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INFLUENCE OF COAL COMPOSITION ON THE FATE OF VOLATILE AND CHAR NITROGEN DURING COMBUSTION

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Fifty coals from North America, Europe, Asia, South Africa and Australia were burned in a 21 kW_t refractory-lined tunnel furnace to determine the influence of coal properties on the fate of volatile and char nitrogen. Excess air fuel NO emissions (as determined by combustion in $Ar/O_2/CO_2$) ranged from 415 ppm to 1380 ppm with a premixed burner. These results correlated with total fuel nitrogen, inert pyrolysis HCN yield, and non-volatile nitrogen content, rather than with the geographic origin of the coal.

Minimum staged NO emissions (at optimum first stage stoichiometry) ranged from 140 ppm to 380 ppm. Detailed in-flame measurements indicated that as first stage stoichiometry (air/fuel) was reduced, first stage NO formation decreased, but was ultimately offset by increases in oxidizable gaseous nitrogen species and solid phase nitrogen retention. TFN ($NH_3 + NO + HCN$) generally increased with increasing fuel nitrogen and the species distribution was dependent upon coal rank. In general, HCN was greater than NH_3 with bituminous coals, but less than NH_3 with subbituminous and lignite coals. Second stage TFN conversion to exhaust NO decreased as the TFN distribution was shifted in favor of HCN and NH_3 . Char nitrogen conversion was generally low (less than 20 percent). Exhaust emissions were correlated in terms of the gas phase TFN and the char nitrogen entering the second stage.

Increasing heat extraction generally reduced exhaust NO emissions via a complex mechanism. Reducing second stage flame temperatures had little effect on the concentration and speciation of the XN species leaving the first stage, and on the conversion of solid phase nitrogen in the second stage. However, it dramatically decreased the second-stage conversion of gas phase TFN to exhaust NO. The controlling mechanism appears to be selective NO reduction by NH_i species. The effectiveness of increased heat extraction rate was also found to depend heavily on the coal composition.

Introduction

Conventional, coal-fired power plants may remain the major source of electricity world wide for decades due to uncertain oil supplies and concern over nuclear generating plants. Many countries without adequate domestic supplies are importing coal from North America, Australia, South Africa, and Eastern Europe. Operational expertise with these coals is limited because they represent newly exploited reserves. Additionally, individual power plants may be required to burn a variety of coals due to supply limitations. Consequently, predicting the combustion and pollutant performance of a coal based on comparative laboratory analysis and bench scale tests with a limited sample is important. This paper summarizes a methodology whereby coals can be ranked according to their nitric oxide (NO) production potential.

The development of NO control strategies for coal-fired boilers has received considerable attention over the past decade. Pilot-scale studies¹ established that fuel/air mixing controlled by burner design dictated the formation of NO in pulverized coal flames and that rapid mixing of coal volatiles and air promoted NO formation. Bench-scale and research studies further established the significance of fuel nitrogen oxidation,² the factors controlling fuel nitrogen evolution,^{3,4} and conditions that affect NO formation from pulverized coal under fuel rich conditions.^{5,6} Burner designs have been demonstrated at various scales,^{7,8,9} which are capable of minimizing emissions from field-operating boilers and more advanced combustion control techniques have been proposed which will substantially change state-of-the art boiler designs.¹⁰ However, little information is currently available regarding fuel property effects on these low emissions concepts.

10. 1 K.

Pulverized coal combustion produces nitric oxide by the fixation of molecular nitrogen (thermal NO) and by the oxidation of coal bound nitrogen (fuel NO). Thermal NO formation is extremely temperature dependent; however, flame temperature has only a minor effect on fuel NO formation. The key parameter controlling fuel NO formation from a given coal is gas-phase reactant stoichiometry. Excess oxygen promotes fuel NO formation. Since fuel nitrogen oxidation is the primary NO formation mechanism, the fate of coal nitrogen must be defined to establish the NO emissions potential of different coals.

When a pulverized coal particle is injected into a flame, it decomposes and the fuel-bound nitrogen splits between the char and the volatile fractions. The volatiles are composed of tars and light gases, and the tars further decompose after ejection from the coal particle producing gas phase nitrogen compounds and soot. Char nitrogen is defined as that which is associated with a solid, either as a pyrolysis product of the tars or as the original coal char; gas phase volatile nitrogen is that which is produced from the volatile coal fractions and reacts in the gas phase forming N_2 , NO, HCN, or NH₃.

This study assessed the impact of coal properties on the fate of both char and volatile (fuel-bound) nitrogen under excess air and fuel rich (staged) combustion conditions. A total of 48 coals from 5 continents were burned in a 21 kW_t refractorylined tunnel furnace using air and nitrogen free mixtures as the oxidant. Exhaust and in-flame measurements were made to quantify the influence of coal properties, thermal environment, and stoichiometry on the amount and speciation of volatile and char nitrogen at the exit of the first stage and on the conversion of the fuel nitrogen fragments in the second stage.

Experimental

A complete description of the experimental system and the analytical techniques used in this study is available elsewhere¹¹ and only a brief summary will be presented below.

Furnace System

The investigations were carried out in a 15.2 cm diameter by 2 m long, vertical refractory-lined reactor which consisted of five separate sections and was fired at a rate of 21 kW_t (approximately 5 lbs/ hr coal). The furnace entry diverged from 5.1 cm to the full 15.2 cm diameter in 30.5 cm.

Pulverized coal was supplied pneumatically from a hopper-fed screw feeder to the premixed burner. Premixing was achieved by direct impingement of the coal jets with the main combustion air supply in a premixing chamber. This chamber was separated from the combustion zone by a series of watercooled tubes which prevented flashback. The coal/ air mixture burned in a plug-flow mode with the ignition zone situated in the divergent entry section.

During the staging experiments a refractory choke was inserted to isolate the fuel rich first stage from the second, burnout stage. Second stage air was injected radially immediately after the choke through a ring.

Analytical Methods

Exhaust samples were withdrawn from the reactor stack with a stainless steel, water-jacketed probe and analyzed using standard continuous instrumentation (chemiluminescent NO, paramagnetic O₂, and NDIR CO and CO₂). A water-jacketed probe with an internal water quench spray near the front end was used for extracting in-flame samples.¹¹ Gas phase HCN and NH3 species were collected in a gas washing unit which consisted of an impinger in series with a bubbler containing a fritted glass cylinder. The sample solutions were subsequently analyzed for CN⁻ and dissolved ammonia using specific ion electrodes. A solution of lead carbonate and sodium carbonate was used in both the impinger and the bubbler to remove sulfide ions. The probe and analysis systems were validated by sampling gases of known composition.

Solid samples were withdrawn isokinetically from the combustion zone with a water-spray probe. Their ultimate composition was determined with a Perkin-Elmer 240 B Elemental Analyzer.

Fuels

Table 1 gives the composition information on the 48 coals used in this study. They ranged from anthracite through lignite and were all pulverized so that 65 ± 7 percent of the mass passed through a 200 mesh (74 micron) screen.

Overall Results

Figure 1 shows fuel NO emissions (excess air) from the 48 coals and the minimum NO (staged)

	Fuel analysis							
Symbol	Source	Rank (ASTM-D388)	HHV Btu/lb (as received)	Volatile matter (daf)	% N (daf)	Pyrolysis HCN ppm equiv.	Modified ASTM solid N ppm equiv.	
\otimes	Utah Char		II,185	12.79	1.48			
\mathbf{X}	Coed Char		12,105	9.35	1.95			
D	Hazellon, PA.	Α	13,124	4.93	0.84	43	1267	
¢	Upper Cliff, Ala.	MVB	13,254	23.36	1.63			
Ō	Rosa, Alabama	MVB	13,394	25.60	1.88	642	2272	
0	Black Creek, Ala.	MVB	14,284	30.31	1.88			
\diamond	W. KY.	HVAB	12,082	43.42	1.68			
\triangle	W. VA.	HVAB	12,228	36.23	1.59			
\diamond	Elkay, W. VA.	HVAB	13,115	37,99	1.57			
0	Gauley Eagle, W. VA.	HVAB	10,110	38.41	1.87			
0	Price, Utah	HVBB	12,340	45.11	1.67	1267	1762	
$\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ $	Price, Utah	HVBB	11,877	46.37	1.71			
\oslash	Utah	HVBB	11,718	49.86	1.67			
D	Cadiz, Ohio	HVBB	11,038	44.90	1.32			
Φ	Four Corners, N.M.	HVCB	9,425	50.83	1.65			
∇	Colstrip, MT.	SBB	9,169	44.57	1.57			
0	Hardin, MT.	SBB	8,603	47.25	1.11			
D	Hardin, MT.	SBB	9,339	46.89	1.11	770	1107	
D	Texas	SBC	8,131	54.75	1.31			
\diamond	Scranton, N.D.	LA	6,446	50.14	0.94			
0	Beulah, N.D.	LA	7,245	47.93	1.11			
	Beulah, N.D.	LA	7,245	44.74	1.04	520	1084	
\triangle	Savage, MT.	LA	6,995	48.25	1.08			
\oplus	N.C. Peat	LA	7,703	63.76	1.40			
	Morwell, Australia		10,051	55.73	0.68	752	556	
	Australia	MVB	11,875	30.57	1.81	823	2302	
	Australia	HVAB	12,683	36.44	1.89	1148	1788	
•	Australia	HVAB	12,005	36.40	2.07	742	1878	
•	Canada	LA	6,107	50.65	0.80			
	Canada	SBC	7,488	46.78	1.22	434	1221	
	Canada	SBB	8,356	45.86	1.55	919	1268	
	Canada	HVCB	10,811	40.78	1.07	675	918	
	Blended/US Canada	HVBB	11,882	40.32	1.34			
•	Canada	HVAB	11,862	37.62	1.75			
•	Canada	HVAB	14,000	36.99	1.81			
	Canada	MVB	11,839	24.04	1.15	448	1276	
	Canada	MVB	12,920	24.30	1.19	540	1357	
	Poland	HVBB	10,995	37.93				
+	Russia	HVAB	11,597	35.60	2.46	740	2323	
	Australia	NVBB	11,888	33.41	1.86	874	1895	
	Australia	MVB	11,938	30.60	1.83			
	Australia	MVB	11,661	32.18	1.66			
•	S. Africa	HVBB	11,394	36.59	1.57			
	China	HVBB	12,005	32.49	0.93	564	856	
	Norway	HVAB	13,948	41.77	1.81	614	1543	
▼	England	HVBB	11,719	33.57	1.81			
	W. Germany	MVB	12,622	28.97	1.69			
•	Australia	HVAB	11,725	34.15	1.84	921	1668	

TABLE 1



FIG. 1. NO emissions under excess air and staged combustion conditions as a function of coal nitrogen content.

as a function of the coal nitrogen (dry, ash free). (Open symbols represent American coals.) Fuel NO was defined by burning each coal in a nitrogen free oxidant $(Ar/O_2/CO_2)^{11}$ and air was used as the oxidant in the staged combustion experiments. In both instances, the overall excess oxygen was 5%.

Excess Air

Fuel NO emissions generally increased with increasing fuel nitrogen content. The geographic source of coal had little impact upon fuel NO production; non-U.S. coals behaved similarly to U.S. coals. The highest nitrogen coal tested was Russian (N DAF) which also gave the highest NO emissions. Low rank coals usually contained less nitrogen and produced less fuel NO than high volatile bituminous coals. The North Dakota lignites (\Box, \diamondsuit) contained less than 1.12% nitrogen and gave very low emissions. However, within any rank, properties other than total fuel nitrogen influenced fuel NO. For example, the Savage (Δ) and Beulah (\Box) lignites both contained approximately 1.05% nitrogen, yet their emissions differed by more than 60%. Lowest overall emissions were from Pennsylvania anthracite (\mathcal{D}) ; highest (relative) emissions were from North Carolina peat (Φ) . The anthracite contained virtually no volatile nitrogen whereas the peat nitrogen was all highly volatile. These results suggested that fuel NO formation is highest with fuels which evolve the most reactive volatile nitrogen and lowest when the nitrogen is retained in the solid phase until the char burnout regime.

In an attempt to quantify these effects, Solomon and co-workers¹² determined the reactive volatile nitrogen content of the 19 most diverse coals by pyrolyzing them in vacuum of 1370 K and measuring the HCN yield by FTIR. The tendency of each coal to retain nitrogen in the solid phase was characterized by conducting a standard ASTM proximate analysis and subsequently measuring the nitrogen content of the residual char. These results are contained in Table 1 and a multi-variable regression algorithm yielded the following equation:

$$NO = 318 + 702 [N] + 0.188 [HCN]$$

- 0.347 [non-volatile N]



	4.5		
[N]	4	=	wt. % nitrogen in original
			coal (daf)
[HCN]		=	inert pyrolysis HCN yield,
			ppm equivalent
[non-vol	atile N]	=	modified ASTM solid nitro-
			gen, ppm equivalent

Figure 2 compares the results of the empirical correlation with the experimental measurements. The high correlation coefficient ($r^2 = 0.9$) was encouraging because the fuels tested ranged from the 2.5 nitrogen, high volatile Russian bituminous coal to the 0.68% nitrogen, pre-dried Australian brown coal and included the anthracite. The actual numerical constants in the equation are unimportant; they are clearly a function of the burner system and the time-temperature profile within the furnace. However, the form of the correlation is consistent with the physical understanding. The first two terms represent the mean behavior with respect to total nitrogen content and reflect the decreasing fuel nitrogen conversion with increasing



FIG. 2. Correlation of NO emissions with coal nitrogen content, pyrolysis HCN yield, and nonvolatile nitrogen content.

Staged Combustion

Figure 1 also shows the minimum NO emissions achieved under staged conditions. (All minimums were not achieved at the same first-stage stoichiometry.) In general minimum NO emissions increased with increasing nitrogen content and again depended on factors other than total nitrogen. These data do not correlate directly with volatile and char nitrogen because the controlling processes are extremely complex as will be discussed in the following sections.

Influence of Fuel Properties on Staged Combustion Effectiveness

First Stage Process

Staged combustion minimizes NO emissions because the initial fuel-rich conditions promote the



FIG. 3. Exhaust NO, XN, and Char N as a function of SR_1 .



FIG. 4. TFN partition as a function of coal rank.

formation of N_2 from volatile nitrogen species. Exhaust NO levels depend upon the conversion and level of the reduced nitrogen species and char nitrogen which exit the first stage and experiments were conducted to quantify the relationships between nitrogen species and coal type. The second stage air was added 1.2 m from the burner and the first stage stoichiometry (SR₁) (moles O₂ supplied/moles O₂ required for complete combustion) was varied while maintaining excess oxygen at 5%.

Figure 3 shows typical results for bituminous and lignite coals. As SR_1 was reduced, the exhaust NO decreased, reached a minimum, and then increased. The primary-zone stoichiometry at the minimum exhaust NO and the NO/SR₁ gradient were dependent upon coal characteristics. No minimum in exhaust NO was observed with anthracite or gasification chars. Char-nitrogen concentrations increased with decreasing primary zone stoichiometry. The major gas-phase nitrogen species were NO, NH₃, and HCN (collectively termed TFN; lower levels of N₂O were also observed.¹³ Decreasing SR₁ decreased the NO exiting the first stage,



FIG. 5. Second stage conversion of XN species and Char N.

but ulitmately increased other TFN species. This behavior is analogous to that reported previously for gas and liquid fuel flames.^{14,15} In general, the TFN exiting the first stage increased with increasing coal nitrogen content but TFN did not correlate with inert pyrolysis HCN yield.

Figure 3 also indicates that gas phase nitrogen speciation depends on coal rank. Figure 4 summarizes the partition of TFN as a function of rank at the first stage exit. The fraction of coal nitrogen converted to NH₃ increased with decreasing rank. First stage NO exhibited the reverse trend; decreasing rank decreased NO. In general, HCN concentrations were small. Only the Utah bituminous coal (\bigcirc) produced a significant amount of HCN at $SR_1 = 0.6$. The differences in TFN partition with decreasing rank may be attributed to variations in hydrocarbon volatiles which control local O2 availability and provide a path for CN and ultimately NH, formation from NO,¹⁶ and to increased volatile nitrogen yields which ultimately result in increased NH, concentrations.

Second Stage Processes

The second stage of a staged-combustion system is analogous to an excess air flame burning partial oxidation-products produced in the first stage. The ultimate NO yield depends upon the TFN and char nitrogen conversion. Figure 5 presents results obtained to assess the conversion of gaseous and char nitrogen species to NO in the second stage flame. Tests were conducted (Figure 5a) with C₃H₈/NH₃ and C₃H₈/NO flames in the first stage (no solid phase present. First stage residence time = 1.0 sec @ $SR_1 = 0.6$, 1.41 wt % N in fuel, 70,000 Btu/ hr.) The percent TFN conversion in the second stage was computed based upon detailed species measurements at the first stage exit and in the exhaust. When NO was the dominant TFN species $(SR_1 > 0.75)$, the second stage conversion (retention) of TFN to NO was very high (approximately 90%) and relatively insensitive to total TFN level. Under these conditions, only limited heat release in the second stage occurred and the second stage "fuel" was primarily CO. As SR₁ was reduced further and the dominant TFN species became NH₃ and HCN, the second stage conversion decreased dramatically and was inversely dependent on the TFN level. Figure 5a also shows data on second stage TFN conversions in Char/C₃H₈/NH₃ flames. Similar trends were observed; the solid phase had relatively little effect on TFN conversion in the second stage.

Second stage char nitrogen conversion to NO was defined by burning COED char/ C_3H_8 in a nitrogen free oxidant. This system provided a second stage reactant stream with minimal TFN species. Figure 5b shows the calculated conversion data based on the TFN and exhaust NO. (The error bars are uncertainty due to limited TFN conversion.) Char nitrogen conversion to NO in the second stage was 20% or less and it increased slightly with decreasing SR₁. A multi-variable non-linear regression was used to calculate exhaust NO concentrations with the amount and speciation of the TFN and char nitrogen entering the second stage. The resulting correlation was:

$$NO_{EX} = 0.87*SR*(NO) + \frac{0.67}{1 + 0.004(HCN + NH_3)} (HCN + NH_3) + 0.27(1 - SR)^{1/2}(Char N)$$
(2)

and the overall correlation coefficient (r^2) was 0.9 based on 26 data sets.

Practical Implications

Minimum exhaust NO data (Figure 1) emphasized the importance of coal characteristics: the



FIG. 6. Predicted conversion of XN and Char N to NO.

Norway (\blacktriangle) and Alabama (\square) bituminous coals both contain approximately 1.85% N (DAF) but their minimum NO emissions differed by 45%. The previous discussions have indicated that coal properties influence staged combustion effectiveness by altering:

- The partition of nitrogen between the volatile and char phases. Nitrogen remaining in the char during the first, fuel rich stage reduces the TFN available for N₂ formation. Since char nitrogen conversion is non-negligible, as the TFN tends to zero, it sets a limit on minimum achievable exhaust NO.
- Gas Phase Speciation. Second stage processing of TFN is species dependent: high levels of NO are undesirable because a large fraction is retained through the second stage flame.

Figure 6 summarizes the relative contribution of each nitrogen component (leaving the first-stage) to exhaust NO emissions. These results were derived by using the correlation (Equation 2) and the internal measurements for the Alabama and Norway coals. Norway coal has a lower minimum NO because the first-stage NO is low due to high volatilehydrocarbon evolution and because less char nitrogen is available in the second stage. At SR₁ = 0.6, char nitrogen produced 200 ppm NO with Alabama and 115 ppm with Norway. Thus, staged combustion technologies will be least effective with coals which strongly retain their nitrogen in the solid phase.

Role of Thermal Environment

Controlling Mechanisms

Increasing primary zone temperature should reduce exhaust NO because it:



FIG. 7. The impact of first stage heat removal.



FIG. 8. Influence of cooling on second-stage TFN conversion.

- Accelerates the rate of TFN decay, and
- Reduces the amount of char nitrogen.

However, unlike liquid fuels¹⁵ when heat is extracted from the primary zone of a staged coal flame, exhaust emissions decrease rather than increase (Figure 7). These data are in agreement with the observations of Johnson, et al.¹⁰ The detailed internal measurements shown in Figure 7 indicate that decreasing the first stage exit temperature ca. 200 K (by inserting a water cooling coil in the first stage) had little effect on the amount and speciation of the TFN or char nitrogen. Additional studies with COED char/C₃H₈ flames burning in Ar/O₂ indicated that heat extraction rate also had little effect on the oxidation of solid nitrogen in the second stage flame. Therefore, reducing the second stage flame temperature must have decreased TFN conversion.

Figure 8 shows the results of an experimental series where NO or NH_3 was injected into the second stage flame (with the staging air) to define the influence of cooling on second stage TFN conversion. When the added fuel N was NO (\bigcirc), thermal environment had essentially no effect on the conversion (retention) in the second stage flame; however, when NH_3 was added (\triangle) cooling signifi-



FIG. 9. The impact of cooling for low rank coals.



FIG. 10. The impact of cooling for high volatile bituminous coals.

cantly decreased TFN conversion. Thus, the reduction in exhaust NO emissions with increased heat extraction appears to be due to the reduction of NO by NH_i in the second stage flame. The composition and thermal conditions (cooled = 1150 K at the second stage inlet) are essentially analogous to those defined by Lyon¹⁷ for external "De-No_x."

Coupling with Fuel Chemistry

Figure 9 shows the influence of heat extraction rate on the Canadian lignite coal. These data (typical of low rank coals) show that increasing heat extraction only reduced exhaust NO at high stoichiometries (SR₁ > 0.7). Figure 9 also presents detailed in-flame measurements. Increased cooling had little effect on TFN; however, at rich conditions (SR₁ < 0.7) it increased the carry over of solid nitrogen. Thus, decreased emission associated with a reduced gas phase conversion was somewhat mitigated by an increased contribution from char nitrogen. Figure 10 shows typical results for a high volatile bituminous coal. At high stoichiometric ratios (SR₁ > 0.7) reducing first stage temperature increased first stage NO. Thus, there was essentially no effect of decreasing temperature on exhaust NO at $SR_1 > 0.7$ because of a decrease in the first stage NO decay rate and the low NH₃ concentrations.

Conclusions

The results of this investigation with fifty coals from five continents indicate that rank and nitrogen content are more significant than geographic origin of the coal. Excess air, fuel NO emissions varied from 415 ppm (0.84% N anthracite) to 1380 ppm (2.46% N HVA bituminous) and correlate with total fuel nitrogen, inert pyrolysis HCN yield, and non-volatile nitrogen content.

Minimum staged NO emissions ranged from 140 ppm (0.68% N brown coal) to 380 ppm (1.88% N MV bituminous). As first stage stoichiometry is reduced, first stage NO formation decreases, but other oxidizable gaseous nitrogen species increase as does solid phase nitrogen retention. TFN (NO + NH₃ + HCN) generally increases with increasing fuel nitrogen.

The distribution of TFN species depends heavily on coal composition. Low volatile fuels form essentially no NH₃ or HCN. First stage NO percentage decreases significantly with decreasing coal rank from bituminous to lignite. Conversely, the relative importance of NH₃ grows with decreasing coal rank. In general, HCN is greater than NH₃ with bituminous coals, but less than NH₃ with subbituminous and lignite coals.

Second stage TFN conversion decreases as the TFN distribution shifts in favor of HCN and NH_3 (and as the hydrocarbon content of the second stage reactants increases¹¹). Second stage char nitrogen conversion to NO is low (less than 20%) and inversely proportional to SR_1 . Exhaust emissions can be correlated with gas phase TFN and char nitrogen.

Increasing heat extraction generally reduces exhaust NO by dramatically decreasing gas phase TFN conversion to NO. If the second stage reactants are cooled to approximately 1150 K, it is possible to enhance the reduction of NO (probably by NH_i species) in the second stage flame. However, the concept's effectiveness depends on the combustor design and fuel chemistry. Increasing heat extraction appears most favorable with low rank coals, because they produce large amounts of NH_3 and relatively less first stage NO. It should be noted that heat extraction from the primary zone can introduce practical problems because of reduced carbon burnout.

Nomenclature

Char N	Nitrogen remaining in the solid at any point in the combustion process, usu- ally the first stage (rich zone) evit
det	dry ash from
uai	uly, ash nee
Fuel NO	NO formed from fuel nitro-
	gen as defined by AR/O ₂ /
	CO ₂ replacement experi-
	ments
Non-volatile N	Nitrogen remaining in the
	solid phase after the ASTM
	proximate (volatile) deter-
	mination at 1373 K

Stoichiometric Ratio	Moles of O ₂ supplied/moles
	O ₂ required for complete
	combustion
SR ₁	Stoichiometric ratio in the
•	first (fuel rich) stage
TFN	Total fixed nitrogen species
	$(NO + NH_3 + HCN)$ (gas
	phase)
Thermal NO	Difference between emis-
	sions with air (total NO)
	and emissions with $Ar/O_2/$
	CO ₂
XN	A reactive, gas-phase, nitro-
	geneous species (e.g.,
	HCN, NH _i , etc.)

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