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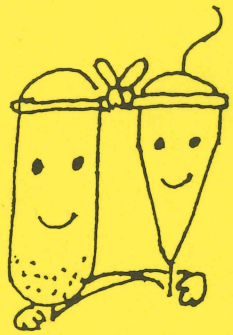
Sven Andersson

3rd INTERNATIONAL CONFERENCE ON CIRCULATING FLUIDIZED BEDS



October 15–18, 1990
Nagoya, JAPAN

Organized by
The Society of Chemical Engineers Japan
In Cooperation with the Secretariat of ICCFB

Modelling of NO_x Formation in a Circulating Fluidized Boiler

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Abstract

A detailed kinetic model for the oxidation of NH_3 and reduction of NO in FBC is used to model the NO concentration profile in an 8 MW CFB. Three different fuels were burned in the full scale tests: Bituminous coal, brown coal and petroleum coke. Kinetics were measured in a laboratory reactor using samples of char and bed material from the boiler. The simulation results show that char is an important catalyst for the oxidation of NH_3 and reduction of NO when burning bituminous coal and petroleum coke. The char content in the brown coal bed is low and very active bed material with a high ash content is the important catalyst in this case. Homogeneous gas phase reactions were found to have only a minor influence. The levels of NO concentration calculated are in agreement with the experimental results. It is concluded that modelling the fuel-N conversion using kinetics measured for the specific chars and bed materials is a considerable step towards a better understanding of the formation and reduction of NO in FBC.

Introduction The paths of formation and reduction of NO in fluidized bed combustion (FBC) are complex and not fully understood. As a consequense it is often difficult to explain the variation in NO_x emission observed for different operating conditions and different fuel types. A simplified reaction scheme for the conversion of fuel-N in FBC is shown in Fig. 1. The nitrogen content of the fuel is split in char-N and volatile-N and subsequently converted to NO, N_2, N_2O, and NH_3 by a large number of heterogenous and homogeneous reactions as described by Johnsson (1989). These reactions have been used to explain qualitatively the emissions of NO_x observed in full scale tests by Leckner and Åmand (1987), Åmand and Leckner (1988) and Hirama et al. (1987), but modelling of the fuel-N conversion was not possible because of lack of reliable kinetic data.

The aim of this work is to model the formation and reduction of NO in an 8 MW circulating fluidized bed boiler (CFB) burning three different fuels, and to evaluate the relative importance of the many reactions. In order to do this, the kinetics of the heterogenous catalytic reduction of NO and oxidation of NH_3 on char and bed material has been measured in the laboratory using samples of solids from the boiler.

CFB-tests

The CFB boiler used in this study has a thermal power of 8 MW and was built by Götaverken in 1981, Fig. 2. The height of the combustion chamber is 8.5 m and the cross section is 1.8 m^2. The fluidizing velocity is normally in

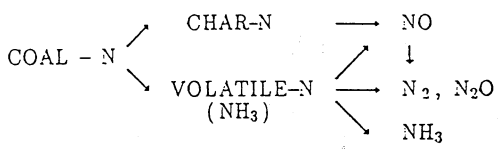

Figure 1. Principal steps in formation and reduction of NO in fluidized bed combustion.

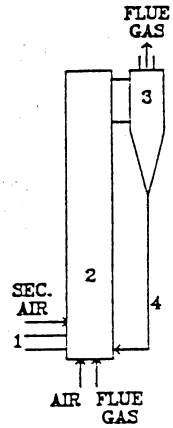

Figure 2. Schematic picture of the boiler. 1: Fuel feed screw, 2: Combustion chamber with fluidized bed, 3: Cyclone, 4: Particle return leg.

the range from 3 to 6 m/s. The fuel is fed with a screw feeder into the lower part of the combustion chamber close to the bottom. Secondary air is introduced through an air register located 1 m above the bottom of the combustion chamber. Silica sand was used as a bed material and no limestone was added during the test program. The three fuels burned were bituminous coal, brown coal and petroleum coke, and so the volatile content varied between 53.1 and 14.3 % maf. The fuel characteristics are listed in Table 1.

The primary parameters in the test series were the bed temperature, the excess air ratio and the primary air stoichiometry. A reference case was defined as a run with a bed temperature of around 1120 K, an excess air ratio of around 1.25 and a primary air ratio of 0.75. From these conditions one parameter at a time was varied to lower and higher values, keeping the two others constant. The variation was carried out for all three fuels. Figure 3 shows the result for variation of the temperature. The conversion of fuel–N to NO was extremely low in all tests, and from Fig. 3 it can be seen that the

Table 1. Fuel characteristics

Type	Brown coal	Bituminous coal	Petroleum coke
Volatiles % maf	53.1	35.5	14.3
Proximate analysis %			
Combustibles	80	87	91
Ash	5	7	2
Moisture	15	6	7
Ultimate analysis % maf			
C	67.1	82.7	89.8
H	4.9	5.2	4.1
O	25.9	8.8	2.7
S	0.8	1.6	2.0
N	0.9	1.7	1.4
Volatile nitrogen % maf	49.0	39.3	25.9

Table 2. Experimental values of parameters used in modelling the fuel–N conversion

Parameter	Brown coal	Bit. coal	Pet. coke
Char content in bed wt%	0.3	7.5	19.5
CO concentration vol%			
at 2.8 m	5.0	3.5	1.2
at 8.5 m	1.1	1.0	0.3
Temperature, top K	1086	1083	1083
Density, top kg/m³	2.8	2.9	2.6

partly due to the low char content (0.3 wt%) and partly due to the very active bed material when burning brown coal. This material has about 25 times the activity of bed material from burning bituminous coal or petroleum coke for the catalytic reduction of NO by CO, and it is responsible for most of the NO reduction in the brown coal bed. This high activity was explained by the high content of CaO and Fe_2O_3 in the ash and the high ash content in the brown coal bed material, Johnsson (1990).

The relative importance of char for the reduction of NO is about the same in the cases of bituminous coal and petroleum coke, even though the char content is about twice as high in the petroleum coke bed. The reason is the lower activity of the petroleum coke char. The conversion of volatile–N is dominated by reactions with char as a catalyst for these two fuels. This effect

Table 3. Reactions and kinetics for the reduction of NO and oxidation of NH_3.

No.	Reaction			Catalyst	Reaction Rate
R1	$NO + CO$	$\rightarrow$	$1/2N_2 + CO_2$	char	$-r_{NO}=kC_{NO}^{a}C_{CO}^{b}$
R2	$NO + CO$	$\rightarrow$	$1/2N_2 + CO_2$	bed material	$-r_{NO}=kC_{NO}^{a}C_{CO}^{b}$
R3	$NO + 2/3NH_3$	$\rightarrow$	$5/6N_2 + H_2O$	hom. gas phase	$-r_{NO}=kC_{NO}C_{NH_3}$
R4	$NH_3 + 5/4O_2$	$\rightarrow$	$NO + 3/2H_2O$	char	$r_{NO}=kC_{NH_3}C_{O_2}$
R5	$NH_3 + 5/4O_2$	$\rightarrow$	$NO + 3/2H_2O$	bed material	$r_{NO}=kC_{NH_3}$
R6	$NH_3 + 5/4O_2$	$\rightarrow$	$NO + 3/2H_2O$	hom. gas phase	$r_{NO}=kC_{NH_3}C_{O_2}$
R7	$2NH_3 + 3/2O_2$	$\rightarrow$	$N_2 + 3H_2O$	char	$-r_{NH_3}=kC_{NH_3}$
R8	$2NH_3 + 3/2O_2$	$\rightarrow$	$N_2 + 3H_2O$	bed material	$-r_{NH_3}=kC_{NH_3}$

Table 4. The calculated fractional conversion of NO and NH_3 in each reaction and the fuel–N conversion to NO in both cases given as percantage of total fuel–N. R1 to R8 are given in Table 3.

Reaction			Bituminous coal		Brown coal		Petroleum coke	
Type	Catalyst	No	a)	b)	a)	b)	a)	c)
Reduction of NO	char	R1	71.4	62.8	0.9	0.4	41.7	66.3
	bed mat	R2	15.4	13.8	78.1	75.7	7.0	12.1
	–	R3	0.2	1.6	0.4	0.4	0.3	1.3
Oxidation of NH_3 to NO	char	R4	33.8	15.5	5.1	0.1	23.1	12.5
	bed mat	R5	0.2	4.8	16.4	18.8	0.07	2.0
	–	R6	0.03	0.4	0.4	0.4	0.01	0.2
Oxidation of NH_3 to N_2	char	R7	0.3	6.9	0.1	0.1	0.2	5.5
	bed mat	R8	0.3	5.6	16.8	19.2	0.08	2.4
Fuel–N conversion to NO	simulation		12.9	8.2	3.2	3.1	50.6	11.5
	experimental		4.6	4.6	4.4	4.4	4.0	4.0

a) Standard simulation
b) The catalytic oxidation of NH_3 to NO is zero order in O_2
c) Like b), but the CO concentration is 5 vol% in the whole bed

may be overestimated in the simulations because of the first order dependence in O_2 concentration for the oxidation of NH_3 to NO. The kinetics could not be measured at O_2 levels above 0.5 vol% because of the fast combustion of the char, and the reaction order may be lower at higher concentrations. Simulations assuming zero order dependence in O_2 concentration for the char catalyzed oxidation of NH_3 to NO are shown for comparison. It is seen that the relative importance of R7 (oxidation to N_2) compared to R4 (oxidation to NO) increases. The selectivity for volatile–N oxidation to NO with char as a catalyst, i.e. R4/(R4+R7), decreases from about unity to about 0.6 in this case. At the same time the difference between simulated and measured fuel–N conversion to NO is diminished.

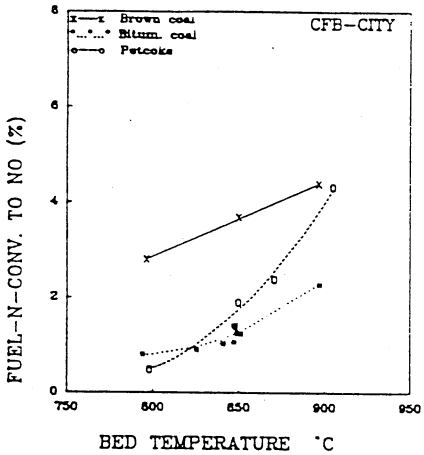

Figure 3. Fuel–nitrogen conversion to NO vs. bed temperature. Primary air ratio = 0.75. Excess air ratio = 1.25.

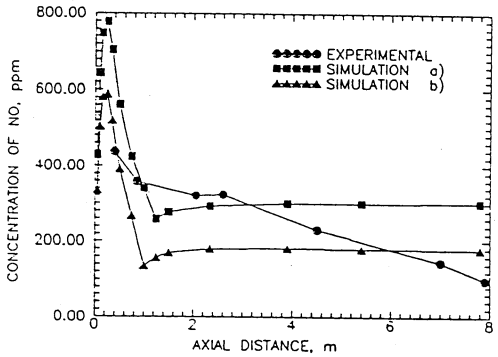

Figure 4.Experimental and simulated NO profile in the bed for bituminous coal combustion. For legend, see Table 4.

Figure 4 shows a comparison of simulated and measured axial NO profiles for bituminous coal. The model fails to predict a decreasing NO concentration in the upper part of the boiler, but the simulated and experimental levels of NO concentration are in good agreement. A possible explanation for the discrepancy is, that the simplified reactor model does not take the stratification in the combustion chamber into account.

For petroleum coke the calculated fuel–N conversion to NO is very high compared to the experimental value. There are of course many possible explanations for this deviation, because there are many assumptions and uncertainties in the model. The most important reason is probably the assumption of uniform NO and CO concentrations in the char particles, where most of the NO reduction takes place. The CO concentration in the bulk phase is relatively low for this fuel, about 1.5 vol% in the dense bed. Detailed modelling of single char particle combustion and simultaneous NO reduction indicates that the CO concentration inside the char particle can exceed the bulk concentration by a factor of 3 to 4, Jensen (1989). This will have the largest impact on the simulation results in the case with petroleum coke, because most of the fuel–N is released as NO in the pores of the char particle for this low volatile fuel. At the same time the measured bulk CO concentration is so low, that an increase of this by a factor of 3 will greatly increase the reduction of

NO by CO catalyzed by char. The result of the simulation with a CO concentration of 5 vol% is much closer to the experimental value.

In general the reduction of NO may be underestimated for several reasons. It was observed that the char looses activity during storage, and the first activity measurements were done about 10 months after sampling. The catalytic reduction of NO by H_2 was not included in the model because of lack of H_2 concentration measurements. The catalytic reduction of NO by NH_3 was not included and the activity of char and bed material is high for this reaction when O_2 is absent, Johnsson (1990). This may be the case in parts of the dense bed, but the NH_3 concentration is predicted to be below 30 vppm in all simulations, and so this reaction is probably of minor importance.The same is true for the homogeneous gas phase reduction of NO by NH_3, which contributes less than 2% to the reduction of NO. This indicates that in general, volatile–N is not beneficial for the reduction of NO, because of the oxidation to NO, which more than outsets the NO reduction.

Conclusions

The simulations show that the heterogenous catalytic reactions for reduction of NO and oxidation of volatile–N, (NH_3) are very important for the fuel–N conversion to NO. The kinetics must be measured for the specific chars and bed materials, because the catalytic activity varies with fuel type. Even if there are still many uncertainties in the kinetics and several assumptions were needed in the reactor model, this approach for modelling the fuel–N conversion leads to a better understanding of the formation and reduction of NO in fluidized bed combustion.

Acknowledgements

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MODELLING OF NO_x FORMATION IN A CIRCULATING FLUIDIZED BED BOILER

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ABSTRACT

A detailed kinetic model for the oxidation of NH_3 and reduction of NO in FBC is used to model the NO concentration profile in an 8 MW CFB. Three different fuels were burned in the full scale tests: Bituminous coal, brown coal and petroleum coke. Kinetics were measured in a laboratory reactor using samples of char and bed material from the boiler. The simulation results show that char is an important catalyst for the oxidation of NH_3 and reduction of NO when burning bituminous coal and petroleum coke. The char content in the brown coal bed is low and very active bed material with a high ash content is the important catalyst in this case. Homogeneous gas phase reactions were found to have only a minor influence. The levels of NO concentration calculated are in agreement with the experimental results. It is concluded that modelling the fuel–N conversion using kinetics measured for the specific chars and bed materials is a considerable step towards a better understanding of the formation and reduction of NO in FBC.

KEYWORDS

Circulating fluidized bed boiler, fluidized bed combustion, NO_x, fuel–N conversion, reduction of NO, mathematical modelling.

INTRODUCTION

The paths of formation and reduction of NO in fluidized bed combustion (FBC) are complex and not fully understood. As a consequense it is often difficult to explain the variation in NO_x emission observed for different operating conditions and different fuel types. A simplified reaction scheme for the conversion of fuel–N in FBC is shown in Fig. 1. The nitrogen content of the fuel is split in char–N and volatile–N and subsequently converted to NO, N_2, N_2O, and NH_3 by a large number of heterogeneous and homogeneous reactions as described by Johnsson (1989). These reactions have been used to explain qualitatively the emissions of NO_x observed in full scale tests by Leckner and Åmand (1987), Åmand and Leckner (1988) and Hirama and coworkers (1987), but modelling of the fuel–N conversion was not possible because of lack of reliable kinetic data. Dutta (1985) did model a pilot scale bubbling fluidized bed using a comprehensive kinetic model. The kinetics of the

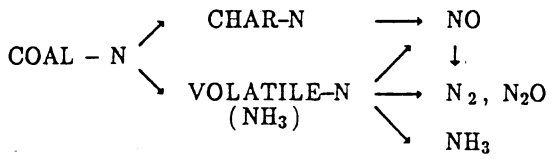

Fig. 1. Principal steps in formation and reduction of NO in FBC.

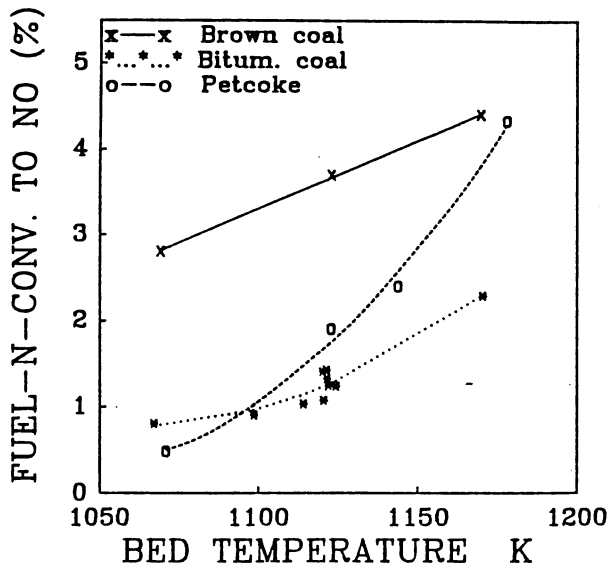

Fig. 2. Fuel–nitrogen conversion to NO vs. bed temperature.

NO–char reaction were found experimentally for the coal. His work identified the important role of char in reduction of NO under fluidized bed combustion conditions. The same was found for NO reduction in the freeboard by Walsh and coworkers (1982).

The aim of this work is to model the formation and reduction of NO in an 8 MW circulating fluidized bed boiler (CFB) burning three different fuels, and to evaluate the relative importance of the many reactions. In order to do this, the kinetics of the heterogeneous catalytic reduction of NO and oxidation of NH_3 on char and bed material has been measured in the laboratory using samples of solids from the boiler.

CFB–TESTS

The CFB boiler used in this study has a thermal power of 8 MW and was built by Götaverken in 1981. The height of the combustion chamber is 8.5 m and the cross section is 1.8 m^2. The fluidizing velocity is normally in the range from 3 to 6 m/s. The fuel is fed with a screw feeder into the lower part of the combustion chamber close to the bottom. Secondary air is introduced through an air register located 1 m above the bottom of the combustion chamber. Silica sand was used as a bed material and no limestone was added during the test program. The three fuels burned were bituminous coal, brown coal and petroleum coke, and so the volatile content varied between 53.1 and 14.3 % maf. The fuel characteristics are listed in Table 1.

TABLE 1 Fuel characteristics

Type	Brown coal	Bituminous coal	Petroleum coke
Volatiles % maf	53.1	35.5	14.3
Proximate analysis %			
Combustibles	80	87	91
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Ultimate analysis % maf			
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O	25.9	8.8	2.7
S	0.8	1.6	2.0
N	0.9	1.7	1.4
Volatile nitrogen % maf	49.0	39.3	25.9

TABLE 2 Experimental values of parameters

Parameter	Brown coal	Bit. coal	Pet. coke
Char content in bed wt%	0.3	7.5	19.5
CO concentration vol%			
at 2.8 m	5.0	3.5	1.2
at 8.5 m	1.1	1.0	0.3
Temperature, top K	1086	1083	1083
Density, top kg/m^3	2.8	2.9	2.6

The primary parameters in the test series were the bed temperature, the excess air ratio and the primary air stoichiometry. A reference case was defined as a run with a bed temperature of around 1120 K, an excess air ratio of around 1.25 and a primary air ratio of 0.75. From these conditions one parameter at a time was varied to lower and higher values, keeping the two others constant. The variation was carried out for all three fuels. Figure 2 shows the result for variation of the temperature. The conversion of fuel–N to NO was extremely low in all tests, and from Fig. 2 it can be seen that the conversion increases for all fuels when the bed temperature is raised, however the bed temperature dependence is different for the different fuels. More details about the full scale tests are published elsewhere, Åmand and Leckner (1990). Measured values of parameters important for the modelling of fuel–N conversion are given in Table 2.

KINETICS AND REACTOR MODEL

A comprehensive kinetic model for the formation and reduction of NO_x in fluidized bed combustion was described and evaluated in Johnsson (1989). Without limestone addition the kinetic model is reduced to six heterogeneous catalytic reactions with char and bed material as catalysts and two homogeneous gas phase reactions as shown in table 3. Kinetic data were obtained in a laboratory fixed bed quartz reactor using samples of char and bed material from the boiler. A detailed description of the kinetic investigations is published elsewhere, Johnsson (1990). The reaction rate expressions are given in Table 3. The kinetics for the homogeneous gas phase reactions were developed from data for Thermal $DeNO_x$, Exxon (1985), and Lyon (1987), corrected for the influence of combustion with data from Duo and coworkers (1989) as described in Johnsson (1990). The kinetics were developed for use in modelling the nitrogen chemistry in fluidized bed combustion in the temperature range 1050 to 1100 K and so they are not generally applicable.

The circulating fluidized bed is treated as a plug flow reactor and the kinetic model includes the nitrogen chemistry. Detailed fluid mechanics, combustion and other parameters of importance for the nitrogen conversion were measured in the boiler and are used as input data in the model. The most important data are: Axial profiles for solids density, temperature and concentrations of char, CO and O_2, boiler configuration, operating conditions (fuel feed rate, air feed rates, flue gas recirculation rates etc.) and fuel composition and volatile nitrogen content.It was assumed that volatile–N is devolatilized as NH_3 and the fraction of volatile–N was set equal to the value measured by standard methods. The remaining fuel–N was assumed to be oxidized to NO during combustion. The release rates for NO and NH_3 were assumed to be proportional to the concentrations of char and oxygen. Intrinsic activity was used for the char catalyzed reactions, because a major part of the NO is formed in the porous structure of the char particle and so the use of an effectiveness factor is not meaningful. The axial concentration profiles for NO and NH_3 in the boiler are calculated using an Euler integration procedure.

RESULTS AND DISCUSSION

The results of simulations for the reference cases with a dense bed temperature of about 1120 K are given in Table 4. The table shows the conversion of NO and NH_3 in each of the reactions calculated as percentage of fuel–N. The calculated total fuel–N conversion to NO is compared to the experimental value from the full scale test. It should be noted that the experimental fuel–N conversion reported in Table 4 is measured at the top of the combustion chamber and so it is higher than the emission values given in Fig. 2, because a considerable reduction of NO takes place in the cyclone.

For bituminous coal most of the fuel–N (99.4%) is first oxidized to NO during combustion of char and catalytic volatile–N oxidation. 12.9% of the fuel–N is emitted as NO, 71.4% is reduced from NO to N_2 by CO with char as a catalyst and 15.4% with bed material as acatalyst. In this case char is a very important catalyst for both volatile–N oxidation and NO reduction. The same is true for petroleum coke. The char plays a minor role in the brown coal bed. This is partly due to the low char content (0.3 wt%) and partly due to the very active bed material when burning brown coal. This material has about 25 times the activity of bed material from burning bituminous coal or petroleum coke for the catalytic reduction of NO by CO, and it is responsible for most of the NO reduction in the brown coal bed. This high activity was explained by the high content of CaO and Fe_2O_3 in the ash and the high ash content in the brown coal bed material, Johnsson (1990).The relative importance of char for the reduction of NO is about the same in the cases of bituminous coal and petroleum coke, even though the char content is about twice as high in the petroleum coke bed. The reason is the lower activity of the petroleum coke char. The conversion of volatile–N is dominated by

TABLE 3 Reactions and kinetics for the reduction of NO and oxidation of NH_3.

No.	Reaction			Catalyst	Reaction Rate
R1	$NO + CO$	$\rightarrow$	$1/2N_2 + CO_2$	char	$-r_{NO}=kC_{NO}^{a}C_{CO}^{b}$
R2	$NO + CO$	$\rightarrow$	$1/2N_2 + CO_2$	bed material	$-r_{NO}=kC_{NO}^{a}C_{CO}^{b}$
R3	$NO + 2/3NH_3$	$\rightarrow$	$5/6N_2 + H_2O$	hom. gas phase	$-r_{NO}=kC_{NO}C_{NH_3}$
R4	$NH_3 + 5/4O_2$	$\rightarrow$	$NO + 3/2H_2O$	char	$r_{NO}=kC_{NH_3}C_{O_2}$
R5	$NH_3 + 5/4O_2$	$\rightarrow$	$NO + 3/2H_2O$	bed material	$r_{NO}=kC_{NH_3}$
R6	$NH_3 + 5/4O_2$	$\rightarrow$	$NO + 3/2H_2O$	hom. gas phase	$r_{NO}=kC_{NH_3}C_{O_2}$
R7	$2NH_3 + 3/2O_2$	$\rightarrow$	$N_2 + 3H_2O$	char	$-r_{NH_3}=kC_{NH_3}$
R8	$2NH_3 + 3/2O_2$	$\rightarrow$	$N_2 + 3H_2O$	bed material	$-r_{NH_3}=kC_{NH_3}$

TABLE 4 The calculated conversion of NO and NH_3 in each reaction and the fuel–N conversion to NO in both cases given as percentage of total fuel–N. R1 to R8 are given in Table 3.

Reaction			Bituminous coal		Brown coal		Petroleum coke	
Type	Catalyst	No	a)	b)	a)	b)	a)	c)
Reduc–	char	R1	71.4	62.8	0.9	0.4	41.7	66.3
tion	bed mat	R2	15.4	13.8	78.1	75.7	7.0	12.1
of NO	–	R3	0.2	1.6	0.4	0.4	0.3	1.3
Oxidation	char	R4	33.8	15.5	5.1	0.1	23.1	12.5
of NH_3	bed mat	R5	0.2	4.8	16.4	18.8	0.07	2.0
to NO	–	R6	0.03	0.4	0.4	0.4	0.01	0.2
Oxidation of	char	R7	0.3	6.9	0.1	0.1	0.2	5.5
NH_3 to N_2	bed mat	R8	0.3	5.6	16.8	19.2	0.08	2.4
Fuel–N								
conver–	simulation		12.9	8.2	3.2	3.1	50.6	11.5
sion	experimental		4.6	4.6	4.4	4.4	4.0	4.0
to NO								

a) Standard simulation
b) The catalytic oxidation of NH_3 to NO is zero order in O_2
c) Like b), but the CO concentration is 5 vol% in the whole bed

reactions with char as a catalyst for these two fuels. This effect may be overestimated in the simulations because of the first order dependence in O_2 concentration for the oxidation of NH_3 to NO. The kinetics could not be measured at O_2 levels above 0.5 vol% because of the fast combustion of the char, and the reaction order may be lower at higher concentrations. Simulations assuming zero order dependence in O_2 concentration for the char catalyzed oxidation of NH_3 to NO are shown for comparison. It is seen that the relative importance of R7 (oxidation to N_2) compared to R4 (oxidation to NO) increases. The selectivity for volatile–N oxidation to NO with char as a catalyst, i.e. R4/(R4+R7), decreases from about unity to about 0.6 in this case. At the same time the difference between simulated and measured fuel–N conversion to NO is diminished.

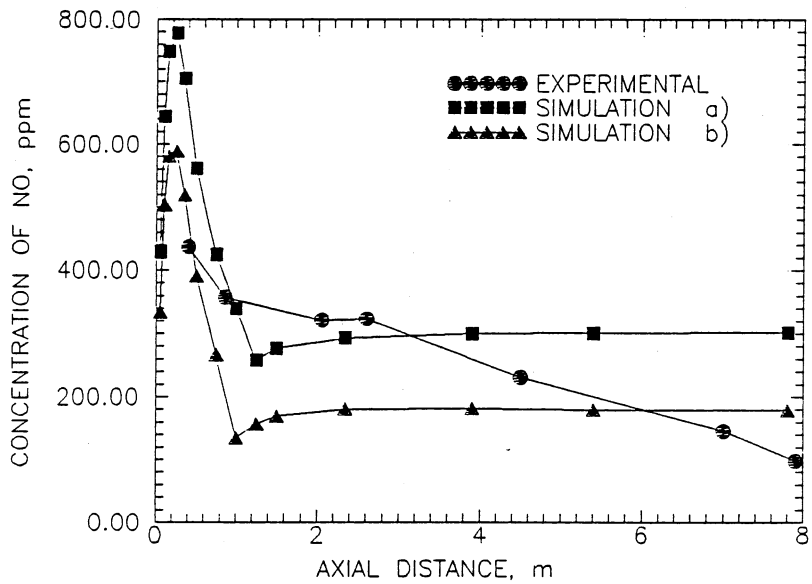

Fig. 3. Experimental and simulated NO profile in the bed for bituminous coal combustion. For legend, see table 4.

Figure 3 shows a comparison of simulated and measured axial NO profiles for bituminous coal. There was no measurement of NO concentration below 0.4 m to compare with the predicted peak in the bottom of the boiler. The simulated and experimental levels are in good agreement, but the model fails to predict a decreasing NO concentration in the upper part of the boiler. A possible explanation for this discrepancy is, that the simplified reactor model does not take the stratification in the combustion chamber into account.

For petroleum coke the calculated fuel–N conversion to NO is very high compared to the experimental value. There are of course many possible explanations for this deviation, because there are many assumptions and uncertainties in the model. The most important reason is probably the assumption of uniform NO and CO concentrations in the char particles, where most of the NO reduction takes place. The CO concentration in the bulk phase is relatively low for this fuel, about 1.5 vol% in the dense bed. Detailed modelling of single char particle combustion and simultaneous NO reduction indicates that the CO concentration inside the char particle can exceed the bulk concentration by a factor of 3 to 4, Jensen (1989). This will have the largest impact on the simulation results in the case with petroleum coke, because most of the fuel–N is released as NO in the pores of the char particle for this low volatile fuel. At the same time the measured bulk CO concentration is so low, that an increase of this by a factor of 3 will greatly increase the reduction of NO by CO catalyzed by char. The result of the simulation with a CO concentration of 5 vol% is much closer to the experimental value.

In general the reduction of NO may be underestimated for several reasons. It was observed that the char loses activity during storage, and the first activity measurements were done about 10 months after sampling. The catalytic reduction of NO by H_2 was not included in the model because of lack of H_2 concentration measurements. The catalytic reduction of NO by NH_3 was not included and the activity of char and bed material is high for this reaction when O_2 is absent, Johnsson (1990). This may be the case in parts of the dense bed, but the NH_3 concentration is predicted to be below 30 vppm in all simulations, and so this reaction is probably of minor importance.The same is true for the homogeneous gas phase reduction of NO by NH_3, which contributes less than 2% to the reduction of NO. This indicates that in general, volatile–N is not beneficial for the reduction of NO, because of the oxidation to NO, which more than outsets the NO reduction.

CONCLUSIONS

The simulations show that the heterogeneous catalytic reactions for reduction of NO and oxidation of volatile–N, (NH_3) are very important for the fuel–N conversion to NO. The kinetics must be measured for the specific chars and bed materials, because the catalytic activity varies with fuel type. Even if there are still many uncertainties in the kinetics and several assumptions were needed in the reactor model, this approach for modelling the fuel–N conversion leads to a better understanding of the formation and reduction of NO in fluidized bed combustion.

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