

Weak flame responses to octane number and pressure in a micro flow reactor with a controlled temperature profile

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1 Introduction

It is urgently required to develop technologies to control internal combustion devices more efficiently in terms of energy savings. As an example of internal combustion engines with higher efficiency and low emission, Homogeneous Charge Compression Ignition (HCCI) engine should be mentioned. However, HCCI engine has a limited operating range because of the difficulty of controlling the ignition, indicating that understandings of the ignition process of fuel play an important role in the development of HCCI engine technology.

This study focused on ignition characteristics of a blended fuel of n-heptane and iso-octane. The blended fuel of n-heptane and iso-octane is used as the simplest Primary Reference Fuel (PRF), which represents the combustion characteristics of gasoline. In addition, the mixing ratio of n-heptane and iso-octane corresponds to Research Octane Number (RON), which is an index of anti-knock ability. Ignition process of PRF/air has been investigated mainly by using rapid compression machines (RCMs). Time-histories of pressure and species in the RCM chamber are measured. Reaction kinetics models are validated by comparing the predicted ignition delay times and concentration time-histories of reactants, intermediates, and products with the experimental results. As a weak point of RCMs, however, difficulty of accurate tracking of the gas-phase temperature time-history in the chamber should be mentioned. This is caused by heat loss through the wall during auto-ignition and temperature non-uniformity in the combustion chamber due to the roll-up vortices.

Therefore, a well-defined, simple experimental system for investigation of the ignition process is required. For that reason, this study focused on a micro flow reactor with a controlled temperature profile [1] as an alternative experimental method.

In the micro flow reactor, a quartz glass tube with an inner diameter smaller than the ordinary quenching diameter is heated by an external heat source so as to have a stationary temperature profile along the inner surface of the tube in the axial direction. A fuel/air mixture flows into the tube, and

then a flame is formed. Due to the small inner diameter, the temperature of the gas phase in the tube strongly depends on the temperature of the inside surface of the tube. Flow in the tube is laminar and pressure in the tube is constant.

In a previous study using this micro flow reactor, Tsuboi et al. found that there is a lower inlet flow velocity limit of methane/air weak flame and wall temperature at the flame position corresponds to the minimum ignition temperature of the fuel [2]. Oshibe et al. observed weak flames of DME/air in the micro flow reactor and found stabilized multi-stage oxidation including low temperature oxidation [3]. Yamamoto et al. have conducted an investigation on the multi-stage oxidation process of n-heptane which consists of cool, blue, and hot flames [4]. These studies indicated that the weak flame phenomena in the micro flow reactor correspond to multi-stage ignition phenomena of given fuels. Thus, application of PRF as a fuel to the micro flow reactor to examine the capability of the reactor for the clarification of ignition characteristics of practical fuels is also considered to be valuable.

In this study, the weak flame responses to the various RONs and the pressures were investigated. In addition, one-dimensional computations were conducted using a detailed reaction mechanism [5] of PRF. Obtained computational results were compared with experimental results.

2 Experimental / Computational method

2.1 Experimental method

In this study, a quartz glass tube was heated by a H_2 /air premixed burner so as to have a stationary temperature profile (300-1300 K). H_2 /air burner was chosen as an external heat source for better visualization of chemiluminescence from hydrocarbon flames in the micro flow reactor. For experiments under the atmospheric pressure, a quartz glass tube with an inner diameter of 2 mm was employed. A gaseous premixture of PRF/air was produced by injecting liquid PRF with a micro-syringe (Hamilton: 1700 series) into heated air. The flow rate of air was controlled by a mass flow controller and the injection volume of liquid PRF was controlled by a mechanical stage with a stepping motor to maintain the equivalence ratio as unity.

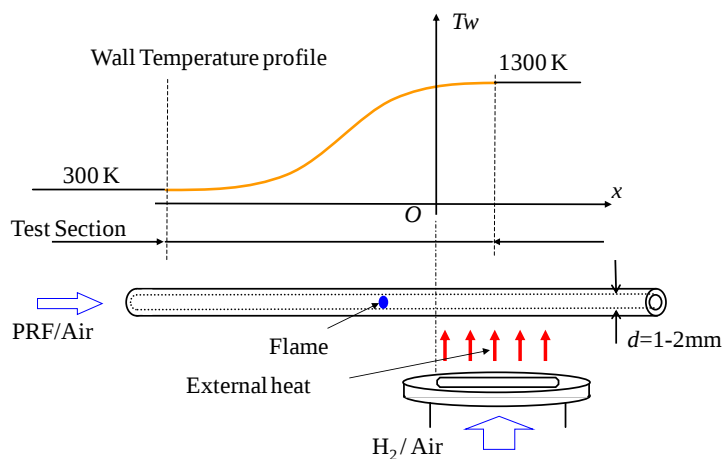


Figure 1. Experimental setup.

In the high pressure experiments, a quartz glass tube with an inner diameter of 1 mm was used. In addition, different mixture supplying method was employed. A gaseous PRF/ N_2 mixture was stored in a tank at 6 atm and 373 K in advance. A gaseous premixture of PRF/air was then produced by mixing PRF/ N_2 and O_2 . Flow rates of the PRF/ N_2 mixture and O_2 were controlled by each mass flow controller and a stoichiometric gaseous PRF/ N_2 / O_2 mixture was fed into the tube. The ratio of N_2 to O_2 was the same as that of air. Pressure in the tube was controlled by a pressure regulator installed downstream of the flow reactor, and it was changed from 1 to 5 atm in this study.

A gaseous PRF/air mixture coming into the quartz tube ignites at the high temperature region and flame is formed at a certain position. Images of this flame were captured with a digital still camera.

The cameras were equipped with optical band-pass filters (transparent wavelength: 431.4 nm, half bandwidth: 6.4nm) for better observation of chemiluminescence from hydrocarbon flames by filtering thermal radiation from the heated tube. Flame location was defined at the peak of the luminosity distribution which was obtained from the captured flame image. The upstream side edge of the H₂/air burner was defined as $x=0$.

After capturing the flame images, wall temperature measurement was conducted under atmospheric pressure with a K-type thermocouple (diameter of 50 μm) inserted from the exit of the tube. Changes of the wall temperature profile due to the pressure increase were confirmed to be negligible because the heat capacity of the tube wall is much larger than the increased heat capacity of the gas phase even under the elevated pressure.

2.2 Computational method

To further examine the experimental results, one-dimensional steady computations were conducted with a code based on PREMIX [6] and the heat convection term between the gas phase and the wall was added to the energy equation [1] as follows.

$$\dot{M} \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \left(\lambda A \frac{dT}{dx} \right) + \frac{A}{c_p} \sum_{k=1}^K \rho Y_k V_k c_{p,k} \frac{dT}{dx} + \frac{A}{c_p} \sum_{k=1}^K \dot{\omega}_k h_k W_k - \frac{A}{c_p} \frac{4\lambda Nu}{d^2} (T_w - T_g) = 0$$

This code models a reactive flow in the micro flow reactor. In the heat convection term, the wall temperature profile from 300 to 1300 K, which is the same as the experimental condition, was given as T_w .

As the reaction scheme, the detailed reaction mechanism of PRF developed by Curran et al. (1034 species, 4236 reactions) [5] was selected. Flame location was defined as the peak of heat release rate (HRR) profile.

3 Results and discussion

3.1 Weak flames response to RONs under the atmospheric pressure

Flame responses to the inlet flow velocity were investigated using PRF100 (iso-octane 100%)/air mixture under atmospheric pressure. Stable flat flame (Normal flame) was observed in a high flow velocity region ($U > 50$ cm/sec). Unstable flames called *flames with repetitive extinction and ignition* (FREI) [1] were observed in an intermediate flow velocity region ($U = 8$ -50 cm/s). Stable flames with weak luminescence (Weak flames) were observed in a lower flow velocity region ($U < 8$ cm/sec). This tendency, that is, the existence of three kinds of flame response observed by changing the inlet flow velocity, agrees with the previous experimental results and theoretical analysis by Minaev et al. [7].

In the weak flames regime, two luminous zones were observed in the flow direction. These luminous zones are thought to be separated hot flames, which have already been realized in a previous study on weak flames of DME/air [3] and n-heptane/air [4]. Observation of weak flames is expected to be efficient for investigation of the ignition process of the fuel in each temperature region. Thus, special attention will be paid to the low flow velocity region from this section.

First, the responses of weak flames to fuels with various RONs under atmospheric pressure were examined. The inlet flow velocity was set to be 1.2 cm/sec, and PRF0 (n-heptane 100%), 20, 50, 100 were used. Figure 2 (Left) shows the images of weak flames with various RONs.

In the case of PRF0 (n-heptane 100%), two luminous zones in the downstream side (high temperature region) and an additional weak luminous zone in the low temperature region were observed. This three-stage oxidation process of n-heptane was previously observed by Yamamoto et al. [4]. According to their study, the weak luminous zone in the low temperature region is confirmed to be cool flame, and two luminous zones in high temperature region are separated hot flames. Very weak luminosity of the cool flame was observed in the case of PRF20, but cool flame was not recognized in the case of PRF50 and PRF100. These findings show that luminosity of cool flame decreases as RON increases. In addition, the second hot flame position shifted to the high temperature region as RON increased.

1-D computation was conducted to investigate the weak flames response to various RONs. Figure 2 (Right) shows the computational HRR profiles of PRF0, 20, 50, and 100, and the given wall temperature profile. Flow velocity was set to be 1.2 cm/sec and equivalence ratio was unity as the same as experiment.

In the case of PRF0, three peaks of the HRR profile were confirmed at $x = 4.25, 4.98$ and 5.33 cm. By conducting the gas sampling analysis [4], it has already been confirmed that these three reactions correspond to the three luminous zones observed in the case of PRF0/air in Fig. 2 (Left). On the other hand, the peak value of cool flame decreases as RON increases, and the peak of cool flame in the case of PRF100 was not confirmed. In addition, the second hot flame position shifts to the high temperature region as RON increases. These tendencies well agree with the experimental result shown in Fig. 2 (Left).

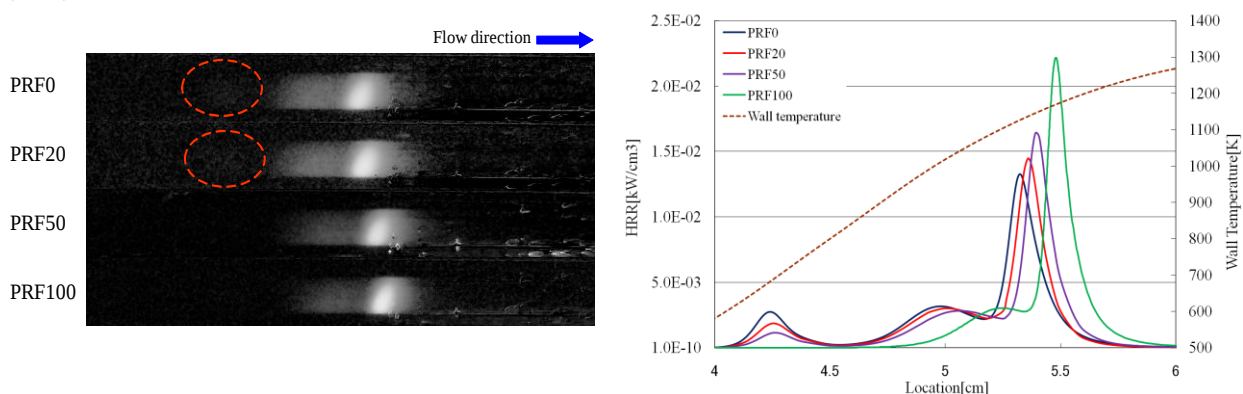


Figure 2. Weak flame response to RONs. Left: Experimentally obtained weak flame images ($U=1.2$ cm/sec). Right: Computational heat release rate profiles and given wall temperature profile.

3.2 Weak flames response to RONs under elevated pressures

Weak flames of PRF0, PRF50, and PRF100 under elevated pressures were investigated to examine the pressure dependence of their ignition characteristics. Pressure range was from 1 to 5 atm. Figure 3 shows the experimentally observed images of weak flames for PRF0/air (Left) and PRF100/air (Right) under atmospheric and elevated pressures ($P=1$ -5 atm). The flow velocity was set to be constant ($U=2.0$ cm/sec).

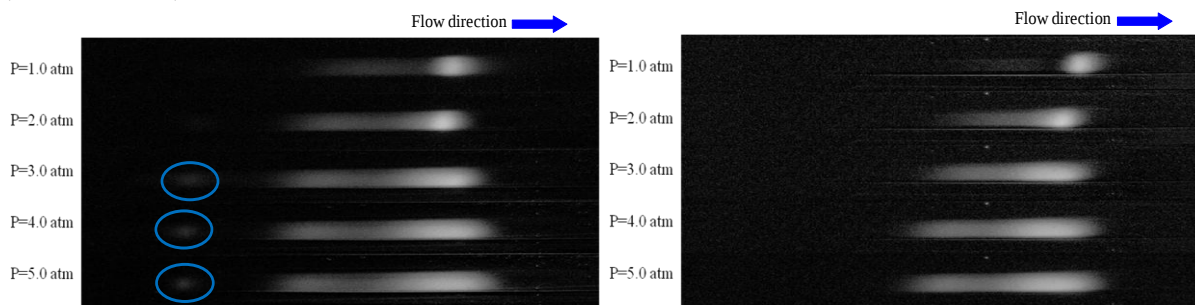


Figure 3. Weak flame images under atmospheric and elevated pressures. Left: PRF0/air. Right: PRF100/air.

In the case of PRF0/air, with the increase of pressure, cool flame appeared and the first hot flame was also intensified, which led to the clear separation of hot flames. As the pressure increases up to 5 atm, the second hot flame appears to be broadened and the cool and first hot flames became stronger. In addition, the positions of the first hot flames shifted to the upstream side with the increase of pressure. On the other hand, the second hot flame shifted to the upstream side from $P=1$ to 2 atm, but tendency is reversed from $P=2$ to 5 atm.

In the case of PRF100/air, cool flame was not captured even under $P=5$ atm. The first and second hot flames exhibited almost the same tendency as the case of PRF0/air, i.e., as pressure increased, the first hot flame shifted to the upstream side and its luminosity became stronger, and the second hot flame shifted to the upstream side from $P=1$ to 3 atm, and the tendency is reversed at higher pressures.

In the case of PRF50/air, very weak chemiluminescence of the cool flame was visible only in the cases of $P=4-5$ atm. Including the first and second hot flames, weak flames which response to pressure change for PRF50/air had intermediate characteristics between those of PRF0/air and PRF100/air.

Figure 4 shows the computational HRR profile of weak flames of PRF0/air and PRF100/air under pressures from 1 to 5 atm. The flow velocity was set to be 1.0 cm/sec. For the case of elevated pressures, the amount of total heat release was normalized to be the same as that of the atmospheric pressure in these figures. In Fig. 4 (Left), there are three HRR peaks in the flow direction, and the HRR peak of second hot flame is strongest under atmospheric pressure. As pressure increases, intensities of the HRR peaks of the cool flame and the first hot flame become stronger and that of the second hot flame is relatively weakened. In addition, the cool and first hot flames shift to the upstream side with increasing pressure.

In the case of PRF100/air, HRR peak of the cool flame was obtained only under elevated pressures. However, the peak value was much smaller than that of PRF0/air. On the other hand, the first and second hot flames showed pressure dependence similar to that of PRF0/air.

In the case of PRF50/air, HRR peak of the cool flame increased as pressure increased. However, it was not so significant as the case of PRF0/air. Overall tendencies of HRR are intermediate between those of PRF0 and PRF100.

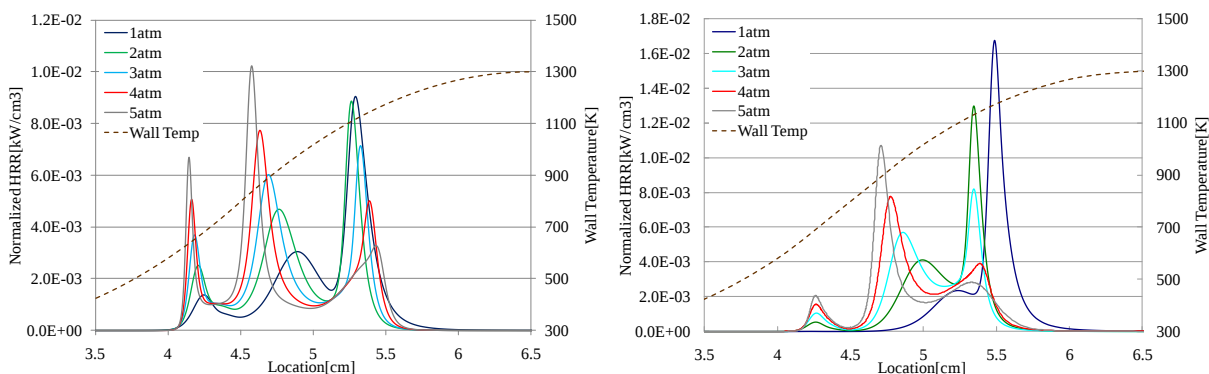


Figure 4. Computational heat release profile under elevated pressure. Left: PRF0/air. Right: PRF100/air.

The experimental and computational results both show that there is only a small pressure dependence of the position of the second hot flame. On the other hand, focusing on the HRR peak value of each flame, the reason why cool flame of PRF100/air was not observed even under the elevated pressure was explained by the computed HRR profile. However, it was not experimentally confirmed that the HRR distribution of each flame, that is, cool and first hot flames increase their HRR significantly under the elevated pressure and that of the second hot flame becomes even lower than them. It should be noted that since luminosity profile of flames observed in experiment and the computed HRR profile are being compared, it is difficult to discuss the quantitative correlation between them.

Computational results show that the difference of the second hot flame position between PRF0 and PRF100 decreases with increasing pressure. Thus, what play a significant role under high pressure are the increasing HRR and the position changes of the cool and the first hot flames to the low temperature region, rather than the position changes of the second hot flame. The same tendency can be expected in the compression ignition-type internal combustion engines which are normally operated under high pressure conditions.

By investigating oxidation characteristics in each temperature region separately for various octane number fuels under elevated pressure, the potential of the micro flow reactor to obtain unique insight

into the ignition characteristics of practical fuels was confirmed. Further investigation may possibly show an alternative index to the octane number which systematizes ignition characteristics of practical fuels.

4. Conclusions

Ignition and combustion characteristics of PRF/air mixtures were investigated using a micro flow reactor with a controlled temperature profile.

Flame responses to various inlet flow velocities were examined using PRF100 (iso-octane 100%) as a fuel. Three different flame patterns were observed: normal propagating flame in a high flow velocity region; FREL in an intermediate flow velocity region; and stable weak flames in a low flow velocity region.

By focusing on weak flames in the low flow velocity region, weak flame responses to various RONs were examined. The cool flame was weakened, and second hot flame shifted to higher temperature region as RON increased. To examine the experimental results, 1-D computations were conducted to investigate the weak flame responses to various RONs. Computed HRR profiles successfully reproduced the experimental results. By conducting the experiments and computations to investigate the weak flames response to RONs, the capability of the micro flow reactor to distinguish and examine the different ignition process for various octane-rated fuels was demonstrated.

In addition, experiment and computation were conducted to investigate the response of weak flames to elevated pressures. It was confirmed that as the pressure increased, cool and first hot flames increased their luminosities and shifted to low temperature region. These tendencies were intensified, especially for the low octane-rated fuels. As a result, it was found that the difference of ignition characteristics with various octane numbers is characterized by low and intermediate temperature oxidation, especially under high pressure.

Results of this study confirmed the possibility of using the micro flow reactor with a controlled temperature profile to investigate the ignition characteristics of practical fuels. The necessity of the investigation of the oxidation process in each temperature region was indicated for a detailed understanding of the ignition phenomena. The obtained results should be useful in various ways, for example, in reaction path analysis, and in the development and validation of reaction kinetics.

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