Effect of alkali metals on nitrogen oxide emission: Role of Na and its occurrence in coal ☆

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Abstract

High-alkali coal contains relatively high contents of alkali metals, which can be usually released in the form of gaseous chlorides and hydroxides during combustion. The effect of alkali metals on NO formation is analyzed in an electrical heated drop-tube furnace at 800–1200 °C during coal combustion. Based on experiments and simulations, the mechanisms underlying the effects of Na salts on NO emission are clarified in $CO/NH_3/O_2/H_2O/Na$ additive (NaCl, Na_2SO_4, and NaAc) systems. The results indicate that the yield of NO initially increases and then decreases as the furnace temperature increased. As the temperature increased from 800 to 1000 °C, NO precursors (HCN and NH_3) undergo accelerated oxidation to form NO. When the furnace temperature is greater than 1000 °C, due to the rapid precipitation of volatiles, a local reducing atmosphere is present around the pulverized coal particles, which inhibits NO formation. NaCl and NaAc addition significantly inhibit NO formation. However, the inhibitory effect is weakened at higher temperatures (>1000 °C). The Na_2SO_4 additive exerts little effect on NO generation during combustion because of its stable chemical properties. The same conclusion is also obtained from gaseous experiments showing that NaCl and NaAc significantly inhibit NH_3 oxidation to form NO. Based on the results of calculations, NaCl and NaAc addition inhibits NO formation by promoting the recombination of H, O and OH and reducing the concentrations of radicals. According to the analysis of chemical reactions, the effect of NaCl and NaAc on NO formation is mainly determined by the competitive relationships among multiple reactions.
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Keywords: Alkali metals; NO formation; Mechanisms; Radicals; Competitive relationships

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1. Introduction

Nitrogen oxides (NO_x) have been recognized as one of the primary pollutants emitted from coal-fired power plants. NO_x emission not only causes serious pollution, but also generates photochemical smog and acid rain, which will cause secondary pollution and a serious threat to the environment and human health [1]. During coal combustion, the main nitrogen oxides are NO and NO_2, and a small amount of N_2O is generated. Generally, NO accounts for 90–95% and NO_2 only accounts for 5–10% of NO_x produced by pulverized coal combustion [2]. Therefore, this paper mainly studies the process of NO formation. Currently, the sources of NO mainly include thermal-N, fuel-N and fast-N, among which fuel-N is the main type, accounting for approximately 75–85%. The fuel-N will first form volatile-N and char-N, and then is further oxidized to form NO or N_2. Volatile-N mainly includes NH_3 and HCN, accounting for about 90–95% of the total volatile-N content [3]. Generally, the NO generated from volatile-N accounts for 60–80% of the fuel-type NO, while the NO generated from char-N accounts for 20–40% during coal combustion. NH_3 mainly forms NO via conversion into NH_2, NH, and HNO, etc. [4]. HCN finally forms NO through intermediate products, such as NCO, HNCO and CN [5]. Char-N directly generates NO through gas-solid reaction on the surface of char. In addition, a heterogeneous reduction reaction of char-N to NO formation has been identified during combustion [6].

The formation of NO is influenced by many factors, such as burner types (fixed bed, fluidized bed, etc.), fuel types, reaction temperature, stoichiometric ratio (oxidation or reduction atmosphere), and impurities (Cl, Br, Ca, Na/K, etc.) [7,8]. Since the impurities are typically present in fairly small concentrations compared to the macro parameters, they are often assumed to exert no effect on the overall combustion process in combustion analysis. However, according to some reports [9,10], the release of trace elements such as alkali metals in high-alkali fuels may affect the generation and transformation of pollutants during thermal utilization. As shown in the study by Cheng et al. [11], Na acetate enhanced the decomposition of nitrogen species, such as protein- and inorganic-N, during sewage sludge pyrolysis. During SNCR process, Hao et al. [12] reported significant effects of Na/K additives on promoting NO reduction and widening the SNCR temperature window. Zhao et al. [13] reported exhibited high catalytic activity of the added Na during coal combustion and NO_x reduction when studying the combustion of Chinese brown coal in a tubular quartz fixed bed reactor. Based on these results, the interactions may occur indirectly through effects of K/Na on the radical pool or through direct reaction.

However, previous studies have mostly focused on the analysis of experimental results, and fewer studies have examined effect mechanisms of alkali metals on NO formation. In addition, some details of the process remain uncertain due to these complicated reaction conditions. Thus, it is necessary to clarify the effect mechanisms of mineral matter such as alkali metals on the NO formation, which will shed light on the understanding of nitrogen oxide chemistry involved in high-alkali fuels combustion.

During the combustion of high-alkali fuels, such as Zhundong coal, Na is usually released as NaCl and NaOH and the stable intermediate Na_2SO_4 is produced in the presence of SO_2, H_2O, and O_2 [14]. Therefore, in this investigation, we first introduce the effect of Na additives (NaCl, Na_2SO_4, and NaAc) on NO formation during coal combustion in a lab-scale electrically heated drop-tube furnace (DTF). Second, the combustion atmospheres are simplified as $CO/NH_3/O_2/H_2O/Na$ additive systems and N_2 as balance gas to reveal the effect mechanisms. Finally, based on the elementary reactions, the effect mechanisms of Na salts on NO formation are analyzed using CHEMKIN. Data from this study will be valuable for the development of new strategies to control NO emission.

2. Experimental section

2.1. Experimental materials

A Chinese coal named Zhundong coal was selected as the experimental coal sample. The sample was pulverized and sieved to particle sizes ranging from 40 to 100 μm. The detailed properties of the raw coal are presented in Tables 1 and 2. The coals of pre- and post-combustion were analyzed through extraction experiments and inductively coupled plasma-optical emission spectroscopy (ICP-OES) to determine the content of alkali metals. According to the results, Na in Zhundong coal is mainly present in water-soluble form. According to the charge conservation of anions and cations in the water solution, the water-soluble Na is considered to exist mainly in the form of crystals or hydrated ions of NaCl, Na_2SO_4, and $NaHCO_3$. In this study, the coal, which was extracted with 1 mol/L HCl soluble, was defined as de-alkali coal due to the removal of most of the Na. By adding NaCl, Na_2SO_4 and NaAc to the de-alkali coal, the real release and migration of Na in the raw coal was simulated.

2.2. Experimental procedures

During pulverized coal combustion, the yield of NO, with or without Na additives, was measured in an electrically heated drop tube furnace (DTF).

Table 1
Ultimate and proximate analyses of tested coal samples.

Proximate analysis (air dry)/wt.%				Ultimate analysis (air dry)/wt.%					
M	A	V	FC	C	H	O*	N	S	Cl
14.1	10.08	26.22	49.6	58.36	2.12	13.48	0.41	1.34	0.11

Table 2
Ash analyses of tested coal samples/wt.%.

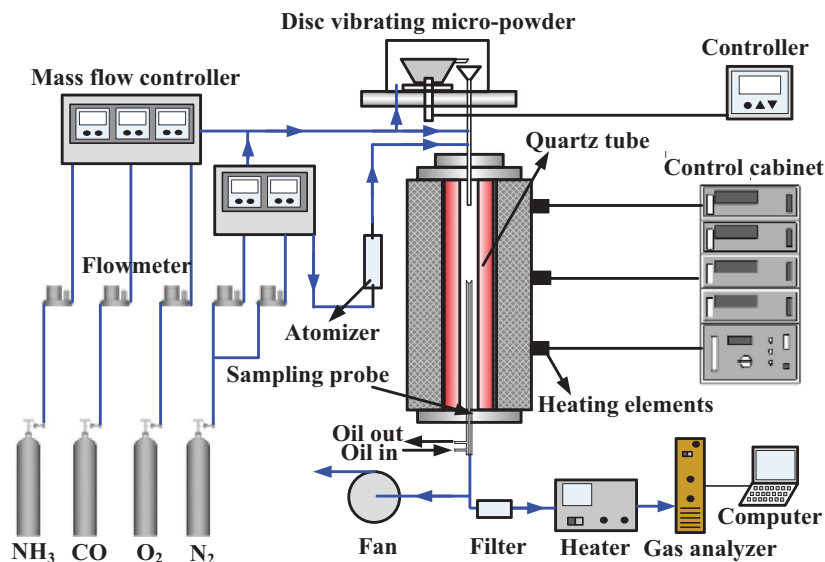| SiO_2	Al_2O_3	Fe_2O_3	CaO	MgO	TiO_2	SO_3	P_2O_5	K_2O	Na_2O
16.61	5.86	14.33	22.66	3.94	0.44	29.18	0.24	0.58	4.97

*The content of O is calculated by subtraction.

Fig. 1. Schematic of the experimental setup of the drop tube furnace (DTF).

As shown in Fig. 1, the DTF consisted of a feed system with a full-scale measurement accuracy of ±5%, an electric heating furnace, a control cabinet, and a gas distributor with a full-scale measurement accuracy of ±1%. The feeder was a disk vibrating micro-powder that continuously fed coal into the furnace at a set rate (2 g/min for coal/coal blend samples). The Na additives with mass fraction of 1% and 3% were physically mixed with de-alkali coal. The samples were burned in the corundum reaction tube inside the furnace body, the length of the reaction zone was 1800 mm, and the inner diameter was 32 mm. The furnace temperature was adjusted from 800 to 1200 °C. The reaction atmosphere was 21% O_2 balanced with 79% N_2 during the combustion experiments, and the flow rate of simulated air was 20 L/min. The simulated air was sent to the feeder to be mixed with the pulverized coal, and then the pulverized coal was carried into the reaction tube. The samples were always nearly burned out under the given reaction conditions.

The concentration of NO was determined using an online gas analyzer (Gasmet DX-4000) with a full-scale measurement accuracy of ±2%. The interference compensation device was added to the gas analyzer to eliminate the error caused by the presence of H_2O since the absorption lines of NO and H_2O coincide. All experiments were carried out thrice and the average of the data collected within 60 s under stable conditions was selected as the reference value, and the difference between the maximum or minimum value and the reference value was set as the value of the error bar.

The $NH_3/CO/O_2/H_2O/N_2$ system was used to simulate coal combustion experiments to reveal the mechanism underlying the effect of Na additives on NO emission. The initial total gas flow rate was maintained at 6 L/min at 25 °C and 0.1 MPa. In the CO/NH_3 combustion system, the mixture of gasses consisted of 3% O_2, 1.5% CO, and 1000 ppm NH_3, and 1% H_2O. N_2 was applied as the gas balance. The NaCl, Na_2SO_4 and NaAc

solution were entrained into the reaction system by N_2 via an atomizer. The concentrations of Na additive vapors in the reaction system were maintained at 25, 50, 75, and 100 ppm, respectively, by adjusting the concentrations of Na salt solutions.

2.3. Kinetic analysis

In the present study, the detailed mechanism and CHEMKIN software were used to calculate the changes in the concentrations of various components during combustion, and the sensitivity analysis, which influenced NO formation, was performed to explain the experimental results in terms of the reaction mechanism. Based on the theory of fluid mechanics, in the initial region, the velocity boundary layer of reaction gas has not yet been completely formed, and the boundary layer is very small. In our study, the initial region length of laminar flow was approximately 56 mm, which was much larger than the distance from the inlet to the reaction region (approximately 5–8 mm gained from simulation results). Thus, the velocity distribution of the reaction region was still close to a uniform distribution and the reaction model could be approximately simplified as a quasi-plug flow reactor (PFR). The program solved the conservation equations for mass and energy, and calculated the temporal evolution of mole fractions of species for a homogeneous mixture in the reactor at 0.1 MPa. The heat loss was considered to ensure that the temperature variation of the simulation was consistent with the experimental conditions, and the heat transfer coefficient was $3 \ J/m^2 \cdot K \cdot s$. The reaction mechanisms included 1112 reversible reactions and 181 species, which consisted of subsets for hydrocarbon, monoxide, hydrogen/oxygen, nitrogen chemistry, chlorine chemistry, and sodium chemistry. The hydrocarbon and monoxide subset [15] and detailed nitrogen subset [15,16] were selected from previous work. The sodium subset, which involved reactions of NaCl, was drawn from the mechanisms of Glarborg and Marshall [17]. The reactions involving NaOH and NaO were referred from the mechanism of Li and Wei [5] and Zamansky et al. [18] and incorporated into the sodium subset.
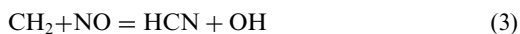
3. Results and discussion

3.1. Effect of the reaction temperature on NO formation during coal combustion

Fig. 2(a) displays the yield of NO as the furnace temperature increased from 800 to 1200 °C during raw coal and de-alkali coal combustion. As the furnace temperature increased from 800 to 1000 °C, the yield of NO emission increases from 1.44 to 1.62 mg/g-coal during raw coal combustion. However, when the temperature increases from 1000

to 1200 °C, the amount of NO released gradually decreases to 1.24 mg/g-coal. This is mainly determined by the atmosphere around the pulverized coal particle. At a furnace temperature less than 1000 °C, the conversion rate of fuel-N to NO accelerates as the furnace temperature increased under an oxidation atmosphere. The main reactions are shown as S1-S7 in the supporting information.

However, according to the report by Zhu et al. [19] and Lenesma et al. [20], CO, H_2 and hydrocarbon species, such as CH_2 and CH, quickly released with the volatiles played an important role in the reduction of NO under high heating rate conditions (or at high temperature). In our experiments, when the furnace temperature exceeds 1000 °C, the total amount and rate of volatiles released gradually increase at higher temperatures, which will change the local atmosphere around the pulverized coal particles from an oxidizable to reducible atmosphere. Meanwhile, as further increased the temperature, the rate of volatiles released will further strengthen, and the local reduction atmosphere will be stronger, which will gradually reduce the yield of NO. The main reactions are expressed as follows:

$$CO + NO = 1/2N_2 + CO_2 \tag{1}$$

$$H_2 + NO = 1/2N_2 + H_2O \tag{2}$$

$$CH_2 + NO = HCN + OH \tag{3}$$

$$CH + NO = HCN + O \tag{4}$$

$$HCN + O = NH + CO \tag{5}$$

$$NH + H = N + H_2 \tag{6}$$

$$N + NO = N_2 + O \tag{7}$$

After extraction, the amount of NO released also initially increases and then decreases with increasing temperature during de-alkali coal combustion. For example, as the temperature increased from 800 to 900 °C, the yield of NO emission increases from 1.65 to 1.77 mg/g-coal. The amount of NO released decreases to 1.34 mg/g-coal when the temperature is 1200 °C. As shown in Fig. 2(b), most Na is released into flue gas at 1000 °C during raw coal combustion, but the content of Na is significantly decreased after extraction with the HCl solution, indicating that minerals such as Na may exert an obvious inhibitory effect on NO formation. This will be discussed in detail in the next section.

3.2. Effects of Na additives on NO formation during de-alkali coal combustion

Fig. 3 shows the effects of different Na additives, including NaCl, Na_2SO_4, and NaAc, on NO emission during de-alkali coal combustion, and the ad-
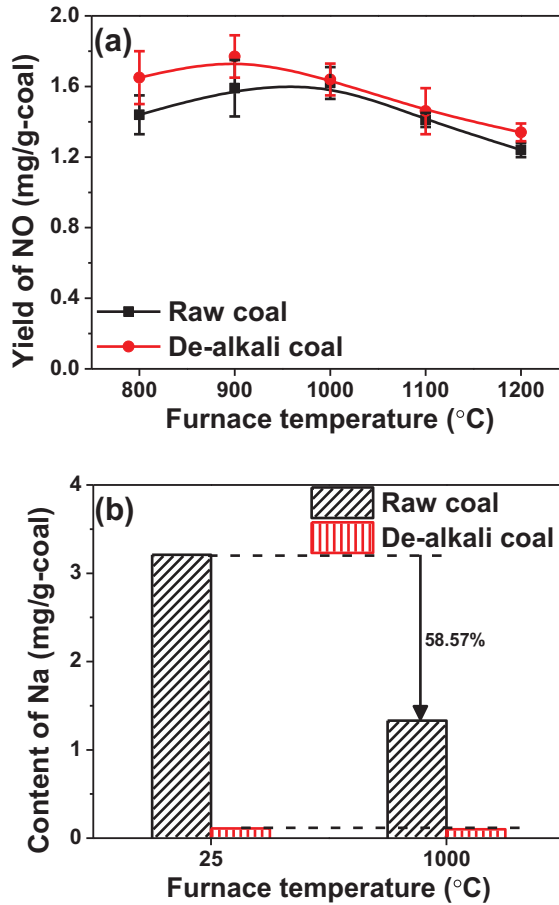
Fig. 2. Processes occurring during raw or de-alkali coal combustion: (a) Effect of temperature on NO formation; (b) amount of Na released.

ditives were introduced into the reaction system by physically mixing with coal. The reduction ratio is defined as ratio of the difference of release amount of NO during de-alkali coal and coal containing Na additives combustion to release amount of NO during de-alkali coal combustion. The experimental results indicate that Na additives significantly reduce NO emission and the inhibitory effects of Na additives on NO emission at lower temperature are much better than at higher temperature. Following the addition of 1% NaCl, Na_2SO_4, and NaAc, the yield of NO decreases to 49.1%, 2.4%, and 19.4% at 800 °C, respectively, suggesting that the ability of the three additives to inhibit NO formation follows the order NaCl > NaAc > Na_2SO_4. The same conclusion is also obtained from the data collected at 1000 and 1200 °C. Among them, NaCl and NaAc exert a strong inhibitory effect on NO production, mainly because they are easily released in the form of NaCl (g) and NaOH (g) during combustion, which play key roles in NO formation. Na_2SO_4 exerts the lowest inhibitory ef-

fect on NO formation, mainly because its chemical properties are relatively stable at high temperatures and it is not easy to decompose. Usually, the effects of Na additives on the formation of NO are explained based on two aspects. On the one hand, Na additives can inhibit fuel-N oxidation by controlling the concentration of radicals. On the other hand, Na additives may also promote the activity of char and the heterogeneous reduction reaction between char and the generated NO is promoted. The major reactions are expressed as follows:

$$Char - N + 1/2O_2 = NO \tag{8}$$

$$(-C) + NO = 1/2N_2 + (-CO) \tag{9}$$
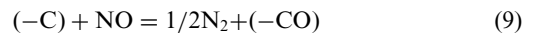
In addition, as shown in Fig. 3(b), the variation in the NO reduction efficiency is less than 5% as the mass fraction of Na additives increased from 1% to 3%, except for the NaAc additive at 800 °C. Thus, the concentration of Na additives has little effect on NO reduction when the mass fraction is greater
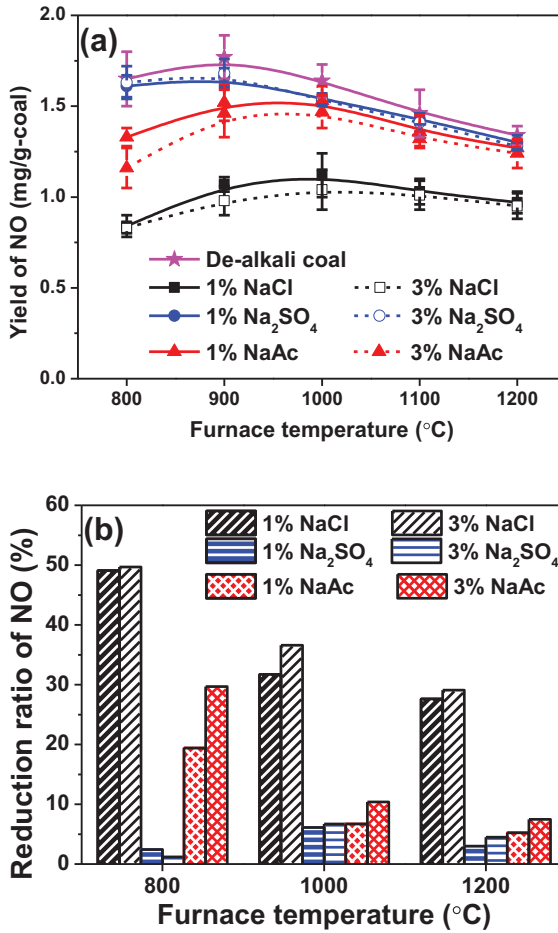
Fig. 3. Effects of Na additives and their mass fractions on NO formation.

than 1%. Under these experimental conditions, the inhibitory effect of 1% Na additives on NO formation has reached saturation in the flue gas.

3.3. Mechanism analysis of the effects of Na additives on No formation

A homogeneous experiment and simulation study were designed and conducted in the DTF at 800 and 1000 °C to reveal the mechanism underlying the effects of Na additives on NO formation in detail. The real atmosphere of coal combustion is complicated, and we simplify the combustion atmosphere as $CO/NH_3/O_2/H_2O/Na$ additive systems and N_2 as the balance gas. As shown in Fig. 4, the results indicate that NaCl and NaAc addition can significantly inhibit NO formation, while Na_2SO_4 addition does not exert a significant effect on NO emission. The measured concentrations of NO are 227.56 ppm without the addition

of Na additives at 800 °C (Fig. 4a). When 50 ppm NaCl and NaAc are added in the gas reaction, NO concentrations gradually decrease to 62.7% and 46.2%, respectively. However, with the further increase in NaCl and NaAc concentrations, their effects on NO production are not significant, which indicates that the inhibitory effect has been close to saturation when the concentrations of NaCl and NaAc are 50 ppm. When the furnace temperature reaches to 1000 °C, as shown in Fig. 4(b), the same conclusion is obtained from measured results. In addition, because the temperature gradually approached to the optimal temperature of $DeNO_x$, the concentration of generated NO decreases via SNCR (S8–S10).

As illustrated in Fig. 5, calculations were performed to explain the measured results obtained for NaCl using the CHENKIN software. The symbols denote the experimental data, while the solid lines denote calculated values. Despite some differences
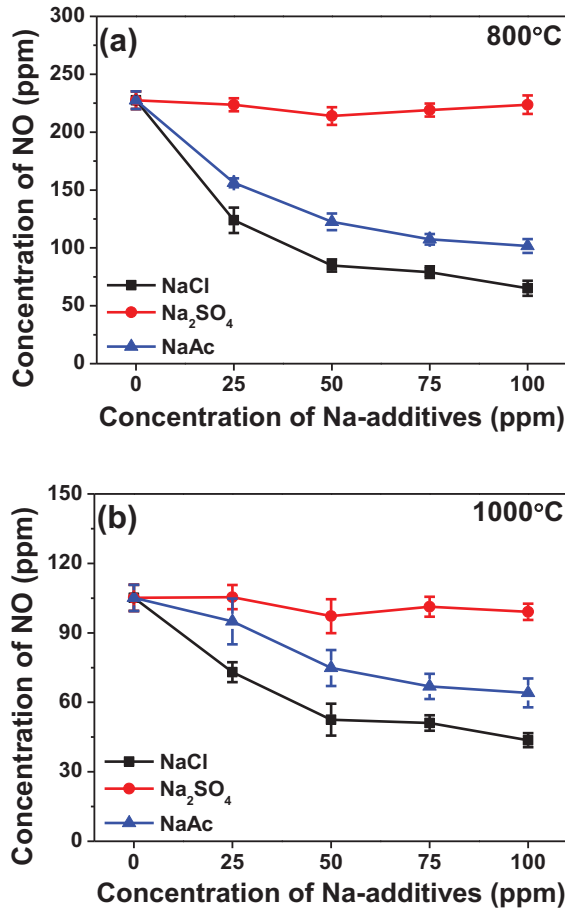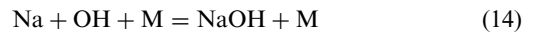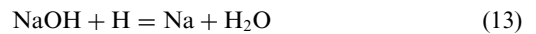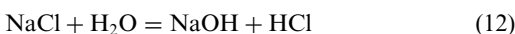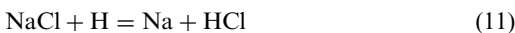
Fig. 4. Effects of Na additives on NO formation at 0.1 MPa, and in the presence of 1.5% CO, 3% O_2, 1% H_2O, 1000 ppm NH_3 and N_2 as the balance gas.
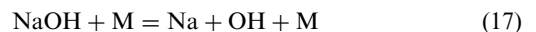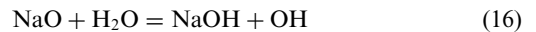
between the measured concentrations of NO and predictions from the model, they exhibit common variation trends as the concentration of NaCl increased. Hence, the experimental results can be explained through detailed reaction mechanisms.

A sensitivity analysis was performed in the presence of 50 ppm NaCl in the reactor at 800 and 1000 °C to determine the key reactions by which NaCl modulates NO formation. The sensitivity coefficient of $H + O_2 = O + OH$ (10) is the largest according to the CHEMKIN analysis. As shown in Fig. 6, the relative sensitivity coefficients of R11-R18 were calculated by comparing the values with R10 (relative sensitivity coefficient of 100%). The inhibitory effect of NaCl on NO formation is determined by the competitive relationships between two groups of reactions.

Inhibitory reactions:

$$NaCl + H = Na + HCl \tag{11}$$

$$NaCl + H_2O = NaOH + HCl \tag{12}$$

$$NaOH + H = Na + H_2O \tag{13}$$

$$Na + OH + M = NaOH + M \tag{14}$$

Stimulatory reactions:

$$NaCl + OH = NaO + HCl \tag{15}$$

$$NaO + H_2O = NaOH + OH \tag{16}$$

$$NaOH + M = Na + OH + M \tag{17}$$

$$NaOH + O_2 = NaO_2 + OH \tag{18}$$

A negative sensitivity coefficient for NO formation is observed for R11-R14, in which the radicals of H and OH are consumed. A positive sensitivity coefficient is observed for R15-R18. The OH radical is generated through R16-R18, which exhibits positive effect on NO formation. Although R15 consumes the OH radical, it also
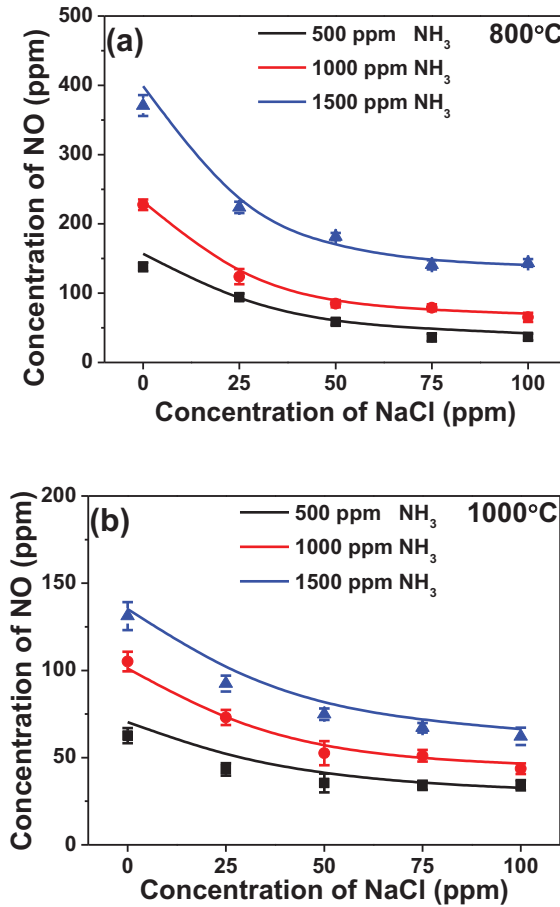
Fig. 5. Effect of NaCl on NO formation, where the symbols denote the experimental data, while the solid lines denote calculated values.

generates the NaO radical and promotes OH formation through R16-R18.The relative sensitivity coefficients of R11-R14 are larger than R15-R18 under these conditions. Therefore, a large number of H and OH radicals are consumed and the oxidation process of NH_3 to NO is inhibited. In addition, the consumption of the H radical also inhibits the R10 reaction to form more O and OH radicals. In an attempt to further explain the results presented in Figs. 4 and 5, it can be seen in Fig. 6 that R11-R14 plays an important role and the radical pool of H, O and OH is consumed when a small amount of NaCl is injected. The inhibitory effect of NaCl is mostly attributed to gas radical removal reactions and it is most likely a simple cycle as follows: $NaOH + H = Na + H_2O$ (13) and $Na + OH + M = NaOH + M$ (14). This indicates that atomic Na inhibits NH_3 oxidation to form NO by reducing H and OH under conditions with high radical concentrations. In addition, as shown in Figs. 3 and 5, the inhibitory effect of NaCl on NO emission is weakened at higher

temperatures ($>1000\,°C$), mainly because R17 ($NaOH + M = Na + OH + M$) may be enhanced at higher temperatures (as shown in Fig. 6(b)), resulting in an increase in the concentration of OH radicals in the flue gas, thereby reducing the inhibition of NaCl on the concentration of radicals.

In the combustion process of high-alkali coal, the mechanism underlying the inhibitor effect of NaAc on radicals is similar to NaCl. First, NaAc will decompose to form Na_2CO_3 at high temperatures, and then Na_2CO_3 will further decompose to form Na_2O at higher temperatures. In the presence of water vapor, NaOH can be formed via the following reactions:

$$2NaAc = CH_3COCH_3 + Na_2CO_3 \qquad (19)$$

$$Na_2CO_3 = Na_2O + CO_2 \qquad (20)$$
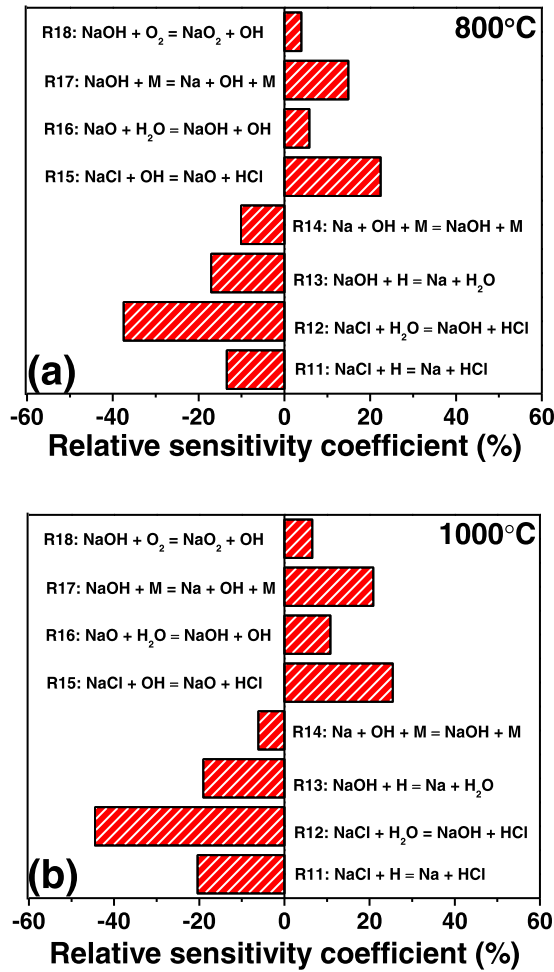
$$Na_2O + H_2O = 2NaOH \qquad (21)$$
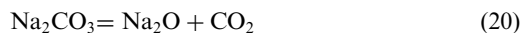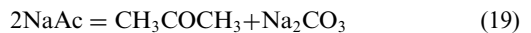
Fig. 6. Relative sensitivity coefficients for NO formation in the presence of 50 ppm NaCl.

Therefore, NaAc can cause a cyclic reaction between R13 and R14 by forming NaOH, thereby promoting the consumption of H and OH radicals. NH$_3$ oxidation to form NO will be inhibited due to the decreased concentration of radicals. In addition, the Na$_2$SO$_4$ additive has little effect on NO generation during coal combustion, mainly because the chemical properties of Na$_2$SO$_4$ are relatively stable and Na$_2$SO$_4$ does not readily react with other substances or radicals. According to the chemical equilibrium analysis, Na$_2$SO$_4$ is not easily decomposed at the experimental temperatures and it cannot also react with H$_2$O to form NaOH as NaCl does.

The effects of NaCl on the concentrations of H, O, and OH radicals are shown in Fig. 7. NaCl addition results in a decrease in the concentration of the OH radical from 70 to 32 ppm, a decrease in the concentration of the O radical from 50 to 16 ppm, and a decrease in the concentration of the H radi-

cal from 8.5 to 1.5 ppm. The concentration of OH is less than half of the value of the reaction conducted without NaCl, and the concentration of O is three times higher than the value obtained with 50 ppm NaCl. In particular, the concentration of the H radical decreases to approximately six times following NaCl addition. Therefore, NO formation will be significantly inhibited due to reduced concentration of H, O, and OH radicals. In addition, as displayed in Fig. 7(a), in the absence of NaCl, the concentrations of the H, O, and OH radicals reach peak values at approximately 0.035 s. However, in Fig. 7(b), the peak time for the generation of OH radical is delayed to 0.05 s. This indicates that NaCl not only suppresses the peak concentrations of the radicals but also delays the ignition of CO. In addition, the generated NaOH can also maintain high concentration of radicals for a longer time in the late combustion phase. At the same time, Fig. 7(b) also indicates that the rapid conversion of NaCl
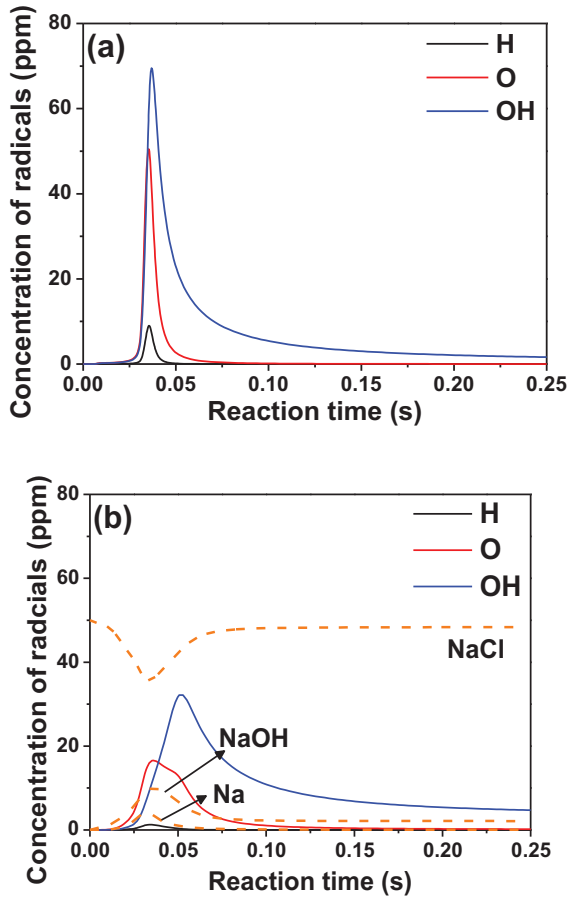
Fig. 7. Effects of NaCl addition on the concentrations of H, O, and OH radicals at 800 °C: (a) without NaCl addition; (b) with 50 ppm NaCl addition.

into NaOH and Na, which can significantly decrease the concentrations of H, O, and OH radicals via R11-R14. The conclusion is consistent with the results of the relative sensitivity analysis shown in Fig. 6.

4. Conclusions

Based on the experiments and calculations, the effect of Na and its occurrence in coal on NO formation were investigated systematically in an electrically heated drop tube furnace. The main conclusions are described below.

(1) With increasing temperature, the yield of NO initially increases and then decreases. The conversion rate of fuel-N to NO is accelerated with the increase in the furnace temperature under an oxidation atmosphere. When the furnace temperature exceeds 1000 °C, NO emission is inhibited due to the formation of a local reducing atmosphere.

(2) During coal combustion, the addition of Na salts tends to inhibit NO formation, and the inhibitory effects observed at lower temperatures are stronger than those at higher temperatures. Under the premise of the same mass fraction, the inhibitory effects of the three additives are ordered as follows: NaCl > NaAc > Na_2SO_4.

(3) A detailed kinetic mechanism is employed to analyze the experimental results of CO/NH_3 combustion when NaCl is added. A rational conclusion is that NaCl decreases the concentrations of H, O, and OH radicals, and subsequently affects NH_3 oxidation to NO via competitive relationships among multiple reactions. The inhibitory effects of NaCl and NaAc are mainly attributed to gas radical removal reactions and are most likely a simple cycle of $NaOH + H = Na + H_2O$ (13) and $Na + OH + M = NaOH + M$ (14).

(4) The inhibitory effects of NaCl and NaAc on NO emission are weakened at higher tem-

peratures ($>1000\,°C$), mainly because R17 (NaOH + M = Na + OH + M) may be enhanced at higher temperatures, resulting in an increase in the concentration of OH radicals in the flue gas and a reduction in the inhibitory effects of NaCl and NaAc on the concentrations of radicals.

Declaration of Competing Interest

None.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.proci.2020.06.052.

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