

Parametric Numerical Studies on Auto-Ignition around a Single Fuel Droplet

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Detailed numerical simulations of the auto-ignition of single methanol droplets embedded in quiescent air have been performed in a closed volume. The influence of ambient air temperature, pressure, droplet radius and global equivalence ratio on the auto-ignition delay time of the droplet is investigated. The result of the parametric study is presented. Furthermore the results of the detailed study are used to identify regions in parameter space where a simplified treatment of droplet ignition is possible. This is the case, when the droplet lifetime and the time required for mixing between fuel vapor and ambient air (mixing time) are much smaller than the ignition delay time and hence can be decoupled. Under this case, droplet ignition can be treated as the corresponding ignition of a homogeneous reactor with same global enthalpy and equivalence ratio, or as ignition in the inhomogeneous gas phase.

1. Introduction

Spray combustion is used in various engineering applications like diesel and jet engines, gas turbines and furnaces. The understanding of ignition in sprays involves convective flows and influence from the neighboring droplets, which further complicates understanding of the phenomena. Numerical simulation of auto-ignition in a spray in full detail, at full spatial and temporal resolution, is computationally prohibitive. Simplified models are needed which capture essential properties of ignition in sprays, without causing exhaustive computational effort. A first step for such models is the study of auto-ignition on single fuel droplets. In these studies, the complex coupling of various underlying physical and chemical processes like fuel vaporization, transport and chemical kinetics can still be treated in full detail.

Single droplet ignition and combustion have been investigated by various research groups in the past. Pioneer work by Spalding [1] and Godsave [2] resulted in the d^2 law which was validated experimentally by Kumagai et al. [3, 4]. Law [5] and Faeth [6] presented their review on the development and details of droplet combustion. Sirignano [7] presented a review on the interactive modeling of various droplets in an artificial array and droplet streams. More recently Nakanashi et al. [8] and Tanabe et al. [9] performed an experimental study on the ignition of single droplets at high ambient temperatures and pressures. Schnaubelt et al. [10, 11] investigated ignition of n-heptane and n-decane droplets both experimentally and numerically. Aouina et al. [12] used a two-dimensional mathematical model for simulating the heating, evaporation, ignition and subsequent combustion of a single and two droplets injected in a hot gas flow. The study was performed using detailed reaction chemistry and the influence; particularly of the distance between the neighboring droplets on the ignition delay times have been investigated. Moriue [13] studied detailed simulation of a single n-heptane droplet in a closed volume. Cuoci et al. [14] studied the mathematical modeling of isolated n-decane droplets with the investigation of ignition delays and burning rates in both hot and cold environment. Stauch et al. [15, 16] performed detailed numerical simulation to investigate auto ignition around a single fuel droplet of n-heptane and n-heptane/octane. Ulzma and Specht [17] investigated the effectiveness of an analytical model which combines a quasi-steady and a transient

process to describe the combustion of a single droplet under microgravity.

In this paper, we focus on detailed parametrical numerical simulations of single droplets of methanol in order to identify regimes in parameter space where auto-ignition delay times of fuel-droplets is approximately equal to certain simple cases, e.g. homogeneous ignition, ignition in an inhomogeneous fuel-vapor air mixture, or the case of ignition delay being much larger than droplet evaporation time and mixing time. These results will be used in future work to infer coupled models for a simplified description of droplet ignition, which can be used, e.g., in conjunction with statistical models of spray combustion.

2. Numerical model

The detailed ignition around a single methanol droplet in quiescent air is simulated with our numerical code INSFLA. The governing unsteady conservation equations are solved in radial coordinates and time, assuming spherical symmetry and uniform pressure in space and time. The resulting partial differential equations were solved using a finite difference method. The code solves for detailed transport and kinetics in the both liquid and gaseous phase, taking into account the phase transition at the liquid/gas interface. Neumann-type boundary conditions are defined for the species and temperature at the outer boundary of the computational domain, with a gradient of zero, so that no heat or mass can be exchanged with the surroundings. A more detailed description of the code and the governing equations is available at Stauch et al. [15].

For comparison with the droplet ignition delay times, simulations of auto-ignition in homogeneous systems were additionally performed with our numerical code HOMREA. HOMREA solves time dependent species and energy conservation equations accounting for detailed chemistry. More detailed description of code and the governing equations can be obtained from [18].

A detailed chemical reaction mechanism of methanol from Chevalier [19] with 23 species and 166 elementary reactions was used to model chemistry for both droplet and homogeneous ignition.

3. Methodology

In this study, the initial droplet temperature was set to 320K. Simulations were performed on methanol fuel for a range of initial droplet radii r_0 between 25 and 100 μm , ambient air temperature T_{air} between 900 K and 1400 K and pressure p from 5 bar to 20 bar.

Droplet and homogeneous ignition simulations were performed for closed volume and hence there was no exchange of mass and energy with the surroundings. The closed volume around the droplet introduces an additional parameter called global equivalence ratio (Φ_{global}), defined as the equivalence ratio obtained after the complete vaporization of fuel and mixing of the fuel vapor into the volume.

In this study, some characteristic time scales are studied. We define the ignition delay time t_{ign} for both homogeneous and heterogeneous simulations as the time when the temperature rises by 400K over the initial ambient air temperature; the mixing time t_{mix} is the time when the spatial mean of mixture fraction (including the droplet) is less the 10 % of its maximum value. Finally, the droplet life time t_{drp} is defined as the time when the droplet has evaporated completely.

The results of the detailed simulations were used to generate libraries of ignition scenarios, which provide an account for ignition delay times, evaporation times, thermo-kinetic states and chemical source terms as a function of mixture fraction and a reaction progress variable for reactive scalars.

4. Results and Discussion

Based on the droplet ignition library, a global overview over the characteristics of droplet ignition can be obtained. In particular, the library gives an overview of important characteristic time scales associated with important governing processes, namely evaporation, mixing and auto-ignition. If the corresponding time scales are strongly separated from each other, ignition scenarios result to cases where a simplified, approximate treatment of droplet ignition becomes possible. Three particularly

interesting cases are as follows:

- $t_{\text{ign}} \gg t_{\text{mix}} > t_{\text{drp}}$. The droplet first evaporates, the fuel vapor mixes completely with air, and much later auto-ignition takes place. The auto-ignition then occurs essentially under homogeneous conditions.
- $t_{\text{mix}} > t_{\text{ign}} \gg t_{\text{drp}}$. The droplet first evaporates, and the fuel vapor/air mixture auto-ignites at some location, before the fuel is completely mixed with air. This scenario can be treated like gas-phase auto-ignition in an inhomogeneous fuel/air mixture.
- $t_{\text{mix}} > t_{\text{drp}} \gg t_{\text{ign}}$. Ignition occurs while the droplet still exists. Chemical reactions are fast compared to the physical time scales (evaporation- and mixing time scale).

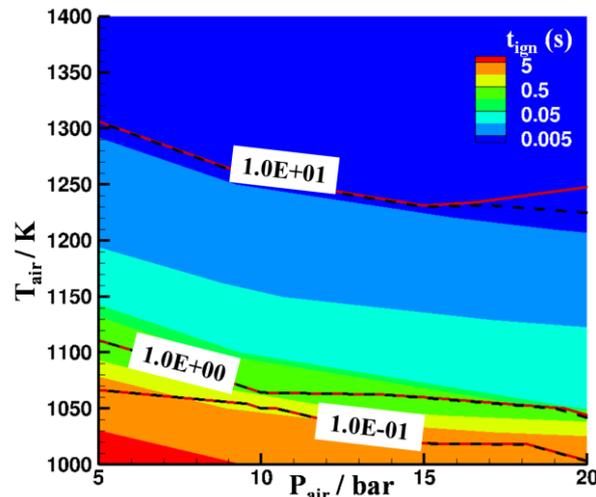


Figure 1. t_{ign} as a function of pressure and ambient air temperature for a droplet with $r_0 = 50 \mu\text{m}$ and $\Phi_{\text{global}} = 1.0$ (colored, filled contour field). Iso-lines of the ratios of mixing time and ignition delay times (red solid lines) as well as droplet lifetime and ignition delay times (black dashed lines) are also plotted. Note the overlap of the red and black curves for $t_{\text{drp}}/t_{\text{ign}} = t_{\text{mix}}/t_{\text{ign}} = 0.1$ and 1.0 .

To identify these regions in parameter space, Figure 1 shows contours of droplet ignition delay time as a function of pressure and ambient air temperature for a droplet with $r_0 = 50 \mu\text{m}$ and $\Phi_{\text{global}} = 1.0$. Only temperatures exceeding 1000 K are shown here; for larger droplets, even at lower temperatures, auto-ignition can occur. Iso-lines of the ratios $t_{\text{mix}}/t_{\text{ign}}$ (red) and $t_{\text{drp}}/t_{\text{ign}}$ (black) are also plotted to indicate regions where a simplified description of droplet ignition is applicable, e.g., region a) ($t_{\text{drp}}/t_{\text{ign}} < 0.1$), and region c) ($t_{\text{drp}}/t_{\text{ign}} > 10$). At low pressures, the iso-lines of $t_{\text{drp}}/t_{\text{ign}}$ and $t_{\text{mix}}/t_{\text{ign}}$ nearly coincide: the droplet lifetime and the mixing time are similar. The fuel evaporating from the droplet is released into the gas phase at a relatively slow rate, allowing newly released fuel to mix nearly completely. At higher pressures, the difference between droplet and mixing time increases, as is seen from the diverging red and black lines in the diagram in regions of higher pressures. This is due to the slower gas-phase transport at higher pressures. Cases where region b) ($t_{\text{mix}} \gg t_{\text{ign}} > t_{\text{drp}}$) prevails can, therefore, occur at higher pressures. The ignition delay time is only a weak function of pressure, as seen from the near-horizontal iso-lines of the t_{ign} field.

The library reveals some nonlinear effects, which lead to a non-monotonic dependence of ignition delay time on some parameters. Figure 2 shows, for instance, droplet ignition delay times as a function of reciprocal ambient air temperature, for various global equivalence ratios (color-coded, as indicated in the legend), and for different droplet sizes, at a pressure of 20 bar. For $T_{\text{air}} = 1000 \text{ K}$, at $\Phi_{\text{global}} = 1.0$ (red curves), a droplet with $r_0 = 50 \mu\text{m}$ (open circles) ignites much slower than a droplet with $r_0 = 100 \mu\text{m}$ (open square). In contrast, at $\Phi_{\text{global}} = 0.3$, the larger droplet ignites slower than the smaller droplet. At low temperature chemistry is rate limiting but chemistry depends both on the local equivalence ratio and temperature. The smaller droplet ignites slower for Φ_{global} values of 1.0 and 0.7

because it first evaporates and then ignites while the bigger droplet offers better local equivalence ratio and hence ignites before it has evaporated completely. The bigger droplet ignites slower for Φ_{global} values of 0.5 and 0.3 because they act as a bigger heat sink when compared to smaller droplets. At high temperatures ($1000\text{ K} / T < 0.9$), the ignition delay time is a function only of air temperature and droplet size, with practically no dependence on Φ_{global} ; at lower temperatures, however, there is an additional dependence on Φ_{global} .

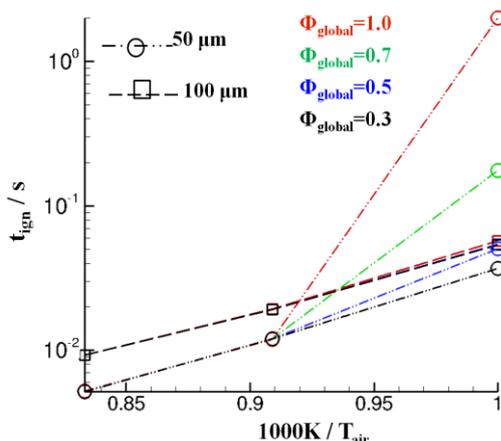


Figure 2. Ignition delay times vs. reciprocal of ambient air temperature for two droplet sizes and for different global equivalence ratios (Φ_{global}) and at a pressure of 20 bar.

The reason is that for high temperatures, the chemistry is very fast, so that the droplet has only little exchange of mass with the surroundings; the droplet, under these conditions, “sees” only its immediate neighborhood before auto-ignition occurs. The global equivalence ratio (which implicitly is a spatially averaged quantity) then cannot have a significant influence. At lower temperatures, ignition delay time is longer, and a larger volume in the droplet’s neighborhood “communicates” with the droplet via transport effects; Φ_{global} then becomes increasingly important.

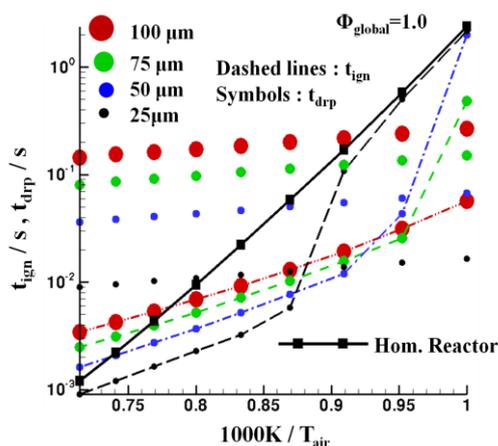


Figure 3. Ignition delay times vs. reciprocal of ambient air temperature for droplets of different size (dashed lines), and for the corresponding homogeneous reactor (solid). Isolated circles represent the droplet lifetimes. Global equivalence ratio (Φ_{global}) is 1.0 and pressure is 20bar.

Another view into the ignition library is provided by Figure 3. Ignition delay times (dashed lines with circular symbols) and droplet life times (isolated circular symbols) are shown as a function of reciprocal air temperature, for various droplet sizes (indicated by the symbol size and color), along with ignition delay times of a homogeneous reactor (black solid line with squares). For smaller droplets ($r_0 = 25\text{ mm}$) and at low air temperatures, the droplet ignition delay time is larger than t_{drp} , and

nearly equal to the homogeneous reactor ignition delay time. At higher air temperatures, t_{drp} is larger than the ignition delay time. For larger droplets, the ignition delay time is smaller than droplet life time at all temperatures. The ambient air temperature shows only a weak influence on droplet life time. For smaller droplets, the difference between the ignition time scales and t_{drp} time varies significantly and hence the ignition delay times are better represented with the corresponding delay times from a homogeneous reactor.

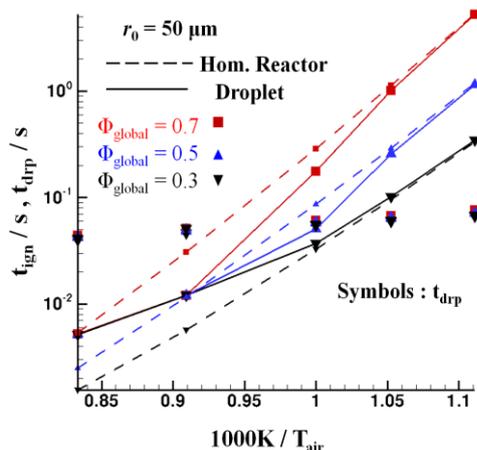


Figure 4. Ignition delay times vs. reciprocal of ambient air temperatures for droplet radius $r_0 = 50 \mu\text{m}$, and various Φ_{global} . The symbols connected by solid lines represent the droplet ignition delay times while the dashed lines represent the corresponding homogeneous ignition delay times. The isolated symbols represent the droplet life times. The ambient air pressure is 20 bar.

Figure 4 shows ignition delay times of droplet for different Φ_{global} (solid dashed lines with different colors), corresponding to homogeneous ignition delay times (solid lines with different colors) and the droplet lifetime (isolated symbols with different colors) as a function of reciprocal air temperature. At low temperature, the droplet ignition delay is much longer than the droplet life time, and also longer than the mixing time; correspondingly, the droplet ignition delay is close to the ignition delay of the corresponding homogeneous reactor. The ignition delay times of droplets and of homogeneous reactor decrease with Φ_{global} at low air temperatures. At high temperatures, there is a transition to the mode $t_{\text{ign}} \ll t_{\text{drop}}$, and the droplet ignition delay times are essentially independent of Φ_{global} . This is the same behavior as seen in Figure 2. At intermediate air temperatures, the droplet ignition delay can be smaller than in the homogeneous case, because pre-ignition chemistry can already be active before complete evaporation and mixing occurs; then, the chemical and physical processes can not be decoupled. For very high temperatures, $t_{\text{ign}}(\text{drop}) > t_{\text{ign}}(\text{hom})$, because the chemistry then is very fast, evaporation and transport become limiting.

5. Conclusion

The present parametric studies show the influence of ambient temperature, ambient pressure, initial droplet radius and global equivalence ratio on auto-ignition delay times of single fuel droplets. Based on the ratio of characteristic time scales (of droplet life time, mixing time auto-ignition delay time), parameter space regions can be identified in which a simplified treatment of the auto-ignition process is possible. These include the limits of homogeneous gas phase ignition, of ignition delay times which are small compared to the droplet lifetime and mixing time, and the case where ignition occurs after the droplet has evaporated, but before the fuel vapor has mixed completely with air.

When the time scales differs strongly, a reduced description of ignition delay becomes possible. When $t_{\text{ign}} \ll t_{\text{drp}}$, the dependence of ignition delay time on ϕ_{global} disappears. If $t_{\text{ign}} \gg t_{\text{mix}} > t_{\text{drp}}$, the ignition becomes independent on the initial droplet radius. The result shows the effectiveness of detailed simulations as a tool to develop reduced models.

The results will be useful for developing coupled computational models for the treatment of sprays, which can make use of the ignition library and the simplified, efficient models derived from it.

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