Verification of a Numerical Simulation Model of Fuel Droplet Ignition through Microgravity Experiments and its Further Application

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Abstract

A fully transient numerical model of spontaneous ignition of single fuel droplets was developed. A physical part of the model is one-dimensional, and therefore it can easily employ a detailed chemical reaction model, which is necessary to reproduce complicated spontaneous ignition process of hydrocarbon fuels. The model simulates an isolated droplet in an open ambient at constant pressure. It was verified through microgravity experiments for relatively large (~0.7 mm) droplets, and was successful in quantitative reproduction of ignition delays of cool and hot flames. With the verified numerical model, ignition of relatively small (< 100 μm) droplets can be numerically observed. However, an isolated droplet in an open ambient that is smaller than a certain initial diameter does not ignite unlike droplets in a spray. The model was modified to handle a droplet in a closed cell so that single droplets could be compared to sprays. Two-stage ignition behavior (cool- and hot-flame ignitions) was observed even for such fine droplets. There was transition from heterogeneous ignition to homogeneous ignition with decreasing initial droplet diameter. The effect of ambient temperature on two-stage ignition was examined in terms of ignition delays, total heat release and cool flame temperature.

1. Introduction

As a fundamental study of fuel spray ignition, fuel droplets have been studied both experimentally and theoretically [1-6]. A single fuel droplet is the simplest model of a fuel spray. Now the question is how to relate the knowledge from the droplet researches to spray ignition problems.

Numerical simulation model is nowadays a useful tool to predict physical phenomena, and the establishment of a reliable model is required also for droplet ignition. Most hydrocarbon fuels that are contained in petroleum have low-temperature reactions, which cause cool flame and are dominant for spontaneous ignition. Detailed reaction models are required to reproduce such complex ignition phenomena though they need long calculation time when they are coupled with a three-dimensional transport model. Single droplet model has an advantage that it requires relatively short calculation time and small memory because of its simplicity of the physical transport model. Droplet ignition model, which is the combination of transport model and detailed reaction model, can be verified through the comparison with experiments. Large (diameter: ~1 mm) droplets are handled in such a comparison so that both spatial and temporal resolutions are high enough. Such large droplets are largely affected by natural convection though fine droplets (diameter: <100 μm), which compose a spray in a practical use, are affected only little. Therefore the droplet ignition model does not consider gravity, and microgravity experiments are necessary for large droplets. Once a reliable numerical model for droplet ignition is established, behaviors of fine droplets, which are difficult to observe experimentally, are also predictable with it.

The single droplet model does not consider the droplet-interaction effects, since it handles a single droplet placed in an ambient gas with an infinite volume. This yields deviation from a spray. For example, a single droplet has a minimum initial droplet diameter for the ignition [1, 2], while a spray can ignite even with the smaller droplet diameters when the overall equivalence ratio of the system is large enough. This is because the characteristic time for physical transport becomes shorter compared with the characteristic time for chemical reactions as the initial droplet diameter decreases in the case of the single droplet. It is also because the gasified fuel dissipates to the faraway in the case of the single droplet. In this meaning, the overall equivalence ratio of the single droplet in an open ambient is zero. The simplest way to compare a single droplet to a spray ignition is to set a droplet in a closed cell [6]. In this case, gasified fuel vaporized from the droplet stays inside an imaginary cell, and therefore the ignition occurs even for very fine droplets if the overall equivalence ratio of the system is a proper value. This model simulates a droplet in a spray, where the gasified fuel from other droplets affects

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the ignition of the droplet, and compares the ignition of the simplest one-dimensional model directly to that of a mono-disperse spray with spatially uniform distribution. Thus, direct application of the knowledge on droplet ignition to a spray is possible.

In this study, a transient numerical simulation model for the spontaneous ignition of fuel droplets were developed and verified through the comparison with microgravity experiments with large droplets. Next, the model was further modified so that it can handle a droplet in a closed cell, and applied to individual conditions.

2. Numerical Model and Experiments

The model simulates spontaneous ignition of a cold fuel droplet placed in a quiescent hot ambient gas. Radial coordinate is employed with a spherical symmetry. The model is fully transient and based on mass-, species- and energy-conservation equations as follows:

$$\frac{\partial}{\partial t}\rho + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\rho v\right) = 0 \qquad (1)$$

$$\frac{\partial}{\partial t}\left(\rho Y_i\right) + \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\rho Y_i\left(v + V_i\right)\right] = w_i \qquad (2)$$

$$\frac{\partial}{\partial t}\left(\rho h\right) + \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\sum_i \rho Y_i h_i\left(v + V_i\right)\right]$$
$$= -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 q_T\right) \qquad (3)$$

Here, t is the time, r radial coordinate, ρ density, v mass-averaged velocity, Y mass fraction, V diffusive velocity, w mass production by reactions per unit volume and time, h specific enthalpy, q_T conductive heat flux. Subscript i denotes species i.

Pressure is assumed to be constant, and momentum conservation is neglected. Thermal diffusion, radiant heat flux, kinetic energy term, viscosity and body force are not taken into account. Only fuel exists in the liquid phase. Boundary conditions at the droplet surface are based on mass-, species- and energy-flux continuity and fugacity equilibrium. The properties of each chemical species are calculated as temperature- and pressure-dependent. A linear grid is employed in the liquid phase, and a droplet-surface-fixed exponential grid is employed in the gas phase to have a high spatial resolution near the droplet surface. At the outer boundary of the calculation field, temperature and mass factions of species are constant. The outer boundary must be far enough so that the mass-averaged velocity there should be almost zero. Spatial discretization was done with second order central difference scheme, and temporal discretization was with implicit multi-order backward differentiation method. The droplet has initial temperature of 300 K. Initially the calculation field is filled with quiescent air of uniform high temperature. Thus, mass fraction of each species Y_i in the gas phase and temperature T in the gas and liquid phases are calculated as a function of time t
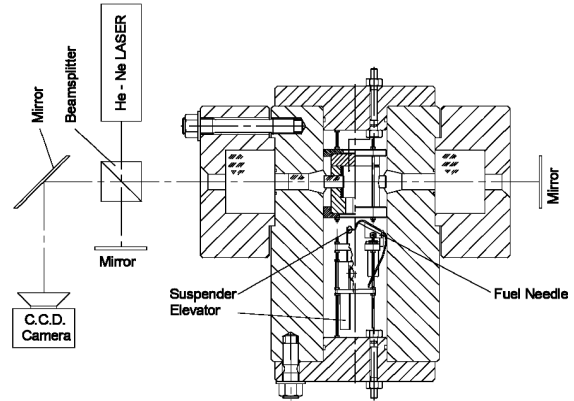

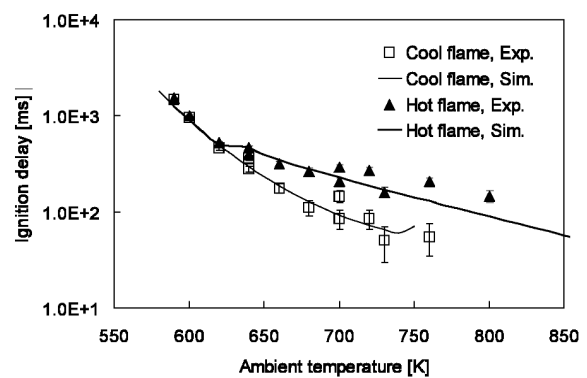
Fig. 1 Experimental apparatus

Fig. 2 Comparison between microgravity experiments and numerical simulations in ignition delays of cool and hot flames. *n*-heptane, 0.5MPa, 0.7 mm droplets.

and radial coordinate r.

Microgravity experiments were done at Drop Tower Bremen at ZARM, University of Bremen. The experimental apparatus is shown in **Fig. 1**. In a pressurized chamber, a suspended fuel droplet with a diameter of 0.7 mm generated at room temperature was suddenly brought into an electric furnace filled with high-temperature air. The inside volume of the electric furnace is 30 mm in diameter and 40 mm in height, which is large enough compared to the size of the droplet. Observation with a Michelson interferometer realized the detection of appearance of cool flame as well as that of hot flame. Thus, ignition delays of cool and hot flames were measured from the video images.

Figure 2 shows the ambient-temperature dependences of ignition delays of cool and hot flames compared between the experiments and the numerical simulations. Fuel was *n*-heptane, and pressure was 0.5 MPa. A reduced reaction model with 437 reactions and 92 species for *n*-heptane [5] was employed for numerical simulations. The numerical simulations reproduce the two-stage ignition behaviors quantitatively well. Two ignition delays were compared between the experiments and the numerical simulations even at 0.3, 1.0 and 2.0
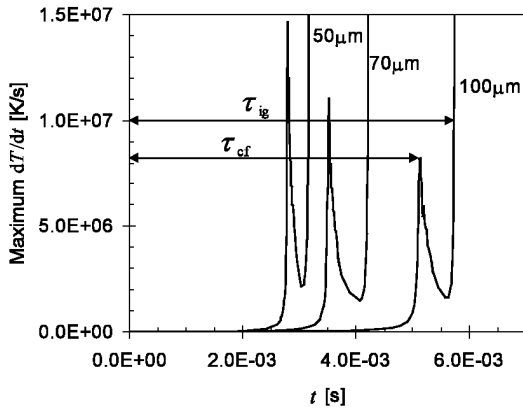
Fig. 3 Histories of maximum temperature rise rate for several initial droplet diameters. *n*-heptane, 3.0MPa, 773K, Overall equivalence ratio was unity.
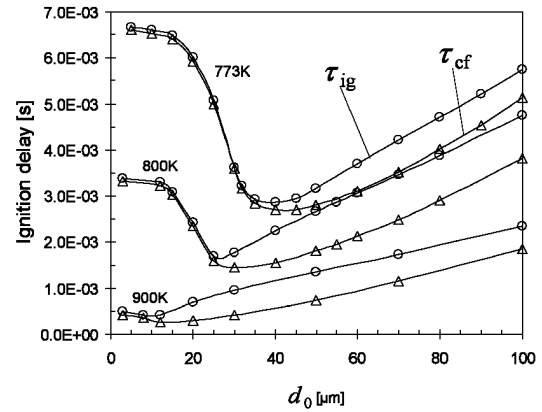
Fig. 4 Ignition delays of cool and hot flames against initial droplet diameters for several initial ambient temperatures. *n*-heptane, 3.0MPa,Overall equivalence ratio was unity.

MPa, and the reasonable reliability of the numerical model was confirmed.

3. Further Application of the Numerical Model

The numerical model was modified so that it can handle a droplet in a closed constant-volume cell. The outer boundary of the calculation field is closed against mass and heat transfer, and its location is arbitrary adjustable for each ignition. Pressure is assumed to be spatially uniform and time-dependent, and momentum conservation is neglected again. Now the energy-conservation equation should contain a pressure term as follows:

$$\frac{\partial}{\partial t}(\rho h) - \frac{\partial P}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 \sum_i \rho Y_i h_i (v + V_i)\right] \quad (4)$$

$$= -\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 q_T\right]$$

Here, P is the pressure. The boundary conditions at the cell boundary are as follows:

$$\frac{\partial T}{\partial r} = 0, \quad \frac{\partial Y_i}{\partial r} = 0, \quad v = 0 \quad (5)$$

With the model, two-stage ignition behaviors were observed even for fine (diameter: <100 μm) droplets as shown in **Fig. 3**. Initial conditions of the ambient gas were 0.3 MPa and 773 K, and overall equivalence ratio ϕ, which is an equivalence ratio in a closed cell after the complete vaporization of the droplet without reactions, was unity. The definitions of ignition delays of cool and hot flames, τ_{cf} and τ_{ig}, are also shown in Fig. 3. Cool flame ignition is defined as the moment when the maximum value of the temperature rise rate caused by chemical reactions among all the grid points takes a temporal maximal value. Hot flame 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 after cool flame ignition, which is a typical value corresponding to a rapid temperature increase.

When the initial droplet diameter d_0 is relatively small, ignition delay could be longer than droplet lifetime. In such a case, ignition takes place as premixed gas ignition. In order to reproduce such cases, the model was further modified. When the droplet diameter becomes smaller than a certain value that is small enough to be regarded as zero, the droplet diameter is held to be constant, and the same boundary conditions as those at the outer boundary are applied at the droplet surface.

Figure 4 shows τ_{cf} and τ_{ig} against d_0 for several initial ambient temperatures. Initial pressure was 3.0 MPa, and ϕ was unity. For all initial ambient temperatures, no ignition limit was observed either for cool flame or for hot flame. Both ignition delays take a minimum value at a certain initial droplet diameter. This is because of two counteracting effects. Smaller droplets need shorter heat-up period, which leads to shorter ignition delay in terms of droplet heating, while they cool down the hot air around them faster through their fast evaporation caused by larger surface-volume ratio. Note that the droplet is initially at room temperature. The latter effect leads to longer induction time in terms of chemical reactions. Though droplet lifetime is not shown in Fig. 4, it increases with increasing d_0 and intersects τ_{ig} around d_0 at which τ_{ig} takes a minimum value for all initial ambient temperatures. That is, droplets initially smaller than this d_0 ignite after the droplet has completely vaporized. Thus, as d_0 decreases, there occurs the transition from heterogeneous ignition (droplet / spray ignition) to homogeneous ignition (premixed gas ignition). As d_0 decreases, τ_{cf} and τ_{ig} increase because of the reason mentioned before. This tendency becomes smaller as the initial ambient temperature increases. This is because the cooling effect of the droplet becomes smaller as initial ambient temperature increases.

In order to examine the two-stage ignition behavior quantitatively, accumulative heat release integrated with time and space at the moment of cool
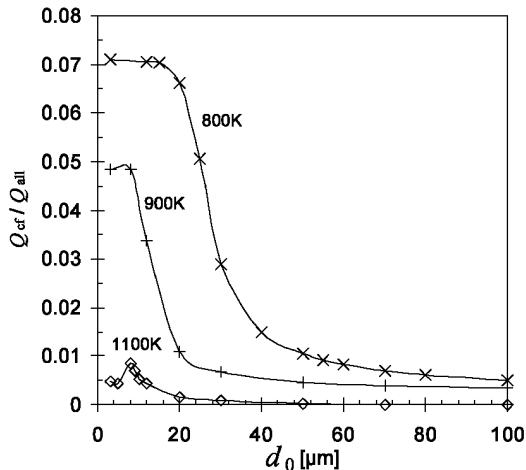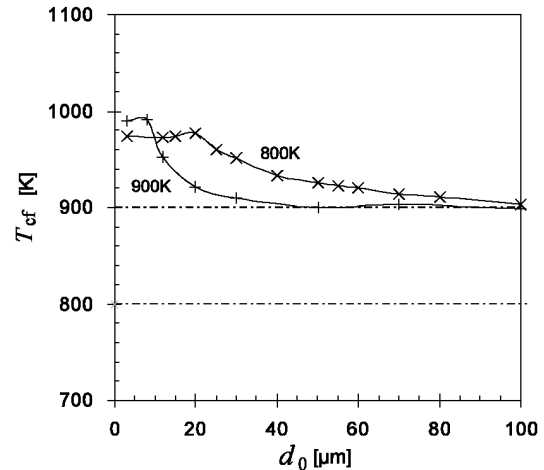
Fig. 5 Accumulative heat release at the moment of cool flame ignition divided by the potential heat release of the droplet for several initial ambient temperatures. *n*-heptane, 3.0MPa, Overall equivalence ratio was unity.

Fig. 6 Cool flame temperatures for several initial ambient temperatures. *n*-heptane, 3.0MPa,Overall equivalence ratio was unity.

flame ignition Q_{cf} was calculated and is shown in **Fig. 5**. Here Q_{cf} is divided by the potential heat release of the droplet Q_{all} and normalized. As d_0 decreases, Q_{cf}/Q_{all} increases. This is because of the transition from heterogeneous ignition to homogeneous ignition. When d_0 is relatively large, heat of reaction is released only locally, i.e., only in the relatively narrow reaction zone where fuel and oxidizer meet. In such a case, the contribution of cool flame to accumulative heat release is not large though cool flame plays a great role to induce hot flame ignition. When d_0 is relatively small, ignition occurs after fuel and oxidizer are well mixed, and heat of reaction is released uniformly inside the cell. As initial ambient temperature increases, Q_{cf}/Q_{all} decreases. This is supposed to be because of the characteristics of low-temperature reactions to induce cool flame ignition, which are suppressed with higher temperature [7].

Cool flame temperature T_{cf} for several initial ambient temperatures is shown in **Fig. 6** with the straight lines to indicate each initial ambient temperature. Here, T_{cf} is defined as the maximum gas-phase temperature when the temperature rise rate there caused by chemical reactions takes a temporal minimal value after cool flame ignition. The effect of cool flame on hot flame ignition in terms of T_{cf} is larger for lower initial ambient temperature and smaller d_0, since higher T_{cf} should lead to shorter induction time of hot flame after cool flame ignition.

4. Conclusions

Transient numerical model to predict spontaneous ignition of single fuel droplets was developed and verified through the comparison with microgravity experiments. Next, the model was modified to simulate a droplet in a closed cell so that it can be compared to a spray. Two-stage ignition

was numerically observed even for fine droplets. Low-temperature reactions are dominant even in the conditions of a spray in a practical use. Two-stage ignition behavior was examined for several initial ambient temperatures in the case where ϕ was unity. Both ignition delays of cool and hot flames took a minimum value at a certain d_0. There was transition from heterogeneous ignition to homogeneous ignition with decreasing d_0. Cooling effect of the droplet becomes smaller as initial ambient temperature increases. Accumulative heat release at the moment of cool flame ignition and cool flame temperature were larger and higher, respectively, for lower initial ambient temperature and for smaller d_0.

References
1) Saitoh, T., Ishiguro, S. and Niioka, T., *Combust. Flame*, **48**, 27-32, 1982.
2) Tsukamoto, T., Okada, H. and Niioka, T., *Trans. Japan Soc. Aero. Space Sci.*, **35** (110), 165-176, 1993.
3) Bergeron, C. A. and Hallett, W. L. H., *Combust. Sci. Technol.*, **65**, 181-194, 1989.
4) Tanabe, M., Bolik, T., Eigenbrod, C., Rath, H. J., Sato, J. and Kono, M., *Proc. Combust. Inst.*, **26**, 1637-1643, 1996.
5) Schnaubelt, S.,Moriue, O., Eigenbrod, C. and Rath,H. J., *Proc. Combust. Inst.*, **28**, 953-960, 2000.
6) Moriue, O., Mikami, M., Kojima, N. and Eigenbrod, C., *Proc. Combust. Inst.*, **30**, 1973-1980, 2005.
7) Compton, R. G., Hancock, G. and Pilling, M. J., "Comprehensive Chemical Kinetics - Low-Temperature Combustion and Autoignition", Elsevier Science B. V., 1997.