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Extinction limits and structure of counterflow nonpremixed hydrogen-doped ammonia/air flames at elevated temperatures



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ABSTRACT

The present study demonstrates the potential of hydrogen (H₂)-doped ammonia (NH₃) as a carbon-free fuel. The extinction limits, flame temperature and morphology of the counterflow nonpremixed NH₃ -H₂/air flames at elevated temperatures and normal pressure are experimentally determined. Also, the detailed flame structure and the extinction limits are computed using a detailed kinetic mechanism. Results show that the blow-off limits, the concentration of radicals H, OH and O and the maximum flame temperature are enhanced with H₂ substitution in NH₃/air flames. This supports the potential of H₂ as an additive for improving the reactivity and ignition of nonpremixed NH₃/air flames and thus the potential of H₂-doped NH₃ as a carbon-free fuel. Meanwhile, the extinction limits (in terms of the mole fraction of NH₃ in the fuel gas) and the maximum flame temperature are reduced with increasing strain rates, indicating that flames can sustain more NH₃ at low strain rates. Also, it is observed that the blow-off limits and the maximum flame temperature for various conditions show encouraging agreement, but quantitative discrepancies among the measurements and predictions merit additional consideration in boundary condition modeling and the reaction mechanism.

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1. Introduction

Despite increased interest in the use of hydrogen (H_2) in combustion devices due to its unique features, e.g., no carbon dioxide (CO_2) emissions and high reactivity in a spark-ignition engine [1] and a compression ignition engine [2], the considerable technological problems related to safety [3], transport [4] and storage [5] should be resolved. Recently, an alternative approach has been suggested to enable H₂ utilization and to overcome the associated problems using ammonia (NH₃) since NH₃ is easily storable with high hydrogen content [4]. Burning NH₃ still involves only nitrogen (N₂) and water (H₂O) vapor as the final products. Recent studies on the use of NH₃ in internal combustion engines also show that NH₃ is cheaper than gasoline and CNG (compressed natural gas) in terms of specific energetic cost (price/GJ) and cost per 100 km driving range [6]. It is not practical to burn NH₃ alone because of its low

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burning intensity and high ignition energy, but these problems can be resolved if H_2 is added to NH_3 . Actually, H_2 has been used as an additive or a blend for hydrocarbon fuel, e.g., CNG and H_2 blends in spark-ignition engines [7], nonpremixed H_2 -methane (CH₄)/N₂oxygen (O₂) flames [8] and H_2 -added CH₄-O₂ jet flames [9].

Previous studies in this laboratory have shown the potential of NH₃ as a carbon-free fuel [10] or additive [11]. A computational and experimental study of outwardly-expanding spherical premixed H₂-added NH₃/air flames shows substantial increases in laminar burning velocities with H₂ substitution, which demonstrates the potential of NH₃ as a clean fuel and H₂ as an additive for improving the combustion performance in premixed NH₃/air flames [10]. Meanwhile, a computational study of the effects of NH₃ substitution on the structure and extinction limits of counterflow nonpremixed H₂/air flames shows that the chemical effects of NH₃ substitution on flame structure are more dominant than the thermal effects [11]. However, NH₃ burning has not been extensively studied because it has not been used as a fuel. The earlier investigations of NH₃ burning in this laboratory are also limited to the predicted nonpremixed NH₃-added H₂/air flames and the premixed H₂-added NH₃/air flames. Thus, the fundamental combustion characteristics of the nonpremixed H₂-doped NH₃/air flames still





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need to be investigated experimentally and computationally. In general, turbulent nonpremixed flames can be considered as an ensemble of strained, one-dimensional, laminar flamelets, being represented by a counterflow nonpremixed flame configuration [12]. Thus, most fundamental studies of the structure and extinction limits of nonpremixed flames have been conducted using the counterflow configuration.

Considering these, in this study we aim to demonstrate the potential of using NH₃ as a clean fuel, and particularly study to improve NH₃ burning performance by doping H₂ to nonpremixed NH₃/air flames, with the following specific objectives. The first objective is to investigate the morphology of the counterflow nonpremixed H₂-substituted NH₃/air flames at NTP (normal temperature and pressure), observing the unique behavior. The second objective is accurately measuring and predicting the blow-off (i.e., high-stretch extinction) limits of the H₂-substituted NH₃/air flames to provide the fundamental combustion database of NH₃ as a fuel and to quantify the extent of flammable range enhancement because of H₂ addition. We would also examine the effects of H₂ substitution on the flame structure, including distributions of temperature and species concentrations. The third objective is to observe the consequences of strain rates and air temperature on the structure and extinction limits of the H₂-substituted NH₃/air flames to elucidate the combustion characteristics of the flames under more practical circumstances. The study would be conducted for a wide range of strain rates, air temperature and the extent of H₂ substitution.

We subsequently presents the morphology of counterflow nonpremixed H_2 -doped NH_3 /air flames and the effects of the extent of H_2 substitution, strain rates and air temperature on the structure and extinction limits of NH_3 - H_2 /air flames, with the descriptions of the experimental and computational methods used in this study.

2. Experimental and computational methods

The counterflow nonpremixed flame is considered for this study since the flame configuration represents a strained, onedimensional, laminar flamelet and its dynamics are also well defined. A diagram of the present experimental apparatus is provided in Fig. 1. The apparatus consists of a counterflow burner with a pair of main converging nozzles (stainless steel SUS316L) and concentric, converging nozzles (SUS316L) surrounding the main nozzles to provide sheath N_2 coflow which prevents burning of fuel with the ambient air, a fuel (NH_3-H_2 blends) supply system, a N_2 supply system, an air supply system with an electric furnace for preheating air, thermocouples for measuring the temperature distribution in the flame and the gas temperature at the nozzle exit. A digital camera (Sony A65) records flame images to assess the visible flame appearance.

Air and fuel are issued from the top and bottom nozzles, respectively, with an inner diameter (*d*) of 15.0 mm and a nozzle separation distance (L) of 20.0 mm. To obtain stabilized, uniform flow at the nozzle exit, the flows issue through three layers of stainless steel honeycombs and stainless steel beads with an average particle diameter of 2.0 mm. The lower and upper inner nozzles are aligned so that their centerline is along the same axis. To isolate the flame from laboratory drafts the burner is placed inside a semi-closed, plexi-glass chamber. Fuel mixes with air near a stagnation plane between the nozzles. A flat, laminar nonpremixed flame is initiated by a spark-igniter. Typical counterflow flame images are shown in Fig. 2. The N₂ coflow to prevent burning of fuel with the ambient air also prevents heating the upper nozzle and dilutes the products. The coflow injection velocity u_{C} is adjusted to be the same as the respective air and fuel injection velocities u_0 and u_F . NH₃ (purity > 99.9999%)-H₂ (purity > 99.999%) mixtures, approximate air (21% O2/79% N2 in volume, purity > 99.9%) and N_2 are delivered using commercial mass flow controllers (Aera and MKP: 0-200 slm) with accuracy $\pm 1.0\%$ of full scale which are calibrated using a bubble meter. Air passes through an electric furnace (maximum heating temperature of 1373 K). The temperature distribution in the flame is measured using micropositioning stage-mounted R-type thermocouples with a bead diameter of $152 \pm 20 \,\mu\text{m}$ and an accuracy of $\pm 0.25\%$, identifying the maximum flame temperature and its location. To prevent sagging when thermocouples are inserted into the flame, tension is added to the bead. To confirm thermal boundary conditions, the air nozzle exit temperature is measured using K-type thermocouples with a



Fig. 1. Schematics of experimental apparatus and counterflow nonpremixed flame.

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