Available online at www.sciencedirect.com
ScienceDirect
Proceedings of the Combustion Institute 31 (2007) 1197–1204
Proceedings of the Combustion Institute
www.elsevier.com/locate/proci

The effect of reformate gas enrichment on extinction limits and NO_X formation in counterflow CH_4/air premixed flames

Hongsheng Guo [a,*], Gregory J. Smallwood [a], Ömer L. Gülder [b]

[a] *Institute for Chemical Process and Environmental Technology, National Research Council Canada, 1200 Montreal Road, Building M-9, Ottawa, Ont., Canada K1A 0R6*

[b] *Institute for Aerospace Studies, University of Toronto, 4925 Dufferin Street, Toronto, Ont., Canada M3H 5T6*

Abstract

The reformate gas enriched counterflow lean premixed CH_4/air flames were studied by numerical simulation in this paper. The reformate gas was assumed to be the product of partial oxidation of methane by air, and it consists of H_2, CO and N_2. Detailed chemistry and complex thermal and transport properties were employed. The results indicate that the addition of the reformate gas enlarges the flammable region, and extends the lean flammability limit of counterflow CH_4/air premixed combustion. When the reformate gas is added, the formation of NO is reduced in a near-stoichiometric flame, and increased in an ultra-lean flame at a constant equivalence ratio. The more significant advantage of the reformate gas enriched lean premixed combustion is that it greatly reduces the formation of NO by allowing a combustor to operate at leaner condition without any effect on flammable range. Further, the addition of the reformate gas decreases the formation of NO_2 and N_2O at a constant equivalence ratio.

Keywords: Lean premixed combustion; Fuel enrichment; NO_X; Extinction limit; Reformate gas

1. Introduction

Lean premixed combustion is a promising concept for substantial reduction in fuel consumption and emissions of greenhouse gases and pollutants. It involves operation at lower equivalence ratios to reduce flame temperatures. At these lower temperatures and equivalence ratios, NO formation from thermal and prompt routes can be effectively suppressed. Emission of soot, the predominant source of particulate matter and a major global warming contributor, can also be essentially eliminated in these flames.

However, lean premixed combustion has some intrinsic weaknesses. One of the weaknesses is that at a lower equivalence ratio, the lean flammability limit is approached and flames become less stable. A strategy to overcome this weakness is to adopt fuel enrichment, i.e., adding a small amount of other fuel, to extend the flammability limit and improve the flame stability, while maintaining the advantages of lean premixed combustion. Our previous study [1] has shown that hydrogen enrichment can extend the flammability limit and reduce NO formation in counterflow

* Corresponding author. Fax: +1 613 957 7869.
E-mail address: hongsheng.guo@nrc-cnrc.gc.ca (H. Guo).

1540-7489/$ - see front matter © 2006 The Combustion Institute. Published by Elsevier Inc. All rights reserved.
doi:10.1016/j.proci.2006.07.205

CH_4/air premixed flames by allowing a combustor to operate at leaner condition.

Hydrogen can be produced by reforming hydrocarbon fuels. The product of fuel reforming, known as reformate gas, contains not only hydrogen, but also carbon monoxide and some other components, depending on the method of reforming. Instead of hydrogen, if the reformate gas of a hydrocarbon fuel can be directly used as the enrichment component, the fuel enrichment combustion technology will be more practical and economical.

The extinction characteristics of stretched premixed flames have been extensively studied for different fuels [2–6]. Similarly, many researchers have investigated the formation of NO_X in various flames [7–12]. The influence of hydrogen addition on flame extinction and NO_X formation in CH_4/air premixed flames has also been studied in [1,13–15]. However, only one study [14] has been reported on the effect of the addition of carbon monoxide, another main component of a reformate gas, on extinction limits in lean premixed flames. If partial oxidation method is employed for reforming, the reformate gas usually contains certain amount of nitrogen that also affects the extinction and NO_X formation. Besides, no study has presented any details of NO_X formation under reformate gas enrichment condition. Therefore, it is of great interest to understand the combustion and pollutant formation characteristics of reformate gas enriched lean premixed flames.

The purpose of this paper is to numerically investigate the extinction and NO_X formation characteristics in reformate gas enriched lean CH_4/air premixed flames. The reformate gas was assumed to contain H_2, CO and N_2. The effect of reformate gas addition on extinction limits and NO_X formation is analyzed and discussed.

2. Numerical model

The flame configuration studied is an axisymmetric counterflow laminar flame, stabilized near the stagnation plane of two opposed-jets.

The governing equations can be found elsewhere [16]. The calculations were carried out with a code used previously [1,4–6]. Upwind and center difference schemes were used for the convective and diffusion terms, respectively, in all the governing equations. Adaptive refinement of meshes was done to obtain grid independent result. The arc-length continuation method [16] was employed to get extinction limits. The pressure and the fresh mixture temperature are, respectively, 1 atm and 300 K.

Two different free stream conditions—potential and plug flow—were alternately used in the literature for counterflow flame simulation. They produce similar qualitative results [17]. As a pure numerical study, the potential boundary condition was used in this paper.

The optically thin radiation model [3] was used to save the computational cost, since the reabsorption has little influence on extinction limits and temperatures in most lean CH_4/air premixed flames [18]. The reaction mechanism used is GRI-Mech 3.0 [19]—an optimized mechanism for methane combustion. The thermal and transport properties were obtained by using the database of GRI-Mech 3.0 and the algorithms given in [20,21].

3. Results and discussion

The reformate gas was assumed to be the product of partial oxidation of methane by air via the reaction

$$2CH_4 + O_2 + \frac{79}{21}N_2 = 2CO + 4H_2 + \frac{79}{21}N_2$$

Therefore, the volume composition of the reformate gas is $(42CO + 84H_2 + 79N_2)/205$.

The fraction of the added reformate gas is defined as $\alpha_{rg} = V_{rg}/(V_{rg} + V_{CH_4})$, with V_{rg} and V_{CH_4} are, respectively, the volume flow rates of the reformate gas and methane. The complete combustion of the fuel mixture goes via the reaction

$$(1-\alpha_{rg})CH_4 + \alpha_{rg}\left(\frac{42}{205}CO + \frac{84}{205}H_2 + \frac{79}{205}N_2\right) + \left(2 - 2\alpha_{rg} + \frac{63\alpha_{rg}}{205}\right)O_2 = \left(1 - \alpha_{rg} + \frac{42\alpha_{rg}}{205}\right)CO_2 + \left(2 - 2\alpha_{rg} + \frac{84\alpha_{rg}}{205}\right)H_2O + \frac{79\alpha_{rg}}{205}N_2$$

Nitrogen in this reaction is from the fuel reforming, while that contained in air does not explicitly appear here, since it does not affect the calculation of fuel–oxidant ratio. Therefore, the stoichiometric fuel–oxidant ratio in a reformate gas enriched mixture is:

$$(F/O)_{st} = (1 - \alpha_{rg} + 126\alpha_{rg}/205)/(2 - 2\alpha_{rg} + 63\alpha_{rg}/205) \quad (1)$$

The equivalence ratio is defined as the ratio of actual fuel–oxidant ratio to the stoichiometric value, i.e.,

$$\phi = (F/O)/(F/O)_{st} \quad (2)$$

In all the figures, the quantity a represents stretch rate.

3.1. Extinction limits

It has been well known that at a constant equivalence ratio, a counterflow premixed flame is extinguished by a high stretch rate due to the shortened residence time. This high stretch rate is called stretch extinction limit. On the other side, for an ultra-lean counterflow premixed flame, a low stretch rate also results in the flame extinction because of radiation heat loss. The low stretch rate at extinction is named as radiation extinction limit. If all these stretch and radiation extinction limits are plotted versus equivalence ratio, a C-shaped curve can be obtained. The upper branch of the curve is the stretch extinction limit branch, and the lower branch is the radiation extinction limit branch. The two branches merge at a critical equivalence ratio, which is the lean flammability limit [4]. The region bounded by this C-shaped curve is the flammable region. Figure 1 displays the C-shaped curves for pure CH_4/air flame, 40% reformate gas enriched CH_4/air flame and pure reformate gas/air flame. For comparison, the C-shaped curves of 40% H_2 and 40% CO enriched CH_4/air premixed flames are also shown in Fig. 1. The definition of the added H_2 and CO fractions is similar to that of the reformate gas.

It is observed that the addition of the reformate gas increases the stretch extinction limit and reduces the radiation extinction limit at a constant equivalence ratio. As a result, the flammable region of CH_4/air premixed flame is enlarged and the flammability limit is extended to leaner side, due to the addition of the reformate gas. The effect of the reformate gas addition is enhanced with the increase in the fraction of the reformate gas. When 40% reformate gas is added, or all the fuel is replaced by the reformate gas, the flammability limit of CH_4/air premixed flame is extended from 0.42 to 0.38 or 0.2. The stretch extinction limit of the 40% reformate gas enriched flame at equivalence ratio of 0.73 is the same as that of pure CH_4/air at equivalence ratio of 0.9. This means that the addition of 40% reformate gas allows the operation equivalence ratio of a combustor to be moved from 0.9 to 0.73 without any effect on flammable range. Therefore, similar to the addition of hydrogen [1], the addition of the reformate gas can significantly improve the flame stability of lean premixed CH_4/air combustion.

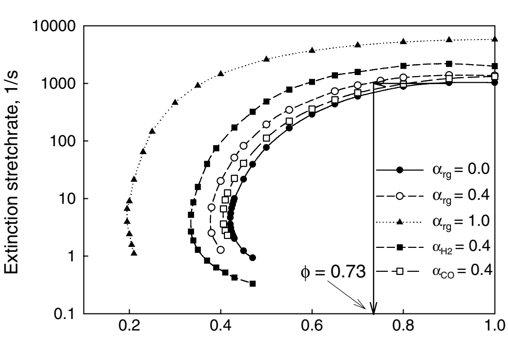

Fig. 1. Effect of the addition of reformate gas, H_2 and CO on C-shaped curves.

Compared to the addition of H_2 and CO, the effect of the reformate gas addition is less effective than that of H_2 addition, but more significant than that of CO addition. This is because the reformate gas is a mixture of H_2, CO and N_2. Our previous study [1] has shown that the addition of H_2 can significantly enlarge the flammable region of CH_4/air premixed flame. The addition of CO also enhances the combustion intensity of a CH_4/air premixed flame due to the reaction $CO + OH = H + CO_2$ and the rise in temperature. However, the effect of CO addition is not as effective as that of H_2 addition. In addition, the reformate gas also contains nitrogen that is basically an inert species for primary combustion reactions. Thus the addition of the reformate gas enlarges flammable region of CH_4/air premixed flame, but the effectiveness is between those of H_2 and CO addition.

In real applications, a reformate gas also contains small amount of CO_2 and H_2O that may slightly narrow the flammable region. However, the formation of CO_2 and H_2O in fuel reforming process increases the reformate gas temperature, which tends to enlarge the flammable region. Therefore, the existence of CO_2 and H_2O in a reformate gas should not significantly change the above conclusion.

3.2. NO formation

The distributions of NO mole fraction in two typical flames at various reformate gas fractions are shown in Fig. 2. The stretch rate of these two flames is the same, 30 s^{-1}, and the equivalence ratios are, respectively, 0.9 and 0.65. These two equivalence ratios were selected because the former represents a near stoichiometric value, whereas the latter is an ultra-lean one. The effects of stretch rate and equivalence ratio will be discussed later. The dash-dot curve in this figure, which is almost the same as the solid one, will be explained below.

It is observed that the addition of the reformate gas enlarges the NO distribution region for both equivalence ratios. This is because the addition of the reformate gas increases the flame speed, leading to a longer distance between the primary reaction zone and the stagnation plane at a constant stretch rate. However, the peak NO mole fraction is reduced in the flame with equivalence ratio of 0.9, while it is increased in the flame of equivalence ratio 0.65, when the reformate gas is added.

To check further the effect of the reformate gas addition on NO formation, we analyze the mechanism of NO formation now. In a hydrocarbon flame, NO can be formed through the thermal, the prompt, the N_2O and the NNH intermediate routes [1,7–9,12]. In our previous study [1], a

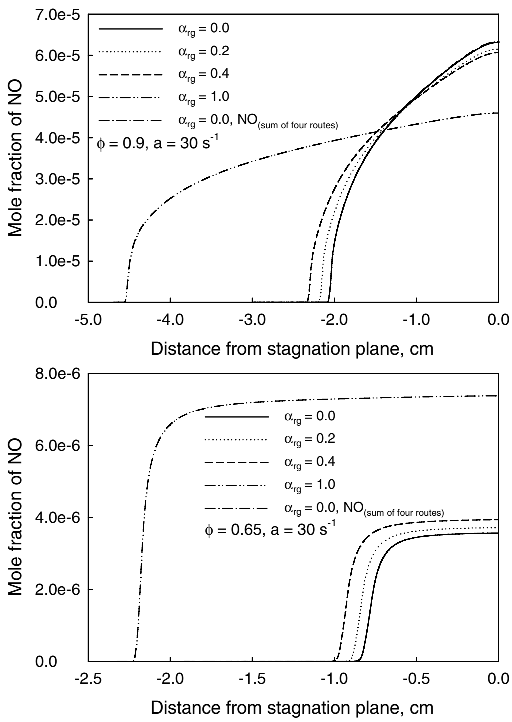

Fig. 2. Distributions of NO mole fraction.

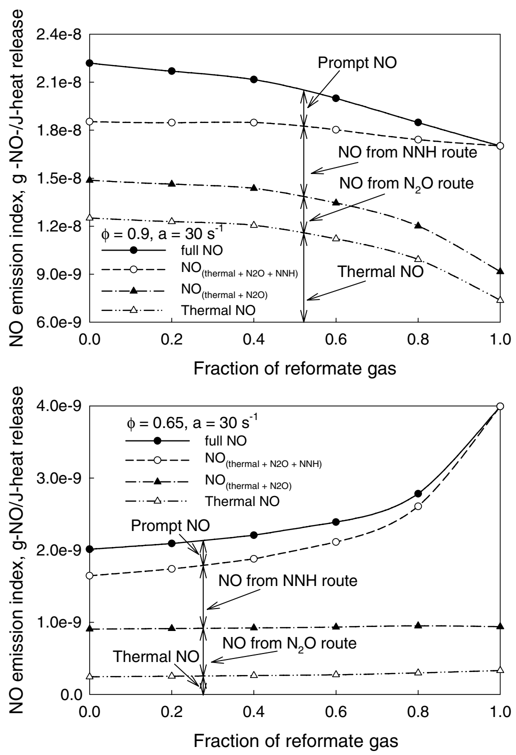

Fig. 3. Variation of NO emission index.

method, in which the initial reactions converting molecular nitrogen to atomic nitrogen and species containing nitrogen element were gradually switched off, was employed to identify the relative contributions of different NO routes. Some researchers argued that due to the complexity of NO formation, the initial reactions of the four routes might not be independent. To verify our approach, in addition to the simulations using the full Gri-Mech 3.0 reaction scheme, we did four extra calculations for the two pure CH_4/air flames with equivalence ratios 0.9 and 0.65. The reaction scheme in each of these four extra simulations only contains the initial reactions converting molecular nitrogen from one route. The NO mole fraction obtained by summing the NO from these four extra simulations is also shown in Fig. 2. No discernible difference can be observed between the curves obtained from the full Gri-Mech 3.0 chemistry (solid line) and the summation (dash-dot line) of the four extra simulations. The flames of other equivalence ratios have similar result. This suggests that any interactions among the four NO formation routes are negligible in a lean premixed flame. The method used in [1] does properly identify the relative contributions of the four routes, and thereby was used again in this paper.

Figure 3 illustrates the variations of NO emission indices from different routes. The definition of NO emission index is the ratio of total formed NO to total heat release in a flame. It first shows that the addition of the reformate gas decreases the formation of NO (full NO) in the flame with equivalence ratio of 0.9, whereas the reformate gas addition increases NO in the flame with equivalence ratio of 0.65. Further, the addition of the reformate gas reduces the contribution of the prompt route in each flame. This is because the addition of the reformate gas decreases the concentration of radical CH, which is the most important radical to initiate NO formation through the prompt route.

For the contribution of the thermal route, the contradictory phenomena are observed for the two equivalence ratio flames. The addition of the reformate gas reduces the contribution of the thermal route in the flame with equivalence ratio of 0.9, but slightly increases that in the flame with equivalence ratio of 0.65. It is caused by the different effects of the reformate gas addition on temperature for the two flames, as shown in Fig. 4. The addition of the reformate gas decreases the peak temperature in the flame of equivalence ratio 0.9, while increases that in the flame of equivalence ratio 0.65. When the reformate gas is added, the decrease in temperature of the near stoichiometric flame ($\phi = 0.9$) is due to the lower heat release of the reformate gas, since part of the energy is released during the reforming process. At a lower equivalence ratio, such as $\phi = 0.65$, the air requirement of the reformate gas

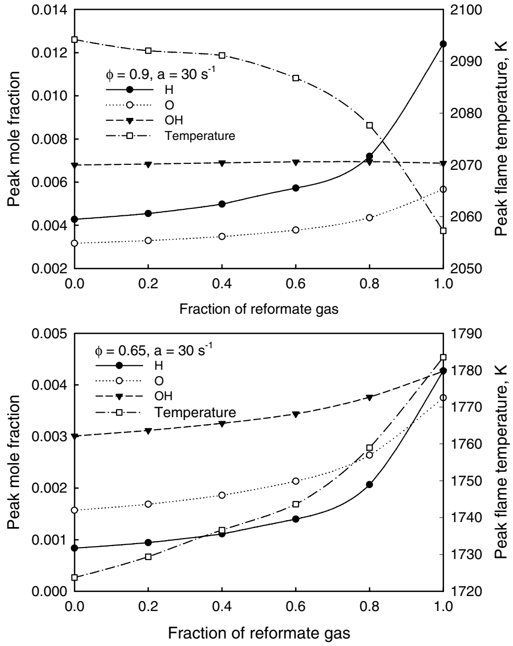

Fig. 4. Variations of peak temperature and peak mole fractions of H, O, and OH.

combustion is less than that of pure methane combustion and therefore less excess air exists when the reformate gas is added, which results in higher temperatures for reformate gas enriched ultra-lean premixed flames. It should be pointed out that although the peak temperature rises significantly in the flame of equivalence ratio 0.65, the contribution of the thermal route only increases slightly, with the addition of the reformate gas. This is because the temperature level in this flame is so low that the contribution of the thermal route is very small.

The contribution of the N_2O intermediate route changes little, while that of the NNH intermediate route increases in each flame, when the reformate gas is added. A pathway analysis indicates that the most significant initiation reactions of the NNH intermediate route are $NNH = N_2 + H$ and $NNH + M = N_2 + H + M$, and the most important NNH destruction reaction is $NNH + O_2 = HO_2 + N_2$. Therefore, the variation in the concentration of radical H affects the formation of NNH.

Figure 4 also shows the variations in peak concentrations of H, O and OH. With the addition of the reformate gas, the main H formation reactions $OH + H_2 = H + H_2O$ and $OH + CO = H + CO_2$ are intensified, leading to the increase in the concentration of H. This raises the formation rate of NNH and thus the following conversion rate of NNH to NO. Consequently, the contribution of the NNH intermediate route in a flame is increased, when the reformate gas is added.

The rise in the concentration of H causes the increase in the concentration of radical O, since the rate of the chain branching reaction $H + O_2 = OH + O$ is also intensified. As for OH, the addition of the reformate gas causes that more OH is needed to complete the reactions $OH + H_2 = H + H_2O$ and $OH + CO = H + CO_2$, but more OH may be produced by the reaction $H + O_2 = OH + O$. As a result, the variation of OH concentration depends on the balance between these reactions. This is the reason that the concentration of OH changes very slowly or even keeps constant with the increase in the fraction of the reformate gas. The variations in the concentrations of these radicals affect the formation of NO through the N_2O intermediate route.

In the N_2O intermediate route, molecular nitrogen is first converted to N_2O, and then the formed N_2O is partly converted to NO. The most important formation and destruction reactions of N_2O are, respectively, $N_2O\,(+M) = N_2 + O\,(+M)$ and $N_2O + H = N_2 + OH$. When the reformate gas is added, the concentrations of both H and O increase, but the increase rate of H concentration is a little higher. Consequently, the net formation rate of N_2O slowly decreases, as will be discussed later. The conversion of N_2O to NO are mainly through paths: $N_2O \rightarrow NO$ and $N_2O \rightarrow NH \rightarrow HNO \rightarrow NO$. The conversion rates of these two paths slightly increase due to the rise in the concentrations of H and O, with the addition of the reformate gas. The comprehensive effects of these factors lead to that the contribution of the N_2O intermediate route keeps almost constant or slightly decreases in a flame, when the reformate gas is added.

Therefore, we conclude that the addition of the reformate gas reduces the formation of NO in a near stoichiometric flame, mainly due to the decrease in the contributions of the prompt and thermal routes. However, the addition of the reformate gas increases the formation of NO in an ultra-lean premixed flame, primarily because the contribution of the NNH intermediate route is increased.

3.3. Effect of stretch rate

Figure 5 shows the effect of stretch rate on NO formation in pure CH_4/air and 40% reformate gas enriched CH_4/air premixed flames. The maximum stretch rates investigated are close to the stretch extinction limits of pure CH_4/air flames for both equivalence ratios. It is noted that at all stretch rates, the addition of the reformate gas reduces NO formation in the flame with equivalence ratio of 0.9, while increases that in the flame with equivalence ratio of 0.65. This is consistent with that previously observed for flames at stretch rate of 30 s^{-1}.

With the increase of stretch rate, NO emission indices monotonically decrease for the flames of

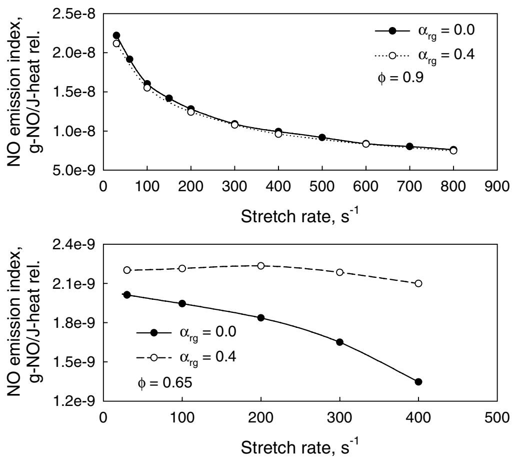

Fig. 5. Effect of stretch rate on NO formation.

equivalence ratio 0.9, either with or without the reformate gas addition. However, when equivalence ratio equals 0.65, NO emission index monotonically decreases for the flame without the reformate gas addition, but first slightly increases and then decreases for the flame with 40% reformate gas addition.

The variation of stretch rate effect on NO formation in different flames is caused by the preferential diffusion of hydrogen. The Lewis number of pure CH_4/air flame is slightly less than, but close to, unity. Therefore, the increase of stretch rate reduces the formation of NO due to the decrease in flame thickness in pure CH_4/air flames. Hydrogen has significantly high diffusion coefficient. When the reformate gas is added, the preferential diffusion of hydrogen tends to cause the rise of flame temperature, as stretch rate is increased. This preferential diffusion effect becomes more significant with the decrease in equivalence ratio. When equivalence ratio equals 0.9, although the preferential diffusion slightly increases temperature in the reformate gas enriched flame, the reduction in flame thickness still causes the monotonic decrease in NO emission index, when stretch rate is increased.

However, for equivalence ratio 0.65, the preferential diffusion of hydrogen becomes so significant that the effect of temperature increase exceeds that of the reduction in flame thickness in the 40% reformate gas enriched flame. This leads to a slight rise in NO emission index, as stretch rate is increased from a low value to 200 s^{-1}. With the further increase in stretch rate, flame temperature rises slowly or even decreases, due to the shortened residence time. Together with the reduction in flame thickness, NO emission index finally decreases when stretch rate is further increased to more than 200 s^{-1} for the 40% reformate gas enriched flame at equivalence ratio of 0.65.

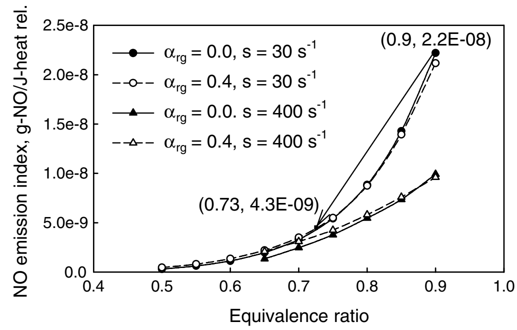

Fig. 6. Variation of NO emission index with equivalence ratio.

3.4. Effect of equivalence ratio

Figure 6 displays the variations of NO emission indices for the flames without reformate gas addition and with 40% reformate gas addition at stretch rates of 30 and 400 s^{-1}, when equivalence ratio is changed. It is illustrated that the decrease of equivalence ratio significantly reduces the formation of NO in a flame. This is easy to understand and an advantage of lean premixed combustion.

Although the addition of the reformate gas suppresses the formation of NO at a constant equivalence ratio for a near stoichiometric flame, more significant benefit can be observed from Fig. 6. As we stated before, the addition of the reformate gas enlarges the flammable range and thus allows a combustor to operate at leaner conditions. For example, with the addition of 40% reformate gas, the equivalence ratio of a combustor can be moved from 0.9 to 0.73 without any effect on flammable range. Then it can be found from Fig. 6 that NO emission index can be reduced from 2.2E−08 to 4.3E−09 g-NO/J-heat release at stretch rate of 30 s^{-1}. Although the reduction in NO emission is decreased at stretch rate of 400 s^{-1} due to the preferential diffusion of hydrogen, it is still very significant, if the equivalence ratio is moved from 0.9 to 0.73 with the addition of 40% reformate gas. Therefore, we can conclude that, like the addition of hydrogen [1], the addition of the reformate gas also significantly reduces the formation of NO by allowing a combustor to operate at leaner condition. This is the biggest advantage of the fuel enriched lean premixed combustion technology. Considering the lower cost of the reformate gas enrichment than that of hydrogen, it is more practical and economical in the application.

3.5. NO_2 formation

Figure 7 shows the variation of NO_2 emission index with the addition of the reformate gas for flames with stretch rate of 30 s^{-1} and equivalence

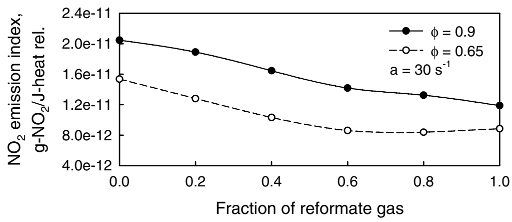

Fig. 7. Variation of NO_2 emission index.

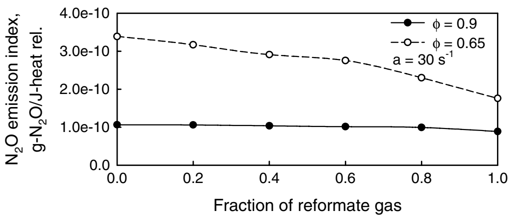

Fig. 8. Variation of N_2O emission index.

ratios of 0.9 and 0.65. The definitions of NO_2 and N_2O emission indices are similar to that for NO.

It is found that the addition of the reformate gas monotonically decreases the formation of NO_2 for the flame of equivalence ratio 0.9. When equivalence ratio equals 0.65, the formation of NO_2 decreases until the fraction of the reformate gas 0.6 is reached. Then with the further rise of the reformate gas addition, the formation of NO_2 slightly increases.

A sensitivity analysis indicates that the main formation and destruction reactions of NO_2 are, respectively, $HO_2 + NO = NO_2 + OH$ and $NO_2 + H = NO + OH$. As discussed before, the addition of the reformate gas reduces the formation of NO and increases the concentration of H for the flame of equivalence ratio 0.9. This tends to reduce the formation rate and increase the destruction rate of NO_2, when the reformate gas is added. Therefore, the addition of the reformate gas monotonically reduces the formation of NO_2 in this flame.

When equivalence ratio equals 0.65, the addition of the reformate gas increases both the formation of NO and the concentration of H, as shown in Figs. 3 and 4, leading to the increase in both formation and destruction rates of NO_2. The formation rate increase is slower than that of the destruction rate when the fraction of the reformate gas is increased from 0 to 0.6, resulting in the decrease of NO_2 formation. However, with the further addition of the reformate gas to over 0.6, the quick increase in the formation of NO causes that the NO_2 formation rate exceeds the destruction rate. Consequently, NO_2 formation slightly increases, when the fraction of the reformate gas is increased from 0.6 to 1.0.

3.6. N_2O formation

Figure 8 shows the variation of N_2O emission index for the flames with stretch rate 30 s^{-1} and equivalence ratios of 0.9 and 0.65, when the reformate gas is added. Other flames have similar result.

It is illustrated that the addition of the reformate gas decreases the formation of N_2O for both flames. As we discussed before, the main formation and destruction reactions of N_2O are, respectively, $N_2O(+M) = N_2 + O(+M)$ and $N_2O + H = N_2 + OH$. Destruction rate of N_2O becomes faster than its formation due to a faster increase in H concentration when the reformate gas is added.

It is also noted that the formation of N_2O in the flame of equivalence ratio 0.65 is greater than that in the flame of equivalence ratio 0.9. This is consistent with that observed in hydrogen enriched lean premixed flames [1]. It implies that the formation of N_2O will be an issue in ultra-lean premixed combustion technology. However, the addition of the reformate gas can reduce the formation of N_2O at a constant equivalence ratio. This is another advantage of the reformate gas enrichment combustion.

4. Conclusions

The extinction and NO_X formation in reformate gas enriched lean premixed methane/air flames have been investigated by numerical simulation. The results indicate that the addition of the reformate gas enlarges the flammable region and extends the lean flammability limit of premixed CH_4/air flames. The addition of the reformate gas reduces the formation of NO for a near-stoichiometric flame, and increases that for an ultra-lean flame at a constant equivalence ratio. However, the addition of the reformate gas can greatly reduce the formation of NO by allowing a combustion system to operate at leaner condition without any effect on flammable range. This is a significant advantage of the reformate gas enriched combustion technology. Moreover, the addition of the reformate gas decreases the formation of NO_2 and N_2O at a constant equivalence ratio.

References

[1] H. Guo, G.J. Smallwood, F. Liu, Y. Ju, Ö.L. Gülder, *Proc. Combust. Inst.* 30 (2005) 303–311.
[2] J.S. Tien, *Combust. Flame* 65 (1986) 31–34.
[3] K. Maruta, M. Yoshida, Y. Ju, T. Niioka, *Proc. Combust. Inst.* 26 (1996) 1283–1289.

[4] H. Guo, Y. Ju, K. Maruta, T. Niioka, F. Liu, *Combust. Flame* 109 (1997) 639–646.
[5] Y. Ju, H. Guo, K. Maruta, F. Liu, *J. Fluid Mech.* 342 (1997) 315–334.
[6] H. Guo, Y. Ju, T. Niioka, *Combust. Theory Model.* 4 (2000) 459–475.
[7] Y. Ju, T. Niioka, *Combust. Theory Model.* 1 (1997) 243–258.
[8] J. Wang, T. Niioka, *Proc. Combust. Inst.* 29 (2002) 2211–2218.
[9] M. Nishioka, S. Nakagawa, Y. Ishikawa, T. Takeno, *Combust. Flame* 98 (1994) 127–138.
[10] S.V. Naik, N.M. Laurendeau, *Combust. Flame* 129 (2002) 112–119.
[11] R. Fuse, H. Kobayashi, Y. Ju, K. Maruta, T. Niioka, *Int. J. Thermal Sci.* 41 (2002) 693–698.
[12] G.J. Rørtveit, J.E. Hustad, S. Li, F.A. Williams, *Combust. Flame* 130 (2002) 48–61.
[13] G.S. Jackson, R. Sai, J.M. Plaia, C.M. Boggs, K.T. Kiger, *Combust. Flame* 132 (2003) 503–511.
[14] J.Y. Ren, W. Qin, F.N. Egolfopoulos, H. Mak, T.T. Tsotsis, *Chem. Eng. Eng. Sci.* 56 (2001) 1541–1549.
[15] G.J. Rørtveit, K. Zepter, Ø. Skreiberg, M. Fossum, J.E. Hustad, *Proc. Combust. Inst.* 29 (2002) 1123–1129.
[16] V. Giovangigli, M.D. Smooke, *Combust. Sci. Tech.* 53 (1987) 23–49.
[17] R. Chen, R.L. Axelbaum, *Combust. Flame* 142 (2005) 62–71.
[18] H. Guo, Y. Ju, K. Maruta, T. Niioka, F. Liu, *Combust. Sci. Technol.* 135 (1998) 49–64.
[19] G.P. Smith, D.M. Golden, M. Frenklach, et al. Available at: <http://www.me.berkeley.edu/gri_mech>.
[20] R.J. Kee., J. Warnatz, J.A. Miller, Report No. SAND 83-8209, Sandia National Laboratories, 1983.
[21] R.J. Kee., J.A. Miller, T.H. Jefferson, Report No. SAND 80-8003, Sandia National Laboratories, 1980.