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Study on octane number dependence of PRF/air weak flames at 1–5 atm in a micro flow reactor with a controlled temperature profile

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ABSTRACT

Combustion and ignition characteristics of a stoichiometric gaseous Primary Reference Fuel (blended fuel of *n*-heptane and iso-octane, PRF)/air mixture were investigated by using a micro flow reactor with a controlled temperature profile.

By changing the mixture flow velocity at the inlet of the reactor, three kinds of flames were observed: normal propagating flame in a high flow velocity region; unstable flames, named *flames with repetitive extinction and ignition* (FREI), in an intermediate flow velocity region; and stable multiple weak flames in a low flow velocity region. In the weak flame phenomenon, multi-stage oxidation process of the fuel in a wide temperature range from 600 to 1200 K can be observed as separated multiple stationary flames. Focusing on this low flow velocity condition, weak flame responses to octane number under atmospheric pressure were examined using PRFs with various octane numbers. As octane number increased, luminosity from low temperature oxidation was decreased and the main reaction shifted to the high temperature region. The capability of the present reactor for examination of the general ignition characteristics of various fuels was demonstrated.

In addition, pressure dependence of the weak flames was investigated using PRFs with various octane numbers. Low temperature oxidation exhibited more significant heat release under elevated pressure, and this change was dependent on the octane number.

To examine the experimental results, one-dimensional steady computation was conducted using detailed reaction kinetics. Computational results reproduced the tendencies of the experimental results qualitatively.

Both the experimental and computational results indicate the advantage of the separate investigation of the oxidation process in each temperature region, which can be realized only by the present micro flow reactor, to obtain a detailed understanding of the ignition characteristics of practical fuels.

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1. Introduction

1.1. Motivation

It is urgently required to develop technologies to control internal combustion devices more efficiently in terms of energy savings. Especially for improving the efficiency of compression ignition engines, the understanding of the ignition process of various fuels would play an important role.

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.

The 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 [1–3]. Ignition delay times of two-stage ignition [4] and concentration time-history of formaldehyde, which is a typical product of kinetic processes associated with cool flame [1], have also been investigated.

As a weak point of RCMs, however, difficulty of accurate tracking of the gas-phase temperature history in the chamber should be mentioned. Sources of errors cannot be fully eliminated due to, e.g., heat loss through the wall during auto-ignition and temperature non-uniformity in the combustion chamber.

Therefore, a well defined, simple experimental system for investigation of the ignition process is required. For that reason, this

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Nomenclature

A	cross-sectional area
c_p	specific heat at constant pressure
d	inner diameter of tube
h	specific enthalpy
$\dot{M}$	mass flow rate
Nu	Nusselt number
P	pressure
T	temperature
U	mean flow velocity
V	diffusion velocity
W	molecular weight
x	spatial coordinate
Y	mass fraction
λ	thermal conductivity
ρ	density
$\dot{\omega}$	molar production rate

Subscripts

k	species index
w	wall

study focused on a micro flow reactor with a controlled temperature profile [5,6] as an alternative experimental method.

1.2. Micro flow reactor with a controlled temperature profile

In the context of fundamental studies on microcombustion [7–9], combustion in a heated channel with an inner diameter smaller than the ordinary quenching diameter for room temperature condition was conducted [5,6]. Some studies were conducted with the similar configuration [10–13]. Recently, it is recognized that such configuration can be utilized as micro flow reactor with temperature gradient for examining ignition and combustion characteristics of given fuels [14–17].

In the micro flow reactor, quartz glass tube with an inner diameter smaller than the ordinary quenching diameter for room temperature condition 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. Effect of surface reaction on the flame behavior was confirmed to be negligible in our previous study [16].

In previous studies using this micro flow reactor, Tsuboi et al. found that there is a lower inlet flow velocity limit of methane/air weak flame and that wall temperature at the flame position corresponds to the minimum ignition temperature of the fuel in a given condition [14,15]. Oshibe et al. observed weak flames of DME/air in the micro flow reactor and found stabilized multi-stage oxidation including low temperature oxidation [16]. Yamamoto et al. have conducted an investigation on the multi-stage oxidation process of *n*-heptane/air, which consists of cool and separated hot flames [17]. These studies have clearly indicated the capability of the micro flow reactor as a method to investigate general ignition characteristics of fuels. 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.

This study focused on the investigation of combustion and ignition characteristics of gaseous blended fuel of iso-octane and *n*-heptane (PRF) by using a micro flow reactor with a controlled temperature profile. The weak flame response to the various RONs was investigated by varying the mixing ratio of *n*-heptane and iso-octane. The pressure dependences of the weak flame were also investigated using PRF/air with various RONs.

In addition, one-dimensional computations were conducted using a detailed reaction mechanism [18,19] of PRF. Obtained computational results were compared with experimental results.

2. Experimental and computational methods

2.1. Experimental method

A schematic of the experimental setup is shown in Fig. 1. A quartz glass tube was heated by a H_2/air premixed burner so as to have a stationary temperature profile (300–1300 K) along the inner surface of the tube in the axial direction. H_2/air burner was chosen as an external heat source for better visualization of chemiluminescence from hydrocarbon flames in the micro flow reactor. The maximum wall temperature and temperature profile can be adjusted by changing the equivalence ratio, the flow velocity of an H_2/air mixture, and the distance between the tube and the burner.

For experiments under 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. Air temperature at the upstream side of the injection position was controlled to be 300–323 K by an electric heater to assure vaporization. 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. *n*-Heptane and iso-octane were blended in the required ratio in the liquid state beforehand. Purities of both *n*-heptane and iso-octane are higher than 99% (Wako Pure Chemical Industries).

In the elevated pressure experiments, a quartz glass tube with an inner diameter of 1 mm was used. This is because the quenching diameter becomes smaller under elevated pressure. In addition, a different mixture supplying method was employed because of difficulties of using the syringe for elevated pressure setups. A gaseous PRF/N_2 mixture was stored in a tank at 6 atm and 373 K in

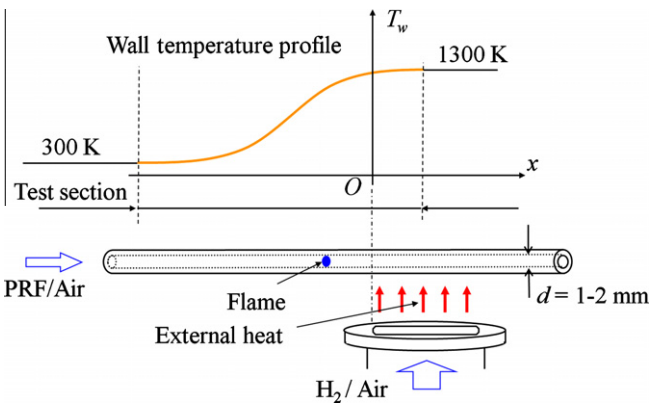

Fig. 1. Experimental setup.

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