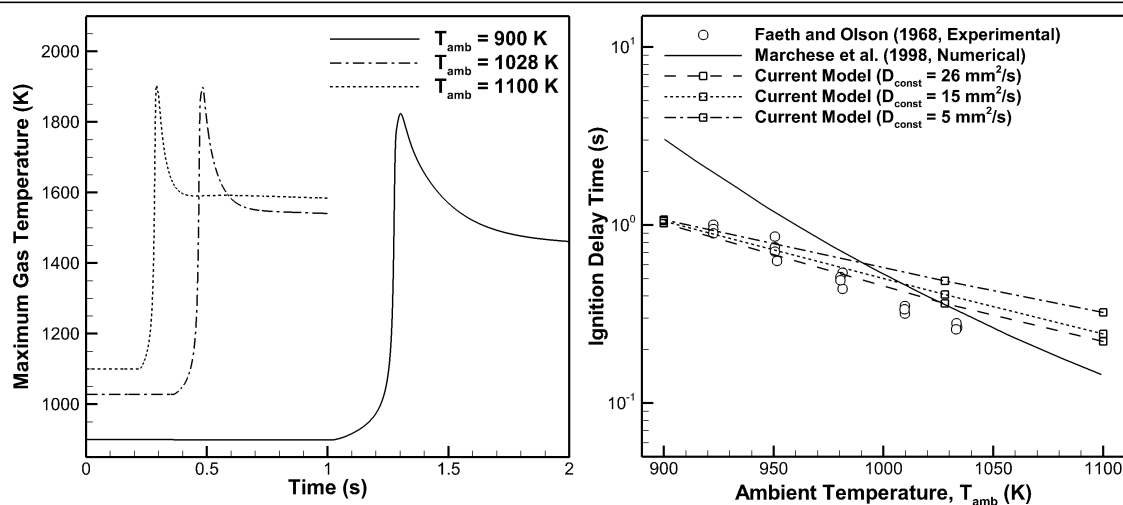


Figure 2: Maximum temperature traces (left) and comparison of ignition delay times to literature data (right) for 1.3 mm *n*-heptane droplets in air. The maximum gas temperature plot is computed with a uniform diffusivity of 26 mm²/s. Literature data [4, 11] was taken as reported by Marchese et al. [4].

shows transient surface and centre temperatures for 1.0 mm droplets and particles, and compares this to the respective gasification rates. The maximum gasification rate occurs when the fuel reaches the boiling temperature at ambient pressure (101.325 kPa). The melting process and higher boiling temperatures significantly delay gasification and increase ignition delay. The impact of initial diameter on ignition delay is given in the right side of Figure 3. Decreasing the initial diameter has a larger impact on particle ignition than droplet ignition as heating is the rate limiting process for the solid fuel. An increased ambient temperature of 1500 K was used for these simulations to avoid the minimum “ignitable diameter” where the condensed fuel fully gasifies before ignition [10]. The current model was able to capture this minimum diameter although its investigation is left for future work.

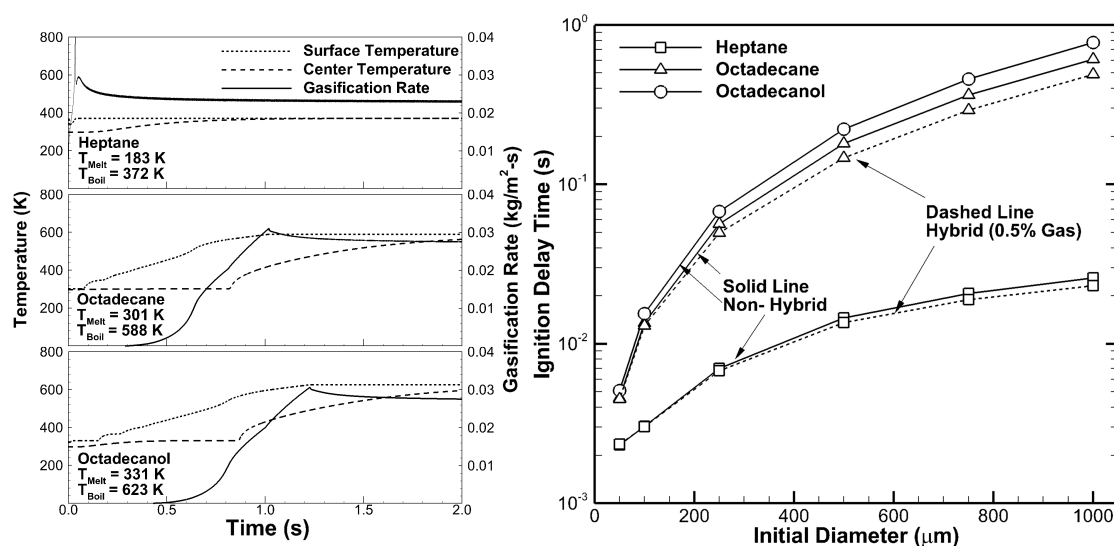


Figure 3: Surface temperature, centre temperature, and gasification rate for 1.0 mm droplets and particles immersed in air at 1500 K (left). Ignition delay time as a function of diameter for air-only (non-hybrid) and hybrid conditions with an ambient temperature of 1500 K (right).

The hybrid simulations completed in this work are also shown in Figure 3 and Figure 4 along with the non-hybrid results computed in ambient environments with air only. The left side of Figure 4 shows maximum gas temperature under hybrid and air-only conditions. Particle combustion is much slower than the flammable vapour while droplet combustion is on the same order of magnitude. In general the addition of reactive gas to the ambient atmosphere decreases the ignition delay time, although this has a larger impact when the gas combustion is much faster than the condensed fuel.

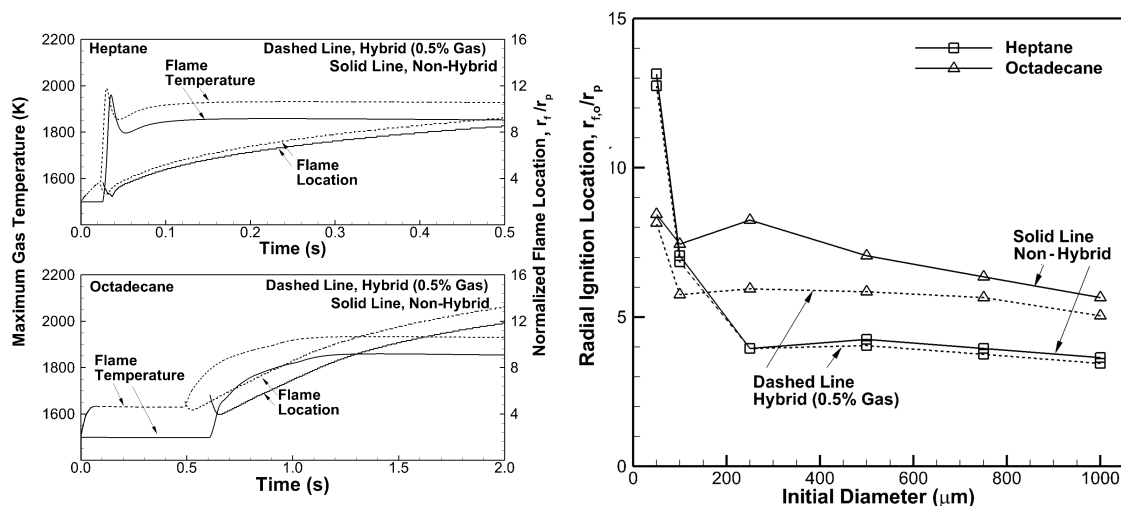


Figure 4: Maximum gas temperature and flame location for 1.0 mm *n*-heptane droplets and *n*-octadecane particles immersed in hybrid flammable gas/air mixtures and in air only, both at 1500 K (left). Flame location at ignition for a range of particle and droplet diameters (right).

The flame ignition location is taken as the location of the maximum gas temperature at ignition and is summarized in the right of Figure 4. The ignition location for octadecanol was very similar to octadecane and is not included. As the droplet and particle diameter is reduced, the ignition location relative to the initial diameter generally increases. This has been shown previously [10] and is due to the relatively faster gasification and diffusion present with smaller droplets and particles. Hybrid conditions decrease ignition delay and reduce the amount of time fuel has to diffuse into the surroundings. All simulations demonstrated a local minimum in ignition flame radius in the smaller diameter range (250 μm for heptane and 100 μm for octadecane). It is currently unclear if this is related to the approach used to indicate when ignition occurs or a feature of the rapid gasification near the minimum ignitable diameter limit.

6 Conclusion and Future Work

The results of this investigation demonstrated the differences between isolated droplets and particles during the early stages of combustion. Increased ignition delay times for solid particles were shown due to longer heating, melting, and gasification timescales. Decreasing the diameter also had a significant impact on particle ignition delay compared to a more moderate impact for droplets as heating is the controlling factor for combustion.

Isolated droplet and particle combustion in flammable gas/air mixtures was also investigated. The droplets demonstrated combustion timescales on the order of the vapour reaction rate and had marginal decreases in ignition delay. Larger particles which did not ignite until significantly after vapour combustion had the largest decrease in ignition delay times.

Future work will include further verification of the numerical model and implementation of more sophisticated reaction kinetics and gas diffusion. With the single-step global reaction mechanism there is limited feedback from particle combustion to gas combustion. With more sophisticated kinetics the lower flammability limit of the gas could be better represented and further interaction with the condensed fuel combustion may be investigated. Moving forward a larger focus will be placed on the smaller diameter ranges typically associated with industrial explosion of particulates in oxidising and hybrid reactive environments.

Acknowledgement

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