

# Flame Structure and Thermal NO<sub>x</sub> Formation in Hydrogen Diffusion Flames with Reduced Kinetic Mechanisms

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Structure and thermal NO<sub>x</sub> formation of hydrogen diffusion flames are studied numerically, by adopting a counterflow as a model problem. Detailed kinetic mechanism having twenty-one step hydrogen oxidation is systematically reduced to a two-step mechanism while five-step thermal NO<sub>x</sub> chemistry of the extended Zel'dovich mechanism is reduced to one-step. Results show that the extinction strain rates are much higher than those for hydrocarbon flames and the NO<sub>x</sub> production can be controlled by increasing strain rates which results in the decrease of flame temperature significantly. Comparison between the results of the detailed and reduced mechanisms demonstrates that the reduced mechanism successfully describes the essential features of hydrogen diffusion flames including the flame structure, extinction strain rate and NO<sub>x</sub> production.

**Key Words:** Hydrogen, Diffusion Flame, Thermal NO<sub>x</sub>, Extinction, Reduced Mechanism

## 1. Introduction

One-step overall reaction has been frequently adopted as a chemistry modeling in analyzing diffusion and premixed flames. As a result, only qualitative predictions can be made. For quantitative predictions, however, a set of multi-step elementary reactions should be accounted for. Recently, due to the advent of powerful computing capability, a detailed chemistry modeling of flame structure has been introduced. Methane/air diffusion flame structure was numerically studied by Dixon-Lewis et al.(1984) for the Tsuji burner geometry and the results are in good agreement with experiment. Dixon-Lewis and Missaghi(1988) analyzed the flame structure and extinction of hydrogen/air diffusion flames, and Pitz and Westbrook(1986) studied the autoignition of butane fuel in engine considering over 200 reaction steps.

Detailed chemistry modeling, however, is still

impractical in applying to multi-dimensional or turbulent flames because of excessive computation time arising from many species involved in chemical reaction. Thus, reduced kinetic mechanisms have been developed by adopting proper steady-state approximations for reaction intermediaries and/or partial equilibrium assumptions for suitable reaction steps. Peters(1985) derived a four-step reduced kinetic mechanism for methane/air premixed flame and calculated the flame speed which was in good agreement with experiment. This four-step reduced mechanism has also been applied to the analysis of diffusion flame structure(Peters and Kee, 1987). The efforts to reduce the reaction steps are extended to the various kinds of fuels including the heavier hydrocarbon(Chung et al., 1993).

As a reduced kinetic mechanism predicts well the flame structure, matched asymptotic analyses have been performed to understand flame characteristics. Chung and Williams(1990) derived a two-step reduced mechanism for diffusion flames of CO/H<sub>2</sub> mixture as a model for a low calory fuel and analyzed the flame structure asymptotically. Lee and Chung(1994) analyzed the hydrogen diffusion flame asymptotically with

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two-step reduced mechanism.

These studies suggest that since the reduced mechanism depends on fuels, the application of a reduced mechanism should be developed for each fuel. Thus, the present study is focused on hydrogen fuel which is used as a liquid propellant and is considered to be a suitable fuel for a hypersonic flight. Due to the increasing awareness on environmental issues, hydrogen fuel is also considered as an alternative clean fuel for automotive use in the future. Thus, the objective of the present study is to analyze the flame structure and investigate the NO<sub>x</sub> formation of hydrogen diffusion flames using reduced kinetic mechanism.

## 2. Formulation and Numerical Schemes

We consider a counterflow system, in which a nitrogen-diluted hydrogen jet impinges on a jet of air, and subsequently mixed stoichiometrically and reacted near the stagnation plane, having a planar diffusion flame stabilized. In a boundary layer approximation, counterflow system has a similarity solution by defining a stream function  $f$  and the mass flux  $V$  as

$$f' = \frac{u}{u_\infty}, \quad V = \rho v \quad (1)$$

The transformed governing equations of continuity, momentum, species, energy, and mixture fraction are as follows:

$$\frac{dV}{dy} + (j+1)\alpha\rho f' = 0 \quad (2)$$

$$\frac{d}{dy} \left( \mu \frac{df'}{dy} \right) - V \frac{df'}{dy} + a[\rho_e - \rho(f')^2] = 0 \quad (3)$$

$$-\frac{d}{dy} (\rho Y_i V_{iy}) - V \frac{dY_i}{dy} + \omega_i W_i = 0, \quad (4)$$

$$i = 1, 2, \dots, N$$

$$\frac{d}{dy} \left( \lambda \frac{dT}{dy} \right) - C_p V \frac{dT}{dy} - \sum_{i=1}^N \rho Y_i V_{iy} C_{pi} \times \frac{\partial T}{\partial y} - \sum_{i=1}^N \omega_i W_i h_i = 0 \quad (5)$$

$$\frac{d}{dy} \left( \frac{\lambda}{C_p} \frac{dZ}{dy} \right) - V \frac{dZ}{dy} = 0 \quad (6)$$

where  $T$  is the temperature,  $\rho$  the density,  $Y_i$ ,  $W_i$ , and  $\omega_i$  are the mass fraction, molecular weight, and reaction rate of  $i$ -th species, respectively,  $u$

and  $v$  the transverse and axial velocities, respectively,  $C_{pi}$  and  $h_i$  the specific heat and enthalpy of  $i$ -th species, respectively,  $C_p$  the specific heat of mixture,  $Z$  the mixture fraction,  $a$  the stretch factor defined in the free stream condition denoted by the subscript  $e$ ,  $j$  the geometric factor for  $j = 0$  and 1 for two-dimensional and axisymmetric cases, respectively, and  $N$  the total number of species involved.  $V_{iy}$  is the diffusion velocity of  $i$ -th species in axial direction determined from the Curtis-Hirschfelder approximation and  $\lambda$  and  $\mu$  the thermal conductivity and viscosity of a mixture determined from Wilke's formula. And the equation of state is

$$\rho = pW/RT \quad (7)$$

where  $p$  is the pressure,  $W$  the molecular weight of mixture, and  $R$  the gas constant.

These equations are subject to the following boundary conditions at the free stream.

$$y = -\infty: \quad V = V_{-\infty}, \quad f' = \sqrt{\rho_\infty/\rho_{-\infty}},$$

$$T = T_{-\infty}, \quad Y_i = Y_{i,-\infty},$$

$$i = 1, \dots, N \quad (8)$$

$$y = \infty: \quad f' = 1, \quad T = T_\infty,$$

$$Y_i = Y_{i,\infty}, \quad i = 1, \dots, N \quad (9)$$

To account for the infinite boundary conditions at  $\pm\infty$ , the calculation domain is selected at  $y = -L_F$  and  $y = L_O$  which are sufficiently far from the boundary layer.

Thermodynamic properties and state equations are calculated from CHEMKIN(Kee et al., 1980) and transport properties from TRANSPORT package(Kee et al., 1983).

The starting mechanism is listed in Table 1 where the specific reaction rate constant  $k_k$  of the  $k$ -th reaction step is

$$k_k = B_k T^{a_k} \exp(-E_k/RT). \quad (10)$$

The reaction rate of  $i$ -th species  $\omega_i$  is the summation over all  $k$ -th steps involving  $i$ -th species. The mechanism contains 12 species and 21 reaction steps for H<sub>2</sub>/O<sub>2</sub> reactions and 5 steps for thermal NO<sub>x</sub> chemistry of the extended Zel'dovich mechanism corresponding to the steps N1 through N5.

Numerical calculation is based on Smooke's code(Smooke et al., 1986) by discretizing the governing equations into algebraic relations and

**Table 1** Specific reaction-rate constants for starting mechanism of H<sub>2</sub>-O<sub>2</sub>-N<sub>2</sub> reaction system (Units: kJ/mol, mol/cm<sup>3</sup>, s<sup>-1</sup>)

No.	Reaction	A <sub>j</sub>	α <sub>j</sub>	E <sub>j</sub>
1	H + O <sub>2</sub> ↔ <sup>b</sup> OH + O	2.0E14	0.0	70.30
2	H <sub>2</sub> + O ↔ OH + H	5.06E4	2.67	26.30
3	H <sub>2</sub> + OH ↔ H <sub>2</sub> O + H	1.0E8	1.6	13.80
4	OH + OH ↔ H <sub>2</sub> O + O	1.5E09	1.14	0.42
5 <sup>a</sup>	H + O <sub>2</sub> + M → <sup>c</sup> HO <sub>2</sub> + M	2.3E18	-0.8	0.00
6	H + HO <sub>2</sub> → OH + OH	1.5E14	0.0	4.20
7	H + HO <sub>2</sub> → H <sub>2</sub> + O <sub>2</sub>	2.5E13	0.0	2.90
8	OH + HO <sub>2</sub> → H <sub>2</sub> O + O <sub>2</sub>	6.0E13	0.0	0.00
9	H + HO <sub>2</sub> ↔ O + H <sub>2</sub> O	3.0E13	0.0	7.20
10	HO <sub>2</sub> + O ↔ OH + O <sub>2</sub>	1.8E13	0.0	-1.70
11	HO <sub>2</sub> + HO <sub>2</sub> → H <sub>2</sub> O <sub>2</sub> + O <sub>2</sub>	2.5E11	0.0	-5.20
12 <sup>a</sup>	OH + OH + M ↔ H <sub>2</sub> O <sub>2</sub> + M	3.25E22	-2.0	0.00
13	H <sub>2</sub> O <sub>2</sub> + H ↔ H <sub>2</sub> O + OH	1.0E13	0.0	15.00
14	H <sub>2</sub> O <sub>2</sub> + OH ↔ H <sub>2</sub> O + HO <sub>2</sub>	5.4E12	0.0	4.20
15 <sup>a</sup>	H + H + M → H <sub>2</sub> + M	1.8E18	-1.0	0.00
16 <sup>a</sup>	H + OH + M → H <sub>2</sub> O + M	2.2E22	-2.0	0.00
17 <sup>a</sup>	O + O + M ↔ O <sub>2</sub> + M	2.9E17	-1.0	0.00
18 <sup>a</sup>	H + O + M ↔ OH + M	6.2E16	-0.6	0.00
19	H <sub>2</sub> O <sub>2</sub> + H ↔ HO <sub>2</sub> + H <sub>2</sub>	1.7E12	0.0	15.75
20 <sup>a</sup>	O + OH + M ↔ HO <sub>2</sub> + M	1.0E16	0.0	0.00
21	H <sub>2</sub> + O <sub>2</sub> ↔ OH + OH	1.7E13	0.0	200.70
Thermal NO <sub>x</sub> mechanism				
N1	O + N <sub>2</sub> ↔ N + NO	1.9E14	0.0	319.03
N2	N + O <sub>2</sub> ↔ O + NO	1.129E10	1.0	27.83
N3	N + OH ↔ NO + H	4.795E13	0.0	5.23
N4	NO + HO <sub>2</sub> ↔ NO <sub>2</sub> + OH	3.E12	0.5	10.08
N5	NO + OH ↔ NO <sub>2</sub> + H	5.9E12	0.0	129.49

<sup>a</sup> Chaperon efficiencies H<sub>2</sub>O/6.5/H<sub>2</sub>/1.0/O<sub>2</sub>/0.4/N<sub>2</sub>/0.4

<sup>b</sup> Reversible reaction

<sup>c</sup> Forward reaction

solving it with Newton method and Euler time integration. Adaptive grid is employed since the reaction zone is very thin. The solution procedure is summarized in the following. For the grid point system  $M$  of

$$M = \{-L_F = y_0 < y_1 < \dots < y_n = L_o\} \quad (11)$$

the finite differencing of the governing equations of Eqs. (2)~(6) leads to the following nonlinear algebraic equations.

$$F(U_k) = 0 \quad (12)$$

where  $U_k$  is a dependent variable. To solve this, the following linear system is devised

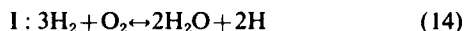
$$J(U_k)(U_{k+1} - U_k) = -\lambda_k F(U_k), \quad k=1, \dots, n-1 \quad (13)$$

which are to be solved by using iteration method, where  $J(U_k)$  is the Jacobian matrix and  $\lambda_k$  the damping factor. Since factoring the matrix takes much time, we used the modified Newton method which determines the Jacobian periodically. Since the Newton method is sensitive to initial condi-

tions in convergence that the Euler time integration is also used to refine initial conditions.

### 3. Reduced Mechanism

Twenty-one steps of  $H_2$ - $O_2$  chemistry and five steps of nitrogen chemistry are adopted as a starting mechanism as is listed in Table 1. This starting mechanism can be reduced systematically as follows. Reaction rates of O, OH,  $HO_2$  and  $H_2O_2$  are orders of magnitude larger than the transport rates of these species and thus steady-state can be assumed for these species. This results in four algebraic equations which can be used to eliminate reaction steps of 2, 3, 7 and 12 in the balance equations for the remaining non-steady state species. Consequently, the starting mechanism is reduced to a two-step mechanism for hydrogen oxidation, given by



which are hydrogen oxidation and radical generation (I) and radical recombination (II).

Preliminary numerical results indicate that the concentrations of N and NO are much lower than that of  $NO_2$ . Thus, one-step reduced  $NO_x$  mechanism can be derived from the extended Zel'dovich mechanism by using the steady-states for N and NO as



The reaction rates of these reduced mechanisms are as follows.

$$\begin{aligned} \omega_I &= \omega_1 + \omega_6 + \omega_9 + \omega_{11} - \omega_{14} - \omega_{17} - \omega_{19} \\ &\quad - \omega_{20} + \omega_{21} (-\omega_{N1} + \omega_{N2} - \omega_{N5}) \\ \omega_{II} &= \omega_5 - \omega_{11} + \omega_{13} + \omega_{14} + \omega_{15} + \omega_{16} \\ &\quad + \omega_{17} + \omega_{18} + \omega_{19} + \omega_{20} \\ \omega_{III} &= \omega_{N1} \end{aligned} \quad (17)$$

Here the terms in the parenthesis can be considered only in predicting  $NO_x$  formation. The overall flame structure including flame extinction is influenced little by neglecting these terms.

The steady-state approximations relate the concentrations of steady-state species with other species concentrations. Since these relations are algebraically complex, it is quite cumbersome to

calculate the concentrations of the steady-state species and express them explicitly. Concentration of some steady-state species can be approximated from the corresponding partial equilibrium. Especially, the concentration of OH can be reasonably approximated from a partial equilibrium of step-3. This result can be fed into other steady-state relations to determine the concentrations such as O,  $HO_2$  and  $H_2O_2$ . And then, the steady-state OH relation can be used for the refinement.

The partial equilibrium of step-3, i.e.,  $\omega_3 \approx 0$ , dictates

$$[OH] = \frac{[H][H_2O]}{K_3[H_2]} \quad (18)$$

where  $K_k$  is the equilibrium constant of step- $k$ . By neglecting the minor radicals of  $HO_2$  and  $H_2O_2$  in the steady-state relation for O, the concentration of O can be approximated as

$$[O] = \frac{\omega_{1f} + \omega_{2b} + \omega_{4f}}{k_{1b}[OH] + k_{2f}[H_2] + k_{4b}[H_2O]} \quad (19)$$

Then, the steady-states of  $HO_2$  and  $H_2O_2$  show the following relations.

$$\begin{aligned} [HO_2] &= (b_1^2/4 + a_1)^{1/2} - b_1/2 \\ a_1 &= \{ \omega_5 + \omega_{9b} + \omega_{10b} + \omega_{20f} + (Z_{14f} + Z_{19f}) \\ &\quad \times (\omega_{12f} + \omega_{13b}) \} / \{ k_{11}(2 - Z_{14f} - Z_{19f}) \} \\ b_1 &= \{ (k_6 + k_7 + k_{9f})[H] + k_8[OH] + k_{10f}[O] \\ &\quad + (k_{14b}[H_2O] + k_{19b}[H_2])(1 - Z_{14f} \\ &\quad - Z_{19f}) + k_{20b}[M] \} / \{ k_{11}(2 - Z_{14f} - Z_{19f}) \} \\ Z_{14f} &= k_{14f}[OH] / (k_{12b}[M] + k_{13f}[H] \\ &\quad + k_{14f}[OH] + k_{19f}[H]) \\ Z_{19f} &= k_{19f}[H] / (k_{12b}[M] + k_{13f}[H] \\ &\quad + k_{14f}[OH] + k_{19f}[H]) \end{aligned} \quad (20)$$

$$[H_2O_2] = \frac{\omega_{11} + \omega_{12f} + \omega_{13b} + \omega_{14b} + \omega_{19b}}{k_{12b}[M] + k_{13f}[H] + k_{14f}[OH] + k_{19f}[H]} \quad (21)$$

For the refinement of O and OH concentrations, the steady-state relations of O and OH yield the following expressions.

$$\begin{aligned} [O] &= (b_2^2/4 + a_2)^{1/2} - b_2/2 \\ a_2 &= (\omega_{1f} + \omega_{2b} + \omega_{4f} + \omega_{9f} + \omega_{10b} \\ &\quad + 2\omega_{17b} + \omega_{18b} + \omega_{20b}) / 2k_{17f} \\ b_2 &= \{ (k_{1b} + k_{20f})[OH] + k_{2f}[H_2] \\ &\quad + k_{4b}[H_2O] + k_{9b}[H_2O] + k_{10f}[HO_2] \\ &\quad + k_{18f}[H] \} / 2k_{17f} \end{aligned} \quad (22)$$

$$\begin{aligned}
 [\text{OH}] &= (b_3^2/4 + a_3)^{1/2} - b_3/2 \\
 a_3 &= (\omega_{1f} + \omega_{2f} + \omega_{3b} + 2\omega_{4b} + 2\omega_6 \\
 &\quad + \omega_{10f} + 2\omega_{12b} + \omega_{13f} + \omega_{14b} \\
 &\quad + \omega_{18f} + \omega_{20b} + 2\omega_{21f}) \\
 &\quad / 2(k_{4f} + k_{12f}[\text{M}] + k_{21b}) \\
 b_3 &= ((k_{1b} + k_{20f}[\text{M}])[\text{O}] + (k_{2b} + k_{16}[\text{M}]) \\
 &\quad \times [\text{H}] + k_{3f}[\text{H}_2] + k_8[\text{HO}_2] \\
 &\quad + k_{13b}[\text{H}_2\text{O}] \\
 &\quad + k_{14f}[\text{H}_2\text{O}_2] \\
 &\quad + k_{18b}[\text{M}] + k_{10b}[\text{O}_2]) \\
 &\quad / 2(k_{4f} + k_{12f}[\text{M}] + k_{21b}) \quad (23)
 \end{aligned}$$

Concentrations of N and NO are also determined from their respective steady-states as follows.

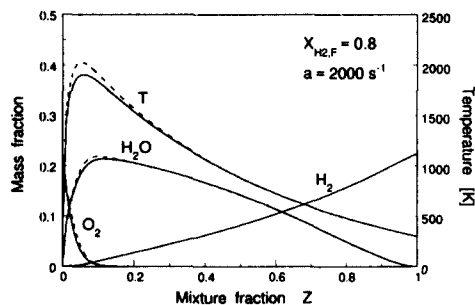
$$\begin{aligned}
 [\text{N}] &= (\omega_{N1f} + \omega_{N2b} + \omega_{N3b}) \\
 &\quad / (k_{N1b}[\text{NO}] + k_{N2f}[\text{O}_2] \\
 &\quad + k_{N3f}[\text{OH}]) \quad (24)
 \end{aligned}$$

$$\begin{aligned}
 [\text{NO}_2] &= (\omega_{N4f} + \omega_{N5f}) \\
 &\quad / (k_{N4b}[\text{OH}] + k_{N5b}[\text{H}]) \quad (25)
 \end{aligned}$$

#### 4. Results and Discussions

Two-dimensional ( $j=0$ ) counterflow system is adopted as a model problem in the present study. Air is assumed a mixture of 79% N<sub>2</sub>/21% O<sub>2</sub> and the fuel is hydrogen diluted with nitrogen. The pressure is 1 atm and the initial temperatures on both sides of fuel and air free streams are 298 K.

Figure 1 demonstrates the temperature and concentrations of major species as a function of mixture fraction for the free stream conditions of  $a=2000 \text{ s}^{-1}$  and the hydrogen mole fraction on the fuel side of  $X_{\text{H}_2,\text{F}}=0.8$ . The solid lines are the

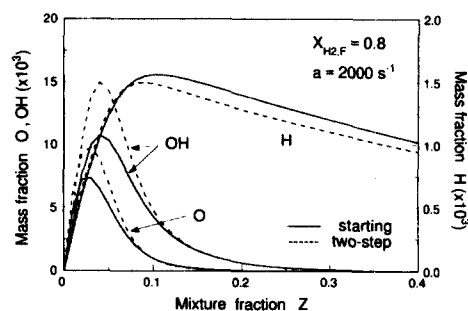


**Fig. 1** Profiles of temperature and major species with mixture fraction for starting (solid line) and two-step reduced (dashed line) mechanisms

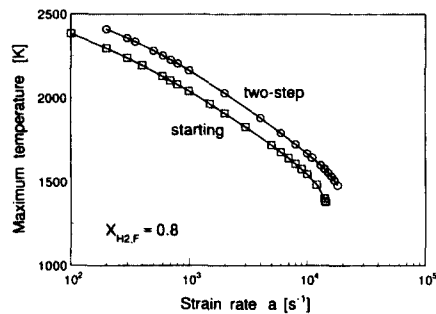
results from starting mechanism and the dotted lines from reduced mechanism. The temperature and concentrations of major species agree well except the high temperature region where the results from the reduced mechanism slightly overpredict the temperature, O<sub>2</sub> and H<sub>2</sub>O.

Radical profiles of O, OH and H are shown in Fig. 2. These profiles are in qualitative agreement, and the concentrations of O and OH are overpredicted in the reduced mechanism. On the other hand, better agreement for radical H can be seen since H is not assumed in steady-state. The reason of the overprediction of the temperature and species concentrations can be attributed to the steady-state approximations of radicals except H, such that the transport effect of diffusion and convection is not accounted for in the reduced mechanism, resulting in the overprediction.

Variations of the flame temperature with stretch are shown in Fig. 3. In general, flame temperature



**Fig. 2** Profiles of H, O and OH mass fractions with mixture fraction for starting and two-step reduced mechanisms



**Fig. 3** Variations of maximum temperature as a function of strain rate for starting and two-step reduced mechanisms

should approach the adiabatic one when the stretch approaches zero if all the Lewis numbers are unity. This is because the characteristic flow time becomes long enough that the reaction reaches an equilibrium in the small stretch regime, that is, the reaction time is shorter than the fuel and oxidizer mixing time. As a result, the fuel and oxidizer at the reaction zone maintain low concentrations. As stretch is increased, due to the reduction in the characteristic flow time, chemical reaction can not be completed and leakages of fuel and oxidizer through the reaction zone increase, leading to the decrease in the flame temperature. As the stretch is further increased over  $a=14300\text{ s}^{-1}$ , flame can not exist since the flow time becomes too short to sustain the flame.

The flame structure of hydrogen diffusion flame is quite different in nature, compared to that of hydrocarbon fuels such as methane. For methane, the flame structure in the reaction zone is composed of three zones; the methane fuel consumption layer, water-gas shift reaction zone and oxidation layer of  $\text{H}_2$  and  $\text{CO}$ . Even for the stretch near extinction for hydrocarbons, fuel leakage does not occur since the fuel is almost completely consumed in the fuel consumption layer, whereas significant amount of oxidizer leaks through the flame. However, for hydrogen flames, the fuel, i. e., hydrogen, leaks through the flame. This is demonstrated by the existence of the appreciable amount of hydrogen in the region between the flame and oxidizer boundary as can be seen in Fig. 1. This is partly because of the mass diffusivity and because the fuel to oxidizer mass ratio for stoichiometry are quite different between hydrogen and hydrocarbon fuels. The extinction strain rate for the present hydrogen fuel is an order of magnitude higher than that of hydrocarbon fuels, meaning that the hydrogen diffusion flame is difficult to extinguish.

For the entire range of the stretch, the prediction of flame temperature from the reduced mechanism is approximately 100 K higher than that from the starting mechanism. For  $X_{\text{H}_2,\text{F}}=0.8$ , the extinction strain rate  $a_E$  is  $14300\text{ s}^{-1}$  and  $18000\text{ s}^{-1}$  from the starting and reduced mechanisms, respectively.

The extinction strain rates as a function of nitrogen dilution are shown in Fig. 4, indicating that the extinction strain rate decreases with the dilution. The extinction strain rates agree well for the reduced and the starting mechanisms considering the variations with dilution. Thus the two-step reduced mechanism based on the approximation of steady-states of all the radicals except H can adequately represents the flame structure and the flame extinction.

Hydrogen fuel is considered as a clean fuel without generating such pollutants as unburnt hydrocarbon, carbon monoxide and soot. However, since the flame intensity of the hydrogen fuel is much stronger than hydrocarbon fuels, appreciable amount of nitrogen oxides are expected to be produced. To develop an efficient way of  $\text{NO}_x$

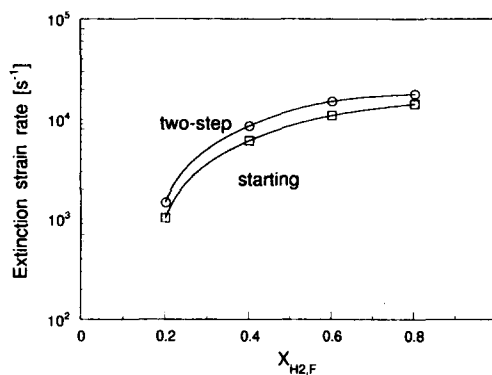


Fig. 4 Extinction strain rates as a function of fuel dilution for starting and two-step reduced mechanisms

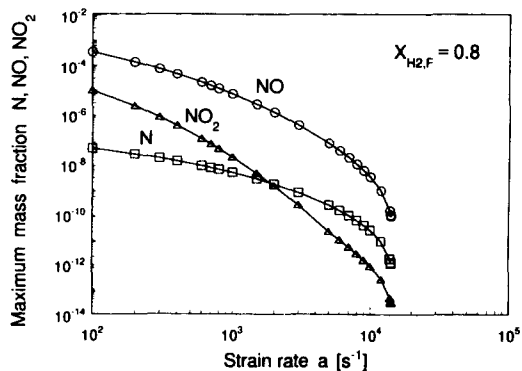


Fig. 5 Variations of N, NO and  $\text{NO}_2$  as a function of strain rate for starting mechanism

control, understanding of the production of NO<sub>x</sub> in hydrogen diffusion flames is essential.

Figure 5 shows the maximum mass fractions of N, NO and NO<sub>2</sub> as a function of strain rate for  $X_{H_2,F}=0.8$  calculated from the starting mechanism. It demonstrates that the production of NO is several orders of magnitude greater than that of N and NO<sub>2</sub>. This leads to the steady-state approximations for N and NO<sub>2</sub>. The decrease in the production of NO<sub>x</sub>, especially NO<sub>2</sub> is significant as the strain rate is increased, caused by the large activation energies associated with the thermal NO<sub>x</sub> mechanism shown in Table 1. As the strain rate is increased, the flame temperature decreases, thereby the nitrogen oxides production is greatly reduced. Since the flame can be sustained up to very high strain rate for hydrogen flames, the production of nitrogen oxides can be lower than that from hydrocarbon fuels, because the flame temperature of hydrogen at high strain rate is about several hundred degrees lower than that of hydrocarbon. Since the strain rate in the present study can be related to a scalar dissipation rate for turbulent diffusion flames, method of increasing turbulence in a combustor could be a measure of reducing nitrogen oxides for hydrogen diffusion flames.

As an indication of NO<sub>x</sub> production in turbulent diffusion flames, Peters and Donnerhack(1981) proposed the integration of NO<sub>x</sub> production rate divided by density over the mixture fraction as

$$I_{NO_i} = \int_0^1 \frac{\omega_{NO_i}(Z)}{\rho(Z)} dZ. \quad (26)$$

Figure 6 demonstrates the integral of  $I_{NO}$  as a function of stretch for various dilution in fuel hydrogen. Since  $I_{NO_2}$  is approximately two orders lower than  $I_{NO}$ , only  $I_{NO}$  is plotted. The results indicate that NO<sub>x</sub> formation is greatly reduced by increasing stretch. Comparison of the reduced one-step NO<sub>x</sub> mechanism with the starting mechanism shows that the prediction from the reduced mechanism is somewhat higher, again due to the overprediction of the flame temperature. Considering NO<sub>x</sub> production with stretch which covers several orders, the prediction with one-step

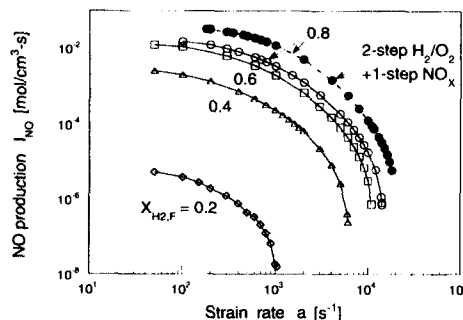


Fig. 6 Comparison of NO<sub>x</sub> production as a function of strain rate(open symbol ; starting mechanism, closed symbol ; reduced mechanism)

NO<sub>x</sub> mechanism is satisfactory. This indicates the potential applicability of the reduced mechanism for both the flame structure and the formation of thermal NO<sub>x</sub>.

## 5. Concluding Remarks

The structure and thermal NO<sub>x</sub> formation of hydrogen diffusion flame with stretch including flame extinction conditions have been analyzed numerically for both the starting mechanism and the reduced mechanism of two-step H<sub>2</sub>/O<sub>2</sub> and one-step NO<sub>x</sub> mechanisms. The agreement between these results are satisfactory.

For the hydrogen diffusion flames, the extinction stretch is much higher and the flame can survive at much lower flame temperature than hydrocarbon flames. The flame temperature and extinction characteristics can be quantitatively predicted from the two-step reduced H<sub>2</sub>-O<sub>2</sub> reactions and the NO<sub>x</sub> production can be predicted with the one-step NO<sub>x</sub> mechanism, based on the assumption of the steady-state of all the radicals except H and NO.

Major source of the NO<sub>x</sub> is from NO, because NO<sub>2</sub> production can be negligible for hydrogen diffusion flames. This characteristics is different from the thermal NO<sub>x</sub> production for the methane/ethane mixture fuel where the NO and NO<sub>2</sub> productions are comparable(Chung et al., 1993). As a possible NO<sub>x</sub> reduction, hydrogen diffusion flame can be burnt at very high turbulence intensity flow field, thereby reducing flame tempera-

ture and NO production while maintaining stable combustion since the flame is difficult to extinguish.

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