行政院國家科學委員會專題研究計畫 成果報告

過氧化氫輔助次極限貧油燃燒之實驗與數值研究
研究成果報告(精簡版)

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過氧化氫輔助次極限貧油燃燒之實驗與數值研究
Experimental and Numerical Investigations of Hydrogen Peroxide Assisted Sub-lean Limit Combustion

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行政院國家科學委員會99年度專題研究計畫成果報告

過氧化氫輔助次極限貧油燃燒之實驗與數值研究
Experimental and Numerical Investigations of Hydrogen Peroxide Assisted Sub-lean Limit Combustion

1. 摘要

本計畫主要是以發展應用過氧化氫作為反應的促進劑或取代空氣當作氧化劑，輔助次極限貧油燃燒，進而達到節能與降低污染物生成的目標。由於目前正在使用之工業燃燒爐、渦輪引擎燃燒室、內燃機引擎等燃燒器之設計尚無法完全採用次極限貧油燃燒，因此，利用高濃度過氧化氫的特性來輔助燃燒，使其達到次極限貧油燃燒的操作條件是一值得研究的主題。因此，本計畫將以實驗與數值方法分年研究過氧化氫作為燃料添加劑或氧化劑對貧油燃燒特性之影響。本年度的工作將利用 CHEMKIN Collection 軟體結合 GRI-Mech 3.0 完整化學反應機構，探討添加過氧化氫對化學反應路徑、層流燃燒速度、火焰結構及污染生成之影響。本計畫有關實驗部分原安排於第 2 及第 3 年，惟因計畫僅核准一年，故本報告將僅呈現第 1 年之數值研究成果。

關鍵字：過氧化氫、次極限貧油燃燒、觸媒分解、數值模擬

2. Abstract

The main objective of this research project is to employ the purified hydrogen peroxide (H_2O_2) as a reaction stimulator or oxidizer for assisting sub-lean limit combustion and to achieve the goal of energy savings and pollutant reductions. However, the applications of hydrogen peroxide assisted sub-lean limit combustion to practical combustion systems strongly rely on fundamental understanding of the characteristics of hydrogen peroxide combustion. The main focus of the present proposal is to thoroughly investigate the detailed chemical kinetics, flame stability limits, flame structures, and pollutant formation mechanisms of hydrogen peroxide assisted lean combustion through experimental investigations and numerical simulations. The work of this year is to numerically investigate the effects of hydrogen peroxide addition on the reaction path, laminar burning velocity, flame structure, and pollutant formation using the CHEMKIN Collection in conjunction with GRI-Mech 3.0 chemical kinetic mechanisms. Experimental investigations will be performed in the second and third years.
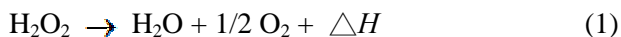
Keywords: Hydrogen peroxide, Sub-lean limit combustion, Catalytic decomposition, Numerical simulation

3. Introduction

Lean combustion is generally considered as one of the timely solutions for the more stringent environmental regulations and global warming concerns in the new century. However, lean combustion suffers from combustion instability, such as flame pulsation, flame flickering and blowout, due to low heat release rate and high local extinction. In addition, it is generally accompanied with incomplete combustion with high CO and UHC (unburned hydrocarbon) emissions in most lean combustion applications. Therefore, the key problem for lean combustion applications is to enhance combustion for flame stabilization and for complete combustion to avoid high CO and UHC emissions [1-2]. Some strategies for stabilizing lean premixed flames and extending lean flammability limit have been proposed and extensively studied for decades [1-3]. Particularly, feasible and pragmatic approaches to extend lean flammability limit can be roughly summarized into three categories: (i) flow structure adjustment [3-5], (ii) increase in temperature and pressure of flow fields [6-8], and (iii) alteration in flame chemical properties [9-14]. Utilizing swirler and bluff body to generate recirculation zone for enhancing flow residence time and fuel-air mixing is a promising

manner by means of flow structures modification. Heat exchanger, flue gas recirculation mechanism as well as turbocharger are generally applied in engines and furnaces to enhance temperature and pressure in the flow field, and to extend flammability limits. As to chemical characteristics alteration in flames, employing catalyst to accelerate chemical reaction [7, 9] and inducing active chemical radicals (H, OH) by imposing microwave [10] or plasma [11] in the flame have received increasing attention recently. Nevertheless, these approaches generally have to further assemble extra mechanical auxiliaries and modify combustor configuration, so that thorough mechanical retrofit design and accurate fabrication are necessitated.

Employing active fuels (such as hydrogen, [12, 13]) or adding strong oxidants [14] to fuels is an attractive alternative to enhance lean flame combustion without involving any moving part or configuration modification. Hydrogen peroxide (H_2O_2) is an environmentally friendly oxidant with strong oxidability. The oxidizing power of hydrogen peroxide is just inferior to that of fluorine [15], which has the strongest electronegativity in the periodic table. Hydrogen peroxide under normal temperature is in liquid state, so that it is easy to store and handle. After chemical dissociation, hydrogen peroxide produces only oxygen and steam, and plus exothermicity (approximately 2884.6 kJ/kg) without toxic products. The decomposition reaction may be facilitated by heating or using catalyst and it is defined as:

$$H_2O_2 \rightarrow H_2O + 1/2\ O_2 + \triangle H \qquad (1)$$

When temperature achieves $450℃$, hydrogen peroxide will decompose with fierce exothermic heat release. Due to its inherently high decomposition temperature and high energy release, hydrogen peroxide with high concentration is often considered as a monopropellant [16]. It can also combine with hydrocarbon fuels to be bipropellants [17]. As to combustion applications, hydrogen peroxide can be used to replace air for reducing NO_x emission and increasing combustion temperature.

A few recent studies have indicated potential promises in utilizing hydrogen peroxide for improving practical combustion process. Golovitchev et al. [18] examined the possibility of promoting methane auto-ignition in air using 5-10% hydrogen peroxide. Ting and Reader [19] used PREMIX code to investigate the effects of hydrogen peroxide on the premixed methane-air flame under atmospheric conditions. The maximum hydrogen peroxide concentration used to replace air was 6.25%. Hydrogen peroxide was found to be effective in enhancing the burning velocity, and this was particularly true for the richer mixtures considered. Kim et al. [20] discovered that hydrogen peroxide assisted the conversion of harmful nitric oxide to nitrogen dioxide in diesel exhaust gas. In addition, Born and Peters [21] found that proper injection of hydrogen peroxide into a diesel engine reduced soot and NO_x drastically. Martinez et al. [22] reported that the concentrations of UHC, CO and NO_x from their industrial pilot plant combustion chamber fueled with natural gas were lowered significantly by injection of a few hundred ppm of hydrogen peroxide. Based on the above studies, promotion to stable lean combustion seems effective with the addition of hydrogen peroxide than that with hydrogen. Hydrogen is usually considered as an easily ignitable fuel and helpful for enhancing combustion. Nevertheless, hydrogen peroxide was also shown to act as a gas catalyst, to shift chemical pathways, and to further enhance chemical radicals [18].
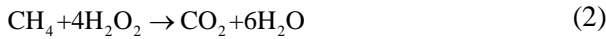
Although the effects of hydrogen peroxide on combustion enhancement have been reported, systematic studies of the roles of hydrogen peroxide in combustion enhancement have not yet been conducted. Therefore, in the present study, the effects of hydrogen peroxide on premixed methane/air reaction pathway, laminar burning velocity, adiabatic flame temperature, and species formation are investigated numerically using the PREMIX code of Chemkin collection 3.5 with the GRI-Mech 3.0 chemical kinetic mechanisms [23] and detailed transport properties.

4. Numerical model

In this work, the PREMIX code of CHEMKIN Collection is used to calculate the adiabatic, unstrained, free propagation velocities of the laminar premixed $CH_4/air/H_2O_2$ flames. It solves the equations governing steady, isobaric, quasi-one-dimensional flame propagation. To obtain the accurate flame speed, the boundaries should be sufficiently far from the flame to avoid temperature and species gradients at the boundaries. Firstly, an initial run is performed with a computational domain just wide enough to encompass the flame. Then, the domain is gradually expanded until the solution is domain-independent. In addition, the adiabatic flame temperature is calculated by using the EQUIL code of the Chemkin Collection. An initial reactant mixture is specified and equilibrium of constant enthalpy and constant pressure is constrained. To obtain accurate adiabatic flame temperature, besides reactants and products, all radical species that might occur in the flame are also included.

The GRI-Mech 3.0 chemical kinetic

mechanism composing of 53 chemical species and 325 reaction steps and detailed transport properties are used without any modifications. The reaction mechanism also includes the formation of NO_x. This mechanism has been used satisfactorily to simulate non-catalytic H_2O_2 decomposition [24]. At the cold boundary, the unburned reactants are supplied at 423 K and 1 atm. This temperature presets at the boiling temperature of H_2O_2 and it is expected that all reactants are in gas phase. To further study into the role of hydrogen peroxide in the combustion enhancement of premixed methane flames, numerical simulations are performed for two different characteristic types of hydrogen peroxide addition: (1) as the oxidizer substituent by partial replacement of air (2) as the oxidizer supplier by using different concentrations of H_2O_2. Decomposition of one mole H_2O_2 can produce half mole O_2 and one mole H_2O. Therefore, the stoichiometric CH_4/H_2O_2 ratio is 0.25 and the global reaction is defined as:

$$CH_4 + 4H_2O_2 \rightarrow CO_2 + 6H_2O \qquad (2)$$

In the case of partially replacing air by H_2O_2, the total O_2 amount is maintained to keep the equivalence ratio constant. Therefore, the reduced amount of O_2 from air is supplied from the decomposition of H_2O_2. For a stoichiometric condition, the reaction is defined as:

$$CH_4 + 4\alpha H_2O_2 + (2-2\alpha)(O_2 + 3.76N_2) \rightarrow CO_2 + (4\alpha+2)H_2O + \\ 3.76(2-2\alpha)N_2 \qquad (3)$$
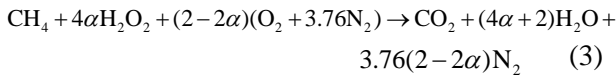
where α is the replacement percentage of air by H_2O_2. The reduction of air leads to reduction of N_2 in the oxidizer stream. For cases of using H_2O_2 as the oxidizer, the volumetric concentration of H_2O_2 is considered ranging from 30% to 100%.

5. Results and Discussion

5.1 Effects of H_2O_2 on combustion characteristics

In order to examine the effects of H_2O_2 on enhancement of premixed methane flames and to study further into the modification of combustion characteristics, the results of premixed stoichiometric CH_4/air and CH_4/80% air + 20% H_2O_2 are compared for illustration. The spatial coordinate ranges from cold boundary to 0.4 cm within the flame. The resultant temperature and species concentration profiles are shown in Fig. 1. Results indicate that the premixed flame with 20% air replaced by hydrogen peroxide has a higher adiabatic flame temperature due to the reduction of nitrogen dilution and heat release from thermal decomposition of hydrogen peroxide. The temperature increases approximately by 140 K as compared to the pure air case. For pure air case, the reactant CH_4 is completely consumed within 1.0 mm of the spatial coordinate but 0.85 mm for the 20% H_2O_2 replacement case. Hydrogen peroxide dedicates to enhance the methane consumption. In addition, the increase of H_2O_2 content in air obviously results in an increase of H_2O production due to the product of H_2O_2 decomposition. It appears to slightly decrease CO_2 formation and increase CO formation. Besides, some intermediate radicals, such as OH, H and O, show increasing trends with hydrogen peroxide addition. Especially, the increasing trends of HO_2, HCO, CH_2O and CH_3O are more significant. These facts suggest that the dominant reactions of methane combustion are altered by H_2O_2 addition. Hydrogen peroxide decomposition increases the active radicals, enhances the reaction rate, and then accelerates the laminar burning velocity. The computed laminar burning velocity of stoichiometric CH_4/air with the inlet temperature 423 K is about 0.71m/s, while the flame speed is increased to about 1.25 m/s when 20% air is replaced by H_2O_2.
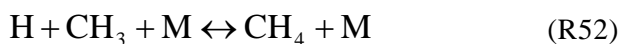
5.2 Laminar burning velocity

Figure 2 shows the effect of partial replacement of air by H_2O_2 on the laminar burning velocity and adiabatic flame temperature for three different equivalence ratios (ER). The maximum percentage of air replaced by H_2O_2 is 100%. It can be seen that the laminar burning velocity is increased with increasing the equivalence ratio and the percentage of hydrogen peroxide replacement. However, the effect of equivalence ratio on flame speed becomes mild for high hydrogen peroxide replacement percentage cases. When air is completely replaced by H_2O_2, the laminar burning velocity approaches 4.7 m/s for all equivalence ratio conditions. This is because that the oxidizer is completely provided from decomposition of hydrogen peroxide and hydrogen peroxide dominates the reaction rate of methane oxidation. Figure 2 also shows that the adiabatic flame temperature increases with increasing the percentage of H_2O_2 replacement. The temperature increase for fuel lean conditions is larger than that for stoichiometric condition. The maximum temperature increase is up to 900 K for ER = 0.6, but 680 K and 520 K for ER = 0.8 and 1.0, respectively. The effect of temperature increase is primarily induced from the heat release of hydrogen peroxide decomposition since it is much higher than that released from methane reactions. Table 1 shows the maximum heat release rates (HRR) for different reactant conditions. The maximum heat release rates are about 6.09×10^9 J/m³-s and 1.04×10^9 J/m³-s for ER = 1.0 and 0.6 CH_4/air flames, respectively. For the case of CH_4/50% H_2O_2 + 50% air the

maximum heat release rates are about 5.42×10^{10} J/m^3-s and 2.77×10^{10} J/m^3-s for ER = 1.0 and 0.6, respectively. Similarly, when air is completely replaced by H_2O_2, the maximum heat release rate approaches 4.49×10^{11} J/m^3-s and 4.37×10^{11} J/m^3-s, respectively. From Table 1 it is also noted that equivalence ratio contributes less significantly to the maximum heat release rate when air is replaced or partially replaced by hydrogen peroxide, but their HRR values are two orders of magnitude higher than that for CH$_4$/air case. This "orders of magnitude" difference comes from hydrogen peroxide decomposition. It proves that the decomposition of H_2O_2 dominates the heat release and then determines the adiabatic flame temperature.

To investigate the characteristics of CH$_4$/H$_2$O$_2$ flames, the volumetric concentration of H_2O_2 is varied from 30 to 100% while ER is kept at 0.6, 0.8, and 1.0. Figure 3 shows the laminar burning velocity and adiabatic flame temperature of the CH$_4$/H$_2$O$_2$ flames with ER = 0.6, 0.8, and 1.0. Results show that both laminar burning velocity and adiabatic flame temperature increase with increasing H_2O_2 concentration. With 30 vol.% of H_2O_2 the laminar burning velocity is higher than that of CH$_4$/air flame for three different equivalence ratios, but the adiabatic flame temperature is lower than that of CH$_4$/air flame. For the case of ER = 1.0 the temperature difference between two cases is about 250 K. However, for the case of ER = 0.6, the adiabatic flame temperature is almost the same as that of CH$_4$/air flame and the temperature difference is only 10 K. In addition, the laminar burning velocity is increased to 0.63 m/s, which is much higher than that of CH$_4$/air flame (0.27 m/s). When the H_2O_2 concentration is increased to 40 vol.%, the adiabatic flame temperature is higher than that of pure CH$_4$/air flame for three different equivalence ratios. Comparisons of Fig. 2 and Fig. 3 suggest that using H_2O_2 with various concentrations as an oxidizer the role of fuel equivalence ratio on the laminar burning velocity and adiabatic flame temperature becomes less important.

In order to understand the effect of chemical reaction on the flame speed of CH$_4$/air/H$_2$O$_2$ flames, the first-order sensitivity analysis of laminar burning velocity is shown in Fig. 4 for different reactant compositions at stoichiometric condition. In the case of pure air, the dominant reactions for laminar burning velocity are,

$$O_2 + H \leftrightarrow O + OH \qquad (R38)$$

$$H + CH_3 + M \leftrightarrow CH_4 + M \qquad (R52)$$

$$OH + CO \leftrightarrow H + CO_2 \qquad (R99)$$

For the hydrogen peroxide replacement cases, the dominant reactions shift to the following chemical steps:

$$O_2 + H \leftrightarrow O + OH \qquad (R38)$$

$$2OH + M \leftrightarrow H_2O_2 + M \qquad (R85)$$

$$OH + H_2O_2 \leftrightarrow HO_2 + H_2O \qquad (R89)$$

$$OH + CH_4 \leftrightarrow CH_3 + H_2O \qquad (R98)$$
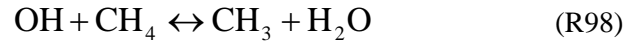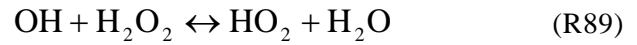
Among these reactions, (R85) and (R89) are the most important chemical reactions, so that hydrogen peroxide modifies the reaction pathway, and significantly enhances the reaction rate leading to flame speed enhancement.

6. Conclusions

In the present study, the effects of hydrogen peroxide on methane/air premixed flames are systemically and numerically investigated under the atmosphere condition with GRI-Mech 3.0 mechanism. Hydrogen peroxide is used as the oxidizer for two different conditions: (1) replacing partial air by H_2O_2 and (2) using H_2O_2 as an oxidizer but with different concentrations. Especially, the characteristics of laminar burning velocity, adiabatic flame temperature and species concentration are studied. The following findings are obtained from this study.

1. The laminar burning velocities and the adiabatic temperature are obviously increased with the addition of H_2O_2. When air is completely replaced by H_2O_2, the laminar burning velocity is almost not affected by the equivalence ratio. The decomposition of H_2O_2 dominates the net heat release rate and then affects the adiabatic flame temperature.

2. When the concentration of H_2O_2 increases, the dominant reactions for laminar burning velocity are shifted. Hydrogen peroxide affects the reaction pathway, enhances the reaction rate, and then increases the flame speed.

3. Hydrogen peroxide affects the species concentration and production/consumption rate. CH$_4$ are completely consumed more upstream as H_2O_2 is added. H_2O_2 addition increases H_2O concentration. However, CO emission is increased and CO$_2$ concentration is decreased. Using H_2O_2 with a lower concentration will help to control CO emission.

4. When air is partial replaced by H_2O_2, N$_2$ reactant concentration is decreased. However, H_2O_2 enrichment enhances NO production reaction and NO emission concentration is increased due to the high flame temperature.

4

7. Self Evaluation

In this project, numerical investigations of the effects of hydrogen peroxide addition on the reaction path, laminar burning velocity, flame structure, and pollutant formation have been made as they were proposed in the proposal. Numerical simulations used the CHEMKIN Collection in conjunction with GRI-Mech 3.0 chemical kinetic mechanisms. Results of this year's research have been published in International Journal of Hydrogen Energy (see Appendix). Experimental investigations will be performed in the second and third years.

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Table 1 Maximum Heat release rate for different reactant conditions

Reactant	HRR(J/m³-s) (ER = 1)	HRR(J/m³-s) (ER = 0.6)
CH_4/air	6.09×10^9	1.04×10^9
CH_4/50% H_2O_2 + 50% air	5.42×10^{10}	2.77×10^{10}
CH_4/50% H_2O_2 + 50% H_2O	7.38×10^{10}	5.27×10^{10}
CH_4/H_2O_2	4.49×10^{11}	4.37×10^{11}

(b) CH_4/80% air/20% H_2O_2.

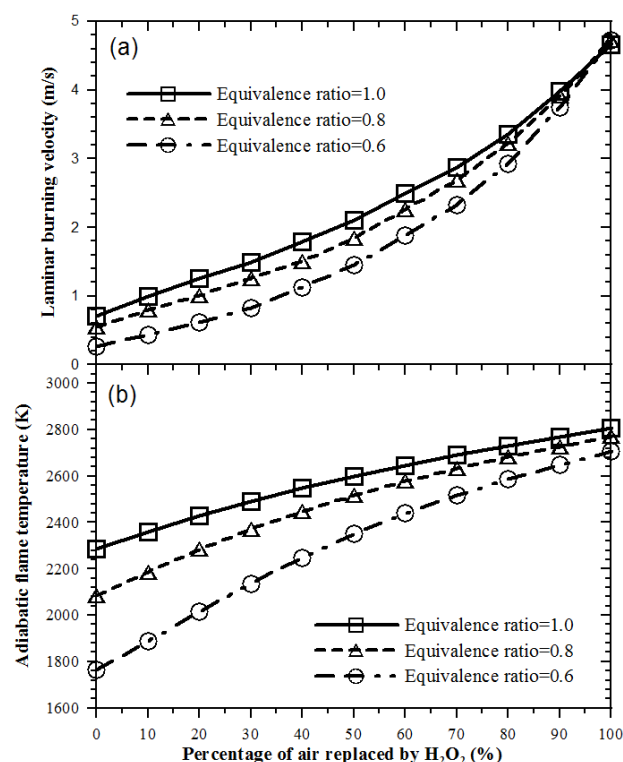Fig. 1. Profiles of temperature and species concentration of stoichiometric CH_4/air/H_2O_2 flames. (a) CH_4/100% air.

Fig. 2. Computed laminar burning velocity and adiabatic flame temperature of methane/air flames with different percentages of air replaced by H_2O_2.
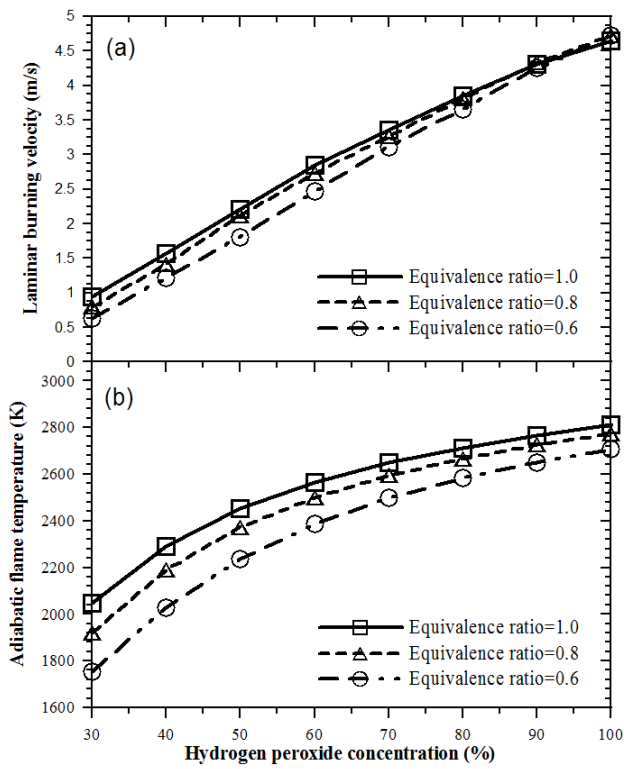
Fig. 3. Computed laminar burning velocity and adiabatic flame temperature of methane/H_2O_2 flames with various H_2O_2 concentrations.
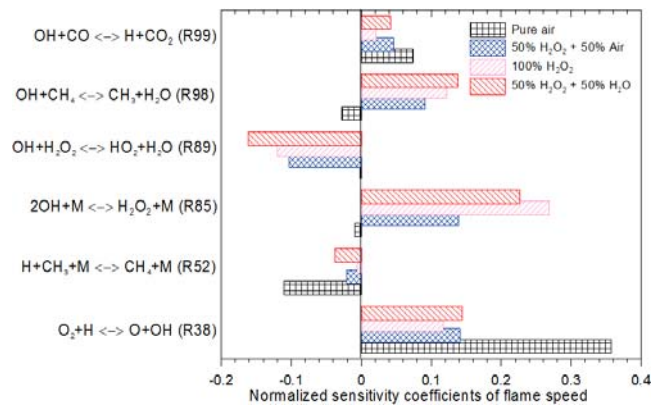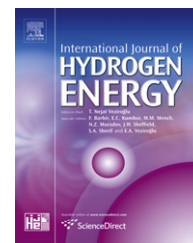

Fig. 4. Sensitivity analysis of laminar burning velocity for CH_4/air/H_2O_2 flames (ER = 1.0).

Appendix

Effects of hydrogen peroxide on combustion enhancement of premixed methane/air flames

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ABSTRACT

Hydrogen peroxide is generally considered to be an effective combustion promoter for different fuels. The effects of hydrogen peroxide on the combustion enhancement of premixed methane/air flames are investigated numerically using the PREMIX code of Chemkin collection 3.5 with the GRI-Mech 3.0 chemical kinetic mechanisms and detailed transport properties. To study into the enhancement behavior, hydrogen peroxide is used for two different conditions: (1) as the oxidizer substituent by partial replacement of air and (2) as the oxidizer supplier by using different concentrations of H_2O_2. Results show that the laminar burning velocity and adiabatic flame temperature of methane flame are significantly enhanced with H_2O_2 addition. Besides, the addition of H_2O_2 increases the CH_4 consumption rate and CO production rate, but reduces CO_2 productions. Nevertheless, using a lower volumetric concentration of H_2O_2 as an oxidizer is prone to reduce CO formation. The OH concentration is increased with increasing H_2O_2 addition due to apparent shifting of major reaction pathways. The increase of OH concentration significantly enhances the reaction rate leading to enhanced laminar burning velocity and combustion. As to NO emission, using H_2O_2 as an oxidizer will never produce NO, but NO emission will increase due to enhanced flame temperature when air is partially replaced by H_2O_2.

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1. Introduction

Lean combustion is generally considered as one of the timely solutions for the more stringent environmental regulations and global warming concerns in the new century. However, lean combustion suffers from combustion instability, such as flame pulsation, flame flickering and blowout, due to low heat release rate and high local extinction. In addition, it is generally accompanied with incomplete combustion with high CO and UHC (unburned hydrocarbon) emissions in most lean combustion applications. Therefore, the key problem for lean combustion applications is to enhance combustion for flame stabilization and for complete combustion to avoid high CO and UHC emissions [1,2]. Some strategies for stabilizing

lean premixed flames and extending lean flammability limit have been proposed and extensively studied for decades [1–3]. Particularly, feasible and pragmatic approaches to extend lean flammability limit can be roughly summarized into three categories: (i) flow structure adjustment [3–5], (ii) increase in temperature and pressure of flow fields [6–8], and (iii) alteration in flame chemical properties [9–14]. Utilizing swirler and bluff body to generate recirculation zone for enhancing flow residence time and fuel-air mixing is a promising manner by means of flow structures modification. Heat exchanger, flue gas recirculation mechanism as well as turbocharger are generally applied in engines and furnaces to enhance temperature and pressure in the flow field, and to extend flammability limits. As to chemical characteristics alteration in flames, employing catalyst to accelerate chemical reaction [7,9–11] and inducing active chemical radicals (H, OH) by imposing microwave [12] or plasma [13] in the flame have received increasing attention recently. Nevertheless, these approaches generally have to further assemble extra mechanical auxiliaries and modify combustor configuration, so that thorough mechanical retrofit design and accurate fabrication are necessitated.

Employing active fuels (such as hydrogen [14–16],) or adding strong oxidants [17] to fuels is an attractive alternative to enhance lean flame combustion without involving any moving part or configuration modification. Hydrogen peroxide (H_2O_2) is an environmentally friendly oxidant with strong oxidability. The oxidizing power of hydrogen peroxide is just inferior to that of fluorine [18], which has the strongest electronegativity in the periodic table. Hydrogen peroxide under normal temperature is in liquid state, so that it is easy to store and handle. After chemical dissociation, hydrogen peroxide produces only oxygen and steam, and plus exothermicity (approximately 2884.6 kJ/kg) without toxic products. The decomposition reaction may be facilitated by heating or using catalyst and it is defined as:

$$H_2O_2 \rightarrow H_2O + 1/2\,O_2 + \Delta H \tag{1}$$

When temperature achieves 450 °C, hydrogen peroxide will decompose with fierce exothermic heat release. Due to its inherently high decomposition temperature and high energy release, hydrogen peroxide with high concentration is often considered as a monopropellant [19]. It can also combine with hydrocarbon fuels to be bipropellants [20]. As to combustion applications, hydrogen peroxide can be used to replace air for reducing NO_x emission and increasing combustion temperature.

A few recent studies have indicated potential promises in utilizing hydrogen peroxide for improving practical combustion process. Golovitchev et al. [21] examined the possibility of promoting methane auto-ignition in air using 5–10% hydrogen peroxide. Ting and Reader [22] used PREMIX code to investigate the effects of hydrogen peroxide on the premixed methane-air flame under atmospheric conditions. The maximum hydrogen peroxide concentration used to replace air was 6.25%. Hydrogen peroxide was found to be effective in enhancing the burning velocity, and this was particularly true for the richer mixtures considered. Kim et al. [23] discovered that hydrogen peroxide assisted the conversion of harmful nitric oxide to nitrogen dioxide in
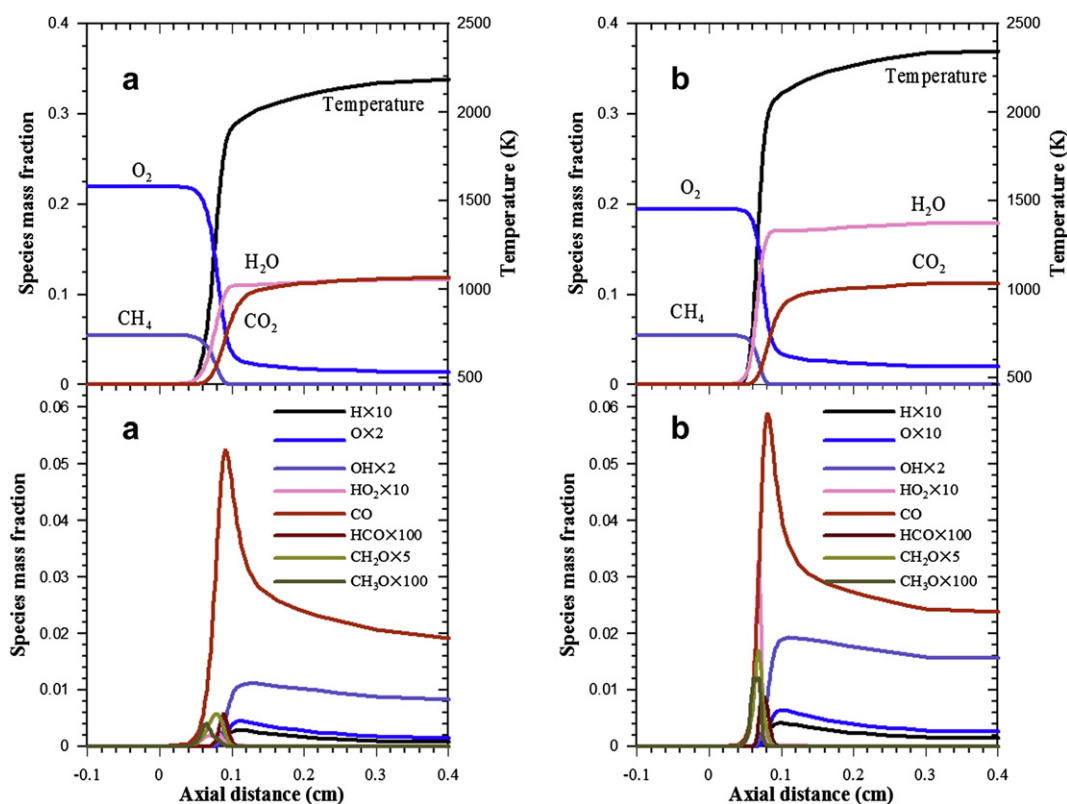

Fig. 1 – Profiles of temperature and species concentration of stoichiometric $CH_4/air/H_2O_2$ flames. (a) CH_4/100% air, (b) CH_4/80% air/20% H_2O_2.
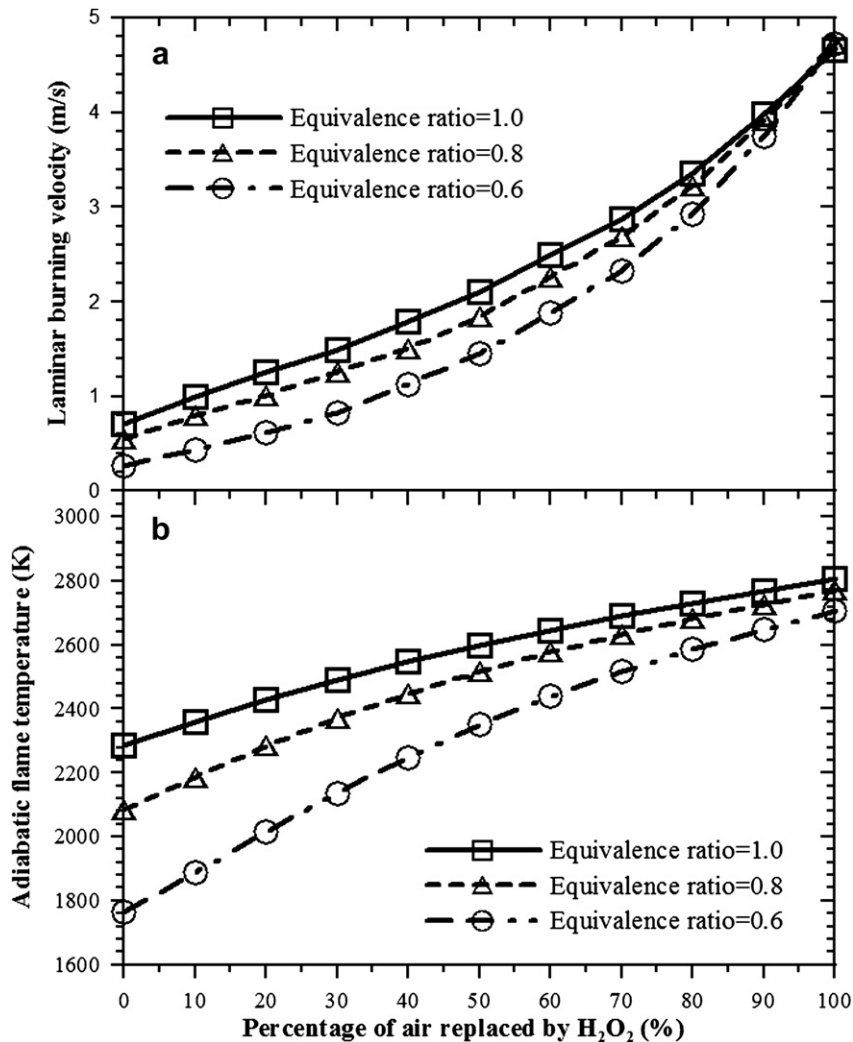
Fig. 2 – Computed laminar burning velocity and adiabatic flame temperature of methane/air flames with different percentages of air replaced by H₂O₂.

diesel exhaust gas. In addition, Born and Peters [24] found that proper injection of hydrogen peroxide into a diesel engine reduced soot and NO_x drastically. Martinez et al. [25] reported that the concentrations of UHC, CO and NO_x from their industrial pilot plant combustion chamber fueled with natural gas were lowered significantly by injection of a few hundred ppm of hydrogen peroxide. Based on the above studies, promotion to stable lean combustion seems effective with the addition of hydrogen peroxide than that with hydrogen. Hydrogen is usually considered as an easily ignitable fuel and helpful for enhancing combustion. Nevertheless, hydrogen peroxide was also shown to act as a gas catalyst, to shift chemical pathways, and to further enhance chemical radicals [21].

Although the effects of hydrogen peroxide on combustion enhancement have been reported, systematic studies of the roles of hydrogen peroxide in combustion enhancement have not yet been conducted. Therefore, in the present study, the effects of hydrogen peroxide on premixed methane/air reaction pathway, laminar burning velocity, adiabatic flame temperature, and species formation are investigated

numerically using the PREMIX code of Chemkin collection 3.5 with the GRI-Mech 3.0 chemical kinetic mechanisms [26] and detailed transport properties.

2.   Numerical model and chemical mechanism

In this work, the PREMIX code of CHEMKIN Collection is used to calculate the adiabatic, unstrained, free propagation velocities of the laminar premixed CH_4/air/H_2O_2 flames. It solves the equations governing steady, isobaric, quasi-one-dimensional flame propagation. The equations are written as follows:

$$\text{Continuity}: \dot{M} = \rho u A \tag{2}$$

$$\text{Energy}: \dot{M}\frac{dT}{dx} - \frac{1}{C_p}\frac{d}{dx}\left(\lambda A\frac{dT}{dx}\right) + \frac{A}{C_p}\sum_{k=1}^{K}\dot{w}_k h_k W_k = 0 \tag{3}$$

Table 1 – Maximum Heat release rate for different reactant conditions.

Reactant	HRR (J/m^3-s) (ER = 1)	HRR (J/m^3-s) (ER = 0.6)
CH$_4$/air	6.09×10^9	1.04×10^9
CH$_4$/50% H$_2$O$_2$ + 50% air	5.42×10^{10}	2.77×10^{10}
CH$_4$/50% H$_2$O$_2$ + 50% H$_2$O	7.38×10^{10}	5.27×10^{10}
CH$_4$/H$_2$O$_2$	4.49×10^{11}	4.37×10^{11}

$$\text{Species}: \dot{M}\frac{dY_k}{dx} + \frac{d}{dx}(\rho AY_kV_k) + A\dot{w}_kW_k = 0 \ (k = 1, ..., K_g) \quad (4)$$

$$\text{Equation of state}: \rho = \frac{P\overline{W}}{RT} \quad (5)$$

In these equations, x denotes the spatial coordinate, $\dot{M}$ is the mass flow rate, ρ is the fluid density, u is the fluid velocity, A is the cross-section of the stream tube encompassing the flame normalized by the burner area, T is the temperature, λ is the thermal conductivity of the mixture, $\dot{w}_k$ is the molar production rate of the kth species, h_k is the specific enthalpy of the k_{th} species, W_k is the molecular weight of the k_{th} species, Y_k is the mass fraction of the k_{th} species, V_k is the diffusion velocity of the k_{th} species, and P is the pressure.
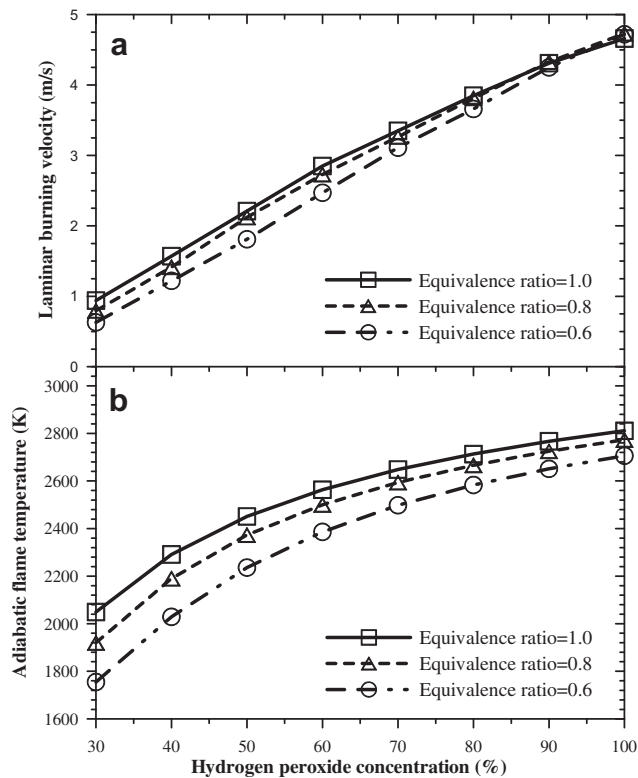

Fig. 3 – **Computed laminar burning velocity and adiabatic flame temperature of methane/H$_2$O$_2$ flames with various H$_2$O$_2$ concentrations.**

For a freely propagation flame, $\dot{M}$ is an eigenvalue and must be determined as part of the solution. The initial guess is set to be 0.04 g/cm^3/s. An additional constraint is required and a flame-fixed coordinate system is established by fixing the temperature at 500 K. To obtain the accurate flame speed, the boundaries should be sufficiently far from the flame to avoid temperature and species gradients at the boundaries. Firstly, an initial run is performed with a computational domain just wide enough to encompass the flame. Then, the domain is gradually expanded until the solution is domain-independent. In addition, the adiabatic flame temperature is calculated by using the EQUIL code of the Chemkin Collection. An initial reactant mixture is specified and equilibrium of constant enthalpy and constant pressure is constrained. To obtain accurate adiabatic flame temperature, besides reactants and products, all radical species that might occur in the flame are also included.

The GRI-Mech 3.0 chemical kinetic mechanism composing of 53 chemical species and 325 reaction steps and detailed transport properties are used without any modifications. The reaction mechanism also includes the formation of NO$_x$. This mechanism has been used satisfactorily to simulate non-catalytic H$_2$O$_2$ decomposition [27]. The reaction rate constant is represented by the modified Arrhenius expression,

$$k = \overline{A}T^b\exp\left(\frac{-E_a}{RT}\right) \quad (6)$$

where $\overline{A}$ is the pre-exponential factor, b is the temperature exponent, and E_a is the activation energy. The chemical kinetics with CHEMKIN format is used in the code. Details of the chemical reaction rate formulation and CHEMKIN format can be found in the user's manual [28].

At the cold boundary, the unburned reactants are supplied at 423 K and 1 atm. This temperature presets at the boiling temperature of H$_2$O$_2$ and it is expected that all reactants are in gas phase. To further study into the role of hydrogen peroxide in the combustion enhancement of premixed methane flames, numerical simulations are performed for two different characteristic types of hydrogen peroxide addition: (1) as the oxidizer substituent by partial replacement of air (2) as the oxidizer supplier by using different concentrations of H$_2$O$_2$. Decomposition of 1 mol H$_2$O$_2$ can produce half mole O$_2$ and 1 mol H$_2$O. Therefore, the stoichiometric CH$_4$/H$_2$O$_2$ ratio is 0.25 and the global reaction is defined as:

$$CH_4 + 4H_2O_2 \rightarrow CO_2 + 6H_2O \quad (7)$$

In the case of partially replacing air by H$_2$O$_2$, the total O$_2$ amount is maintained to keep the equivalence ratio constant. Therefore, the reduced amount of O$_2$ from air is supplied from the decomposition of H$_2$O$_2$. For a stoichiometric condition, the reaction is defined as:

$$CH_4 + 4\alpha H_2O_2 + (2 - 2\alpha)(O_2 + 3.76N_2) \rightarrow CO_2 + (4\alpha + 2)H_2O$$
$$+3.76(2 - 2\alpha)N_2 \quad (8)$$
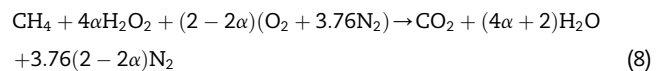
where α is the replacement percentage of air by H$_2$O$_2$. The reduction of air leads to reduction of N$_2$ in the oxidizer stream. For cases of using H$_2$O$_2$ as the oxidizer, the volumetric concentration of H$_2$O$_2$ is considered ranging from 30% to 100%.
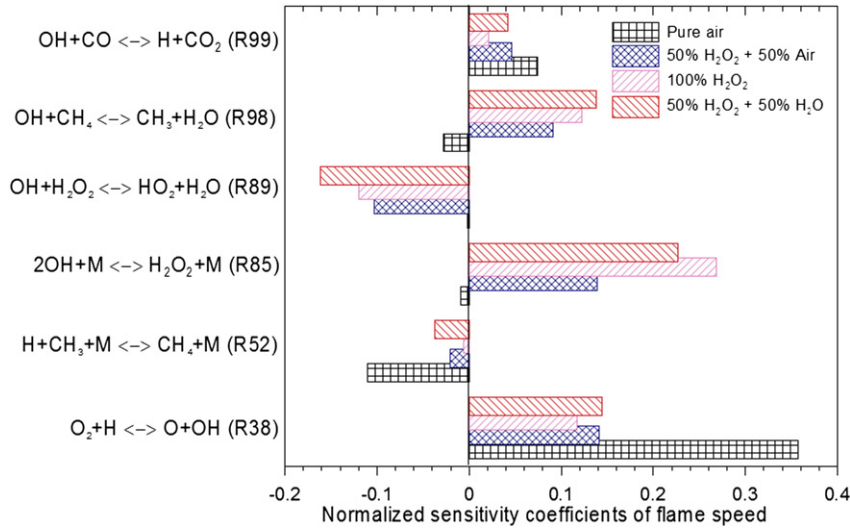
Fig. 4 – Sensitivity analysis of laminar burning velocity for CH$_4$/air/H$_2$O$_2$ flames (ER = 1.0).

3. Results and discussion

3.1. Effects of H$_2$O$_2$ on combustion characteristics

In order to examine the effects of H$_2$O$_2$ on enhancement of premixed methane flames and to study further into the modification of combustion characteristics, the results of premixed stoichiometric CH$_4$/air and CH$_4$/80% air + 20% H$_2$O$_2$ are compared for illustration. The spatial coordinate ranges from cold boundary to 0.4 cm within the flame. The resultant temperature and species concentration profiles

are shown in Fig. 1. Results indicate that the premixed flame with 20% air replaced by hydrogen peroxide has a higher adiabatic flame temperature due to the reduction of nitrogen dilution and heat release from thermal decomposition of hydrogen peroxide. The temperature increases approximately by 140 K as compared to the pure air case. For pure air case, the reactant CH$_4$ is completely consumed within 1.0 mm of the spatial coordinate but 0.85 mm for the 20% H$_2$O$_2$ replacement case. Hydrogen peroxide dedicates to enhance the methane consumption. In addition, the increase of H$_2$O$_2$ content in air obviously results in an increase of H$_2$O production due to the product of H$_2$O$_2$
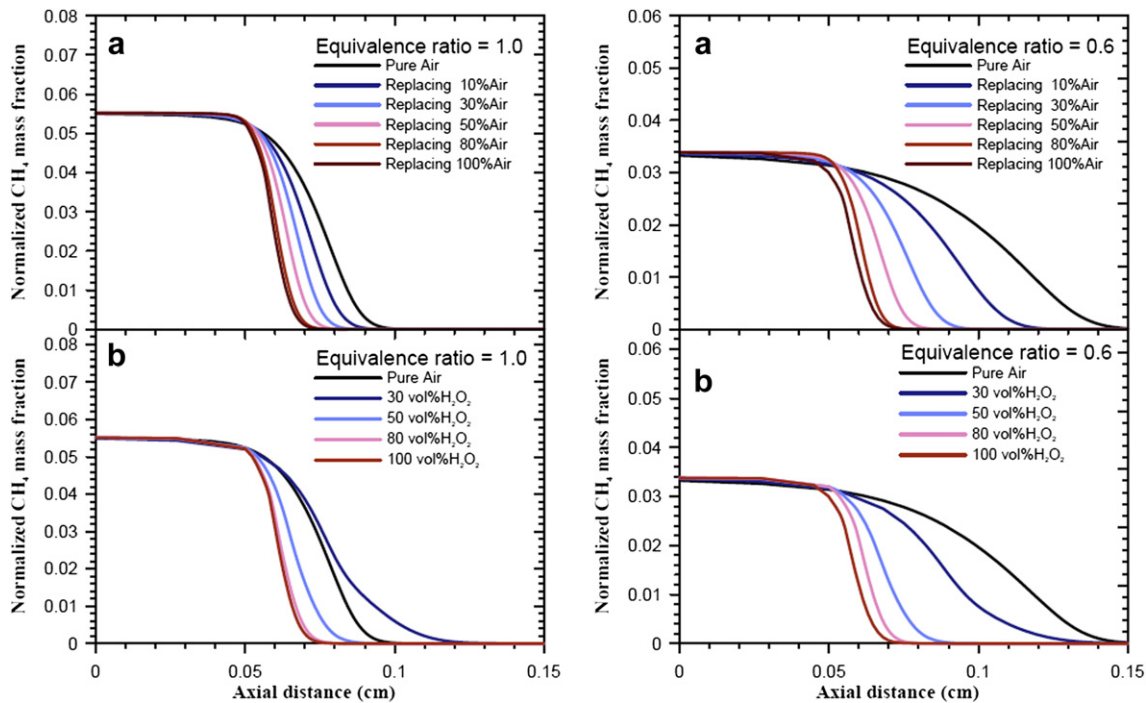

Fig. 5 – Effect of H$_2$O$_2$ on normalized CH$_4$ mass fraction for two cases. (a) replacing partial air by H$_2$O$_2$ and (b) H$_2$O$_2$ as an oxidizer with different concentrations.

decomposition. It appears to slightly decrease CO_2 formation and increase CO formation. Besides, some intermediate radicals, such as OH, H and O, show increasing trends with hydrogen peroxide addition. Especially, the increasing trends of HO_2, HCO, CH_2O and CH_3O are more significant. These facts suggest that the dominant reactions of methane combustion are altered by H_2O_2 addition. Hydrogen peroxide decomposition increases the active radicals, enhances the reaction rate, and then accelerates the laminar burning velocity. The computed laminar burning velocity of stoichiometric CH_4/air with the inlet temperature 423 K is about 0.71 m/s, while the flame speed is increased to about 1.25 m/s when 20% air is replaced by H_2O_2.

3.2. Laminar burning velocity

Fig. 2 shows the effect of partial replacement of air by H_2O_2 on the laminar burning velocity and adiabatic flame temperature for three different equivalence ratios (ER). The maximum percentage of air replaced by H_2O_2 is 100%. It can be seen that the laminar burning velocity is increased with increasing the equivalence ratio and the percentage of hydrogen peroxide replacement. However, the effect of equivalence ratio on flame speed becomes mild for high hydrogen peroxide replacement percentage cases. When air is completely replaced by H_2O_2, the laminar burning velocity approaches 4.7 m/s for all equivalence ratio conditions. This is because that the oxidizer is completely provided from decomposition of hydrogen peroxide and hydrogen peroxide dominates the reaction rate of methane oxidation. Fig. 2 also shows that the adiabatic flame temperature increases with increasing the percentage of H_2O_2 replacement. The

temperature increase for fuel lean conditions is larger than that for stoichiometric condition. The maximum temperature increase is up to 900 K for ER = 0.6, but 680 K and 520 K for ER = 0.8 and 1.0, respectively. The effect of temperature increase is primarily induced from the heat release of hydrogen peroxide decomposition since it is much higher than that released from methane reactions. Table 1 shows the maximum heat release rates (HRR) for different reactant conditions. The maximum heat release rates are about 6.09×10^9 J/m³-s and 1.04×10^9 J/m³-s for ER = 1.0 and 0.6 CH_4/air flames, respectively. For the case of CH_4/50% H_2O_2 + 50% air the maximum heat release rates are about 5.42×10^{10} J/m³-s and 2.77×10^{10} J/m³-s for ER = 1.0 and 0.6, respectively. Similarly, when air is completely replaced by H_2O_2, the maximum heat release rate approaches 4.49×10^{11} J/m³-s and 4.37×10^{11} J/m³-s, respectively. From Table 1 it is also noted that equivalence ratio contributes less significantly to the maximum heat release rate when air is replaced or partially replaced by hydrogen peroxide, but their HRR values are two orders of magnitude higher than that for CH_4/air case. This "orders of magnitude" difference comes from hydrogen peroxide decomposition. It proves that the decomposition of H_2O_2 dominates the heat release and then determines the adiabatic flame temperature.

To investigate the characteristics of CH_4/H_2O_2 flames, the volumetric concentration of H_2O_2 is varied from 30 to 100% while ER is kept at 0.6, 0.8, and 1.0. Fig. 3 shows the laminar burning velocity and adiabatic flame temperature of the CH_4/H_2O_2 flames with ER = 0.6, 0.8, and 1.0. Results show that both laminar burning velocity and adiabatic flame temperature increase with increasing H_2O_2 concentration. With 30 vol.% of H_2O_2 the laminar burning velocity is higher
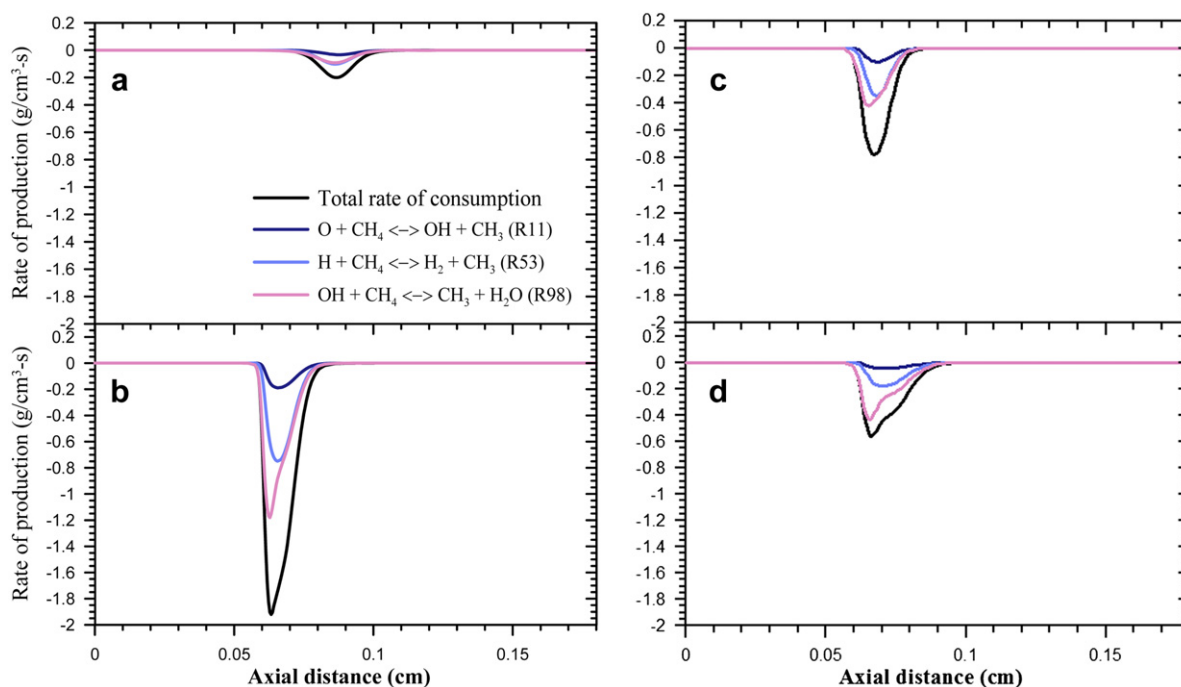

Fig. 6 – Effect of H_2O_2 on normalized CH_4 consumption rate for different reactant conditions. (a) pure air, (b) 100% H_2O_2, (c) 50% air + 50% H_2O_2 and (d) 50% H_2O_2 + 50% H_2O.

than that of CH_4/air flame for three different equivalence ratios, but the adiabatic flame temperature is lower than that of CH_4/air flame. For the case of ER = 1.0 the temperature difference between two cases is about 250 K. However, for the case of ER = 0.6, the adiabatic flame temperature is almost the same as that of CH_4/air flame and the temperature difference is only 10 K. In addition, the laminar burning velocity is increased to 0.63 m/s, which is much higher than that of CH_4/air flame (0.27 m/s). When the H_2O_2 concentration is increased to 40 vol.%, the adiabatic flame temperature is higher than that of pure CH_4/air flame for three different equivalence ratios. Comparisons of Figs. 2 and 3 suggest that using H_2O_2 with various concentrations as an oxidizer the role of fuel equivalence ratio on the laminar burning velocity and adiabatic flame temperature becomes less important.

In order to understand the effect of chemical reaction on the flame speed of CH_4/air/H_2O_2 flames, the first-order sensitivity analysis of laminar burning velocity is shown in Fig. 4 for different reactant compositions at stoichiometric condition. In the case of pure air, the dominant reactions for laminar burning velocity are,

$$O_2 + H \leftrightarrow O + OH \tag{R38}$$

$$H + CH_3 + M \leftrightarrow CH_4 + M \tag{R52}$$

$$OH + CO \leftrightarrow H + CO_2 \tag{R99}$$

For the hydrogen peroxide replacement cases, the dominant reactions shift to the following chemical steps:

$$O_2 + H \leftrightarrow O + OH \tag{R38}$$

$$2OH + M \leftrightarrow H_2O_2 + M \tag{R85}$$

$$OH + H_2O_2 \leftrightarrow HO_2 + H_2O \tag{R89}$$

$$OH + CH_4 \leftrightarrow CH_3 + H_2O \tag{R98}$$

Among these reactions, (R85) and (R89) are the most important chemical reactions. Hydrogen peroxide promotes the product of OH radical, so that hydrogen peroxide modifies the reaction pathway, and significantly enhances the reaction rate leading to flame speed enhancement. The effect of hydrogen peroxide on OH radical is further discussed in the next section.

3.3. Major species and OH radical

The effects of H_2O_2 on the major species and OH radical of the CH_4/air/H_2O_2 premixed flames are investigated. In the study, the CH_4 reactant concentration is changed with different percentages of hydrogen peroxide additions, and it affects the concentration of carbon-related species in the products [29]. Normalization of concentration of the carbon-related species is performed to eliminate this problem by the following formula,
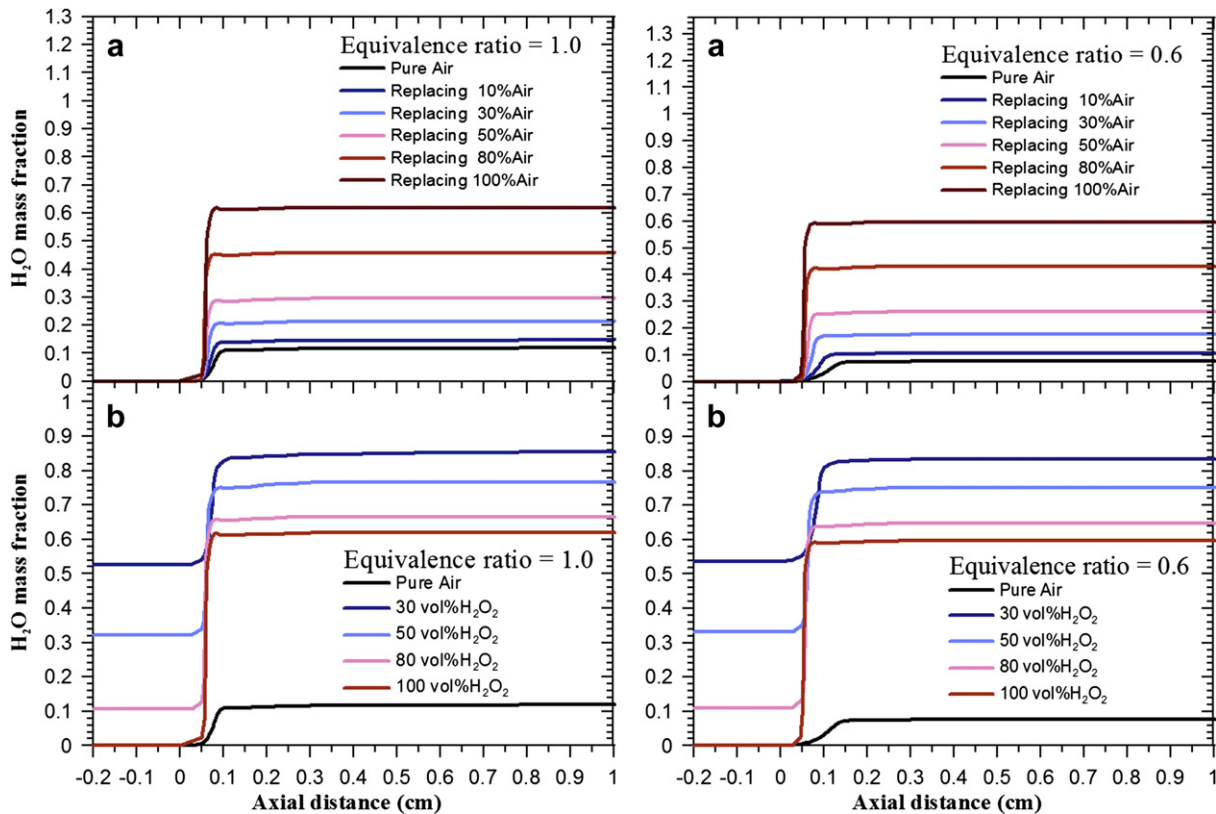

Fig. 7 – Effect of H_2O_2 on H_2O mass fraction for two cases. (a) replacing partial air by H_2O_2 and (b) H_2O_2 as oxidizer with different concentrations.

Fig. 8 – Effect of H_2O_2 on normalized CO_2 mass fraction for two cases. (a) replacing partial air by H_2O_2 and (b) H_2O_2 as oxidizer with different concentrations.

$$y_{k,n} = y_{k,n} \times \frac{y_{CH_4(air)}}{y_{CH_4(n)}} \qquad (9)$$

where $y_{k,n}$ is the mass fraction or the rate of production of the carbon-related species k in flame n, $y_{CH_4}(air)$ is the mass

fraction or the rate of methane in pure air case and $y_{CH_4}(air)$ is in flame n.

Fig. 5 shows the normalized CH_4 mass fraction for ER = 1.0 and 0.6. The normalized CH_4 mass fraction at inlet is the same for different H_2O_2 concentrations and the CH_4 consumption
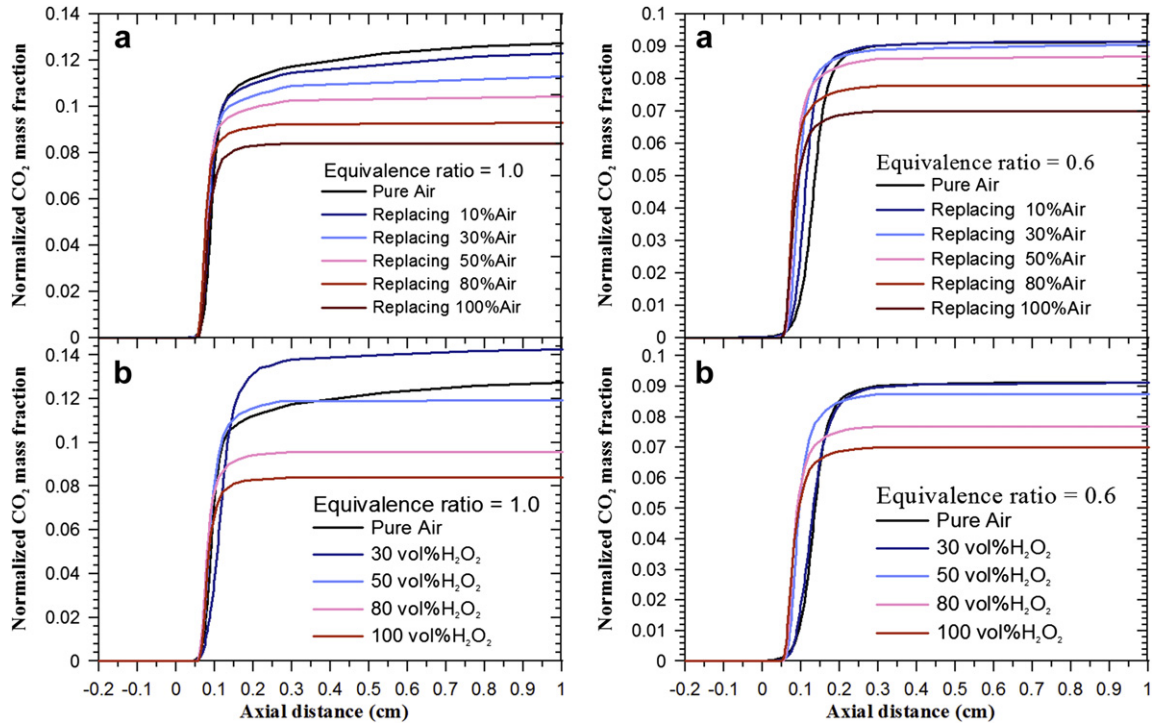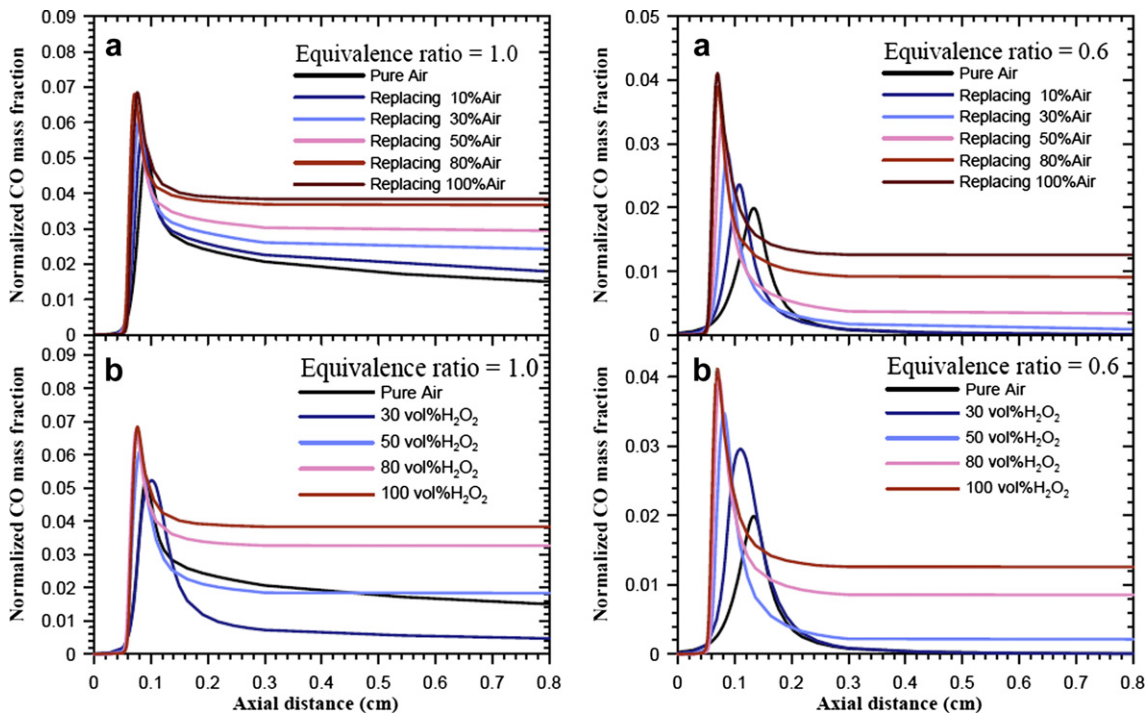

Fig. 9 – Effect of H_2O_2 on normalized CO mass fraction for two cases. (a) replacing partial air by H_2O_2 and (b) H_2O_2 as oxidizer with different concentrations.

trend can be clearly revealed. In stoichiometric (ER = 1.0) and fuel lean (ER = 0.6) conditions earlier accomplishment of complete methane consumptions is noted with increasing hydrogen peroxide replacement percentage. Similarly, increasing the hydrogen peroxide concentration also enhances rapid methane consumption in both stoichiometric and fuel lean conditions, except for the case of 30 vol.% H_2O_2 in stoichiometric condition. Fig. 6 shows the normalized CH_4 consumption rate for different reactant conditions at stoichiometric. With the increase of hydrogen peroxide addition, the total consumption rate of CH_4 is obviously increased. The primary CH_4 consumption reactions are,

$$O + CH_4 \leftrightarrow OH + CH_3 \tag{R11}$$

$$H + CH_4 \leftrightarrow H_2 + CH_3 \tag{R53}$$

$$OH + CH_4 \leftrightarrow CH_3 + H_2O \tag{R98}$$

The main reactions for CH_4 consumption are the abstraction reactions initiated by radicals, such as H, O, and OH and yield CH_3. Reaction (R98) is the principal reaction for CH_4 consumption rate. Since hydrogen peroxide increases the production of O, H, and OH radicals, the reactions (R11), (R53), and (R99) are then enhanced to promote CH_4 consumption.

Fig. 7 shows the effect of H_2O_2 on H_2O mass fraction for ER = 1.0 ad 0.6. Since H_2O_2 decomposes to O_2 and H_2O, the H_2O in product gas is primarily from H_2O_2 decomposition and secondarily from the CH_4 combustion. It appears that the mass fraction of H_2O increases with increasing H_2O_2 in the reactant. However, in the cases of using H_2O_2 as an oxidizer with various concentrations, the lower H_2O_2 concentration means more water vapor will be produced in the product stream. It turns out that H_2O mass fraction increases with decreasing H_2O_2 volumetric concentration.

The normalized CO_2 mass fraction profiles with different H_2O_2 concentrations for ER = 1.0 and 0.6 are shown in Fig. 8. The rise of CO_2 production curve shifts upstream, especially for ER = 0.6. In the case of hydrogen peroxide replacement, the normalized mass fraction of CO_2 is obviously decreased with increasing H_2O_2 for ER = 1.0. Nonetheless, for ER = 0.6, the decrease of CO_2 mass fraction is not obvious when the hydrogen peroxide replacement is below 30% in total air. In the case of using different concentrations of H_2O_2 as the oxidizer, CO_2 mass fraction is also decreased with increasing H_2O_2 concentration. However, CO_2 mass fraction with 30%vol. concentration of H_2O_2 is less than that of pure air case for ER = 1.0. For ER = 0.6, the decrease of CO_2 mass fraction is also not obvious when the hydrogen peroxide concentration is below 30% in volume.

CO and CO_2 are the main carbon-related products in CH_4 flames. The decrease of CO_2 production is often accompanied with the increase of CO production. Both of them have a trade off tendency. Therefore, the normalized CO mass fraction obviously increases with H_2O_2 addition. Fig. 9 shows the effect of H_2O_2 on normalized CO mass fraction or ER = 1.0 and 0.6. Similar to CO_2 effect, with H_2O_2 addition, CO production shifts upstream, especially for ER = 0.6. The CO concentration increases drastically in the preheat zone and then decreases in the reaction zone. The replacement of partial air with H_2O_2 increases the peak of CO concentration. It also increases the CO formation in the post reaction zone except in the lower H_2O_2 concentration (30%). Fig. 10 shows the normalized CO production rate for different reactant conditions. The dominant reactions for CO production are,
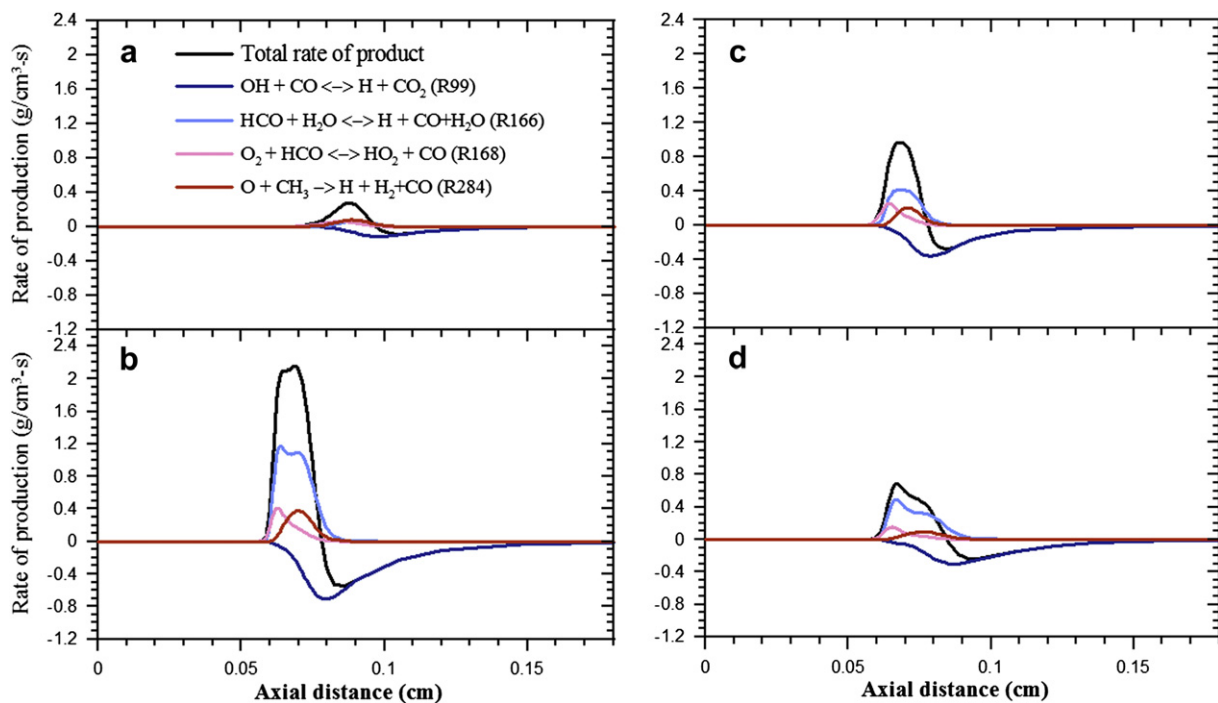

Fig. 10 – Effect of H_2O_2 on normalized CO production rate for different reactant conditions. (a) pure air, (b) 100% H_2O_2, (c) 50% air + 50% H_2O_2, and (d) 50% H_2O_2 + 50% H_2O.

$$HCO + H_2O \leftrightarrow H + CO + H_2O \tag{R166}$$

$$O_2 + HCO \leftrightarrow HO_2 + CO \tag{R168}$$

$$O + CH_3 \leftrightarrow H + H_2 + CO \tag{R284}$$

And the main CO consumption reaction is

$$OH + CO \leftrightarrow H + CO_2 \tag{R99}$$

Reaction (R99) is the most important reaction in CH_4/air combustion and most of the heat release is from this exothermic reaction. According to Fig. 10, these reactions are enhanced with H_2O_2 addition and reaction (R166) is promoted to become the most important reaction in CO formation. This is due to HCO decomposition ameliorated by massive H_2O. With the increase of hydrogen peroxide, the total production rate of CO is obviously increased.

The effects of H_2O_2 on OH mass fraction for ER = 1.0 and 0.6 are shown in Fig. 11. The increase of OH concentration in flames manifests the severe chemical reactions, especially for the case of using H_2O_2 as the oxidizer. OH radicals are significantly yielded upstream and its corresponding concentration obviously increases when H_2O_2 replacement or vol. concentration is increased to 50%. It elucidates that the effect of hydrogen peroxide consists of thermal and chemical effects. When H_2O_2 replacement or vol. concentration is increased to above 80%, the OH concentration is almost unaffected by the equivalence ratio. This is because that under these conditions, OH radicals are primarily yielded from H_2O_2 reaction pathway, instead of from the original CH_4 combustion reactions. Fig. 12

shows the OH production rate for various reactant conditions. In order to clearly display the main reactions, the values of some reactions are reduced several folds. In the case of pure air, the dominant reactions for OH production and consumption are,

$$O_2 + H \leftrightarrow O + OH \tag{R38}$$

$$OH + H_2 \leftrightarrow H + H_2O \tag{R84}$$

The chain branching reaction (R38) is the main reaction for forming OH and (R84) is the main reaction for consuming OH. When hydrogen peroxide enrichment gradually increases, the effect of these above reactions is weakened and the dominant reactions shift to the following mechanisms:

$$2OH + M \leftrightarrow H_2O_2 + M \tag{R85}$$

$$OH + H_2O_2 \leftrightarrow HO_2 + H_2O \tag{R89}$$

Hydrogen peroxide modifies the reaction pathway. With the increase of hydrogen peroxide, the total production rate of OH is increased.

3.4. NO formation

The effect of H_2O_2 on NO mass fraction for ER = 1.0 and 0.6 are sown in Fig. 13. Since the concentration of N_2 is changed with partial replacement of air by hydrogen peroxide, it affects the concentration of NO in the products. Similar to the carbon-related species, the normalized concentration of NO is used to eliminate this effect by the following formula,
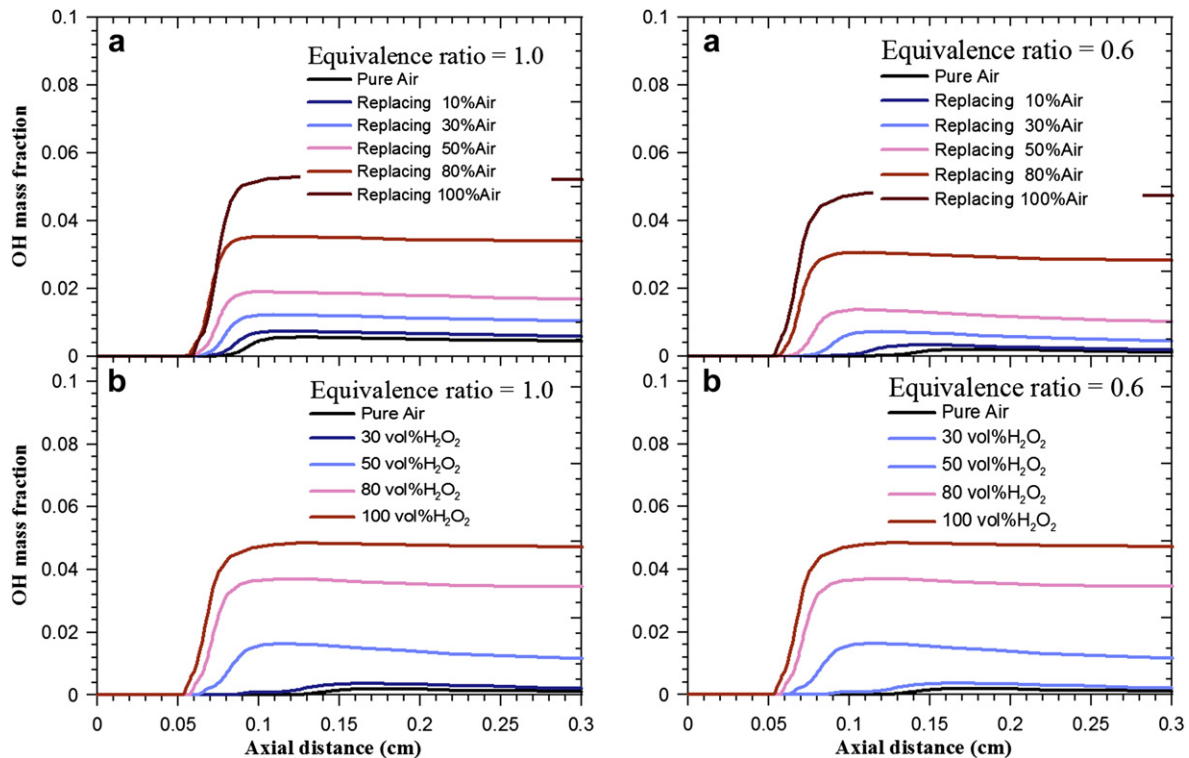

Fig. 11 – **Effect of H_2O_2 on OH mass fraction for two cases. (a) replacing partial air by H_2O_2 and (b) H_2O_2 as oxidizer with different concentrations.**
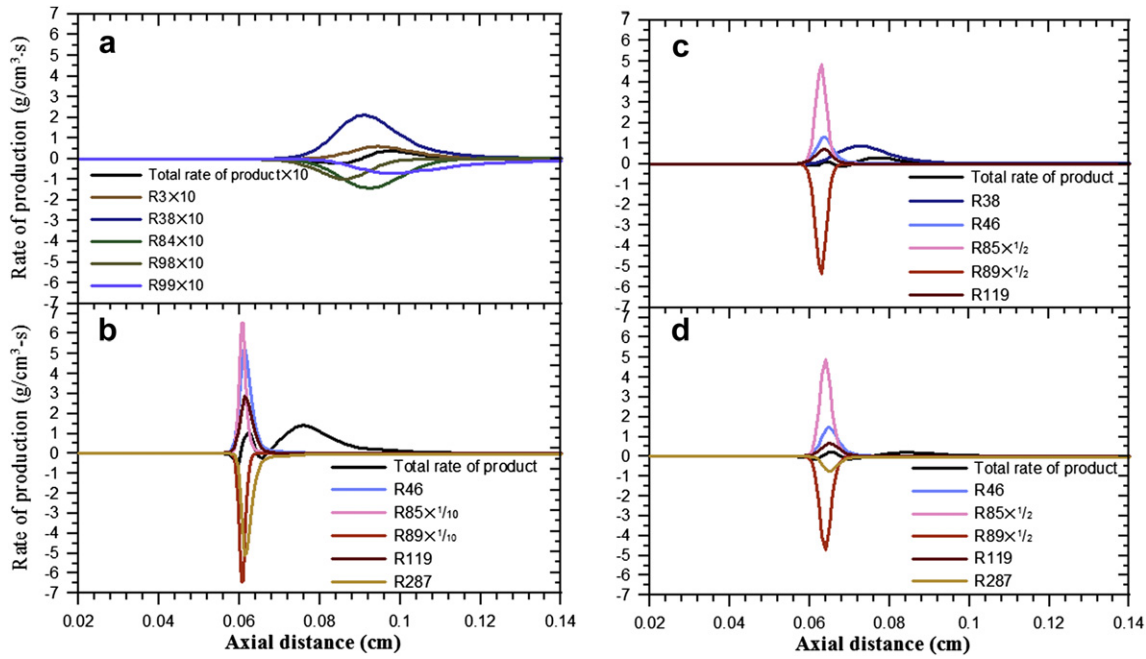
Fig. 12 – Effect of H$_2$O$_2$ on OH production rate for different reactant conditions.

$$y_{\text{NO},n} = y_{\text{NO},n} \times \frac{y_{\text{NO(air)}}}{y_{\text{NO}(n)}} \tag{10}$$

where $y_{\text{NO},n}$ is the mass fraction or the rate of production of NO in flame n, y_{NO} (air) is the mass fraction or the rate of production of NO in pure air case, and $y_{\text{CH}_4}(n)$ is in flame n.

Since there is no nitrogen in the oxidizer, using different volumetric concentrations of H$_2$O$_2$ as the oxidizer is unable to produce NO emission. As to the cases of hydrogen peroxide replacement, NO production increases with H$_2$O$_2$ enrichment. The higher adiabatic flame temperature leads to higher yield of thermal NO$_x$, so that NO emission formation overwhelms the benefit on reduction of N$_2$ reactant reduction. The normalized NO mass fraction always gradually increases with increasing H$_2$O$_2$ addition and it represents the existence of H$_2$O$_2$ in hydrocarbon flame may accelerate thermal NO formation due to inherently high flame temperature.

Fig. 14 shows the normalized NO production rate for various reactant conditions. The total production rate of NO is increased with the increase of H$_2$O$_2$ addition. The dominant reactions for NO production are,

$$N + O_2 \leftrightarrow NO + H \tag{R179}$$

$$N + OH \leftrightarrow NO + H \tag{R180}$$

$$HO_2 + NO \leftrightarrow OH + NO_2 \tag{R186}$$

$$NO_2 + H \leftrightarrow NO + OH \tag{R189}$$

$$O + NH \leftrightarrow H + NO \tag{R190}$$

$$H + HNO \leftrightarrow H_2 + NO \tag{R214}$$

$$CH_2 + NO \leftrightarrow H + HNCO \tag{R249}$$

It can be seen that reactions (R179), (R180), (R190), (R214), and (R249) dominate at high temperature zone and reactions (R186) and (R189) dominate at lower temperature zone. With the addition of H$_2$O$_2$, the flame temperature increases and
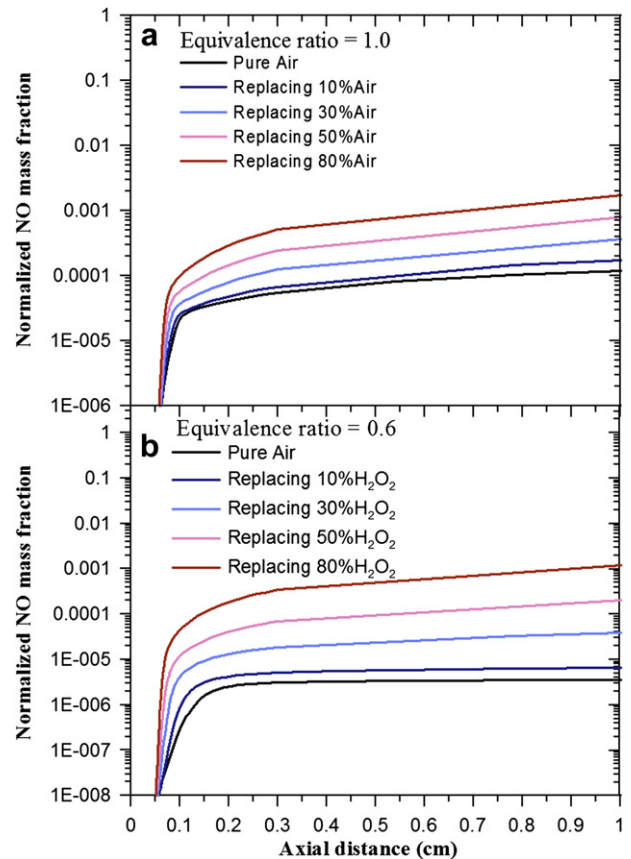

Fig. 13 – Effect of H$_2$O$_2$ on NO mass fraction with replacing partial air by H$_2$O$_2$.
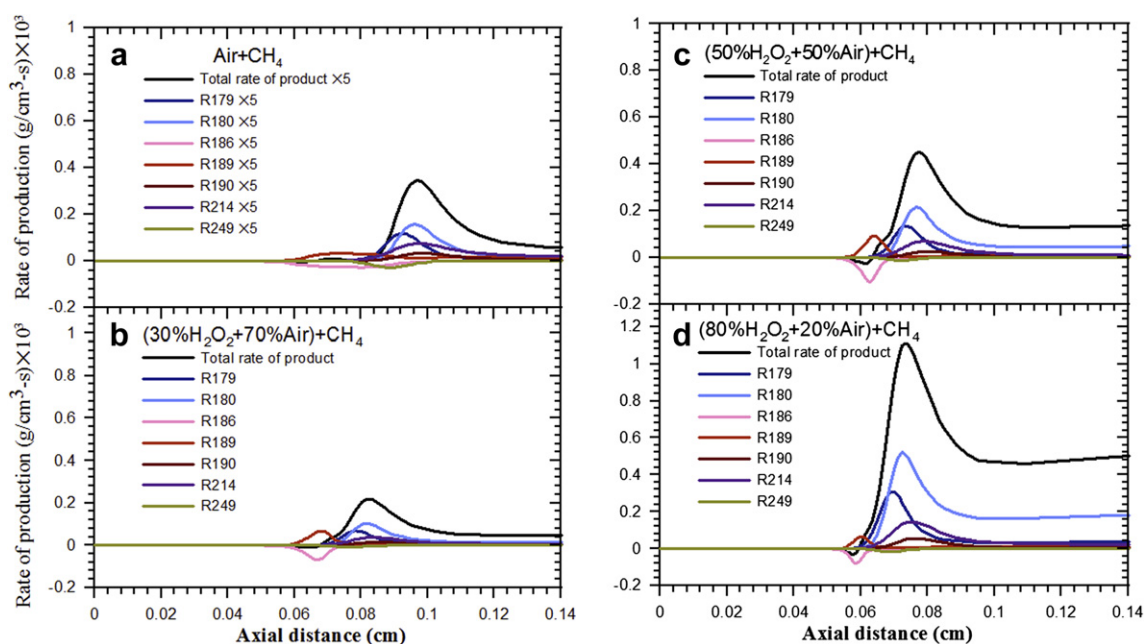
Fig. 14 – Effect of H_2O_2 on NO production rate for different reactant conditions. (a) pure air, (b) 70% air + 30% H_2O_2, (c) 50% air + 50% H_2O_2, and (d) 20% air + 80% H_2O_2.

these reactions are enhanced and (R186) becomes the dominant reaction for NO consumption.

NO production reaction and NO emission concentration is increased due to the high flame temperature.

4.   Conclusions

In the present study, the effects of hydrogen peroxide on methane/air premixed flames are systemically and numerically investigated under the atmosphere condition with GRI-Mech 3.0 mechanism. Hydrogen peroxide is used as the oxidizer for two different conditions: (1) replacing partial air by H_2O_2 and (2) using H_2O_2 as an oxidizer but with different concentrations. Especially, the characteristics of laminar burning velocity, adiabatic flame temperature and species concentration are studied. The following findings are obtained from this study.

1. The laminar burning velocities and the adiabatic temperature are obviously increased with the addition of H_2O_2. When air is completely replaced by H_2O_2, the laminar burning velocity is almost not affected by the equivalence ratio. The decomposition of H_2O_2 dominates the net heat release rate and then affects the adiabatic flame temperature.
2. When the concentration of H_2O_2 increases, the dominant reactions for laminar burning velocity are shifted. Hydrogen peroxide affects the reaction pathway, enhances the reaction rate, and then increases the flame speed.
3. Hydrogen peroxide affects the species concentration and production/consumption rate. CH_4 are completely consumed more upstream as H_2O_2 is added. H_2O_2 addition increases H_2O concentration. However, CO emission is increased and CO_2 concentration is decreased. Using H_2O_2 with a lower concentration will help to control CO emission.
4. When air is partial replaced by H_2O_2, N_2 reactant concentration is decreased. However, H_2O_2 enrichment enhances

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國科會補助計畫衍生研發成果推廣資料表

國科會補助計畫	計畫名稱: 過氧化氫輔助次極限貧油燃燒之實驗與數值研究
	計畫主持人: 鄭藏勝
	計畫編號: 99-2221-E-216-007-　　　　　學門領域: 航太科技

<div align="center">

無研發成果推廣資料

</div>

計畫名稱: 過氧化氫輔助次極限貧油燃燒之實驗與數值研究

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99 年度專題研究計畫研究成果彙整表

成果項目			量化			單位	備註（質化說明：如數個計畫共同成果、成果列為該期刊之封面故事...等）
			實際已達成數（被接受或已發表）	預期總達成數(含實際已達成數)	本計畫實際貢獻百分比		
國內	論文著作	期刊論文	0	0	100%	篇	
		研究報告/技術報告	1	1	100%		
		研討會論文	0	0	100%		
		專書	0	0	100%		
	專利	申請中件數	0	0	100%	件	
		已獲得件數	0	0	100%		
	技術移轉	件數	0	0	100%	件	
		權利金	0	0	100%	千元	
	參與計畫人力（本國籍）	碩士生	1	1	100%	人次	
		博士生	1	1	100%		
		博士後研究員	0	0	100%		
		專任助理	0	0	100%		
國外	論文著作	期刊論文	1	1	100%	篇	
		研究報告/技術報告	0	0	100%		
		研討會論文	1	1	100%		
		專書	0	0	100%	章/本	
	專利	申請中件數	0	0	100%	件	
		已獲得件數	0	0	100%		
	技術移轉	件數	0	0	100%	件	
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	參與計畫人力（外國籍）	碩士生	0	0	100%	人次	
		博士生	0	0	100%		
		博士後研究員	0	0	100%		
		專任助理	0	0	100%		

	成果項目	量化	名稱或內容性質簡述
其他成果 (無法以量化表達之成果如辦理學術活動、獲得獎項、重要國際合作、研究成果國際影響力及其他協助產業技術發展之具體效益事項等，請以文字敘述填列。)	無		

	成果項目	量化	名稱或內容性質簡述
科教處計畫加填項目	測驗工具(含質性與量性)	0	
	課程/模組	0	
	電腦及網路系統或工具	0	
	教材	0	
	舉辦之活動/競賽	0	
	研討會/工作坊	0	
	電子報、網站	0	
	計畫成果推廣之參與（閱聽）人數	0	

國科會補助專題研究計畫成果報告自評表

請就研究內容與原計畫相符程度、達成預期目標情況、研究成果之學術或應用價值（簡要敘述成果所代表之意義、價值、影響或進一步發展之可能性）、是否適合在學術期刊發表或申請專利、主要發現或其他有關價值等，作一綜合評估。

1. 請就研究內容與原計畫相符程度、達成預期目標情況作一綜合評估 ■達成目標 □未達成目標（請說明，以 100 字為限） 　　　□實驗失敗 　　　□因故實驗中斷 　　　□其他原因 　說明：
2. 研究成果在學術期刊發表或申請專利等情形： 論文：■已發表 □未發表之文稿 □撰寫中 □無 專利：□已獲得 □申請中 ■無 技轉：□已技轉 □洽談中 ■無 其他：（以 100 字為限）
3. 請依學術成就、技術創新、社會影響等方面，評估研究成果之學術或應用價值（簡要敘述成果所代表之意義、價值、影響或進一步發展之可能性）（以 500 字為限） 本計畫主要是以發展應用過氧化氫作為反應的促進劑或取代空氣作為氧化劑，以輔助次極限貧油燃燒，進而達到節能與降低污染物生成的目標。本研究初期係以數值方法並利用 CHEMKIN Collection 軟體結合 GRI-Mech 3.0 完整化學反應機構，探討添加過氧化氫對化學反應路徑、層流燃燒速度、火焰結構及污染生成之影響。研究成果已發表於國際著名期刊(International Journal of Hydrogen Energy)，且可作為將來設計貧油燃燒器之參考。後續研究將以實驗方法驗證數值模擬之結果及建構一示範型 CH4/H2O2 燃燒器，以進一步瞭解添加過氧化氫之操作條件，並建立資料庫。