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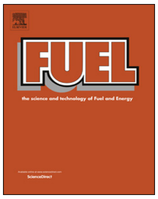

Full Length Article

Experimental and kinetic studies of the effect of CO_2 dilution on laminar premixed *n*-heptane/air flames

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ABSTRACT

In the present study, experimental and kinetic studies of the effect of CO_2 dilution on laminar premixed *n*-heptane/air flames were performed via the outwardly propagating spherical flames and the simulation of one-dimensional planar flames. The laminar flame speeds and Markstein lengths of *n*-heptane/air/CO_2 mixtures at different CO_2 dilution rates were measured and the chemical effect of CO_2 was separated from its total effects by introducing a type of fictitious carbon dioxide (FCO_2) in the simulation. Results show that the laminar flame speeds of *n*-heptane/air/CO_2 mixtures nonlinearly decrease with the increase of CO_2 dilution rate. Moreover, as CO_2 dilution rate increases, the instability of laminar *n*-heptane/air/CO_2 flames decreases due to the decrease of the hydro-dynamic instability. The results of kinetic analysis show the increase of CO_2 concentration in the *n*-heptane/air flames decreases the peaks of mole fractions of the main radical species (OH, O, H, CH_3 and HO_2), net reaction rates of the main elementary reactions and flame temperature. Both the physical and chemical effects of CO_2 suppress the laminar flame speeds and flame temperatures and inhibit the productions of the main radical species and net reaction rates of the main elementary reactions, and the former dominates. The chemical effect of CO_2 remarkably promotes the production of CO via shifting the equilibrium of R24 $CO + OH = CO_2 + H$, and the third-body effect of CO_2 slightly increases the production of H_2O shifting the equilibrium of R8 $H_2O + M = H + OH + M$. The backward reactions of R24 and R8 enhanced by CO_2 addition compete with the important chain branching reaction R1 $H + O_2 = O + OH$ for H atoms, which plays the chemical role in reducing the laminar flame speed and flame temperature.

1. Introduction

Exhaust Gas Recirculation (EGR) is an effective and widely used technique in engines to reduce the NO_x emissions [1–3]. Lots of studies have been focused on the influence of EGR on the combustion and emissions in various engines [4–6]. They concluded that the EGR has significant and different effects on fuel combustion and emissions, and the fundamental impact mechanism of EGR on fuel combustion and emissions is still not perfectly understood. The specific heat capacity of intake mixture can be significantly enhanced by inletting partial exhaust gas to intake air, and under the same heat release of the fuels, it decreases the flame temperature which attributes to the decrease of NO_x emissions. Besides, the O_2 concentration in intake mixtures is also reduced, and it affects the stabilities and velocities of the fuels combustion. Therefore, in order to essentially reveal the effect of EGR on the engines, it is necessary to investigate the influence of EGR gas on the fuel combustion.

Moreover, a detailed chemical kinetic mechanism considered the influence of EGR gas is of great importance to acquire the high-accuracy prediction of combustion process in the engine with EGR system [7]. The experimental data of the premixed flames such as the laminar flame speed plays an important role in validating and developing the chemical kinetic mechanisms [8]. Hence, the original experimental data of the premixed flames with EGR gas dilution is recommended to be measured.

CO_2 is one of the major components of EGR gas. Many researches on the effect of CO_2 dilution on the combustion characteristic of the premixed flames have been carried out in previous studies. Yossefi et al. [9] investigated the combustion of methane and ethane with CO_2 replacing N_2 as diluent. They found that the CO_2 has significant influence in the initial combustion of methane and ethane. Liu et al. [10] emphasized that the chemical effect of CO_2 significantly reduces the flame speed of CH_4 and H_2 premixed flames, and the influence on methane flames is more significant than that in hydrogen flames. Recently, Han et al. [11] measured the laminar flame speeds of H_2/CO with CO_2 dilution at normal and elevated pressures and temperatures. Liu et al.

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Nomenclature

Abbreviations

t	times (s)
R_f	flame radius (m)
A	flame surface area (m^2)
S_b	stretched flame speed (m/s)
K	flame stretch rate (1/s)
S_b^0	unstretched flame speed (m/s)
S_u^0	laminar flame speed (cm/s)
L_b	Markstein length (mm)
Le	Lewis number
T	temperature (K)
P	pressure (MPa)

Subscripts

u	unburned gas
b	burned gas

Greek Symbols

ρ	density (g/cm^3)
δ	laminar flame thickness (mm)
σ	thermal expansion ratio

[12] numerically analyzed the difference in the effect of CO_2 addition on the oxidation of two isomeric oxygenated fuels: ethanol and DME. Li et al. [13] experimentally studied the chemical effects of CO_2 on the oxidation of biodiesel surrogate, methyl butanoate (MB) in the SJTU laminar flow reactor, and their results showed that the presence of CO_2 suppresses the oxidation of MB. In addition, Zhao et al. [14] experimentally and numerically studied the effect of prompt dissociation of formyl radical on 1,3,5-trioxane and CH_2O laminar flame speeds with CO_2 dilution. It is well know that *n*-heptane is one of the representative components of diesel and gasoline surrogates. However, to the best of authors' knowledge, less attention has been paid to the effect of the CO_2 dilution on the laminar combustion characteristics of *n*-heptane/air mixtures. Moreover, CO_2 in premixed flames not only causes the thermal and dilution effects but also directly participates in chemical reactions through $CO + OH = CO_2 + H$, indicating that the impact mechanism of CO_2 on laminar premixed flames is much more complicated. Therefore, differentiating the physical and chemical effects of CO_2 on the laminar premixed *n*-heptane/air flames also contributes to understanding the impact mechanism of EGR gas on fuel combustion and emissions of diesel and gasoline engines.

With these points in mind, in the present study, the outwardly propagating spherical flames were employed to investigate the effect of CO_2 dilution on the laminar combustion characteristics for premixed *n*-heptane/air mixtures at different equivalence ratios under initial pressure and temperature of 0.1 MPa and 358 K, respectively. Meanwhile, the freely propagating one-dimensional planar flames of *n*-heptane/air/CO_2 mixtures were simulated to analyze the kinetic effects of CO_2 on the laminar flame speed of *n*-heptane/air flames. Moreover, a fictitious species FCO_2 having the same thermal and transport properties as normal CO_2 was defined to isolate the chemical effect of CO_2 on *n*-heptane/air mixtures from its total effect.

2. Experimental section

2.1. Experimental apparatus

In the present study, the experimental setup of outwardly propagating spherical flames was employed to perform the related experiments, and the schematic of the experimental setup is shown in Fig. 1. The apparatus mainly consists of a cylinder stainless-steel constant-volume combustion chamber, a heating system, gas and liquid distribution system, an ignition system and a schlieren optical system for observing flame propagation with a high-speed digital camera. The inner diameter of the chamber is 360 mm, and the volume of the chamber is 12.85 ± 0.005 L. Two quartz optical windows of 120 mm diameter are mounted in the both sides of the chamber to provide optical access to observe the spherical flames. The outside chamber surfaces are covered with heating tapes and thermal insulation materials. A thermocouple is mounted into the combustion chamber to monitor the initial temperature, and a pressure transmitter is utilized to measure the partial pressure of each composition of mixtures. Two electrodes of 2 mm diameter are fitted in the center of combustion chamber, and the capacitive ignition system is employed to ignite the prepared mixtures. In the experiments the high-speed digital camera with the frame rate of 10 000 fps is used to record the images of the combustion process of the mixtures, and the resolution rate of the image is 768 × 768 pixels. The detailed error analyses can be referred to the Refs. [15] and [16].

Prior to the experiments, the combustion chamber was heated to that its inner temperature is stabilized at the designed temperature. According to the initial conditions and the Dalton partial pressure law, the partial pressures of CO_2, O_2 and N_2 and the liquid volume of *n*-heptane were calculated initially. During the experiments, the combustion chamber was vacuumed firstly, and then each reactant with appropriate proportion was injected into the combustion chamber. To ensure the homogeneity and motionlessness of the reactants, the mixtures were ignited after the preparation for 15 min. The mixtures were ignited by the ignition system, and the flame propagation image was recorded by the high-speed camera simultaneously.

In the experiments, the air was considered to be a mixture of 21% oxygen and 79% nitrogen in volume. The purities of *n*-heptane and CO_2 are 99.95% and 99.99%, respectively. The purities of O_2 and N_2 are both 99.999%. The dilution rate in the mixture is defined as $R_{\text{diluent}} = n_{\text{diluent}}/(n_{\text{diluent}} + n_{\text{fuel}} + n_{o_2} + n_{n_2}) \times 100\%$. In the present study, experiments were conducted at the initial temperature of 358 ± 2 K and the initial pressure of 0.1 MPa with the equivalence ratio of 0.8–1.5 and the CO_2 dilution rate of 0–15%. The maximum partial pressure of *n*-heptane in the present experiments is 2.785 kPa and its corresponding saturation temperature is 283.4 K. That is to say, when the initial temperature is set as 358 K, the superheat of *n*-heptane

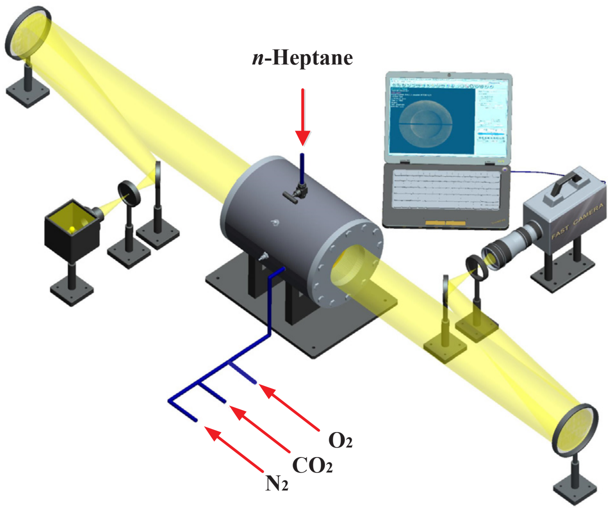

Fig. 1. Schematic of the experimental setup.