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Effects of inert dilution on the propagation and extinction of lean premixed syngas/air flames

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HIGHLIGHTS

- New experimental extinction data for the diluted lean premixed H_2/CO/air flames.
- Detailed simulation on the propagation and extinction of syngas flames.
- Assessment of dilution mechanisms on the propagation of syngas flames.
- Assessment of dilution mechanisms on the extinction of syngas flames.

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ABSTRACT

The dilution effects of inert components N_2 and CO_2 on the propagation and extinction of lean premixed H_2/CO/air syngas flames were experimentally and numerically investigated. Extinction stretch rates were measured using the counterflow technique while laminar flame speed data were obtained from literatures. Numerical simulations were conducted at 1-D freely propagating configuration and opposed-jet configuration with detailed chemistry and molecular transport description. The numerical results well predicted the experimental measurements. Both results revealed that CO_2 dilution had more profound effect on flame propagation and extinction than N_2 dilution. In addition, numerical simulation assessed the preferential importance in a rather quantitative manner among the three effects, i.e., the thermal effect, the diffusivity change effect and the chemical effect with artificial manipulation of mass diffusivities and chemical reactions of CO_2 and N_2. The results showed that the thermal effect dominated the reduction of laminar flame speed and extinction strain rate. The chemical effect caused by CO_2 dilution was slightly stronger to the reduction of extinction limit than to that of laminar flame speed. The diffusivity change effect is negligible for both CO_2 and N_2 dilutions. N_2 only acts as a thermal inert in the propagation and extinction of the H_2/CO/air flames.

1. Introduction

Synthesis gas (syngas) is the gaseous product of coal or biomass gasification. Since most of the harmful contaminants (e.g., H_2S, SO_x, heavy metals and ashes) can be removed during the post-gasification process, syngas is regarded as a promising alternative fuel of natural gas used in industrial furnaces and gas turbines [1]. The design of syngas burners and combustors requires adequate knowledge of the combustion properties of syngas flames.

The main combustible components in syngas are H_2 and CO, besides a small amount of CH_4 and other hydrocarbons. By nowadays, the fundamental combustion properties, the laminar flame speeds (S_u^0's) and extinction strain rates (K_{ext}'s) of H_2/CO/air mixtures, have been studied over a wide range of H_2/CO ratio by a number of researchers [2–11]. It was found that S_u^0 non-linearly varies with H_2/CO ratio [7–10] and the extinction phenomenon of stretched H_2/CO flames was sensitive to not only the chemical kinetics but also the mass transport [11]. Besides, the flammability limits and the associated controlling mechanisms of near-limit syngas flames have been studied over a large range of H_2/CO ratio at different preheat temperatures [12]. Based on experimental data, H_2/CO/air chemistry, the basis for entire hydrocarbon family, has been also validated and updated [13–16].

In addition to the combustible components, syngas usually contains considerable amount of inert diluents, mostly N_2 and CO_2 [1,4,12]. In some practical application, a certain amount of flue gas containing mainly N_2 and CO_2, is deliberately introduced to the fresh unburned mixtures to reduce the flame temperature

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and thereby NO_x formation. Some studies revealed that the inert diluents can noticeably affect the propagation, extinction and flammability limit of syngas/air flames (e.g., [3,4,12]). On one hand, the diluents can introduce a thermal dilution effect, reducing the heat value of the fuel. On the other hand, based on the studies on S_u^0's of some diluted hydrocarbon/air flames (e.g., CH_4/air [17,18], C_3H_8/air [19–21], DME/air [22,23]), the diluents can also introduce a chemical effect, even being "active" reactants in chemical reactions, and an effect in changing the overall diffusivity of the mixture. However, full assessment on the preferential importance of those effects is still lacked. In addition, even though some kinetic models, e.g., the one proposed by Li et al. [15], were well validated by the pure H_2/CO/air flames, none of them has been validated with the presence of considerable amount of inert diluents.

Based on the aforementioned introduction, in this paper, an experimental and numerical study on the propagation and extinction of laminar lean premixed H_2/CO/air flames with the presence of considerable amount of N_2 and CO_2 diluents was conducted. In addition, the effects caused by the dilution were individually assessed by the numerical simulation with artificial manipulation of thermal and chemical properties of CO_2 and N_2 and the dominant effect was discussed.

2. Experimental approaches

The experimental data of S_u^0 were referred from the literatures [3,4]. K_{ext}'s were measured in the present study using the opposed-jet twin-flame counterflow configuration, schematically shown in Fig. 1. Two identical burners with 10 mm exit diameter were installed symmetrically with a separation distance of 10 mm. The flow rates of the fuel and air streams were respectively controlled by adjusting the upstream pressures of the sonic nozzles, which were pre-calibrated using a high-accuracy wet gas meter. The fuels were mixtures of pure H_2 (>99.99%) and CO (>99.95%). Diluents were pure CO_2 (>99.99%) and N_2 (>99.99%). The oxidizer was compressed air, pre-dried by a silica-gel desiccator. The burner nozzles were water-cooled to keep at ambient temperature. N_2 (>99.99%) co-flow was used to isolate the combustible mixture from the ambient air.

After the flames were stabilized at a given equivalence ratio (ϕ), the air flow rate was kept unchanged, while the fuel flow rate was gradually decreased to a constant value at which the flames were right about to extinguish. At this condition, the flow field between the two nozzles was measured using the digital particle image velocimetry (DPIV). The DPIV tracers were silicon oil droplets atomized by a quartz nebulizer, and its flow rate was 0.03–0.05 mL/min, accurately controlled by a syringe pump. The

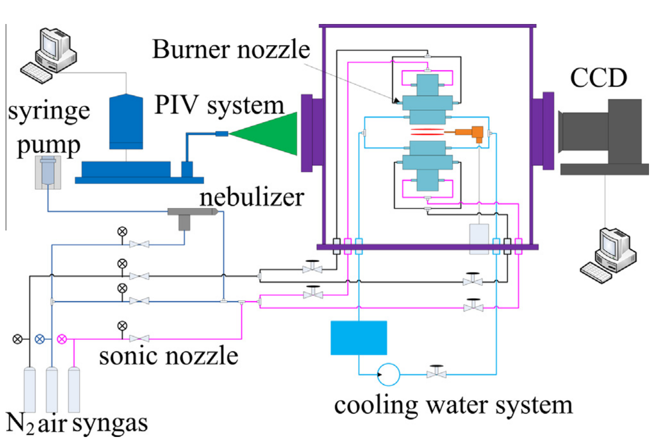

Fig. 1. Schematic of the opposed-jet counterflow flame system.

velocity profile along the centerline was retrieved from the flow field data. The local stretch rate (K) was defined as the absolute maximum axial velocity gradient in the hydrodynamic zone [24] along the centerline. The K value at the condition that the flame was right about to extinguish was defined as the extinction limit (K_{ext}), and the corresponding equivalence ratio (ϕ) was regarded as the extinction equivalence ratio (ϕ_{ext}) [24–26]. All the measurements were conducted at atmospheric pressure and the unburned mixture temperature T_u's were kept at room temperature of 298 K ± 3 K.

The uncertainties of K_{ext} and ϕ_{ext} were carefully considered following the method proposed by Moffat [27]. The uncertainty of K_{ext} was determined by the measurement uncertainties of flow velocity using DPIV, spatial distance, and standard deviation of repeated measurements of K_{ext}. The uncertainty of DPIV measurements was estimated as $\sim\pm$ 1.46 cm/s following the method proposed by Westerweel [28]. Each case was repeatedly at least 30 runs to reduce the random uncertainty caused by the flow fluctuation. The uncertainty of ϕ_{ext} was estimated from the calibration data of the gas flow rates. The confidential interval was 95%. Detailed description of the measurement uncertainty analysis can be found in our previous study [7].

Six kinds of syngases with different fuel composition and inert dilutions were used in the experiments or as references for comparison, as listed in Table 1. Syngas-1, Syngas-2 and Syngas-3 were three syngases with equal H_2/CO volumetric ratio. This ratio was a typical value of industrially-used syngases and commonly used in previous studies [3–5,7,9,10]. Syngas-1 was free of dilution. Syngas-2 and Syngas-3 were with CO_2 dilution and N_2 dilution respectively. Syngas-4, Syngas-5 and Syngas-6 were used for K_{ext} measurements and they had the same H_2/CO volumetric ratio of 1:9 but with no dilution, CO_2 dilution and N_2 dilution respectively. This ratio was convenient to keep all experiments in laminar flow. The molar fractions of N_2 and CO_2 were both set at 20% to keep their dilution effects at the same concentration level. For strong flames close to stoichiometric condition, extinction occurred at a large strain rate in which the flow was in turbulent region. Thus, all extinction experiments were conducted at $\phi < 0.6$ with relatively low H_2/CO ratio.

3. Numerical approaches

S_u^0's were computed using the PREMIX code [29] and K_{ext}'s were computed using the Opposed-Jet code [30]. Both codes were originally developed by Kee and his coworkers, and modified to account for thermal radiation of CO_2, H_2O, CH_4, and CO in the optically thin limit [31]. The codes were integrated with the CHEMKIN-II [32] package and Sandia thermal and transport subroutine libraries [33].

The detailed H_2/CO/C_1 kinetic model proposed by Li et al. [15] with the modification (recommended by the original authors) of the reaction rate constant of CO + HO_2 = CO_2 + OH [34] was used in both S_u^0 and K_{ext} computations. Since H_2 and H have strong mass diffusion capability, full multi-component diffusion formulation was used in the computation along with the Soret effect.

In the S_u^0 calculation, the 1-D computation domain was 17 cm to allow fully developed downstream boundary conditions. Two grid control parameters, GRAD and CURV, were both set at 0.1, and the grid number was assured to be at least 800. In the K_{ext} calculation, the computation domain was 1 cm, consistent with the experimental setting. GRAD and CURV were set at 0.1 and 0.05 respectively and the grid number was around 1500 to precisely capture the thin flame structure at near-extinction condition. Similar to the previous studies [11,12], the one-point continuation approaches was used to solve the singular state near the extinction turning point. According to the recent studies [35,36], the velocity gradient at