The Droplet Ignition in High Pressure Condition with Natural Convection

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Introduction

For some of combustion devices such as liquid-propellant rocket motors, gas turbines and diesel engines, the liquid fuel sprays burn in the high pressure and temperature condition. Therefore, in order to understand the fundamental phenomena involved therein, the research on the combustion of single droplet in the high-pressure environment must be preceded.

A simulation of the droplet combustion in the high-pressure environment often requires including real gas effects on the equation of state and thermo-physical properties that are usually neglected in normal pressure conditions [1]. Based on these facts, many researchers have studied high-pressure droplet combustion as well as vaporization [1-4]. These studies discussed on the high-pressure droplet combustion characteristics focusing their attentions on its vaporization or burning rate. However, there are few studies on the ignition delay times of droplets in high-pressure conditions. Especially, the research on the natural convection effects on the ignition delay time, while considering various high-pressure effects, has not been available yet. The natural convection effect would become important as the ambient pressure rises, since the density of the gas increases. Therefore, to describe the real situation of the normal gravity experiments about high-pressure droplet combustion, the natural convection effects must be considered.

Based on these facts, the objectives of this paper are to investigate the effects of high temperature and pressure on the ignition delay time for a n-heptane droplet, both for normal gravity and microgravity condition, while considering natural convection effects, and to make a bench mark through the comparison with other experimental results.

Formulation

In order to elucidate this transient droplet ignition phenomenon in high pressure condition, the following assumptions are employed: 1) the system is one-dimensional. 2) the droplet shape remains spherical. 3) the ambient pressure is uniform. 4) the radiation effect is negligible. 5) the internal circulation inside the droplet is neglected. Though the gravity effect is not included in the basic governing equations, the natural convection effects are taken into consideration through the time scale correction.

When a liquid fuel droplet is introduced into the quiescent hot air environment, a system of governing equations describing the single droplet ignition in high pressure condition can be constructed as below.

For the gas phase , $r{\geq}R(t)$

Energy equation

$$\rho C_{P} r^{2} \left(\frac{\partial T}{\partial t} + u_{r} \frac{\partial T}{\partial r} \right) = \frac{\partial}{\partial r} \left(k r^{2} \frac{\partial T}{\partial r} \right) + \sum_{i} \rho r^{2} D_{im} C_{Pi} \frac{\partial Y_{i}}{\partial r} \frac{\partial T}{\partial r} + W_{f} \dot{\omega} Q r^{2}$$
(1)

Species equation

$$\rho r^2 \left(\frac{\partial Y_i}{\partial t} + u_r \frac{\partial Y_i}{\partial r} \right) = \frac{\partial}{\partial r} \left(\rho D_{im} r^2 \frac{\partial Y_i}{\partial r} \right) - (v' - v'') W_i \dot{\omega} r^2$$
⁽²⁾

Continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial \rho u r^2}{\partial r} = 0$$
(3)

For the liquid phase analysis ($r \le R(t)$), energy equation and species equation are solved, which neglect the bulk velocity in the liquid field. Since the governing equations are divided into gas and liquid phases, the matching conditions such for energy as well as mass balance at the droplet surface are solved [4]. Thus, the reduction rate of the droplet radius can be determined using the vaporizing mass flux and the density change [4]. The composition of fuel and air at the droplet surface can be determined by the following vapor-liquid equilibrium condition for fugacity

$$f_{i}^{g}(x_{i}^{g}) = f_{i}^{l}(x_{i}^{l})$$
(4)

The fugacity can be related to the Helmholtz free energy and the chemical potential [5]. For the calculation of the fugacity and density Redlich-kwong equation of state is used [5].

In order to calculate the reaction rate, the single-step global reaction model is employed. Model constants of the reaction model are taken from the data used by the Bergeron and Hallet [6].

For considering natural convection effects, it is assumed that the heat required for ignition is approximately equal for the normal gravity and microgravity case.

$$Q_{ig} = \int_0^{t_a} \pi D^2 h(T_a - T_s) dt \cong \pi \overline{D}^2 h(T_a - \overline{T}_s) \times t_{ig}$$
⁽⁵⁾

$$Q_{ig0} = \int_{0}^{t_{ig0}} \pi D^2 h_0 (T_a - T_s) dt \cong \pi \overline{D}^2 h_0 (T_a - \overline{T}_s) \times t_{ig0}$$
(6)

From equating Eq. (6) and Eq. (7), we get

$$t_{ig} = (h_0 / h)t_{ig0} = (Nu_0 / Nu)t_{ig0}$$
⁽⁷⁾

The Nusselt number of a sphere in the natural convection field can be expressed as [7]

$$Nu = 2.0 + 0.6Gr^{1/4} \operatorname{Pr}^{1/3}$$
(8)

This relation was used by Curtis and Farrell [8] and Sato et al. [9] whose results showed a good agreement with the experimental results for high-pressure droplet vaporization and combustion.

Since under the microgravity field the Grashof number, Gr is zero, Eq. (7) is rendered as

$$t_{ig} = 2t_{ig0} / (2.0 + 0.6Gr^{1/4} \operatorname{Pr}^{1/3})$$
(9)

where $Gr = (g\rho^2 d^3 / \mu^2)(T_a - T_s) / T_a$.

Since *Gr* is strongly dependent on the ambient pressure, the natural convection effects would become more severe as the pressure is increased.

Results and discussion

In the below the ignition delay times for n-heptane droplet are discussed under various conditions. The results are calculated for initial droplet temperature, T_{θ} =300K.

Figure 1 shows the unsteady variation of gas phase temperature for D_0 =1.8*mm*, T_a =1000*K*, and *P*=11*atm*. Before an onset of ignition, the gas temperature at the vicinity of the droplet is seen to decrease, due to heat loss from ambient gas to the droplet. However, as time passes, the vaporized fuel is mixed with oxidizer so that the reaction rate progressively increases. At *t*=70 *msec*, it is observed that the gas temperature at r=3R exceeds the initial ambient temperature T_a . Since an increase in gas temperature



Figure 1 Temporal variation of gas temperature along radial direction



Figure 2 Variation of ignition delay time against the inverse of ambient temperature for various ambient pressures without gravity

causes the reaction rate to increase, finally the ignition takes place. In this study, the ignition delay time is defined as the time required for the peak gas-phase temperature to exceed its ambient temperature by 100*K*.

Figure 2 represents a variation of the ignition delay time with different ambient temperature for various pressure conditions without gravity. As seen in the figure, the logarithmic ignition delay time linearly decreases with an increase in the ambient temperature, and the line slopes are almost the same for all ambient pressures. Since their equivalent activation energies are proportional to the slope of each curve, it is concluded in this study that the ambient pressure does not affect the overall activation energy. This fact is also validated by the experiments of Kadota et al. [10] who indicated that the decreasing slope of the logarithmic ignition delay time doesn't change with the ambient pressure. Thus, as the ambient pressure increases, the ignition delay time gets shorter. And, this reduction rate of the ignition delay time with pressure becomes smaller at a higher pressure. These phenomena can be explained as follows. As Jia and Gogos [4] pointed out, the heat of vaporization as well as the mass diffusivity decreases with an increase in ambient pressure. Whereas a decrease in heat of vaporization causes the vaporization rate to increase, a decrease in mass diffusivity tends to decrease the vaporization rate. Therefore, a competition between

these two counter-balancing effects finally determines the droplet vaporization rates. Since the vaporization rate is an important factor for ignition, it is considered that the effect of pressure on the reduction in heat of vaporization decreases the ignition delay time, while its effect on the reduction in mass diffusivity increases.

However, in high-pressure condition, the natural convection effect plays a more important role since the density is higher so that its effect is to be discussed in the below.

In Figure 3, the ignition delays for the case with natural convection effects are presented and compared with experimental results by Kadota et al. [10] as well as those for the case without natural convection. For the case of 1atm, the present numerical results with natural convection are in



Figure 3 Effects of natural convection on ignition delay time



Figure 4 Variation of the Nusselt number with ambient pressure for various ambient temperature under normal gravity condition



Figure 5 Variation of ignition delay time against the inverse of ambient temperature for various ambient pressures with natural convection effect

good agreement with experimental ones, while the case without natural convection yields a little longer ignition delays. For the case of 31*atm*, however, the results without natural convection effects show a severe deviation from experiments, while the results with natural convection show a good agreement. Thereby, the natural convection is considered more important in high pressure condition.

Figure 4 shows a variation of the Nusselt number with the ambient pressure. From Eq. (8), the Nusselt number becomes 2 for the case without gravity. When the gravity is taken into account, the Nusselt number increases with the ambient pressure from the minimal value at P=1atm as seen in the figure. Therefore, the ignition delays become shorter due to an enhanced heat transfer by natural convection as the ambient pressure increases, which concludes that the natural convection effects may not be neglected in this ignition study. In Figure 5 additional calculations for other pressure conditions are presented and compared with the experimental results. It shows a good agreement so that the approach used here to examine the natural convection effects is validated.

Conclusions

In this study the ignition delay times of a n-heptane droplet in high-pressure conditions were investigated. Especially, the natural convection effects on the ignition delay time were considered and discussed by comparison with no-gravity case. As in the results, the natural convection effect becomes important as the ambient pressure rises due to higher gas density.

The summary of the results is as follows:

(1) The logarithmic ignition delay time linearly increases with the inverse of the ambient temperature, and its increasing slope is independent of the ambient pressure. Therefore, the overall activation energy is not influenced by the pressure variation.

(2) As the pressure increases, the ignition delay time becomes shorter because the droplet vaporization rate is found to increase. But, the reduction rate of the ignition delay time with pressure is getting smaller as the pressure increases.

(3) The natural convection effect is observed to reduce the ignition delay time due to the enhanced heat feedback to the droplet.

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References

- [1] S. D. Givler and J. Abraham, Supercritical Droplet Vaporization and Combustion Studies, *Progress in Energy and Combustion Science*, 22(1): 1-28, 1996
- [2] K. C. Hsieh, J. S. Shuen and V. Yang, Droplet Vaporization in High-Pressure Environments I: Near Critical Conditions, *Combustion Science and Technology*, 76: 111-132, 1991
- [3] J. S. Shuen, V. Yang and C. C. Hsiao, Combustion of Liquid-Fuel Droplets in supercritical Conditions, *Combustion and Flame*, 89: 299-319, 1992
- [4] H. Jia and G. Gogos, High Pressure Droplet Vaporization; Effects of Liquid-phase Gas Solubility, International Journal of Heat and Mass Transfer, 36(18): 4419-4431, 1993
- [5] R. C. Reid, J. M. Prausnitz and B. E. Polling, the Properties of Gases and Liquids (4th Edn). McGraw-Hill, New York, 1987
- [6] C. A. Bergeron and W. L. H. Hallet, Ignition Characteristics of Liquid Hydrocarbon Fuels as Single Droplets, *The Canadian Journal of Chemical Engineering*, 67: 142-149, 1989
- [7] W. E. Ranz and W. R. Marshall, Evaporation From Drops, Chemical Engineering Progress, 48(3): 141-146, 1952
- [8] E. W. Curtis and P. V. Farrell, A Numerical Study of High-Pressure Droplet Vaporization, *Combustion and Flame*, 90: 85-102, 1992
- [9] J. Sato, M. Tsue, M. Niwa and M. Kono, Effects of Natural Convection on High-Pressure Droplet Combustion, *Combustion and Flame*, 82: 142-150, 1990
- [10] T. Kadota, H. Hiroyasu and H. Oya, Spontaneous Ignition Delay of a Fuel Droplet in High Pressure and High Temperature Gaseous Environments, *Bulletin of the JSME*, 19(130): 437-445, 1976