

Numerical Simulation of the Ignition of a Single Fuel Droplet in an Air with Finite Volume

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Spontaneous ignition of a single fuel droplet in a hot air with constant volume is numerically simulated with the spherical symmetry. The droplet is positioned at the center of a spherical imaginary vessel, which is closed against energy and mass transfer. The model is fully transient and with the assumption of uniform pressure. It can simulate the ignition after the droplet has completely vaporized. The employed fuel is n-heptane. The influence of the initial droplet diameter and the overall equivalence ratio on the ignition delay is examined for the initial pressure of 3 MPa and the initial ambient temperature of 773 K. When the overall equivalence ratio is fixed to be large enough, there exists no ignitable limit in terms of the initial droplet diameter, and the ignition delay takes a minimum value at a certain initial droplet diameter. When the initial droplet diameter is fixed to be so small that the ignition would not occur in an infinite volume of air, the ignition delay takes a minimum value at a certain overall equivalence ratio.

1. Introduction

The simplest model of the fuel spray ignition is the ignition of a single fuel droplet. If the droplet is placed in an air with ideally infinite volume, which is applicable to the often-conducted single droplet experiments, the droplet smaller than a certain initial diameter does not ignite because of small Damköhler number [1]. However, this is not the case for the spray ignition because the fuel vaporized from the droplet clouds would stay around the clouds. To simulate the ignition of a spray consisting of such small droplets, the single droplet ignition in a closed volume can be calculated [2, 3]. That is, the gasified fuel vaporized from the droplet stays inside an imaginary vessel, and therefore the ignition occurs even for the small droplets if the overall equivalence ratio is a proper value. This model simulates a droplet in a spray, where the gasified fuel from other droplets affects the ignition of the droplet. There is an advantage that the ignition of a mono-disperse spray is directly compared with a simple one-dimensional model though it must be noted that the spatial inhomogeneity of the interaction between the droplets in the spray is not considered because of the one-dimensionality.

In this study, the spontaneous ignition of a single fuel droplet in a closed constant volume is numerically simulated. The calculation is continued even after the droplet has completely vaporized, and the pre-vaporized ignition is also simulated. The influence of the initial droplet diameter and the overall equivalence ratio on the ignition delay is examined.

2. Model description

The model of the present study handles a fuel droplet positioned at the center of a closed spherical vessel with constant volume. The employed program is extended from that of the former works [4, 5]. The model is fully transient and based on mass-, species- and energy-conservation. Mass fraction of each species Y_i in the gas phase and temperature T in the gas and liquid phase are calculated as a function of time t and radial coordinate r . Pressure P is assumed to be spatially uniform and time-dependent. Thermal diffusion, radiant heat flux, kinetic energy term, viscosity and body force are not taken into account, and the one-dimensional calculation is done with spherical symmetry. No transfer of mass or of energy over the boundary of the vessel is allowed. The boundary conditions at the vessel boundary are as follows.

$$\frac{\partial T}{\partial r} = 0, \quad \frac{\partial Y_i}{\partial r} = 0, \quad v = 0 \quad (v: \text{mass-averaged velocity})$$

Thus the total system is closed for mass and heat transfer. Linear grid arrangement is employed in the liquid phase, and exponential in the gas phase, which is fixed at the droplet surface and at the boundary of the vessel. That is, the radial coordinate in the gas phase is given as follows.

$$r[g] = R_s \left(\frac{r_{\max}}{R_s} \right)^{gh}, \quad g = 0, 1, \dots, N_g - 1, \quad h = \frac{1}{N_g - 1}$$

g : number of grid point, N_g : total number of the grid points in the gas phase
 R_s : droplet radius, r_{\max} : radius of the vessel

When the droplet diameter becomes smaller than a certain value that is small enough to be regarded as zero, the evaporation of the droplet is stopped. That is, the droplet diameter is held to be constant, and no transfer of mass or of energy at the droplet surface is allowed. The calculation is continued only in the gas phase, and the ignition can be calculated even after the evaporation of the droplet has been completed. Thus the ignition of the small droplets whose droplet lifetime is shorter than the ignition delay can be also calculated, and the prediction of pre-vaporized and premixed ignition is possible. The ratio of the diameter of the vessel r_{\max} to the initial droplet diameter R_{s0} has a one-to-one correlation to the overall equivalence ratio ϕ at given initial pressure and temperature, which is independent of R_{s0} . That is,

$$\frac{1}{\phi} \propto \left(\frac{r_{\max}}{R_{s0}} \right)^3 - 1$$

Fuel is n-heptane, and its reduced reaction model with 64 reactions and 35 species [6] is employed. The properties of the species are calculated as temperature- and pressure-dependent. The droplet has initial temperature of 300 K. Initially the vessel is filled with quiescent air of uniform high temperature. The calculation is done with 11 and 41 grid points for the liquid and gas phase respectively. Ignition is defined as the moment when the maximum value of the temperature rise rate derived from chemical reactions among all the grid points reaches 10^7 K/s.

For the ignition of a droplet in an infinite volume of air, the parameters to control the ignition delay are ambient temperature, pressure and droplet diameter. In the present model, the overall equivalence ratio (or r_{\max}/R_{s0}) is an additional parameter. In this study, the initial pressure in the vessel and the initial temperature of the air are fixed to be 3 MPa and 773 K respectively in order to focus on the other parameters.

3. Results

3.1. Dependence of ignition delay on initial droplet diameter

The influence of the initial droplet diameter on the ignition delay is examined with r_{max}/R_{s0} fixed. Two values are chosen for r_{max}/R_{s0} . First, r_{max}/R_{s0} is fixed to be 50, with which the overall equivalence ratio is almost zero. Therefore, this case almost corresponds to the droplet in an infinite volume of air. The results are shown in Fig. 1. Droplet lifetime is also shown beside ignition delay for better understanding. However, it is not shown in the case where the ignition occurs before the droplet completely vaporizes, because the calculation is stopped at the moment of ignition. Ignition delay decreases with decreasing initial droplet diameter, and there exists an ignitable limit. It is examined with the resolution of 1 μm , and is 19 μm for this case. The diameter at which the droplet lifetime is almost equal to the ignition delay is 24 μm and slightly larger than the ignitable limit. That means, around the ignitable limit the ignition occurs slightly after the droplet completely vaporizes. The droplets smaller than the ignitable limit do not ignite because the fuel mass flux from the droplet is too fast for the ignition though the place to give proper local equivalence ratio for the ignition exists somewhere in the gas phase. After the droplet disappears, the local equivalence ratio is not large enough for the ignition.

Next, r_{max}/R_{s0} is fixed so that the overall equivalence ratio should be unity. That is, r_{max}/R_{s0} is about 9.12. The results are shown in Fig. 2. There exists no ignitable limit because the mixture in the vessel has a proper value of equivalence ratio to ignite even after the droplet has completely vaporized. The diagram shows the existence of the initial droplet diameter to give a minimum ignition delay. As the initial droplet diameter increases, longer time is needed to heat up the droplet, and it can lead to longer ignition delay. On the other hand, as the initial droplet diameter decreases, fuel and air are more mixed, and therefore the highest temperature in the vessel (at the boundary of the vessel if there is little amount of heat release by reactions) becomes lower. (Note that the initial droplet temperature is a room temperature, and the droplet behaves as heat sink. Therefore, mixing of fuel and air means a descent of pressure and temperature in the gas phase.) This can lead to longer induction time for the reactions. Because of these counteracting effects, there exists a minimum ignition

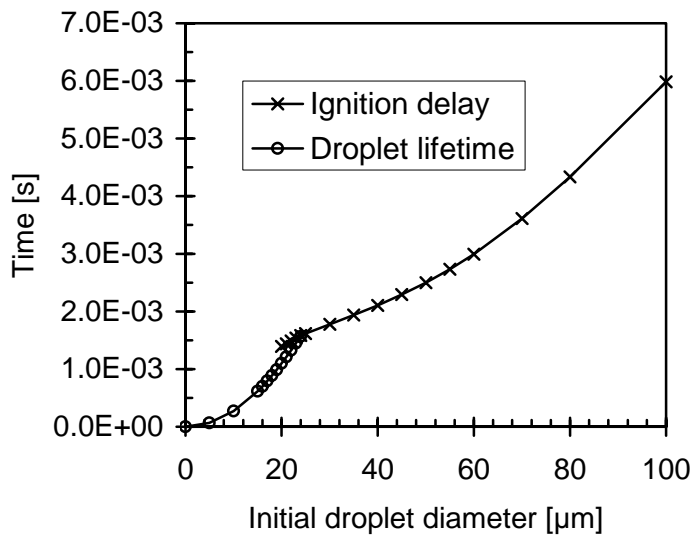


Fig. 1 Influence of initial droplet diameter on ignition delay ($\phi \approx \infty$)

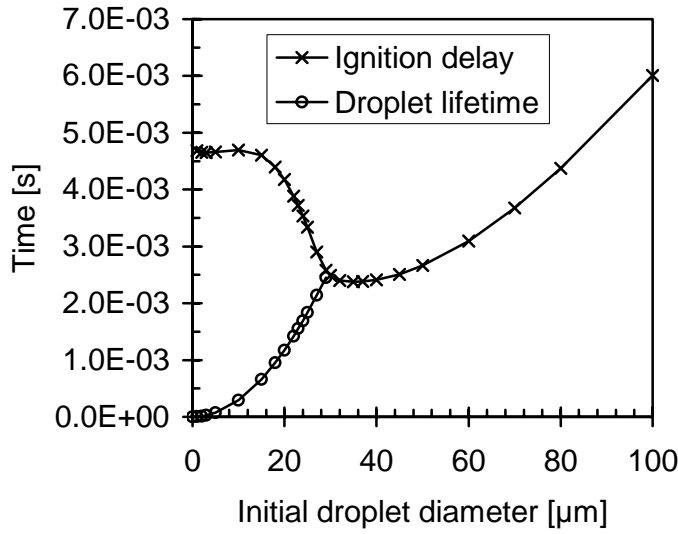


Fig. 2 Influence of initial droplet diameter on ignition delay ($\phi = 1$)

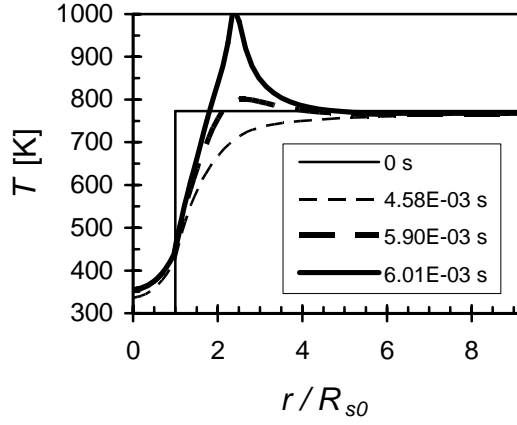
delay at a certain initial droplet diameter. The droplet diameter at which the droplet lifetime and the ignition delay are equal can be interpreted as the maximum droplet diameter to allow pre-vaporized combustion. This (29 μm) is slightly smaller than the diameter to give a minimum ignition delay (35 μm).

Three initial droplet diameters are chosen from Fig. 2, and the temporal development of temperature and fuel distribution for each diameter is shown between Fig. 3 and Fig. 5. The axis of abscissa in each diagram shows the radial position relative to the initial droplet radius. Zero denotes the center of the droplet. Unity denotes the initial position of the droplet surface. The boundary of the vessel is positioned around 9.12. Mass fraction of C and H atoms are chosen as fuel mass fraction so that the gasified fuel may be traced even after n-heptane has reacted.

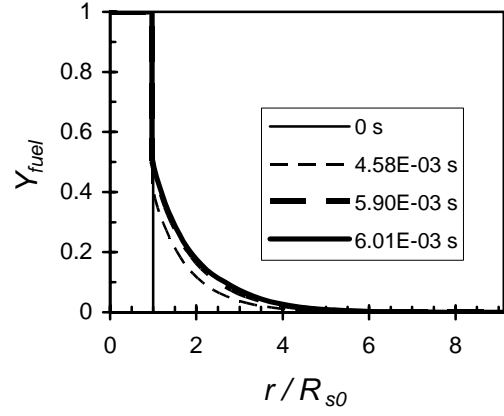
Figure 3 is for the initial droplet diameter of 100 μm . This diameter is much larger than the diameter of ignitable limit. Vaporized fuel does not reach to the boundary of the vessel even at the moment of the ignition (6.01×10^{-3} s), and the temperature there stays to be an initial value. Ignition occurs in the vicinity of the droplet, where gasified fuel exists. Droplet diameter stays almost unchanged.

Figure 4 is for the initial droplet diameter of 29 μm , at which the droplet lifetime and the ignition delay are almost equal. The ignition occurs (2.58×10^{-3} s) slightly after the droplet has completely vaporized (2.45×10^{-3} s). Vaporized fuel reaches to the boundary of the vessel, and the temperature there decreases. It is recognized that the droplet shrinks with time. Though there exists no more liquid fuel at the moment of the ignition, fuel and air are not yet uniformly mixed, and the spatial peak of temperature is observed. However, the gradient is not as steep as that seen in Fig. 3. The place of the ignition is shifted outwards to the stagnation point (the boundary of the vessel) compared with that in Fig. 3.

Figure 5 is for the initial droplet diameter of 20 μm . The evaporation of the droplet is completed (1.17×10^{-3} s) long before the ignition (4.17×10^{-3} s), and there is enough time for non-uniformity of temperature and fuel distribution to be smoothed out. At the moment of the ignition, temperature and fuel mass fraction is spatially uniform, and spatial peak of temperature is not observed. (Note that the ignition is defined for the temporal peak.) In the case like in Fig. 5 where the ignition occurs after the droplet has completely vaporized, as the initial droplet diameter decreases, the time for the evaporation becomes shorter, and the

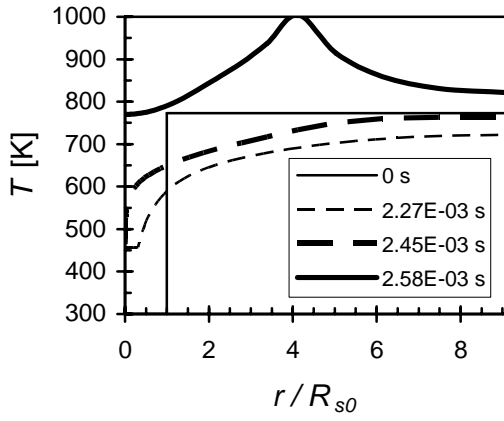


(a) Temperature

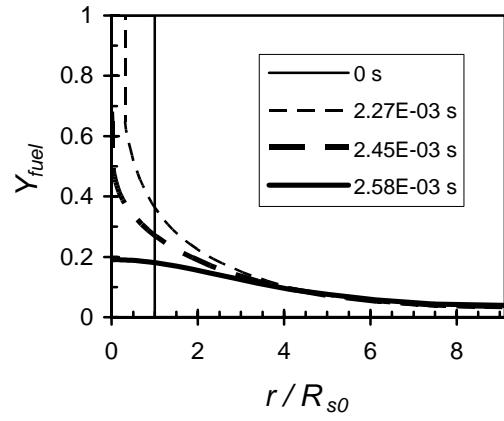


(b) Fuel mass fraction

Fig. 3 Development of distribution of temperature and fuel mass fraction ($\phi = 1$, $2R_{s0} = 100 \mu\text{m}$)

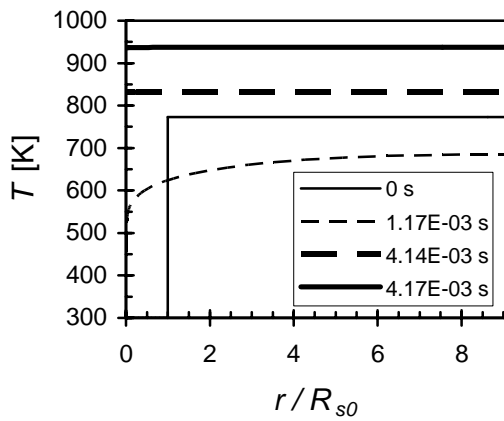


(a) Temperature

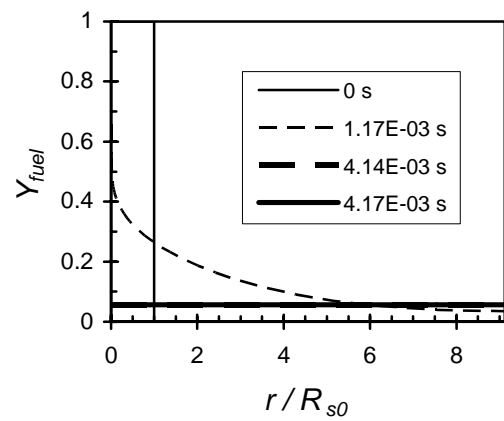


(b) Fuel mass fraction

Fig. 4 Development of distribution of temperature and fuel mass fraction ($\phi = 1$, $2R_{s0} = 29 \mu\text{m}$)



(a) Temperature



(b) Fuel mass fraction

Fig. 5 Development of distribution of temperature and fuel mass fraction ($\phi = 1$, $2R_{s0} = 20 \mu\text{m}$)

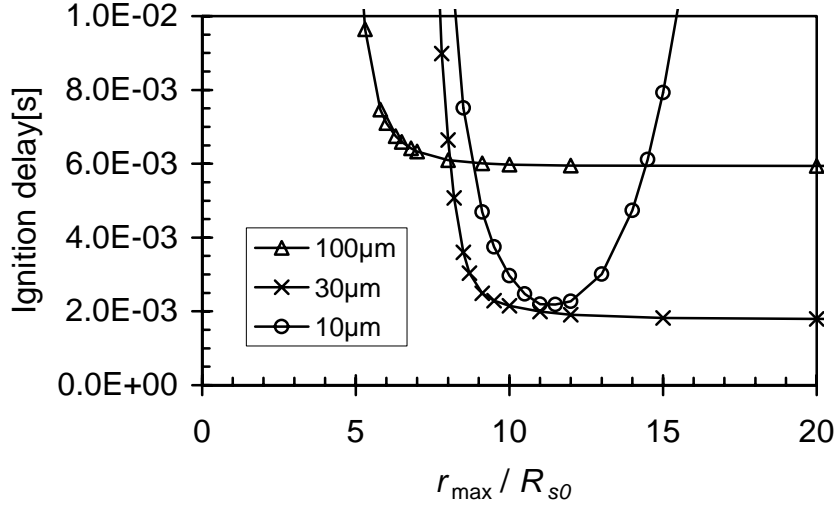


Fig. 6 Influence of r_{max}/R_{s0} on ignition delay

ignition process becomes more like that of homogeneous (zero-dimensional) ignition of premixed gas.

3.2. Dependence of ignition delay on overall equivalence ratio

The influence of r_{max}/R_{s0} (or of the overall equivalence ratio) on the ignition delay is examined for three initial droplet diameters (10, 30 and 100 μm) and shown in Fig. 6. Note that 9.12 on the axis of abscissa corresponds to unity of the overall equivalence ratio. Smaller r_{max}/R_{s0} means larger overall equivalence ratio. For all the three initial droplet diameters, it is observed that the ignition delay increases as r_{max}/R_{s0} decreases (as the total equivalence ratio increases) in the smaller r_{max}/R_{s0} range. This is because of the cooling effect by the cold droplet and the shortage of oxygen. On the other hand, the dependence of the ignition delay on r_{max}/R_{s0} is little in the larger r_{max}/R_{s0} range for 30 and 100 μm , which is not the case for 10 μm . The ignition delay increases as r_{max}/R_{s0} increases (as the total equivalence ratio decreases) for 10 μm . For such large droplets as 30 and 100 μm , the ignition can occur in the vicinity of the droplet, where the local equivalence ratio is large enough, even when the overall equivalence ratio is almost zero. Therefore r_{max}/R_{s0} has almost no influence on the ignition delay if r_{max}/R_{s0} is larger than a certain value. In the case of the 10 μm droplet, the ignition occurs after the droplet has completely vaporized for all the r_{max}/R_{s0} . Therefore the ignition delay increases as the total equivalence ratio decreases as expected for the ignition of premixed gas. Thus there exists an overall equivalence ratio to give a minimum ignition delay for the 10 μm droplet.

4. Summary

When the overall equivalence ratio is fixed to be large enough, there exists no ignitable limit in terms of the initial droplet diameter, and the ignition delay takes a minimum value at a certain initial droplet diameter. The maximum initial droplet diameter to allow pre-vaporized

combustion is slightly smaller than this diameter. Transition from the heterogeneous ignition to the homogeneous ignition with decreasing initial droplet diameter is observed.

When the initial droplet diameter is fixed to be large enough to enable the ignition in an infinite volume of air, the ignition delay increases with increasing overall equivalence ratio in the larger overall equivalence ratio range and shows little dependence on the overall equivalence ratio in the smaller overall equivalence ratio range. When the initial droplet diameter is fixed to be so small that the ignition would not occur in an infinite volume of air, the ignition delay takes a minimum value at a certain overall equivalence ratio.

The influence of pressure, ambient temperature and the volatility of the fuel on the ignition delay remain to be the themes to be studied further.

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