

# Detailed Modeling of NO<sub>x</sub> and SO<sub>x</sub> Formation in Co-combustion of Coal and Biomass with Reduced Kinetics

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**ABSTRACT:** In the paper, the numerical simulation program coupled with the detailed chemical reaction mechanism and computational fluid dynamics software was applied to calculate the concentration profiles of CO, NO<sub>x</sub>, and SO<sub>x</sub> during co-combustion of coal and biomass. The predicted data are compared to experimental results in an entrained flow combustion reactor to validate the numerical method for pulverized coal combustion. The characteristics of pollutant emissions in co-combustion with coal and three typical kinds of biomasses (Swedish wood, Danish straw, and sewage sludge) are also investigated. NO formation is significantly affected by the reactor temperature, and an increasing temperature obviously enhances the NO concentration. In the range of the calculated temperature, the final SO<sub>2</sub> emission level is not obviously influenced by the temperature. Co-combustion technology could effectively reduce the pollutant emissions, and the effect is proportional to the blending ratio of biomass. The biomass with low contents of nitrogen and sulfur and a high volatile content and lower heating value is an ideal co-fired fuel to reduce NO and SO<sub>2</sub> emissions.

## 1. INTRODUCTION

In pulverized coal combustion, fuel N conversion to NO is generally the major source of NO (>80%), with some contribution from thermal NO.<sup>1,2</sup> During coal devolatilization, fuel N is distributed between the volatiles and the solid char. It is generally assumed in modeling that nitrogen-containing volatiles either consist of or are rapidly converted to HCN and/or NH<sub>3</sub>. Subsequently, HCN and/or NH<sub>3</sub> are oxidized to NO via the homogeneous reactions involving the radicals (O, H, OH, and HO<sub>2</sub>), while they are competitively reduced to N<sub>2</sub>. The conversion of nitrogen-containing char occurs via the heterogeneous reactions involving the solid char, which also result in the formation of NO (by oxidation) or N<sub>2</sub> (by reduction).

During solid fuel combustion, the NO<sub>x</sub> formation is influenced by several factors, e.g., temperature, equivalence ratio, mixing, residence time, etc. Traditional global mechanisms are sometimes not able to simulate the process over an adequate range with desired accuracy. On the other hand, a number of comprehensive detailed mechanisms describing hydrocarbon combustion and the related N chemistry have been developed.<sup>3–5</sup> The direct use of these mechanisms in computational fluid dynamics (CFD) modeling of practical problems, however, is usually very expensive or even impossible, owing to the extremely large computing time and costs. Reasonably reduced kinetics based on these mechanisms can retain the important features of the original mechanisms and also greatly reduce the computing time. Reduced schemes in the CFD modeling of NO<sub>x</sub> formation in coal combustion have been reported.<sup>6,7,9–12</sup>

On the basis of the previous work,<sup>6</sup> Xu et al. postulated a simpler 4 steps, 8 species reduced mechanism for the prediction

of nitric oxide concentrations for advanced reburning, i.e., the hybrid reburning/selective noncatalytic reduction (SNCR).<sup>7</sup> A systematic reduction method<sup>8</sup> was used to derive the reduced mechanism, including the selection of the full mechanism, the development of the skeletal mechanism, and the selection of steady-state species. The reduced mechanism was derived from a 62 steps, 20 species skeletal mechanism,<sup>6</sup> which itself was based on a 312 steps, 50 species full mechanism. The 4 step integrated submodel for advanced reburning has been combined with a comprehensive CFD combustion code, PCGC-3. The predicted average axial NO concentration with advanced reburning (NH<sub>3</sub> injection) followed experimental trends.<sup>9</sup>

Han et al. developed a 12 steps, 16 species reduced mechanism for the conditions of CH<sub>4</sub> reburning in the coal-fired furnace.<sup>10</sup> The reduced mechanism was derived from a 137 steps, 43 species skeletal mechanism, which was based on the "GRI 3.0" mechanism with 325 steps, 53 species.<sup>5</sup> The reduced mechanism is then integrated into the three-dimensional (3D) combustion simulation CFD program "AIOLOS". The simulation results agree well with the experimental data for CH<sub>4</sub> reburning during pulverized coal combustion. Further, Han et al. developed a 10 steps, 14 species reduced mechanism for advanced reburning.<sup>11</sup> The reduced mechanism was derived from a 105 steps, 39 species skeletal mechanism, which was based on the "GADM98" mechanism with 438 steps, 64

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species.<sup>4</sup> CFD simulations were performed with the reduced kinetics for pure reburning and hybrid reburn/SNCR in a coal-fired reactor. The comprehensive modeling gave quite satisfactory results for wide ranges of the parameters.

Lv et al.<sup>12</sup> developed a joint mechanism including 44 species and 150 elementary reactions based on the mechanism by Rota et al.<sup>13</sup> and the scheme by Zebetta et al.<sup>14</sup> to predict the hybrid NO<sub>x</sub> control process. The simplification employed related graphs and the rate-of-product method and was validated by comparing to reported experimental data. To handle CFD simulation of practical problems, a reduced mechanism was accordingly established including 18 global steps and 22 species and was tested by comparing its predicted results to those of the joint mechanism. Perfect coherency between them is observed at different operating conditions, and the deviation is negligible compared to the general measuring uncertainty.

In the paper, on the basis of the previous work,<sup>10,11</sup> a reduced mechanism involving NO<sub>x</sub> and SO<sub>x</sub> reaction kinetics was applied to predict the concentration profiles of CO, NO<sub>x</sub>, and SO<sub>x</sub> during pulverized coal combustion. The effect of the combustion temperature on NO and SO<sub>2</sub> formation is analyzed. The characteristics of pollutant emissions in co-combustion with coal and three typical kinds of biomasses (Swedish wood, Danish straw, and sewage sludge) at different blending ratios and temperatures are investigated.

## 2. NUMERICAL SIMULATION METHOD

The detailed modeling method of NO<sub>x</sub> formation in pulverized coal combustion with reduced kinetics has been described in detail elsewhere,<sup>10,11</sup> and in this work, the sulfur chemistry is also integrated into the reduced kinetics. A brief description of the numerical simulation method is given here.

**2.1. Reduction of the Detailed Mechanism.** First, a skeletal mechanism was derived from the full mechanism by eliminating unimportant reaction steps through sensitivity analysis, partial equilibrium analysis, and integral reaction flow analysis.<sup>8,15</sup> Second, the quasi-steady-state (QSS) species are identified from the reactions in the skeletal mechanism, and the reactions including each QSS species are eliminated. Finally, a global reaction mechanism is established, and the global reaction rates are determined by the elementary reaction rates in the skeletal mechanism.

The present work chooses the "GADM98" mechanism<sup>4</sup> as one of the original detailed mechanisms, including NO<sub>x</sub> formation and C<sub>1</sub> and C<sub>2</sub> hydrocarbon fuels chemistry. Another original detailed mechanism is taken from the "GKDCB96" mechanism for SO<sub>x</sub> formation<sup>16</sup> including 66 reactions and 15 species. There are in total 504 reactions and 79 species in the full reaction mechanism. The reduction procedure is performed in conjunction with the SENKIN code<sup>17</sup> in the CHEMKIN package. After the computation, the mechanism reduction program reads data from the CHEMKIN link file and the SENKIN results file that contain the information on the kinetic mechanism and species concentrations, the rates of production, and the sensitivity coefficient of all species with respect to each reaction. The mechanism reduction is performed through analyzing the SENKIN results by means of the developed program.

The skeletal mechanism is derived from the full reaction mechanism by identifying and eliminating unimportant reaction steps through the analysis regarding the major variables under a particular flame condition of interest.<sup>8,15</sup>

The reaction steps having the normalized first-order sensitivity coefficients along the time of the main reaction stretch smaller than a predefined criterion, in this work, 1–5%, will be eliminated

$$S_{k,i}/\max_i(S_{k,i}) < \delta \quad (1)$$

where  $S_{k,i}$  is the sensitivity coefficient of the  $k$ th species with respect to the  $i$ th reaction. The sensitivity coefficient is defined as

$$S_{k,i} = \frac{\partial[X_k]}{\partial A_i} \quad (2)$$

where  $X_k$  is the mole fraction of the  $k$ th species and  $A_i$  is the pre-exponential factor in the Arrhenius expression for the forward rate constant of the  $i$ th reaction [ $k_i = A_i T^b \exp(-E_i/RT)$ ].

In addition, the reaction steps are in partial equilibrium fulfilling the following relation along the time of the main reaction stretch:

$$\frac{|k_{f_i} - k_{r_i}|}{\max(k_{f_i}, k_{r_i})} < \delta \quad (3)$$

where  $k_f$  and  $k_r$  are the forward and reverse reaction rate constants, respectively, and are also omitted from the skeletal mechanism ( $\delta = 5$ –10%).

To avoid some important reactions being eliminated from the mechanism, the strategy is that all reactions that have a great relative integral reaction flow are retained in the skeletal mechanism

$$\frac{\int_0^{\Delta t} q_i dt}{\max_i(\int_0^{\Delta t} q_i dt)} < \delta \quad (4)$$

where the usual value of the criterion  $\delta$  equals 1–5%,  $\Delta t$  is the time of the reaction stretch, and  $q_i$  is the rate of progress of the  $i$ th reaction, which fulfills the following equation:

$$q_i = k_{f_i} \prod_{k=1}^K [X_k]^{\nu'_{ki}} - k_{r_i} \prod_{k=1}^K [X_k]^{\nu''_{ki}} \quad (5)$$

where  $K$  is the total number of the species,  $\nu'_{ki}$  is the stoichiometric coefficient of the  $k$ th species in the  $i$ th forward reaction, and  $\nu''_{ki}$  is the stoichiometric coefficient of the  $k$ th species in the  $i$ th reverse reaction.

According to the above method, the skeletal mechanism is derived containing 242 reactions and 63 species.

In the skeletal mechanism, the species fulfilling the following relation along the whole reaction stretch are identified as the QSS species:<sup>8</sup>

$$[X_k] \frac{|\dot{\omega}_k^p - \dot{\omega}_k^d|}{\max(\dot{\omega}_k^p, \dot{\omega}_k^d)} < \delta \quad (6)$$

where  $\dot{\omega}_k^p$  is the production rate of the  $k$ th species and  $\dot{\omega}_k^d$  is the destruction rate of the  $k$ th species. The usual value of the criterion  $\delta$  equals 0.1–1%.

After the QSS analysis, 15 species are retained, called non-steady state (or major) species. They are O<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, H<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>, NH<sub>3</sub>, HCN, NO, SO, SO<sub>2</sub>, SO<sub>3</sub>, and H<sub>2</sub>S, which will remain in the reduced global mechanism.

The steady-state assumption for a species leads to the algebraic equation

$$\frac{d[X_k]}{dt} = \dot{\omega}_k = \sum_i (\nu''_{ki} - \nu'_{ki}) q_i = 0 \quad (7)$$

between reaction rates. The above equations denote the net production rate of the QSS species. Each of these equations can be used to eliminate a reaction rate (because  $q_i = 0$ ) in the balance equation set for the major species. Principally, the present work selects for each QSS species the least sensitive reaction involving the species. This elimination principle ensures the smallest errors, and the reduced mechanism has lower stiffness.<sup>15</sup> The stoichiometry of the resulting equation system defines the global mechanism between the major species. The rate of each global reaction step can be expressed with the rates of the elementary reactions in the skeletal mechanism. After this eliminating procedure, 10 independent reactions (global reaction scheme) were obtained.

When eq 7 is used to determine the concentration of the QSS species, an algebraic equation set can be obtained that expresses the concentrations of the QSS species in terms of other species (see eq 5). This set of equations is often coupled nonlinearly among those QSS species. Given the concentrations of the major species, the concentrations of QSS species are determined by solving the equation system iteratively. Finally, a Fortran subroutine is automatically generated for calculating the production rate of the major species according to the reduced mechanism. More details about the reduced mechanism and its discussion can be found in refs 10, 11 and 18.

**2.2. Integration into the CFD Code "AIOLOS".** The developed reduced kinetics for  $\text{NO}_x$  and  $\text{SO}_x$  formation under coal-fired conditions was implemented into the 3D furnace simulation CFD program "AIOLOS" developed by the Institute of Combustion and Power Plant Technology at the University of Stuttgart, which mainly deals with pulverized coal combustion. The code "AIOLOS" is based on a conservative finite-volume formulation, using the SIMPLEC or SIMPLE method for velocity–pressure coupling, the standard  $k-\epsilon$  model, or the differential Reynolds stress model for turbulence.<sup>19</sup> Radiative heat transfer is calculated by either a discrete ordinates method or five other different radiation models. The turbulent gas-phase reactions are calculated with the eddy dissipation concept (EDC) model.<sup>20–23</sup> The EDC is a general concept for treating the interaction between turbulence and chemistry in flames.

After the implementation, all of the homogeneous reactions (gas-phase reactions) are calculated with the reduced mechanism. The heterogeneous reactions, i.e., the pyrolysis and char combustion, the heterogeneous sources of N species, the heterogeneous  $\text{NO}_x$  reduction by char, etc., are calculated with the available models in AIOLOS (see ref 24). The composition of the pyrolysis product as well as the distribution of coal nitrogen within the pyrolysis products is predicted using the functional-group, depolymerization, vaporization, cross-linking (FG-DVC) model<sup>25</sup> in a pre-processing step.<sup>24</sup> Char nitrogen is assumed to be released as the primary product  $\text{NH}_3$  during char burnout. To simulate biomass combustion, a model of evaporation of moisture in biomass is used. For both kinds of fuels, the particle shape is assumed to be spheroidal, the size distribution is given using three typical average diameters and proportions according to experimental measurements, and the parameters for pyrolysis and char burnout are also modified for different fuels based on the formula  $k_i = A_i \exp(-E_i/RT)$ . The corresponding information is shown in Table 1. The

**Table 1. Particle Size Distribution and Kinetic Parameters for Pyrolysis and Char Burnout**

	coal		biomass	
particle size distribution	10 $\mu\text{m}$	40%	15 $\mu\text{m}$	20%
	25 $\mu\text{m}$	40%	40 $\mu\text{m}$	40%
	50 $\mu\text{m}$	20%	75 $\mu\text{m}$	40%
Kinetic Parameters for Pyrolysis				
$A_i$ ( $\text{s}^{-1}$ )	$1.5 \times 10^5$		$1.667 \times 10^4$	
$E_i/R$ (K)	8900		9500	
Kinetic Parameters for Char Burnout				
$A_i$ ( $\text{s}^{-1}$ )	208		500	
$E_i/R$ (K)	9553		9553	

heterogeneous reduction of  $\text{NO}$  by soot and char is considered for both coal and biomass with a first-order rate expression as

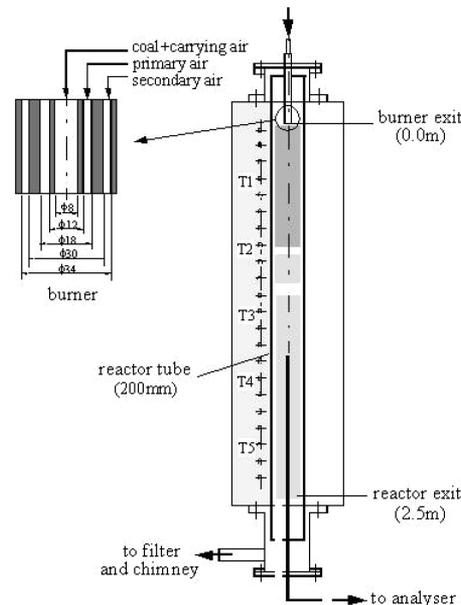
$$\left(\frac{dn_{\text{NO}}}{dt}\right)_i = -A_i \exp(-E_i/RT) X_{\text{NO}} S_e \quad (8)$$

where  $n_{\text{NO}}$  is the mole number of  $\text{NO}$  in kilomoles,  $X_{\text{NO}}$  is the mole fraction of  $\text{NO}$ , and  $S_e$  is the available external surface area of soot or char. The corresponding rate parameters are  $A_i = 4.47 \times 10^{-7} \text{ kmol m}^{-2} \text{ s}^{-1} \text{ Pa}^{-1}$  and  $E_i = 9.65 \times 10^3 \text{ K}$  for soot and  $A_i = 4.18 \times 10^{-4} \text{ kmol m}^{-2} \text{ s}^{-1} \text{ Pa}^{-1}$  and  $E_i = 1.75 \times 10^4 \text{ K}$  for char.<sup>24</sup>

In the present work, seven additional gas species ( $\text{NH}_3$ ,  $\text{HCN}$ ,  $\text{NO}$ ,  $\text{SO}$ ,  $\text{SO}_2$ ,  $\text{SO}_3$ , and  $\text{H}_2\text{S}$ ) over the eight originally existing gas species in

AIOLOS ( $\text{O}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{C}_2\text{H}_6$ ,  $\text{H}_2$ ,  $\text{H}_2\text{O}$ , and  $\text{N}_2$ ) were supplemented into the AIOLOS program. Transport equations for these species are to be solved, and the concentration distribution of the species is obtained.

**2.3. Description of the Experiment.** Tests and simulations are executed for a 20 kW electrically heated pulverized coal-fired entrained flow reactor (EFR). The reactor is schematically shown in Figure 1.



**Figure 1.** Schematic of the pulverized coal-fired EFR.

The combustion air can be heated to 400 °C. A gravimetric screw conveyor supplies a constant coal-feeding rate between 0.5 and 5 kg/h. The electrically heated reactor has five regulated heating zones with a maximum temperature of 1400 °C, measured by PtRh–Pt thermocouples. The ceramic reactor tube has a length of 2.5 m and an internal diameter of 200 mm. The flue gas composition ( $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{SO}_2$ , and  $\text{O}_2$ ) at different positions is measured online using standard instrumentation [paramagnetism for  $\text{O}_2$ , non-dispersive infrared (NDIR) for  $\text{CO}$  and  $\text{CO}_2$ , chemiluminescence for  $\text{NO}_x$ , and infrared photometer for  $\text{SO}_2$ ] through a vertically moveable gas probe cooled with oil. The error of the measuring instrument is 1–5 ppmv.

In the present experiment, a German bituminous coal "Göttelborn" is used as a fuel with a feeding rate of 1 kg/h during the tests, and the coal analysis is listed in Table 2. The carrying air with pulverized coal enters the burner center, surrounded by the primary air and the

**Table 2. Pulverized Coal and Biomass Analysis Data**

	Göttelborn	Swedish wood	Danish straw	sewage sludge
Proximate Analysis (wt %)				
moisture (ar)	1.69	7.80	11.71	5.86
volatile (dry)	31.94	84.10	71.32	48.45
ash (dry)	10.74	0.20	13.42	48.06
fixed carbon (dry)	57.32	15.70	15.26	3.65
LHV (MJ/kg, dry)	30.89	18.52	16.01	10.72
Ultimate Analysis (wt %, dry)				
C	74.16	49.57	41.43	25.77
H	4.42	6.05	4.18	4.31
N	1.18	0.07	1.09	3.02
S	1.12	0.06	0.10	0.81
Cl	0.22	0.01	0.53	0.04
O	8.16	44.04	39.25	17.99

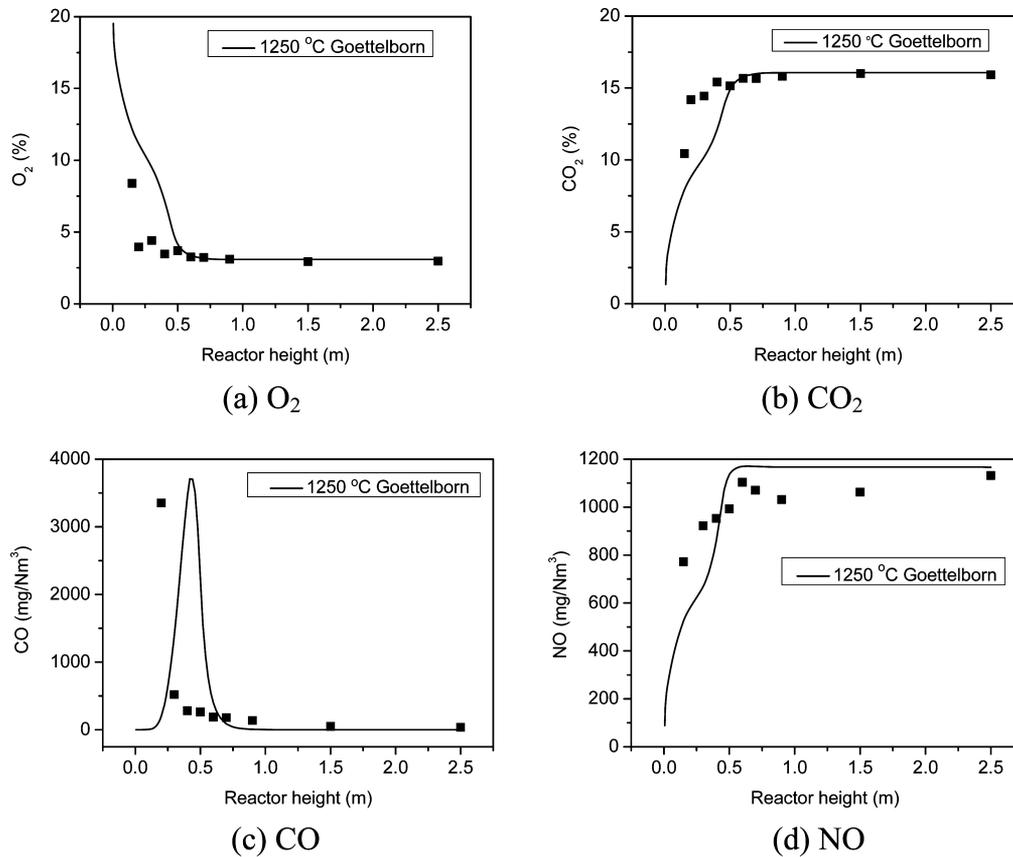


Figure 2. Comparison between the predicted and measured results in EFR (—, predicted result; ■, measured result).

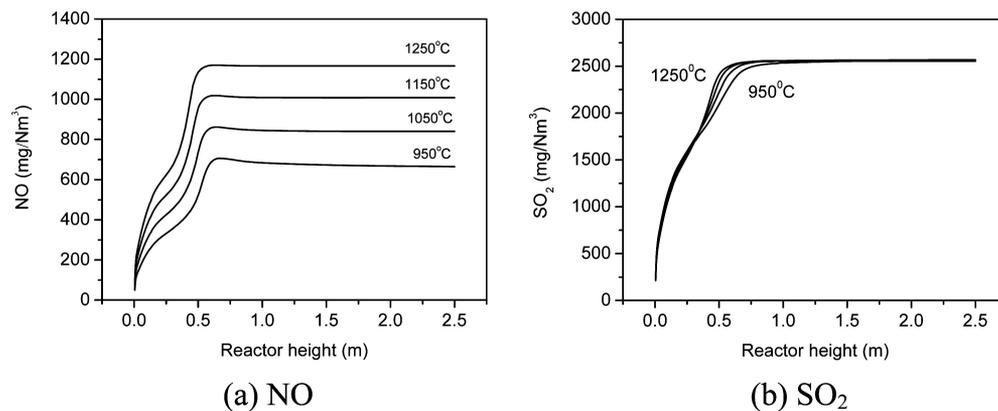


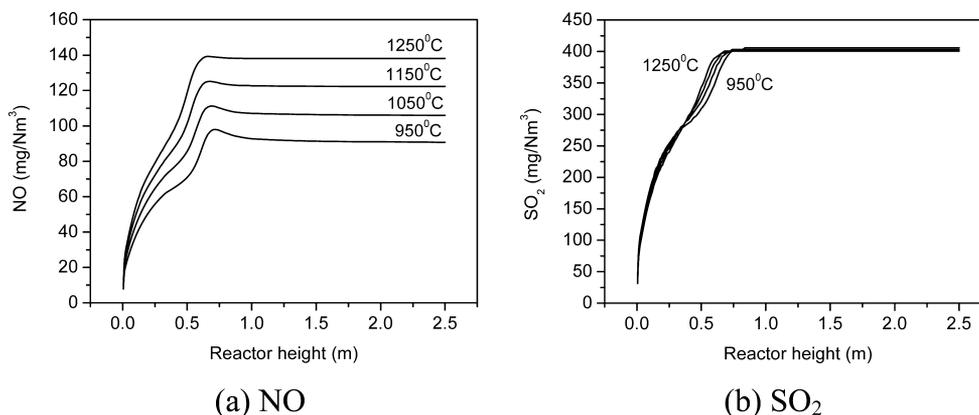
Figure 3. Predicted results of (a)  $NO$  and (b)  $SO_2$  concentration distribution for Götteleborn coal along the reactor height for various wall temperatures.

secondary air. The carrying air flux is  $1.5 \text{ N m}^3 \text{ h}^{-1}$ . The total flux of the primary and second air is  $8 \text{ N m}^3 \text{ h}^{-1}$ , and the ratio between them is 1:2. The air/fuel equivalence ratio  $\lambda$  is 1.15. The wall temperature is  $1250 \text{ }^\circ\text{C}$ .

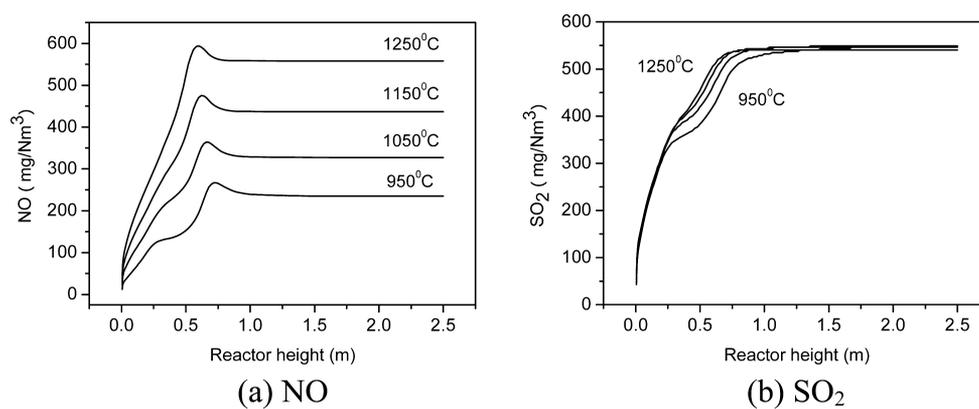
During the tests, it was found that, besides the controllable parameters, pollutant emissions might be influenced by some unexpected incidents, e.g., a slight variation of fuel composition or a fluctuating feeding rate. For example, the results show that the maximum variation of  $NO_x$  under each condition is likely to attain  $\pm 20$  ppmv. However, the averaged emission during a relatively long time period is obviously close to a constant.<sup>26</sup> Therefore, each experimental data point in this paper is an average result of 2–3 times measurements, with a 2 min interval for one time.

**2.4. Model Validation.** The predicted data are compared to experimental results in the entrained flow combustion reactor shown

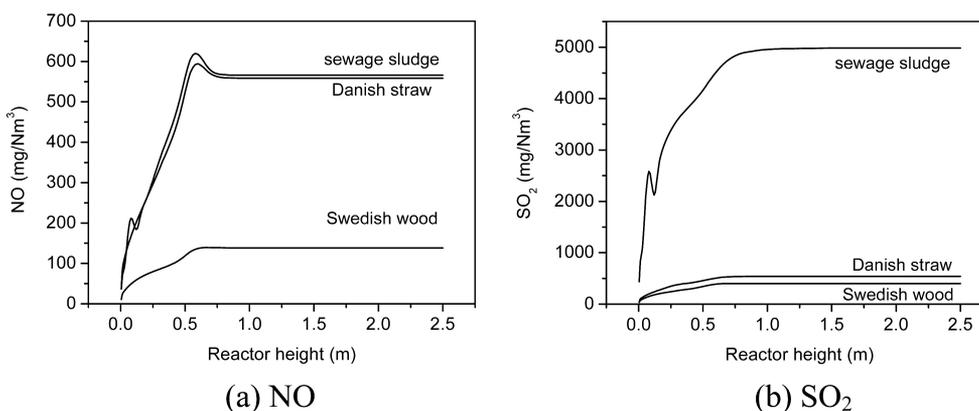
in Figure 1 to validate the numerical method. Figure 2 gives the predicted and measured  $O_2$ ,  $CO_2$ ,  $CO$ , and  $NO$  concentration profiles along the reactor height. It can be seen that both results coincide well for the change trend and final emission of various species. However, in the beginning of the coal flame, the predicted concentration of  $O_2$  is higher than the experimental value and the corresponding calculated  $CO_2$  concentration is less than the test data. Also, the predicted  $CO$  concentration peak delays to occur, and the calculated  $NO$  concentration is lower than the experimental data near the burner. These differences between measured and predicted values might be induced by the ignition delay in the numerical model, or the flow field and coal combustion might be affected by the sampling probe with a relatively big diameter (38 mm) near the burner in the experiments. Nevertheless, the detailed modeling method seems to be able to predict the pulverized coal combustion satisfactorily. For simulating



**Figure 4.** Predicted results of (a) NO and (b) SO<sub>2</sub> concentration distribution for pure Swedish wood along the reactor height for various wall temperatures.



**Figure 5.** Predicted results of (a) NO and (b) SO<sub>2</sub> concentration distribution for pure Danish straw along the reactor height for various wall temperatures.



**Figure 6.** Predicted results of (a) NO and (b) SO<sub>2</sub> concentration distribution for Swedish wood, Danish straw, and sewage sludge along the reactor height at the temperature of 1250 °C.

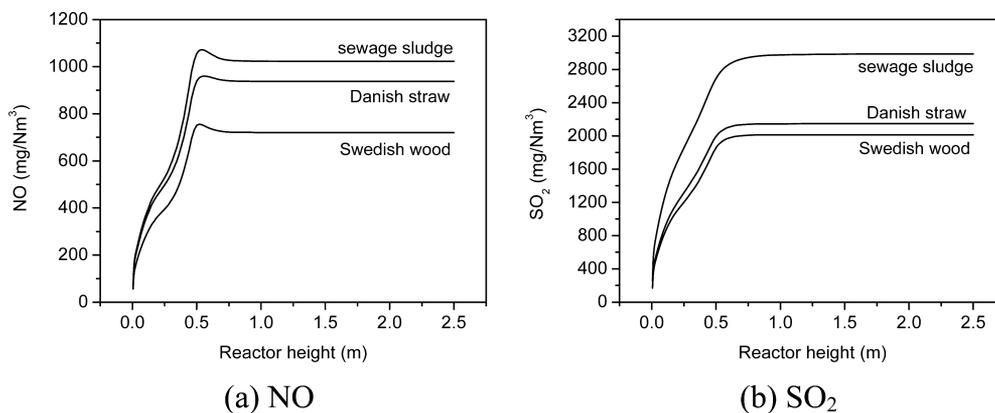
biomass combustion or co-combustion of coal and biomass using AIOLOS, some work has been performed to validate its feasibility and rationality, such as refs 27 and 28.

### 3. PREDICTED RESULTS AND DISCUSSION

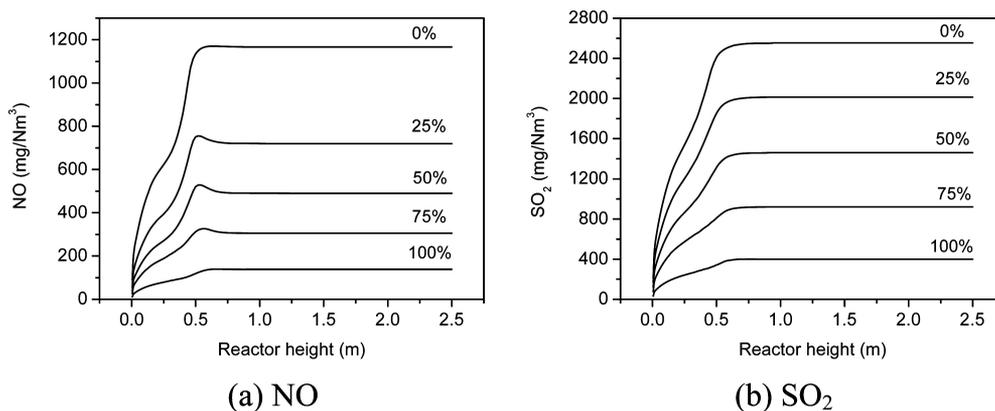
On the basis of the validation of the detailed modeling method, the effect of the combustion temperature on NO and SO<sub>2</sub> formation is analyzed, and the predicted results are shown in Figure 3 for the temperature range from 950 to 1250 °C. The simulation results of the same case published in ref 29 are slightly different, because it shows the values near the axis;

however, in this paper, they are average values of the whole cross-section. Results indicate that the temperature significantly affects NO formation, and increasing the temperature obviously enhances the NO concentration, which coincides with the trend of measurement data.<sup>26</sup> In the range of the calculation, the final concentration level of SO<sub>2</sub> is not obviously affected by the temperature, and all of the concentration lines almost coincide with each other for different temperatures, with a higher temperature only leading to a little faster release process.

The combustion of three kinds of biomass fuels is also investigated. Biomass fuels are Swedish wood, Danish straw,



**Figure 7.** Predicted results of (a) NO and (b) SO<sub>2</sub> concentration distribution for co-combustion with Swedish wood, Danish straw, and sewage sludge along the reactor height (blending ratio, 25%; temperature, 1250 °C).



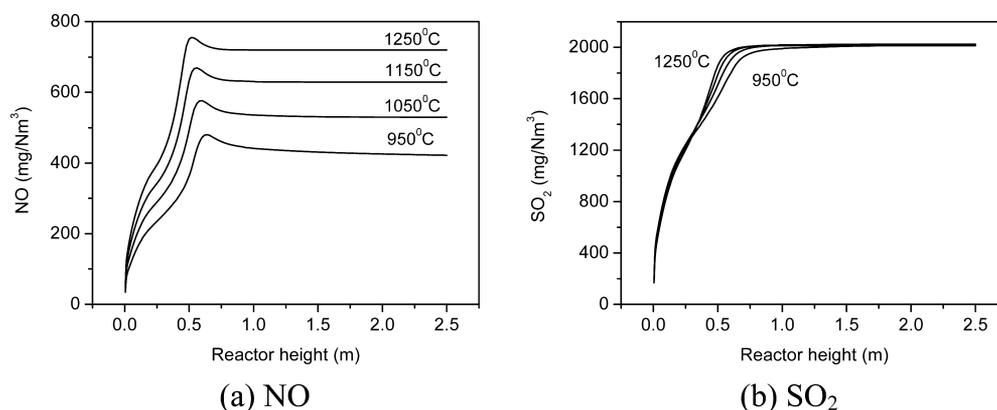
**Figure 8.** Modeling results of (a) NO and (b) SO<sub>2</sub> concentration distribution for co-combustion along the reactor height at the temperature of 1250 °C under different blending ratios of Swedish wood.

and sewage sludge, and the chemical analysis data of fuels are listed in Table 2. To coincide with the actual thermal power input, the simulation is based on the same heat release with 1 kg/h Götteborn coal. Figure 4 shows the concentration profiles of NO and SO<sub>2</sub> emission during pure Swedish wood combustion. Although the trend of the curve is similar to those of coal combustion under various wall temperatures, the concentrations of the pollutant emissions are much lower than those of the coal obviously. This is because the wood has a very low content of nitrogen and sulfur and a high content of volatiles. Similar results can also be observed in Danish straw combustion, which is shown in Figure 5.

As mentioned above, although the combustion of biomass might reduce the pollutant emissions substantially, there are some differences in the chemical composition of biomass, which may influence NO and SO<sub>2</sub> emissions. Figure 6 shows NO and SO<sub>2</sub> concentration distributions during the combustion of the three different biomass fuels at 1250 °C. There are great differences of NO and SO<sub>2</sub> emissions for Swedish wood, Danish straw, and sewage sludge, which are caused by the different chemical composition shown in Table 2. The lower pollutant emissions of Swedish wood compared to those of Danish straw and sewage sludge are caused by its low content of nitrogen and sulfur. In addition, the high content of volatiles might result in an oxygen-poor atmosphere and limit the conversions of fuel N and fuel S to NO<sub>x</sub> and SO<sub>x</sub>. A low value of the lower heating value (LHV) can increase the demand of fuel, which will increase the source of fuel N and fuel S. This is

a reason why the SO<sub>2</sub> emission is very high during sewage sludge combustion.

However, only burning pure biomass in a power plant might result in problems, such as a low LHV compared to coal and the deposition and corrosion possibility caused by alkali metals in biomass. To obtain low-pollutant emissions and good operation of the power plant, the co-combustion technology of coal and biomass is often applied. Because of the different composition of biomass fuels, co-combustion with biomass may influence pollutant emissions. In this paper, during the simulation of co-combustion of two fuels, the fuel with a larger mass flow is fed through carrying air inlet and the other is fed through carrying primary air inlet. The particle size distribution and kinetic parameters of each kind of fuel are given according to Table 1. Figure 7 shows the simulation results of co-combustion of Götteborn coal and biomass fuels at the blending ratio of biomass at 25% and temperature of 1250 °C, where the blending ratio of biomass refers to the percentage of heat release for biomass and not the mass fraction. In comparison to the combustion of Götteborn coal, the NO reductions of Swedish wood and Danish straw at the exit of the reactor are 38.30 and 19.67%, while the SO<sub>2</sub> reductions are 21.16 and 15.90%, respectively. For sewage sludge, the NO formation is reduced by 12.35%; however, the SO<sub>2</sub> formation is increased by 16.91%. The high SO<sub>2</sub> emission of sewage sludge is caused by the high content of sulfur and the low value of the LHV. Thereby, the biomass with low contents of nitrogen and



**Figure 9.** Modeling results of (a) NO and (b) SO<sub>2</sub> concentration distribution for co-combustion along the reactor height at the blending ratio of 25% of Swedish wood for various wall temperatures.

sulfur and a high volatile content and LHV is an ideal co-fired fuel to reduce NO and SO<sub>2</sub> emissions.

The results predicted above indicate that, among the three biomass fuels, Swedish wood is the best fuel to reduce pollutant emissions while co-combusting with coal. Figure 8 is the simulation results of co-combustion of Götteborn coal and Swedish wood at the temperature of 1250 °C. Figure 9 shows the influence of the wall temperature on NO and SO<sub>2</sub> emissions at the blending ratio of 25%. These results indicate that co-combustion is affected by the temperature with the similar trend as the combustion of pure fuel. A low-temperature combustion can effectively reduce the formation of NO; however, the release process of SO<sub>2</sub> only slows, and its emission is not affected. The effect of co-combustion is proportional to the blending ratio of biomass; the higher the blending ratio of biomass, obviously the lower the NO and SO<sub>2</sub> emissions.

#### 4. CONCLUSION

In the present work, a reduced reaction mechanism including N/S chemistry was developed on the basis of the detailed reaction mechanisms of “GADM98” and “GKDCB96” to investigate NO<sub>x</sub> and SO<sub>x</sub> formation in co-combustion of coal and biomass. The reduced mechanism with 15 species was integrated into a 3D combustion CFD program AIOLOS for simulation. The simulation results of coal combustion show good agreement with the experimental data, which provide a good validation for the simulation method and reduced mechanism.

The combustion of coal and biomass and co-combustion of coal and biomass were investigated through a large number of CFD simulations. The results indicate that the combustion of coal or biomass in EFR is affected by the temperature, and a lower temperature combustion can effectively reduce NO formation; however, the final concentration of SO<sub>2</sub> is almost not influenced by the temperature, with a higher temperature only leading to a little faster release process. The same influence can also be found while simulating co-combustion of coal and biomass fuels. Different biomass fuels can lead to different NO<sub>x</sub> and SO<sub>x</sub> emissions because of their chemical compositions. The biomass with low contents of nitrogen and sulfur and a high volatile content and LHV is an ideal co-fired fuel to reduce NO and SO<sub>2</sub> emissions. For co-combustion of coal and this kind of ideal biomass, a high blending ratio of biomass can lead to low NO and SO<sub>2</sub> emissions.

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#### NOMENCLATURE

- $A_i$  = pre-exponential factor of the  $i$ th reaction
- $b$  = temperature exponent
- $E_i$  = activation energy of the  $i$ th reaction
- $K$  = total number of the species in a chemical reaction mechanism
- $k_f/k_r$  = forward/reverse reaction rate constant
- LHV = lower heating value
- $n_{\text{NO}}$  = mole number of NO
- $q_i$  = rate of progress of the  $i$ th reaction
- $R$  = universal gas constant
- $S_e$  = available external surface area
- $S_{k,i}$  = sensitivity coefficient of the  $k$ th species with respect to the  $i$ th reaction
- $T$  = temperature
- $X_k$  = mole fraction of the  $k$ th species
- $\delta$  = predefined criterion
- $\Delta t$  = time of reaction stretch
- $\nu'_{k,i}/\nu''_{k,i}$  = stoichiometric coefficient of the  $k$ th species in the  $i$ th forward/reverse reaction
- $\dot{\omega}_k^p/\dot{\omega}_k^d$  = production/destruction rate of the  $k$ th species

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