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Numerical study on effect of oxygen content in combustion air on ammonia combustion

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ABSTRACT

As a key parameter for a fuel in real combustion development, burning velocity of NH_3 which is usually low limits its application in the energy device. In this study, the combustion of NH_3 at oxygen enriched condition has been proposed as a novel method for improving NH_3 combustion. The oxygen concentration in the combustion air was varied from 21% to 30%. The results show that O_2-enriched combustion has positive effects on both laminar burning velocity and adiabatic flame temperature of NH_3. The maximum burning velocity of NH_3 is 38.6 cm/s at O_2 content of 30%, which is approximately 2.6 times the value obtained at an O_2 content of 21%, mainly due to the increased reaction rates of OH, H, O, and NH_2 radicals in the reaction zone at higher O_2 contents. NO emissions increase with an increase in the O_2 content of the combustion air. Whereas, the reactions between NO and surplus NH_2, NH and N radicals cause more NO consumption especially at fuel-rich conditions, showing the potential in reducing NO emission in NH_3-air combustion. Therefore, O_2-enriched combustion is a suitable method for improving NH_3 combustion when NH_3 is utilized as fuel.

1. Introduction

In the past decade, because of the increasing strictness of governmental regulation of energy and pollutant emissions, the search of alternative fuel becomes important. The use of alternative fuels, such as biofuels, natural gas and H_2, can reduce greenhouse gases and pollutant emissions [1]. NH_3 is regarded as one of the most promising alternatives independent of hydrocarbon-based fuels [2–5], the combustion of NH_3 does not result in the release of CO_2, SO_x and soot [6–8], which makes it a unique fuel. In addition, NH_3 can be synthesized by the Haber-Bosch process from various sources of N_2 and H_2, such as wind, solar energy, waste, and biomass [9,10]. Since it has a liquefaction pressure of about 8.0 atm at room temperature, it is economically viable to store NH_3 in large quantities and transport it in the liquid-form. However, there are many challenges in using NH_3 as a fuel due to its high auto-ignition temperature (903 K), narrow flammability limit (15.5%–27.0%), and low burning velocity (5–13 cm/s) [11,12], which lead to a low combustion rate and limit its application in various energy devices [13–15].

Many methods have been proposed for enhancing NH_3 combustion, including co-combustion of NH_3 with fuel possessing high burning velocity such as H_2 [4,16–18]. Li et al. [16] investigated the combustion characteristics and NO_x formation when use NH_3 and H_2 as dual fuel. They found the burning velocity and NO_x formation of NH_3/H_2-air combustion increased with the increase of H_2 fraction. A novel concept, operating heavy duty engine with H_2-NH_3 dual fuel, was presented by Boretti [4]. The fuel conversion efficiency approached 44% without power turbine, and NO_x emissions were extremely high and needed a proper treatment. However, many challenges are encountered when use H_2 as an alternative fuel. H_2 has a low flash point, which exhibits a high explosion hazard; a low volumetric energy density (5.6 MJ/L at 70 Mpa) and high storage pressure, leading to a high storage and transportation cost [1,4]. Furthermore, the co-combustion of H_2 with NH_3 enhances the combustion temperature, leading to a higher NO emissions [16,18].

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O_2-enriched combustion is considered to be a useful energy-saving technology for fossil fuel combustion systems. It increases the burning velocity of fossil fuels and NO emissions. Therefore, special treatment is needed to decrease NO emissions [19–23]. Wu et al. [19] investigated the effect of O_2 content in the combustion air on the heating rate, NO_x emissions, and temperature distributions of natural gas combustion. They found the heating rate increased by 53.6% as the O_2 content was increased from 21% to 30%, accompanied by a 26.1% reduction in natural gas consumption. However, the amount of NO_x emissions increased because of the higher combustion temperature at high O_2 contents. Sánchez et al. [22] experimentally evaluated the effects of oxygen enrichment on the performance of a flameless combustion furnace equipped with a regenerative burner. Flameless combustion phenomena were obtained at all oxygen enrichment rates, leading to a NO_x emissions below 5 ppm. Furthermore, the global efficiency increased almost 5% for an oxygen enriched level of 30% compared to that of 21%. Bělohradský et al. [23] experimentally studied the influence of O_2 content in the combustion air on the combustion characteristics of a two-gas-staged burner. NO_x emissions in the flue gas were significantly lower in the air oxy/fuel method compared to the premix-enrichment method. When the O_2 content was increased, higher heating intensities were reached owing to higher CO_2 and H_2O concentration. The available heat was also higher by 20% at an O_2 content of 46% compared to that at an O_2 content of 21%, mainly due to more formation of CO_2 and H_2O at the oxygen-enhanced flames, leading a higher heating intensity in the furnace.

The above results show that the combustion of hydrocarbon fuels could be improved under O_2-enriched conditions. However, none of these studies have used O_2-enriched combustion for NH_3 combustion. The effect of O_2 enrichment on NH_3 combustion characteristics and NO emissions were never studied. Moreover, as a typical NO_x formation precursor, the mechanism of NH_3 combustion at O_2-enriched condition is completely different with that of conventional fuels. In this study, we proposed O_2-enriched combustion as a potential method for improving NH_3 combustion, in order to enable the use of NH_3 as a practical fuel. The dependence of parameters, including laminar burning velocity (S_u), and adiabatic flame temperature (T_{ad}), on O_2 concentration in the combustion air is presented. Additionally, the mechanism of major species, free radicals, and nitrogen radicals during NH_3 combustion are clarified. Finally, the detailed combustion and NO emission characteristics of NH_3 at various O_2 concentrations of 21%, 23%, 25%, 27%, and 30% in the combustion air have been numerically investigated.

2. Numerical simulations

The CHEMKIN 4.0 software was used for the numerical simulations. A freely propagating adiabatic, premixed, laminar flame speed calculation model [24] was used. The Millar–Bowman [25] and the Reductive Konnov mechanisms [3,26] were employed, as show in Appendices A1 and A2. The steady–state mass, species and energy conservation equations of the flames were solved using the hybrid time-integration/Newton-iteration technique with adaptive meshes and mixture-averaged transport parameters. With-draw differencing on both the convective and diffusion terms were used in the simulation [27]. In order to control the adaptive grid mesh, the values of adaptive grid control based on the solution gradient and curvature were set to be 0.01 and 0.05, respectively. The calculation domain was from 0.0 cm to 2.5 cm, which was long enough to reach adiabatic equilibrium for NH_3-air combustion downstream of the flames. At the cold boundary, the initial temperature and pressure were set at 298 K and 1 atm, respectively. The initial guess value for the inlet mass flow rate was set as 0.09 g/cm^2 s, for the freely propagating flame. The guess values for the initial, intermediate, and production fractions along with the temperature profiles were also specified at the beginning of the simulations. A new subroutine for calculation of the rate production of all species has been added, which can give a deep analysis of the rate production of nitrogen relating species in NH_3-air combustion.

The initial composition of the NH_3-air flames was defined using equivalence ratio (ϕ) and O_2 content in the combustion air (Ω). The chemical equation for NH_3-air combustion under stoichiometric conditions is given by the following overall reaction (R0):

$$NH_3 + 0.75/\Omega\,(\Omega\, O_2 + (1-\Omega)\, N_2) \rightarrow (1.25-0.75\Omega)\, N_2 + 1.5H_2O \quad (R0)$$

ϕ which was calculated according to R0, ranged from 0.80 to 1.25, whereas Ω ranged from 21% to 30% (molar base), which is defined as follows:

$$\Omega = \frac{X_{O_2}}{X_{O_2} + X_{N_2}}$$

Where, X_{O_2} is the mole fraction of O_2 in the inlet gas, and X_{N_2} is the mole fraction of N_2 in the inlet gas. The initial concentrations of NH_3, O_2, and N_2 corresponding to various O_2 contents in the combustion air are summarized in Tables B1 to B5 in Appendix B.

3. Results and discussion

3.1. Laminar burning velocity

As a key parameter in fuel combustion, the laminar burning velocity of NH_3 at various O_2 concentrations in the combustion air has been computed. The laminar burning velocity is defined as the speed at which unburned gases move through the combustion wave in the direction normal to the wave surface. The laminar burning velocity can be calculated as follows according to Metghalchi and Kech power–law relation [28]:

$$S_u = S_{u0}\left(\frac{T_u}{T_0}\right)^{\alpha}\left(\frac{p}{p_0}\right)^{\beta}$$

where S_u is the laminar burning velocity (m/s), T_u is the unburned temperature (K), $T_0 = 298$ K, p is pressure (atm), $p_0 = 1$ atm, S_{u0}, α, and β are constants.

The model used in this study was verified by comparing the burning velocity in this study with the predicted values by Liu et al. [6], Duynslaegher et al. [17], and the measurement values by Rooney [12], Pfahl et al. [29], Jabbour et al. [30], and Takizawa et al. [31], which is shown in Fig. 1. A strong difference between the calculated and measured results is shown in Fig. 1, mainly because there is no heat loss (adiabatic flame temperature) in the simulation results. The laminar burning velocities calculated in this study based on the Reductive Konnov mechanism [17] were consistent with the previously predicted values, which confirm that the selected mechanisms provide an acceptable and repeatable result for NH_3 combustion. All the simulation results presented in the remainder of the paper were obtained using the Reductive Konnov mechanism.

The effect of O_2 content in the combustion air on the laminar burning velocity and adiabatic flame temperature are shown in Figs. 2 and 3, respectively. O_2-enriched combustion positively affects the laminar burning velocity of NH_3 and enhances the adiabatic flame temperature. The laminar burning velocity increases with an increase in the O_2 content and may be enhanced to the level