NRC Publications Archive
Archives des publications du CNRC

The effect of CO addition on extinction limits and NO_x formation in lean counterflow CH_4/air premixed flames

Guo, Hongsheng; Smallwood, Gregory

This publication could be one of several versions: author’s original, accepted manuscript or the publisher’s version. / La version de cette publication peut être l’une des suivantes : la version prépublication de l’auteur, la version acceptée du manuscrit ou la version de l’éditeur.

NRC Publications Archive Record / Notice des Archives des publications du CNRC :
https://nrc-publications.canada.ca/eng/view/object/?id=a1a4197b-d0b8-4456-8ef0-81104657c70f
https://publications-cnrc.canada.ca/fra/voir/objet/?id=a1a4197b-d0b8-4456-8ef0-81104657c70f

Access and use of this website and the material on it are subject to the Terms and Conditions set forth at
https://nrc-publications.canada.ca/eng/copyright
READ THESE TERMS AND CONDITIONS CAREFULLY BEFORE USING THIS WEBSITE.

L’accès à ce site Web et l’utilisation de son contenu sont assujettis aux conditions présentées dans le site
https://publications-cnrc.canada.ca/fra/droits
LISEZ CES CONDITIONS ATTENTIVEMENT AVANT D’UTILISER CE SITE WEB.

Questions? Contact the NRC Publications Archive team at
PublicationsArchive-ArchivesPublications@nrc-cnrc.gc.ca. If you wish to email the authors directly, please see the first page of the publication for their contact information.

Vous avez des questions? Nous pouvons vous aider. Pour communiquer directement avec un auteur, consultez la première page de la revue dans laquelle son article a été publié afin de trouver ses coordonnées. Si vous n’arrivez pas à les repérer, communiquez avec nous à PublicationsArchive-ArchivesPublications@nrc-cnrc.gc.ca.

National Research Council Canada
Conseil national de recherches Canada

THE EFFECT OF CO ADDITION ON EXTINCTION LIMITS AND NO_X FORMATION IN LEAN COUNTERFLOW CH_4/AIR PREMIXED FLAMES

Hongsheng Guo, Gregory J. Smallwood
hongsheng.guo@nrc-cnrc.gc.ca
Institute for Chemical Process and Environmental Technology
National Research Council of Canada
1200 Montreal Road, Ottawa, Ontario, Canada K1A 0R6

Abstract

The effect of CO addition on flame extinction and NO_X formation in counterflow lean premixed CH_4/air flames was investigated by numerical simulation. Detailed chemistry and complex thermal and transport properties were employed. The results revel that the addition of certain amount of CO can increases the stretch extinction limits and reduces the radiation extinction limits. As a result, the lean flammability limit of CH_4/air premixed flame is extended to the leaner side by the addition of CO. The formation of NO in a flame is increased with the addition of certain amount of CO at a constant equivalence ratio. For an ultra-lean flame, the increase in the formation of NO is mainly because of the increase in the contribution from the NNH intermediate route, while this increase is mainly due to the rise in the contribution from the thermal route for a near stoichiometric flame. With the fraction of added CO being gradually increased, the formation of NO_2 in a flame first decreases, and then increases at a given equivalence ratio. The addition of certain amount of CO reduces the formation N_2O in an ultra-lean flame, while affects little on the formation of N_2O in a near stoichiometric flame.

Introduction

Lean premixed combustion is one of the most promising concepts for substantial reduction in fuel consumption and the emissions of greenhouse gases and pollutants. It involves operation with excess air-fuel ratios to substantially reduce flame temperature. At these low temperatures and excess air-fuel ratios, NO_X formation from the thermal and prompt routes can be effectively suppressed. Emission of soot, the predominant source of particulate matter and a major global warming contributor, can be essentially eliminated in these flames.

Unfortunately lean premixed combustion has some intrinsic weaknesses. One of the weaknesses is that at excessive air-fuel ratios, the lean-flammability limit is approached and the flame becomes less stable. A strategy to overcome this weakness is to adopt fuel enrichment, i.e. adding a small amount of other component to the fuel to enhance the flame stability, while maintaining the advantages of lean premixed combustion. Our previous study [1] has shown that hydrogen enrichment can significantly improve the flammability limit and reduce NO formation in counterflow CH_4/air premixed flames by allowing a combustor to operate under leaner condition. Hydrogen can be obtained by reforming hydrocarbon fuels. However, the reformate gas contains not only hydrogen, but also carbon monoxide and some minor components. It is of interest to understand the effect of carbon monoxide addition on the extinction and NO_X formation characteristics in lean CH_4/air premixed flames. Though the extinction and NO_X formation characteristics of CH_4/air premixed flames have been extensively studied [2-11], to our knowledge, these is no detailed investigation on the effect of carbon monoxide addition on extinction and NO_X formation in CH_4/air premixed flames in the literature.

The purpose of this paper is to numerically investigate the extinction and NO_X formation characteristics in lean CH_4/air premixed flames, when CO is added. Detailed chemistry and complex thermal and transport properties were used. The effect of CO addition on flammable region and flammability limit is discussed, followed by NO_X formation in CO/CH_4/air premixed flames.

Numerical Model

The flame configuration studied is an axisymmetric laminar counterflow premixed flame. The simulations assumed the stagnation point flow approximation. The governing equations can be found elsewhere [12]. The potential boundary conditions were used. Upwind and center difference schemes were respectively used for the convective and diffusion terms in all the governing equations. Adaptive refinement of meshes was done. The arc-length continuation method [12] was employed to obtain the extinction limits. The pressure and the fresh mixture temperature were 1 atm and 300 K, respectively.

A previous investigation [13] showed that the radiation reabsorption has little influence on the extinction limits and temperatures of lean counterflow CH_4/air premixed flames. To simplify the calculation, the optically thin radiation model [1, 4] was used in this paper.

The chemical reaction mechanism used is GRI-Mech 3.0 [14]. The thermal and transport properties were obtained by using the database of GRI-Mech 3.0 and the algorithms given in [15, 16]. The thermal diffusion velocity of H_2 and H was accounted for, while that of other species was ignored.

Results and Discussion

A stretch rate of 40 1/s was used for all the flames, except in the discussion of extinction limits. This is an arbitrary choice. The fraction of added CO is defined as $\alpha_{CO} = V_{CO}/(V_{CO} + V_{CH4})$, with V_{CO} and V_{CH4} being the volume flow rates of CO and CH_4, respectively. The equivalence ratio (represented by ϕ in all the plots) investigated was limited to less than 0.8 and the fraction of CO was varied from 0 to 0.6 for most cases. However for the sake of comparison, a CO fraction of 0.9 was reached in some cases.

Effect of CO Addition on Extinction Limits

A counterflow premixed flame can be extinguished by an extra high or low stretch rate [3-5]. For a given equivalence ratio flame, if stretch rate is increased to a critical value, the flame is extinguished due to the shortened residence time. On the other side, an extra low stretch rate causes a flame to extinguish due to radiation heat loss, if equivalence ratio is low. The two extinction limits are named, respectively, as stretch and radiation extinction limits. If all the extinction limits and the corresponding equivalence ratios are plotted in a stretch rate – equivalence ratio plane, a C-shaped curve is formed [4]. The upper branch of the curve is the stretch extinction limit branch, and the lower branch is the radiation extinction limit branch. The region bounded by the two branches is the flammable region of counterflow lean premixed flames. At a critical equivalence ratio, the two branches merge at one point. This critical equivalence ratio is the flammability limit of counterflow lean premixed flame.

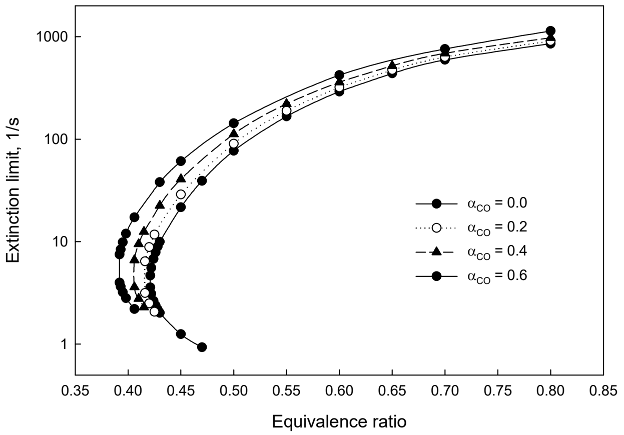

Figure 1. C-shaped curves of lean CH_4/CO/air premixed flames.

Figure 1 shows the C-shaped curves of counterflow lean CH_4/CO/air premixed flames, with the fraction of CO varying from 0 to 0.6. It is observed that if the fraction of added CO is less than or equal to 0.6, the addition of CO does not have any side effect on flammable region and flammability limit of lean CH_4/air premixed flames. The addition of CO actually slightly increases the stretch extinction limits and reduces the radiation extinction limits. As a result, the addition of CO enlarges the flammable region and lowers the lean flammability limit, although it is not as effective as hydrogen addition [1]. The lean flammability limit of CH_4/air premixed flame is extended from 0.421 to 0.406 when 40% CO is added, while this limit can be lowered from 0.421 to 0.335 with the addition of 40% hydrogen [1].

The reason that the addition of certain amount of CO to CH_4/air premixed flames enlarges the flammable region and extend the flammability limit is that it intensifies the reaction OH + CO = H + CO_2. As a result, the concentrations of radicals H and O are increased, when CO is added. This leads to the enhanced combustion intensity, and finally enlarges the flammable region and extends the flammability limit.

Simulations also indicate that when the fraction of CO is greater than 70 ~ 80%, the flammable range of a given equivalence ratio flame may be narrowed with further increasing the fraction of CO. This is because the concentration of radical OH begins to decrease. Since big fraction CO or pure CO flames are beyond the purpose of fuel enrichment combustion and this paper, details of these flames will not be discussed.

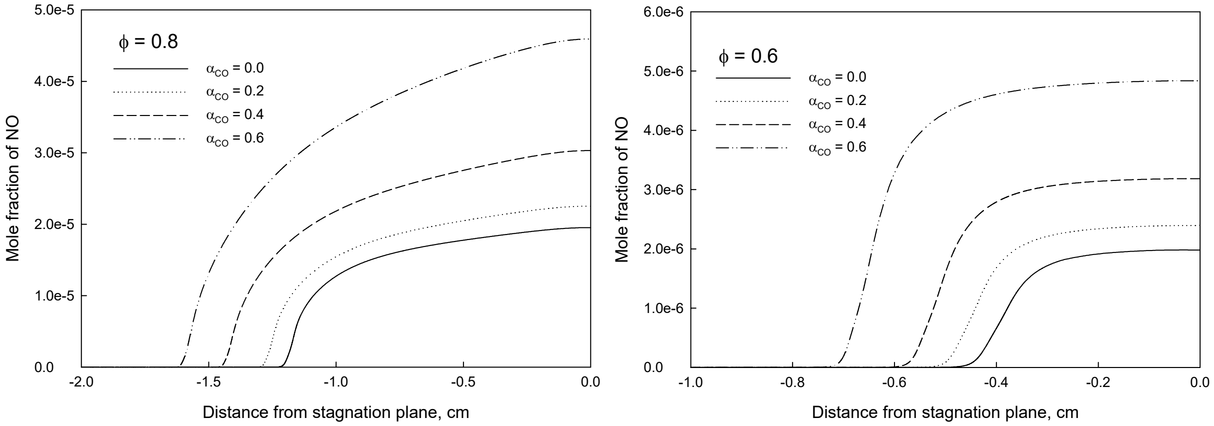

Figure 2. Profiles of NO mole fraction in flames with equivalence ratios of 0.8 and 0.6.

NO Formation

Figure 2 displays NO mole fractions in the flames with equivalence ratios of 0.6 and 0.8 and stretch rate of 40 1/s, when the fraction of CO is changed from 0 to 0.6. The reason to choose these two equivalence ratios is that they represent an ultra lean and a near stoichiometric flame, respectively. The effect of CO addition on NO formation in other flames is qualitatively similar. It is clearly illustrated that the addition of certain amount of CO to a CH_4/air premixed flame increases the formation of NO at a constant equivalence ratio.

To figure out how the addition of CO affects the formation of NO in a flame, we analyze the mechanism of NO formation first. It is known that in a hydrocarbon flame, NO can be formed through the thermal, the N_2O intermediate, and the prompt routes [6, 7], based on the initiation reactions by which molecular nitrogen is converted to atomic nitrogen or other intermediate species containing nitrogen element. Thermal NO formation is comprised of the three reactions: $N_2 + O = N + NO$; $N + O_2 = NO + O$; and $N + OH = NO + H$; of which the first one is the initiation reaction converting molecular nitrogen to NO and atomic N. The N_2O intermediate route is initiated by the reactions: $N_2O (+M) = N_2 + O (+M)$; $N_2O + H = N_2 + OH$; $N_2O + O = N_2 + O_2$; and $N_2O + OH = N_2 + HO_2$; and then the N_2O formed is partially converted to NO. The prompt NO formation is initiated by the rapid reactions of hydrocarbon radicals with molecular nitrogen [6]. In addition, NO formation can also be initiated by the reactions of molecular nitrogen with other hydrocarbon-free radicals, such as H, OH and H_2. These reactions include: $NH + N = N_2 + H$; $NH + NO = N_2 + OH$; $NNH = N_2 + H$; $NNH + M = N_2 + H + M$; $NNH + O_2 = HO_2 + N_2$; $NNH + O = OH + N_2$; $NNH + H = H_2 + N_2$; $NNH + OH = H_2O + N_2$; and $NNH + CH_3 = CH_4 + N_2$. Although the last reaction is initiated by CH_4, we also attribute it to this route due to NNH. This route is known as the NNH intermediate route [17]. In our previous study [1], a method, by 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 routes to NO formation. Some researchers argued that due to the complexity of NO formation reactions, the initial reactions of the four routes may not be independent. To verify this, we did calculations of the pure CH_4/air flame with equivalence ratio of 0.8 by five reaction schemes. The first reaction scheme is the full Gri-Mech 3.0 chemistry, and each of other four schemes contains only the initial reactions converting molecular nitrogen from one route. The NO mole fractions from the calculation using full Gri-Mech 3.0, from each separate route and the summation of NO from the four separate routes are compared in Fig. 3. No discernible difference can be observed between the two curves obtained from the full chemistry and the summation of four separate routes. This suggests that the initial reactions converting molecular nitrogen from different routes are independent. Therefore the method used in [1] does properly identify the relative contributions of the four routes. This method was used again in this paper, i.e four simulations were carried out for each flame. The first simulation (SIM1) was conducted by the full chemistry (GRI-Mech 3.0), while the second (SIM2) was carried out by removing the initiation reactions of the prompt routes. In the third simulation (SIM3), the initiation reactions of both the prompt and the NNH intermediate routes were removed. All the initiation reactions of the prompt, the N_2O and the NNH intermediate routes were removed in the fourth simulation (SIM4). Consequently NO obtained from SIM4 can be attributed to the thermal mechanism. The difference in NO between SIM1 and SIM2 is attributed to the prompt route, and the difference between SIM2 and SIM3 is due to the NNH intermediate route. The NO contributed by the N_2O intermediate route is the difference between SIM3 and SIM4.

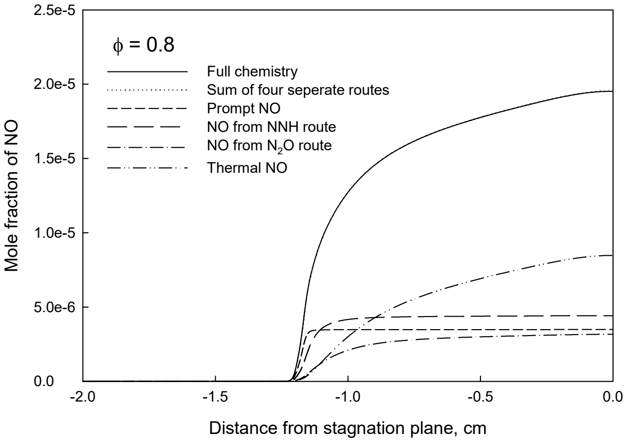

Figure 3. Comparison of NO mole fractions from full chemistry and the sum of four separate routes.

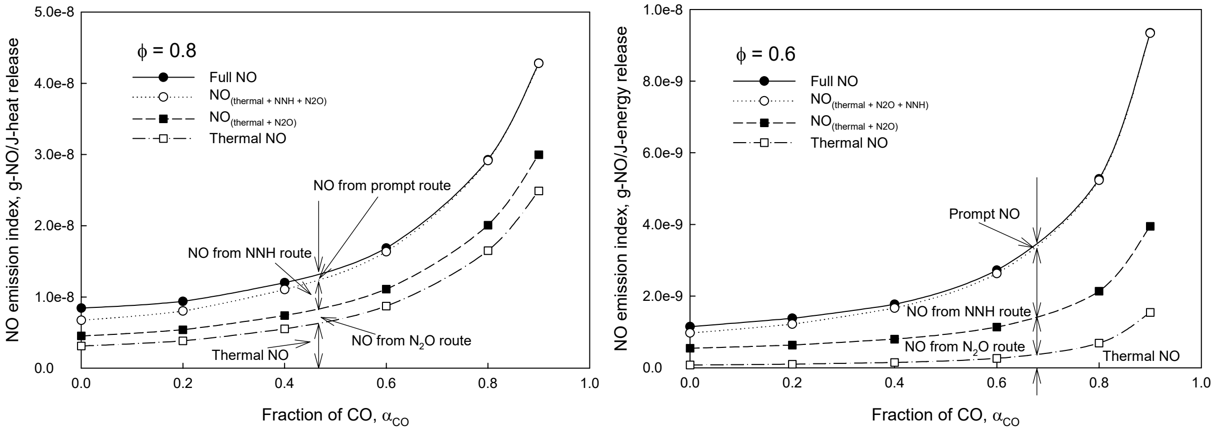

Figure 4. NO emission indices of flames with equivalence ratios of 0.8 and 0.6.

Figure 4 shows the variation of NO emission index with increasing the fraction of CO for flames with equivalence ratios of 0.8 and 0.6. Since the studied fuel is a mixture of CH_4 and CO, the definition of NO emission index is based on the total heat release rather the fuel consumption, i.e. emission index equals the ratio of the total formed NO to the total released energy (g-NO/J-energy release). Similar definition was used for the emission indices of NO_2 and N_2O, as will be discussed later. Being consistent with Fig. 1, it is noted that the addition of certain amount of CO increases the formation of NO in a lean premixed CH_4/air premixed flame.

When equivalence ratio equals 0.8, the biggest contribution to NO formation in the pure CH_4/air (α_{CO} = 0.0) premixed flame is from the thermal route. This agrees with the general understanding of NO formation in a near stoichiometric flame [6]. The contribution of the NNH intermediate route follows, and those of the other two routes are relatively smaller. With increasing the fraction of CO addition, the contribution of the thermal route quickly increases, while that of the prompt decreases. The contributions of the NNH and N_2O intermediate routes slightly rise with the increase of CO addition. When the fraction of CO is raised to 0.8 ~ 0.9, the thermal route dominates the formation of NO, and the contribution of the prompt route almost vanishes.

The quick increase of the contribution from the thermal route with the addition of CO in flames of equivalence ratio 0.8 is because of the rise in flame temperature, as shown in Fig. 5. Although the rise of flame temperature also intensifies the reactions of other routes, they are not as sensitive as the thermal route to temperature. The concentrations of hydrocarbon radicals decrease with the addition of CO, which leads to the reduction of the contribution from the prompt route, when CO is added.

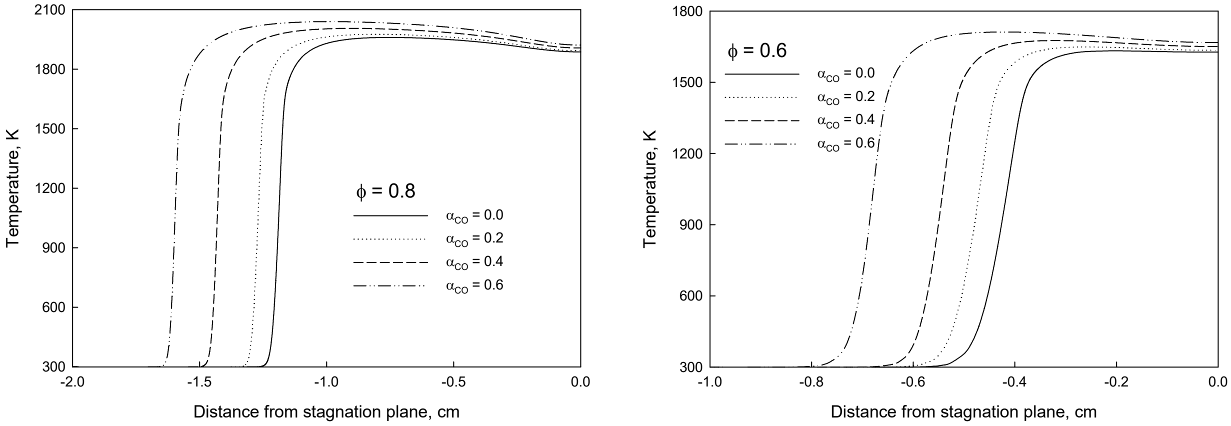

Figure 5. Temperatures in flames with equivalence ratios of 0.6 and 0.8.

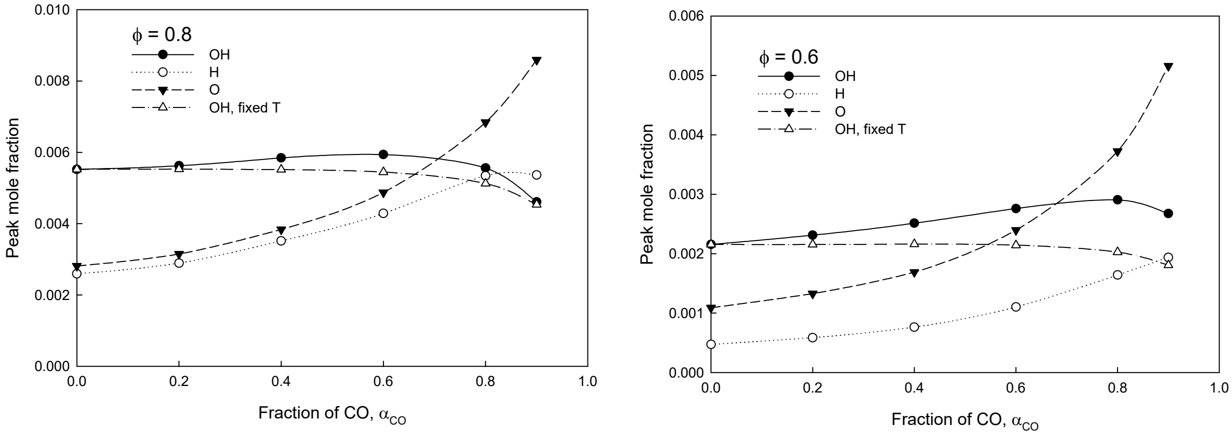

Figure 6. Variations in peak mole fractions of OH, H and O with the addition of CO.

When equivalence ratio equals 0.6, the situation varies. Due to the low flame temperature, as shown in Fig. 5, the contribution of the thermal route is very small for pure CH_4/air flame (α_{CO} = 0.0), Fig. 4. The contribution of the prompt route is also very small in flames with equivalence ratio of 0.6, because of the higher air-fuel ratio. The NNH and N_2O intermediate route contributes most NO formation in pure CH_4/air flame. This is a feature of an ultra-lean CH_4/air premixed flame. With increasing the fraction of CO addition, similar to the flames of equivalence ratio 0.8, the contribution of the prompt gradually reduces. Although the contributions of the other three routes increase, relatively the rise rate of the NNH intermediate route is faster, when the fraction of CO addition is raised from 0.0 to 0.8. With the further rise of the CO fraction to over 0.8, the contribution of the thermal route begins to quickly increase.

The variation of the NO formation mechanism with the addition of CO in flames of equivalence ratio 0.6 is caused by the changes in flame temperature and concentrations of some important radicals, such as H, OH and O. Figure 6 displays the variations of the peak mole fractions of OH, H and O with increasing the addition of CO. It is observed that the concentrations of radicals H and O monotonously increase until the fraction of CO is raised to 0.9. The concentration of OH first increases, and then decreases with raising the fraction of CO. This phenomenon is due to the reaction $OH + CO = H + CO_2$. When CO is added, the rate of this reaction is intensified, and thus the formation rate of H is enhanced. Consequently, the rate of the chain branching reaction $H + O_2 = OH + O$ is also intensified, which leads to the rise in the concentration of radical O. It should be noted that the addition of CO results in that more OH is needed to complete the reaction $OH + CO = H + CO_2$, although more OH may be produced by the reaction $H + O_2 = OH + O$. As a result, the variation of OH concentration with the addition of CO depends on the balance between the two reactions. We also conducted some extra simulations in which the flame temperatures were kept the same as in pure CH_4/air flames. The results indicate that the peak concentrations of O and H also increase with the addition of CO in these extra simulations. However, the peak mole fraction of OH is almost constant until the fraction of CO reaches 0.4. With the further increase of CO, the peak mole fraction of OH begins to decrease, as shown in Fig. 6 (represented by the curve of OH, fixed T). Therefore the increase of peak OH mole fraction in normal simulations is partly caused by the rise of flame temperature. When the fraction of CO is greater than 0.8, the large amount of CO leads to the decrease of OH, even the flame temperature still increases with the addition of CO.

In the NNH and N_2O intermediate routes, molecular nitrogen is first converted to NNH and N_2O. Then NNH and N_2O are converted to NO by some reaction sequences. A sensitivity analysis indicates that the two 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 $NNH + O_2 = HO_2 + N_2$. When CO is added to the flame of equivalence ratio 0.6, the rise in flame temperature and concentration of radical H, as shown in Figs. 5 and 6, causes the increase in the rates of NNH formation and the later NNH conversion to NO. This leads to the quick increase in the contribution of the NNH intermediate route to NO formation, when CO is added. The most important formation and destruction reactions of N_2O are $N_2O\ (+M) = N_2 + O\ (+M)$ and $N_2O + H = N_2 + OH$, respectively. The increase in the concentrations of radicals H and O causes the rise in the rates of both the formation and destruction reactions of N_2O. Therefore the contribution of the N_2O intermediate route to NO formation rises slower than that of the NNH intermediate route, with increasing the fraction of CO. It should be pointed out that the concentrations of O and H in the flames of equivalence ratio 0.8 also increase with the addition of CO, but the high temperature levels cause the increase rates of the contributions from the NNH and N_2O intermediate routes are not as faster as that of the thermal route.

Although the rise of temperature can cause the increase in the contribution of the thermal route, the lower temperature levels in the flames of equivalence ratio 0.6 results in the negligible NO formation by the thermal route until the fraction of CO reaches 0.8. When the fraction of CO increases to greater than 0.8, the flame temperature is raised to a high enough level, so that the

NO from the thermal route becomes significant. Therefore with the further increase of CO fraction, the contribution of the thermal route quickly increases.

The above results and discussion conclude that the addition of certain amount of CO to a lean CH_4/air premixed flame causes the increase in the formation of NO at a constant equivalence ratio. The increase of NO formation is mainly due to the NNH intermediate route in the ultra-lean flames, and due to the thermal route in the near stoichiometric flames.

NO_2 Formation

Figure 7 shows the variations of NO_2 emission indices with increasing the fraction of CO in the flames with equivalence ratios of 0.8 and 0.6. It is observed that at a constant equivalence ratio, the formation of NO_2 first decreases, and then increases, when the fraction of CO is increased.

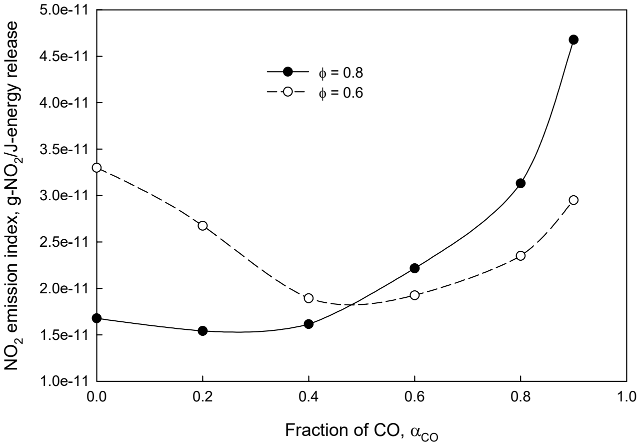

Figure 7. Variation of NO_2 emission index with increasing the fraction of CO.

The main NO_2 formation and destruction reactions are $HO_2 + NO = NO_2 + OH$ and $NO_2 + H = NO + OH$, respectively. The activation energy of the former is negative, and the latter is positive. When equivalence ratio equals 0.6 and the fraction of CO is increased from 0 to 0.5, both flame temperature and NO formation rate gradually increase, as in Figs. 5 and 6, leading to little variation in the formation rate of NO_2, because of the negative activation energy of the main NO_2 formation reaction. On the other hand, the addition of CO increases the concentration of H, as shown in Fig. 6, which causes the rise in the main NO_2 destruction reaction rate. Consequently, the net NO_2 formation rate decreases, when the fraction of CO is increased from 0 to 0.5 for the flame with equivalence ratio of 0.6. However, with the further addition of CO, the formation of NO begins to quickly rise, as in Fig. 6, resulting in the rate of the NO_2 formation reaction begin to rise. Therefore the net NO_2 formation reaches the minimum at α_{CO} equals about 0.5 for the flame of equivalence ratio 0.6.

The situation in the flame with equivalence ratio of 0.8 is similar to that in the flame with equivalence ratio of 0.6, except that the transition of net NO_2 formation from decrease to increase occurs at $\alpha_{CO} = 0.2 \sim 0.3$, when the fraction of CO is gradually increased.

N_2O Formation

Figure 8 displays the variations of N_2O emission indices with changing the fraction of CO. It is noted that with increasing the addition of CO, the variations of N_2O emission indices of the two flames (ϕ = 0.6 and 0.6) differ. For the flame with equivalence ratio of 0.6, the emission index of N_2O first decreases, and finally rises, when the fraction of CO is increased. When equivalence ratio equals 0.8, the emission index of N_2O almost does not change until the fraction of CO reaches 0.6. With the further increase of the CO fraction from 0.6 to 0.9, the emission index of N_2O slightly rises. The difference in the variations of the N_2O emission indices of the two equivalence ratio flames with the addition of CO is caused by the disparity in the temperature levels.

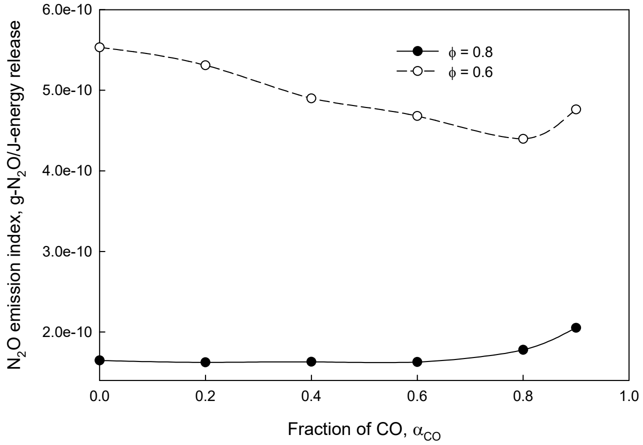

Figure 8. Variation of N_2O emission index with increasing the fraction of CO.

The most important formation and destruction reactions of N_2O are N_2O (+M) = N_2 + O (+M) and $N_2O + H = N_2 + OH$, respectively. The formation reaction has higher activation energy than the destruction reaction. With the addition of CO, the flame temperature and concentrations of O and H increase in both equivalence ratio flames, as in Figs. 5 and 6, which causes the increase in both the formation and destruction reaction rates. Since the temperature level is low in the flame with equivalence ratio of 0.6, the increase of the formation reaction rate is slower than that of the destruction reaction rate, when the fraction of CO is changed from 0 to 0.8, leading to the reduction in the net formation of N_2O. For the flame with equivalence ratio of 0.8, the higher temperature level results in the similar increase in the rates of the N_2O formation and destruction. Consequently, the net N_2O formation rate almost does not change when the fraction of CO is increased from 0 to 0.6 in the flame with equivalence ratio of 0.8.

With the fraction of CO is increased to a higher level, the concentration of H begins to decrease or increase very slowly, as shown in Fig. 6. This causes the slightly increase of the net N_2O formation in flames of both equivalence ratios, with the further addition of CO. However, it should be noted that the higher fraction CO addition rarely happens in applications, and is beyond the purpose of this paper. We will not discuss more details about higher fraction CO addition.

Conclusions

The effect of CO addition on the characteristics of flame extinction and NO_X formation in counterflow lean premixed CH_4/air flames has been examined by numerical simulation. The results indicate that the addition of certain amount of CO slightly increases the stretch extinction limits and reduces the radiation extinction limits. As a result, the lean flammability limit of CH_4/air premixed flame is slightly extended to the leaner side by the addition of CO. The formation of NO in a flame is increased with the addition of certain amount of CO at a constant equivalence ratio. For an ultra-lean flame, the increase in the formation of NO is mainly because of the increase in the contribution from the NNH intermediate route, while this increase is mainly due to the rise in the contribution from the thermal route for a near stoichiometric flame. With the fraction of added CO being gradually increased, the formation of NO_2 in a flame first decreases, and then increases. The addition of certain amount of CO reduces the formation N_2O in an ultra-lean flame, while affects little on the formation of N_2O in a near stoichiometric flame.

References

1. Guo, H., Smallwood, G. J., Liu, F., Ju, Y., and Gülder, Ö.L., Proc. Comb. Inst. 30 (2005) 303-311.
2. Tien, J.S., *Combust. Flame* 65 (1986) 31-34.
3. Maruta, K., Yoshida, M., Ju, Y., and Niioka, T., *Proc. Combust. Inst*. 26 (1996) 1283-1289.
4. Guo, H., Ju, Y., Maruta, K., Niioka, K., and Liu, F., *Combust. Flame* 109 (1997) 639-646.
5. Ju, Y., Guo, H., Maruta, K., and Liu, F., *J. Fluid Mech*. 342 (1997) 315-334.
6. Miller, J.A., and Bowman, C.T., *Prog. Energy Combust. Sci*. 15 (1989) 287-338.
7. Ju, Y., Niioka, T., *Combust. Theory Modelling* 1 (1997) 243-258.
8. Wang, J., Niioka, T., *Proc. Combust. Inst*. 29 (2002) 2211-2218.
9. Atreya, A., Kim, H.K., Shamim, T., and Suh, J., *Proc. Combust. Inst*. 26 (1996) 2181-2189.
10. Naik, S.V., Laurendeau, N.M., *Combust. Flame* 129 (2002) 112-119.
11. Fuse, R., Kobayashi, H., Ju, Y., Maruta, K., and Niioka, T., *Int. J. Therm. Sci.* 41 (2002)693-698.
12. Giovangigli, V., and Smooke, M.D., *Combust. Sci. Tech*. 53 (1987) 23-49.
13. Guo, H., Ju, Y., Maruta, K., Niioka, T., and Liu, F., *Combust. Sci. Technol*. 135 (1998) 49-64.
14. Gregory P. Smith, David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, C. Thomas Bowman, Ronald K. Hanson, Soonho Song, William C. Gardiner, Jr., Vitali V. Lissianski, and Zhiwei Qin http://www.me.berkeley.edu/gri_mech/.
15. Kee., R.J., Warnatz, J., and Miller, J.A., *A Fortran Computer Code Package for the Evaluation of Gas-Phase Viscosities, Conductivities, and Diffusion Coefficients*, Report No. SAND 83-8209, Sandia National Laboratories, 1983.
16. Kee., R.J., Miller, J.A., and Jefferson, T.H., *A General-Purpose, Problem-Independent, Transportable, Fortran Chemical Kinetics Code Package*, Report No. SAND 80-8003, Sandia National Laboratories, 1980.
17. Rørtveit, G. J., Hustad, J.E., Li, S., and Williams, F.A., *Combust. Flame* 130 (2002) 48-61.