

## MODELLING NO<sub>x</sub> EMISSIONS DURING STAGED COMBUSTION

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### SUMMARY

Staged combustion has been accepted as an effective way to reduce NO<sub>x</sub> emission. Based on the comparison of calculated results using Miller and Bowman's (1989, *Progr. Energy Combust. Sci.* **15**, 287) detailed elementary reaction model with experimental data, it is found effective to apply this model in the simulation of NO formation and destruction during staged combustion. Sensitivity analysis shows that C, CH, CH<sub>2</sub> and HCCO play an important role in NO destruction and reduction under fuel staging. NO generated in the primary zone can be reduced greatly by staged combustion. Besides the air–fuel ratio in the primary combustion zone, the combustion temperature in the reburning zone and the mass factor of the reburning fuel in the overall fuel, the main factors which affect NO destruction and reduction are the position where reburning is introduced and the types of reburning fuel. It is found that reburning cannot be introduced too close to the primary combustion zone. The reburning fuels that can effectively stimulate NO to HCN are H<sub>2</sub> and C<sub>2</sub>H<sub>4</sub>. Copyright © 1999 John Wiley & Sons, Ltd.

KEY WORDS: modelling; nitrogen oxides; staged combustion

### INTRODUCTION

Nitrogen oxides (NO<sub>x</sub>) emitted from pulverized coal fired, stationary combustion sources are significant contributors to atmospheric pollution. Combustion modifications involving air and fuel staging techniques each require NO and other nitrogenous species to be destroyed under overall reducing environments. To attain ultra-low-NO<sub>x</sub> emissions, flue gas treatment processes should be used. It is believed that the necessary NO<sub>x</sub> reduction measures can be obtained by a combustion of in-furnace combustion modification (low-NO<sub>x</sub> burners, reburning, etc.) without the need for expensive flue gas treatment processes (Xu, 1992).

NO<sub>x</sub> formation and reduction mechanisms have been investigated by many researchers (Abbas *et al.*, 1991, 1994; De Soete, 1975, 1990; Fenimore, 1976, 1979; Godoy *et al.*, 1991; Hirji *et al.*, 1987; Magnussen and Hjertager, 1976; Mitchell and Tarbell, 1982; Rees *et al.*, 1981; Xu, 1992). A previous study (Penshing and Wendt, 1979) showed that although ~50% of the coal-N was retained in the char under normal pulverized fuel combustion conditions, ~60–80% of the NO<sub>x</sub> produced was derived from the volatile-N. However, for low-NO<sub>x</sub> burners, char-N has been identified as the main contributor to NO (Phong-Anant *et al.*, 1985). It is also generally accepted that the conversion efficiency of volatile-N to NO is higher than it is for char-N. Recent studies (Gavin and Dorrington, 1993; Pels *et al.*, 1993; Shimizu *et al.*, 1992) on both coal- and char-N oxidation and reduction had shown that coal properties are important factors.

A number of techniques available for NO<sub>x</sub> control were highlighted in a table by Williams *et al.* (1994). Combustion-modified low-NO<sub>x</sub> systems have additional benefits of being easy to maintain once installed

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and not requiring the handling of toxic chemicals, such as ammonia, associated with flue gas  $\text{NO}_x$  treatment techniques.

There are two ways for staged combustion, say, air staging and fuel staging or reburning. In the early 1970s, it was found that air staging can reduce  $\text{NO}_x$  emission. The investigations by Wendt *et al.* (1978) and Glass (1981) verified further the effect of air staging on  $\text{NO}_x$  destruction. In air staging, the combustion air is introduced by two stages. First, about 80% of the theoretical air will be used. Since the combustion is under the circumstance of fuel-rich (with excess air less than 1.0), the combustion process goes slowly and the temperature is low. These led to the combustion product of CO. Nitrogen in the fuel will decompose to form HN, HCN, CN,  $\text{NH}_3$  and  $\text{NH}_2$ , etc. These species composite with each other. At the same time, they will destroy  $\text{NO}_x$  formed before and hence reduce the fuel  $\text{NO}_x$ . The remaining air will be introduced as secondary air for the burnout of the fuel. During the second combustion stage, fuel  $\text{NO}_x$  forms not so much because of low temperature under high excess air. Moreover, the formation of thermal  $\text{NO}_x$  is restrained because of low temperature. All these make the air staging an effective technology of low  $\text{NO}_x$  combustion. However, it is verified that the reduction of  $\text{NO}_x$  by air staging is lower than that by reburning. Meanwhile, there is a possibility of slagging and fouling under air staging. This is because the circumstance in the primary zone is fuel rich and may reduce the melting temperature of the ash.

Reburning or fuel staging as an  $\text{NO}_x$  reduction technique in combustion systems was originally developed by the John Zink company (1969) and Wendt *et al.* (1973). However, much earlier studies (Myerson *et al.*, 1957; Patry and Engel, 1950) had shown that  $\text{NO}_x$  could be reduced by reaction with hydrocarbon fragments. More recently, researchers have conducted several fundamental studies on the process, and its potential for large-scale application has been demonstrated (Bose and Wendt, 1988; Chen *et al.*, 1986; Knill and Morgan, 1989; LaFlesh *et al.*, 1991; Lanier *et al.*, 1986; Mereb and Wendt, 1990; Mulholland and Hall, 1985; Newell *et al.*, 1993; Takahashi, 1980). Effectiveness of reburning a primary pulverized-coal flame with a range of fuels including natural gas, coke oven gas, heavy fuel oil and coal was also reported (Kichever *et al.*, 1994; Smart and Morgan, 1994).

A number of computational codes have been developed and used for coal combustion modelling (Fiveland and Wessel, 1991; Lockwood *et al.*, 1984; Schmid *et al.*, 1988; Smith *et al.*, 1981; Truelove, 1984; Visser and Weber, 1989; Xu *et al.*, 1992, 1994, 1996, 1998). Predictions of  $\text{NO}_x$  formation from coal processes using computational programs have also been reported previously (Aguire, 1991; Coimbra *et al.*, 1994; Fiveland and Vessel, 1991; Hill *et al.*, 1984; Miller and Bowman, 1989; Xu *et al.*, to be published) and require the incorporation of thermal, prompt and fuel-NO formation mechanisms. However, reports on predictions of  $\text{NO}_x$  formation from fuel staging combustion systems are very limited. This paper therefore concentrates on the use of computational codes as a method to predict  $\text{NO}_x$  emissions from fuel staging combustion systems.

In fuel staging, the combustion is divided into three zones, say, the primary combustion zone, reburning zone and burnout zone. The primary combustion zone or the main combustion zone is located at the lower part of the furnace. About 80–85% fuel is burning in this zone with a normal excessive air coefficient and yields combustion products such as NO, CO,  $\text{H}_2\text{O}$ , ash, etc. About 80% total heat is released in this zone. If the burning gas does not stay for enough time in this zone, the unburned fuel will go to the following zone, say, the reburning zone. The remaining fuel is sprayed into the reburning zone and forms a fuel-rich combustion zone. The other air required by the combustion is provided by the burnout zone which is located at the upper end of the furnace.

## MATHEMATICAL MODELS

Generally, the fluid flow is simplified and the detailed elementary reactions are considered in the study of the mechanism of  $\text{NO}_x$  formation during combustion process. A gas-phase reaction model in a closed cavity with constant pressure is used in this paper to study the change of temperature and concentration of the species in

the system at different times. In the closed system, the temperature and concentration of each species is assumed to be uniform. If sufficient reaction species such as CH<sub>4</sub>, O<sub>2</sub>, HCN, etc., and energy are put into the system, the combustion will probably occur.

#### Mass balance equation

Based on the above assumption, the mass variation rate of each species  $K$  is completely decided by the formation and destruction of the reactions:

$$\frac{dm_k}{dt} = V\dot{\omega}_k W_k, \quad k = 1, \dots, K \quad (1)$$

Since the reactions are conducted in a closed system, the total mass  $M$  of the system will be constant. Divide equation (1) by  $M$ , we have

$$\frac{dY_k}{dt} = v\dot{\omega}_k W_k, \quad k = 1, \dots, K \quad (2)$$

where

$$Y_k = \frac{m_k}{M}, \quad v = \frac{V}{M}$$

#### Equation of energy conservation

According to the first law of thermodynamics, for the closed adiabatic constant pressure system, we have

$$\frac{dh}{dt} = 0 \quad (3)$$

For ideal gas mixture, the enthalpy is

$$h = \sum_{k=1}^K Y_k h_k \quad (4)$$

where

$$h_k = c_{pk} T$$

thus

$$\sum_{k=1}^K c_{pk} Y_k \frac{dT}{dt} + \sum_{k=1}^K h_k \frac{dY_k}{dt} = 0 \quad (5)$$

since

$$c_p = \sum_{k=1}^K c_{pk} Y_k \quad (6)$$

then

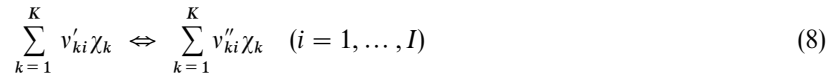
$$c_p \frac{dT}{dt} + v \sum_{k=1}^K h_k \dot{\omega}_k W_k = 0 \quad (7)$$

To solve the species balance equation (2) and the energy conservation equation (7) simultaneously, we can have the temperature and concentration of each species at different time.

#### Calculation of mole formation rate of the species

While solving the species balance equation and the energy conservation equation, the net formation rate of species  $k$ ,  $\dot{\omega}_k$ , needs to be calculated.

A reaction system which consists of  $I$  elementary reactions (reversible or irreversible) and  $K$  species can be expressed as (Lutz *et al.*, 1987):



Generally speaking, an elementary reaction involves only 3–4 species, so that the matrix composed by  $v_{ki}$  is very scattered.

The mole formation rate of species  $k$  can be written as the weighed algebraic sum of the reaction rates of the elementary reactions involving species  $k$ :

$$\dot{\omega}_k = \sum_{i=1}^I v_{ki} q_i \quad (9)$$

where

$$v_{ki} = v''_{ki} - v'_{ki}$$

$$q_i = k_{fi} \prod_{k=1}^K [X_k]^{v'_{ki}} - k_{ri} \prod_{k=1}^K [X_k]^{v''_{ki}}$$

$k_{fi}$  and  $k_{ri}$  is the forward and backward reaction velocity constant of reaction  $I$ , respectively.  $k_{fi}$  has an Arrhenius form as

$$k_{fi} = A_i T^{\beta_i} \exp\left(-\frac{E_i}{R_c T}\right) \quad (10)$$

The backward reaction velocity constant of reaction  $i$  can be solved by the reaction velocity balance constant  $k_{ci}$ :

$$k_{ri} = \frac{k_{fi}}{k_{ci}} \quad (11)$$

#### Calculation of the sensitivity coefficient

Sensitivity analysis can be used to investigate the effect of reaction rate constant on species concentration in complicated reaction system. This is helpful for us to study the reaction mechanism and good for parameter correction in the unperfected reaction model according to the results of sensitivity analysis (Aiken, 1985; Edeson, 1981).

The vector form of equation (2) and (8) is

$$\frac{dZ}{dt} = F(Z, t, A) \quad (12)$$

where

$$Z = (T, Y_1, Y_2, \dots, Y_k)^T$$

The matrix of sensitivity coefficient is defined as (Glarborg *et al.*, 1992; Miller and Bowman, 1989)

$$\omega_{j,i} = \frac{\partial Z_j}{\partial A_i}, \quad i = 1, \dots, I, \quad j = 1, \dots, K + 1 \quad (13)$$

it stands for the effect of the variation of pre-exponential Arrhenius factor for reaction  $i$  on  $Z_j$ . The derivative of equation (13) with respect to time is

$$\frac{d\omega_{j,i}}{dt} = \frac{\partial F}{\partial Z} \omega_{j,i} + \frac{\partial F_j}{\partial A_i} \quad (14)$$

There are many equations when solving equation (14) and (12) simultaneously. For an elementary reaction system which consists of  $I$  reactions and  $K$  species, the total number of the equations will be  $(I + 1) \times (K + 1)$  if the sensitivities of temperature and species concentration are calculated. Furthermore, the difference of the reaction rates of reactions is very big, some of them is up to  $10^4$ – $10^5$  times. In this circumstance, the coupled equations are usually very 'stiff'. To solve the equations, Gear algorithm (Gear, 1971) is applied. This method has a high calculating efficiency since it can change the step size and order of the differential equations automatically so that it is effective in solving 'stiff' coupled differential equations.

#### *Overall nitrogen reaction model*

It is found that the reaction between char and NO<sub>x</sub> is not obvious (Yasuro and Kimishivo, 1981). NO<sub>x</sub> formation and destruction can be described by proper homogeneous reaction model under staged combustion and it is used in this study. The main hydrocarbon substances released in coal combustion are CH<sub>4</sub> and C<sub>2</sub>H<sub>4</sub>, and the flame of C<sub>2</sub>H<sub>4</sub> is more close to the temperature of that of pulverized coal combustion, so that C<sub>2</sub>H<sub>4</sub>/Air flame is modelled. At the same time, all the fuel–N is HCN, it is acceptable to bituminous coal.

The chemical reactions proceed very fast in homogeneous combustion, especially at high temperature. In order to realize the detailed combustion process, the inert gas Ar is filled into the reaction system to dilute the concentration of the reactants to slow down the combustion reactions. Miller and Bowman's (1989) overall elementary reaction model is applied to simulate the homogeneous reactions of NO<sub>x</sub> formation. This model involves 234 elementary reactions and 51 species. It can be used to study the mechanism of NO<sub>x</sub> formation in gas-phase reactions.

## MODELLING OF NO<sub>x</sub> FORMATION AND DESTRUCTION UNDER FUEL-RICH COMBUSTION

#### *Main reactions of NO<sub>x</sub> formation and destruction*

The mechanism of the reaction of NO<sub>x</sub> emission under fuel staging combustion is not understood thoroughly so far. It is generally accepted that the lower NO<sub>x</sub> emission is because the reductant reaction between NO and CH<sub>*i*</sub> ( $i = 0, 1, 2, 3$ ) which is produced by hydrocarbon fuels under oxygen lean circumstance. However, which reactions play a leading role is not clearly known.

From the species mass balance equation (2) we know that the mass variation rate of each species is decided completely by the chemical reactions. Hence, the effect of reaction  $j$  on the mass variation rate of NO,  $dY_{\text{NO}}/dt$ , namely  $(v\dot{\omega}_{\text{NO}}W_{\text{NO}})_j$  stands for the function of reaction  $j$  in the process of NO formation and destruction. Reaction  $j$  makes NO decompose if  $(v\dot{\omega}_{\text{NO}}W_{\text{NO}})_j < 0$  and otherwise makes NO generate. The leading reactions of NO formation and destruction can be decided by putting  $(v\dot{\omega}_{\text{NO}}W_{\text{NO}})_j$  in order.

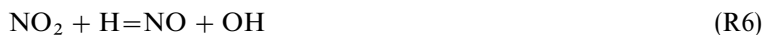
According to the above method, the authors (Xu *et al.*, to be published) calculated a C<sub>2</sub>H<sub>4</sub>/Air/NO flame to investigate the effect of CH<sub>*i*</sub> on reducing NO. The system has a pressure of 1.0 atm, a temperature of 1500 K, the mass fraction of C<sub>2</sub>H<sub>4</sub>,  $Y_{\text{C}_2\text{H}_4}$  1%, the primary mass concentration of NO 500 ppm, and the air–fuel ratio  $\alpha$  of 0.5 and 0.6 respectively. It is found that there are only three reactions which make NO decompose remarkably although there are as many as 28 reactions which directly relate with NO formation and destruction in Miller and Bowman's (1989) detailed elementary reaction model. The three reactions are



Besides R1–R3, the following reaction has an obvious effect on NO destruction as well:



The reactions considerably contributing to NO formation are listed below:

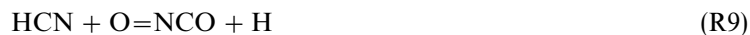


The contribution of the above reactions on NO formation is fairly complicated. R5 and R8 have a remarkable effect on NO formation at  $\alpha = 0.6$ . Compared with R5, the commencement of the effect of R8 on NO formations is later, but it has the effect nearly to the end of the reaction. R6 has an important effect on NO formation at  $\alpha = 0.5$  and the effect is mainly at the early stage of the reaction. R7 plays a notable role at  $\alpha = 0.6$ . It should be noted that R7 has an obvious effect on NO destruction for a long period. This is the reason why NO cannot be decomposed efficiently when  $\alpha$  increases, especially near  $\alpha = 1$ .

#### *Sensitivity analysis of NO<sub>x</sub> formation*

To investigate the mechanism of NO formation and destruction under fuel staging, the sensitivity of NO formation is calculated at  $P = 1.0$  atm,  $Y_{\text{C}_2\text{H}_4} = 1\%$ ,  $\alpha = 0.5$  and the primary mass concentration of NO equals 500 ppm. The objective of the sensitivity calculation is to obtain the key reactions that govern NO formation and destruction.

The profile of NO, HCN concentration at reaction temperature  $T = 1500$  K is illustrated in Figure 1(a). NO decomposes rapidly from  $t = 0.4$ – $0.8$  ms. At the same time, HCN increases significantly. The concentration of NO and HCN remains nearly unchanged as the reaction continues. From the results of sensitivity calculation shown in Figure 1(b), the key reaction of NO formation is



The key reactions of NO destruction are



Figure 2 shows the results of sensitivity calculation at  $T = 1800$  K. With increasing reaction temperature, NO destruction and HCN formation speed up. NO increased remarkably in the later stage of the reaction. This is mainly because some HCN changes to NO at higher temperature. The key reactions of NO formation and destruction at high temperature do not change, as shown in Figure 2. However, the sensitivity of NO formation governed by R9 increases greatly and remains a high value for a long period while that of NO destruction governed by R10–R12 remains unchanged as temperature rises, hence some HCN will change to NO at the later stage of the reaction.

According to the leading reactions and key reactions of NO formation and destruction, the mechanism of NO decomposing under fuel-rich conditions can be analysed as follows: owing to the relative lack of oxygen in the reaction system, NO formation is hindered by R9. At the same time, the relative excess of the fuel leads

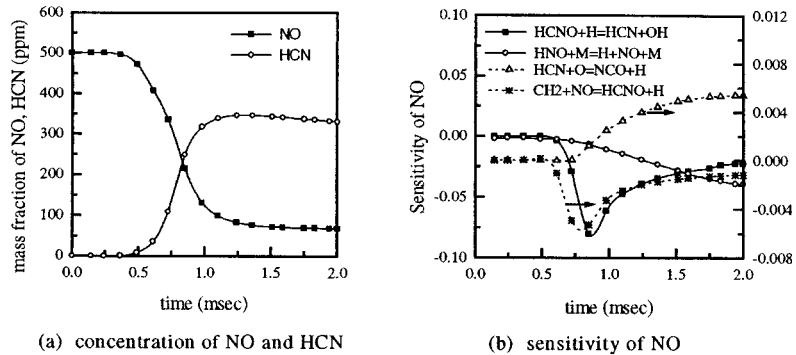


Figure 1. Sensitivity of NO<sub>x</sub> formation and destruction at  $T = 1500$  K: (a) concentration of NO and HCN; (b) sensitivity of NO

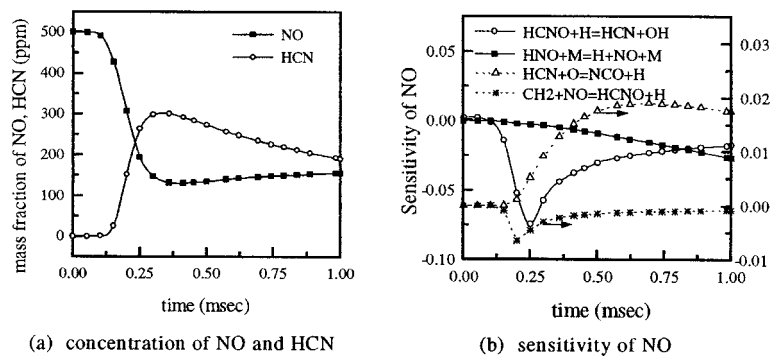


Figure 2. Sensitivity of NO<sub>x</sub> formation and destruction at  $T = 1800$  K: (a) concentration of NO and HCN; (b) sensitivity of NO

to CH<sub>i</sub> in abundance, which makes NO decomposes remarkably by the action of R1–R4. From the key reactions R10–R12 it can be concluded that NO will decompose rapidly as the concentration of CH<sub>2</sub>, NO and HCNO increases.

### NO<sub>x</sub> EMISSION UNDER REBURNING

In a previous study, the authors (Xu *et al.*, 1999) investigated some factors that affect NO reduction. It is found that the air–fuel ratio in the primary combustion zone, the combustion temperature in the reburning zone and the mass factor of the reburning fuel in the overall fuel will play an important role on NO formation and destruction. It is also verified that the best air–fuel ratio in the primary combustion zone for NO reducing in the reburning zone is 1. The raising of the temperature in the reburning zone is good for the reducing of NO. The best mass fraction of the reburning fuel in the overall fuel for NO destruction is 30%. In the present study, some other factors are investigated and found essential on NO emission.

#### *Effects of the introducing time of reburning fuel on NO emission*

To investigate the effect of the introducing time of reburning fuel on NO emission, different times for the introduction of reburning fuel are used. Figure 3 illustrates the calculated results for introduction times of 0.16, 0.20 and 0.24 ms, respectively. It shows the NO concentration is only 252 ppm at 2.0 ms when the

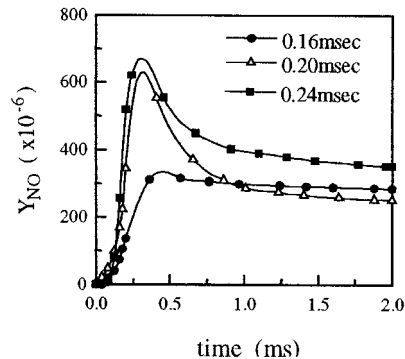


Figure 3. Effects of reburning fuel introducing place on NO concentration ( $T_2 = 1300$  K,  $R = 0.3$ )

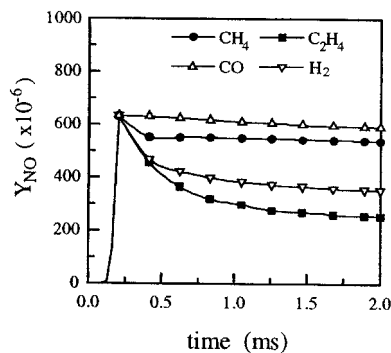


Figure 4. Effects of the type of reburning fuel on NO concentration ( $\phi_1 = 1.0$ ,  $T_2 = 1300$  K,  $R = 0.3$ )

introducing time is 0.20 ms, while the corresponding concentration of NO grows to 286 and 369 ppm for the introducing time of 0.16 and 0.24 ms, respectively. This certified that the introducing time of reburning fuel has a great effect on NO destruction. In fact, if the reburning fuel is introduced too early, the primary combustion zone will merge with the reburning zone. This means the reburning combustion becomes the air staging combustion. Thus NO formation in the primary combustion is low but it will not be reduced again in the further combustion period. These results were also shown in Figure 3.

#### *Effects of the types of reburning fuel on NO emission*

It is known that the reburning fuel can be different from the primary fuel. Several fuels are selected in this study to investigate the effects of the types of reburning fuel on NO emission. Figure 4 illustrates the calculated NO emission for different reburning fuels, say,  $\text{CH}_4$ ,  $\text{C}_2\text{H}_4$ , CO and  $\text{H}_2$ , respectively. It can be concluded that the types of reburning fuel have a remarkable effect on NO reduction. For the calculation conditions considered here, it is found that CO has a negligible effect on NO destruction, the introduction of  $\text{CH}_4$  is beneficial to NO reduction, and  $\text{H}_2$  and  $\text{C}_2\text{H}_4$  can be used to reduce NO to HCN effectively.

## CONCLUSIONS

The following conclusions are made from the modelling of  $\text{NO}_x$  formation and destruction:

1. Based on Miller and Bowman's (1989) overall elementary reaction model, NO formation and destruction during staged combustion is calculated. The calculation results verified the effectiveness of the above model.



- Sensitivity analysis shows that C, CH, CH<sub>2</sub> and HCNO play a key role in NO destruction and reduction under fuel staging.
- NO can be reduced effectively by staged combustion. Besides the air-fuel ratio in the primary combustion zone, the combustion temperature in the reburning zone and the mass factor of the reburning fuel in the overall fuel, the main factors that affect NO reducing are the place where the reburning fuel is introduced and the type of reburning fuel.
- For the calculation conditions considered here, it is found that CO has a negligible effect on NO destruction, the introducing of CH<sub>4</sub> is beneficial to NO reduction, and H<sub>2</sub> and C<sub>2</sub>H<sub>2</sub> can be used to reduce NO to HCN effectively.

### NOMENCLATURE

$A$	= vector composed by temperature and mass fractions
$A_i$	= pre-exponential Arrhenius factor (same dimension as $k$ )
$C_p$	= specific heat of the gas mixture, $\text{J kg}^{-1} \text{K}^{-1}$
$C_{pk}$	= specific heat of species $k$ , $\text{J kg}^{-1} \text{K}^{-1}$
$E_i$	= activation energy, $\text{J kmol}^{-1}$
$h$	= enthalpy of the gas mixture, $\text{J kg}^{-1}$
$h_k$	= enthalpy of the species $k$ , $\text{J kg}^{-1}$
$K$	= number of species or elementary groups in reaction
$k_{fi}$	= forward reaction constant of reaction $i$ (dimension depends on the reaction)
$k_{ri}$	= backward reaction constant of reaction $i$ (dimension depends on the reaction)
$k_{ci}$	= reaction balance constant
$M$	= mass of the system, kg
$M_k$	= mass of species $k$ , kg
$P$	= pressure, atm
$q_i$	= rate of reaction $I$ , $\text{kg m}^{-3} \text{s}^{-1}$
$R_c$	= universal gas constant, $\text{J kmol}^{-1} \text{K}^{-1}$
$R_f$	= mass fraction of reburning fuel in the overall fuel
$T$	= temperature, K
$t$	= time, s
$V$	= volume of reaction system, $\text{m}^3$
$W_k$	= molecular weight of species $k$ , $\text{kmol}^{-1}$
$[X_k]$	= mole concentration of species $k$ , $\text{kmol m}^{-3}$
$Y_k$	= mass fraction of species $k$
$Z$	= vector composed by temperature and mass fractions
$\alpha$	= air-fuel ratio
$\beta_i$	= temperature index
$\phi_i$	= air-fuel ratio in the primary combustion zone
$\omega_{j,i}$	= matrix of sensitivity coefficients
$\dot{\omega}_k$	= mole formation rate of species $k$ in reaction, $\text{kmol m}^{-3} \text{s}^{-1}$
$v$	= specific volume of the gas mixture, $\text{m}^3 \text{kg}^{-1}$
$v_{ki}$	= stoichiometry coefficients of species $k$ in reaction $i$
$\chi_k$	= molecular formula of species $k$

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