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NITROGEN OXIDE EMISSIONS FROM COAL FIRED MHD PLANTS

TOPICAL REPORT

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TABLE OF CONTENTS

	PAGE
ABSTRACT.....	vi
CHAPTER 1 GENERAL NATURE OF NO _x EMISSIONS	
1.0 INTRODUCTION.....	1
1.1 The MHD-Steam Combined Cycle Power Plant.....	1
1.2 General Nature of the Nitrogen Oxide Problem.....	1
CHAPTER 2 THE NO _x EXPERIMENTS	
2.1 The Low Mass Flow (LMF) Train.....	11
2.2 Measurement Methodology.....	12
2.3 NO _x Sampling Locations.....	12
2.3.1 The LMF0 Test.....	12
2.3.2 LMF1 Tests.....	12
2.3.3 LMF 2 & 4 Tests.....	20
2.3.4 LMF5 Tests.....	20
CHAPTER 3 NUMERICAL MODELING OF NITROGEN OXIDE DECOMPOSITION	
.....	25
CHAPTER 4 NITROGEN OXIDE EMISSION ISSUES FOR PLANT DESIGN	
4.1 Parametric Studies.....	34
4.2 Minimization Study.....	40
4.3 Multi-Dimensional Modeling.....	40
5.0 Conclusions.....	40
REFERENCES.....	43

LIST OF FIGURES

	PAGE
1.1-1	Schematic of MHD/Steam Power Plant.....2
1.2-1	Combustor Temperature vs. Oxidant Ratio.....3
1.2-2	Combustor NO _x vs. Oxidant Ratio.....4
1.2-3	NO _x at Radiant Boiler Exit vs. Oxidant Ratio.....5
1.2-4	Combustor Plasma Conductivity vs. Oxidant Ratio.....7
1.2-5	Conductivity at Channel Entrance vs. Oxidant Ratio.....8
1.2-6	Overall Efficiency vs. Primary Stoichiometry.....9
1.2-7	NO _x at Cyclone Exit vs. Oxidant Ratio.....10
2.3.1-1	LMF-O Test Train Configuration.....13
2.3.1-2	NO _x in Radiant Furnace vs. Mass Flow.....14
2.3.1-3	NO _x at Stack vs. Mass Flow Rate.....15
2.3.2-1	Summary of Gas Analysis Operation in LMF1.....16
2.3.2-2	Stoichiometry NO vs. Stoichiometry.....17
3.2.3	NO ₂ and N ₂ O (Equivalent) Levels at Radiant Furnace Inlet.....19
2.3.3-1	Gas Analysis Instrumentation Locations for the LMF3 Series.....21
2.3.3-2	LMF4 Test Train Configuration.....22
2.3.4-1	CFFF NO _x Data.....24
3.1	Calculated and Experimental NO Levels in CFFF Flow Train.....30
3.2	Calculated and Experimental NO Levels in the CFFF Flow Train.....31
3.3	Calculated and Experimental NO Levels in the CFFF Flow Train.....32
4.1-1	Parametric Study, NO _x Emissions.....37
4.1-2	Parametric Study, NO _x Emissions.....38

4.1-3	Parametric Study, NO _x Emissions.....	39
4.2-1	Effects of Cooling Rate and SCI Temperature on NO _x Emissions.....	41
4.3-1	Spatial Character of Computed CFFF Radiant Furnace NO Decomposition.....	42

LIST OF TABLES

	PAGE
2.1-1	CFFF LMF TEST TRAIN CONFIGURATIONS.....11
2.3.2-1	GAS ANALYSIS - LMF1-C TESTS.....18
3.1	KINETIC REACTION DATA.....26
4.1-1	PARAMETRIC STUDY OF EXIT COOLING RATES IN THE RADIANT FURNACE ON NO _x EMISSIONS.....36

FOREWORD

This report is a compilation of relevant reports and technical papers previously published. Most of this work, especially the calculational work was performed by the late Professor Lloyd W. Crawford and is hereby so acknowledged. Portions of the text and many of the illustrations are extracted and quoted from the referenced works of Dr. Crawford.

The reader is also referred to a topical thesis report by Mr. Xiaoliang Lu which was supervised by Dr. Crawford and contains both the experimental and modeling treatment of NO_x for a single MHD POC Test, LMF5-J. That report is "Parameters Affecting Nitrogen Oxides in a Coal-Fired Flow Facility System", DOE/PC/95231-3, dated March 1996.

ABSTRACT

In this topical report, the nitrogen oxide emission issues from a coal fired MHD steam combined cycle power plant are summarized, both from an experimental and theoretical/calculational viewpoint. The concept of staging the coal combustion to minimize NO_x is described. The impact of NO_x control design choices on electrical conductivity and overall plant efficiency are described. The results of the NO_x measurements in over 3,000 hours of coal fired testing are summarized. A chemical kinetics model that was used to model the NO_x decomposition is described. Finally, optimum design choices for a low NO_x plant are discussed and it is shown that the MHD Steam Coal Fired Combined Cycle Power Plant can be designed to operate with NO_x emissions less than 0.05 lbm/MMBTU.

CHAPTER 1

GENERAL NATURE OF NO_x EMISSIONS

1.0 INTRODUCTION

1.1 The MHD-Steam Combined Cycle Power Plant

The prototypical application of MHD to central power generation is in a combined cycle with an MHD generator topping cycle and a steam bottoming cycle. The generic concept for this type plant is shown in Figure 1.1-1.¹ The coal is burned at high temperature (around 2900K or 4760°F) with a potassium seed to produce an electrically conducting gas that is needed for efficient MHD power generation. Once the gases cool to the level where equilibrium ionization is too low for efficient MHD power generation (around 2200K, 3500°F), they are exhausted to a furnace through a diffuser for use in generation of additional power via a steam Rankine cycle. The topping and bottoming cycles are inter-related in a number of ways, of course, including heating air for the primary combustor, integration of topping cycle cooling water into the steam circuit, extraction of energy for coal drying, extraction of steam for compressor drives and extraction of steam for drying regenerated potassium seed.

1.2 General Nature of the Nitrogen Oxide Problem

The MHD primary combustor operates at higher temperature than other existing and proposed coal fired power plants. Since the formation of nitrogen oxides is known to be higher at higher temperatures, this was considered a substantial problem for the development of environmentally acceptable MHD power plant technology. Figure 1.2-1 shows the typical MHD combustion temperatures as a function of stoichiometry. Stoichiometry is defined in this report as the ratio of the amount of oxygen present to the theoretical amount required for complete oxidation of the fuel reactants. As expected, the temperatures peak at fuel rich conditions, stoichiometry about 90%. The level of nitrogen oxides formed (actually almost exclusively NO in the fuel rich condition) is shown in Figure 1.2-2. Note that the amount of NO_x formed is not a strong function of pressure, but is a strong function of stoichiometry. NO_x emission standards in the United States are specified in lbm/million Btu at the exhaust stack. The weight of emitted NO_x is based on the fact that NO is further oxidized to NO₂ when the combustion is completed. The New Source Performance Standards (NSPS) level that was in effect for many years was 0.6 lbm/MMBTU. (There is currently a new standard that lowers this to 0.5 or 0.45 lbm/MMBTU as dictated by the Clean Air Act Amendments of 1990). The 0.6 lbm/MMBTU corresponds to about 600 ppm versus the up to 12,000 ppm formed in the primary combustor. The NO_x control concept developed to solve this problem involves burning the primary combustor fuel rich, allowing the NO_x to decompose in a radiant furnace as the gas cools and performing the secondary combustion at a temperature and in such a way that little additional NO_x is formed. This is the concept that was developed and proven for use in the design of the Low Mass Flow Train in the DOE Coal Fired Flow Facility (CFFF).

Figure 1.2-3 shows the calculated equilibrium NO_x at the radiant furnace outlet as a function of primary stoichiometry for various secondary combustor gas inlet temperatures. Note the strong dependence on primary stoichiometry and gas temperature entering the secondary combustor, but that very low values seem possible with design control of these

MagnetoHydroDynamics

Electric Power Plant

Schematic of MHD/Steam Power Plant

FIGURE 1.1-1

Figure 1.2-1 Combustor Temperature versus Oxidant Ratio. Air Preheated to 1800 K. Illinois #6 Coal Dried to 2 Percent Moisture. One Percent of Coal HHV Lost from Combustor.

Figure 1.2-2 Combustor NO_x Versus Oxidant Ratio.

Figure 1.2-3 NO_x at Radiant Boiler Exit Versus Oxidant Ratio. P = 1.2 atm

variables. A critical issue related to these design choices is how they affect the performance of the plant. One of the principal needs for the topping cycle performance is electrical conductivity of the gas in the MHD generator. The effect of primary stoichiometry on conductivity is shown in Figure 1.2-4 for the primary combustor and in Figure 1.2-5 for the MHD generator entrance, assuming an isentropic expansion to Mach No. 0.9. These calculations show that operation at stoichiometries around 0.85 would be optimum for electrical conductivity and are very favorable for NO_x control. However, there is a performance issue in choosing this stoichiometry since a lower value implies a lower mass flow and thermal input to the more efficient topping cycle and a higher input to the less efficient steam bottoming cycle. Thus, lower stoichiometries tend to reduce overall plant efficiencies. This was studied³ and Figure 1.2-6 shows the overall plant efficiency variation as a function of primary stoichiometry. Capital costs increase with increasing stoichiometry, however, and the most economical design point depends on the fuel price. The study concluded that the stoichiometry should be chosen primarily to meet the NO_x emission criterion.

Prior to finalizing the design of the LMF furnace and secondary combustor, NO_x measurements were made in the UTSI laboratory (the Cell III apparatus that was used to develop the design data for the steam bottoming plant simulator) as a function of stoichiometry. The data are shown in Figure 1.2-7⁴ and generally confirm the nature of the equilibrium calculations of Figure 1.2-3 although there was insufficient residence time in this test cell to approach equilibrium at the higher stoichiometries. Pepper⁵ also found primary stoichiometry in the upper 80% range was most economical and reduced NO_x , but he was advised to use a higher primary stoichiometry to reduce corrosion in the radiant furnace. The UTSI design used studded, refractory covered walls to eliminate this corrosion problem.

Figure 1.2-4 Combustor Plasma Conductivity Versus Oxidant Ratio. Air Preheated to 1800K. Illinois #6 Coal Dried to 2 Percent Moisture. One Percent of Coal HHV Lost from Combustor.

Figure 1.2-5 Conductivity at Channel Entrance Versus Oxidant Ratio.
Entrance Mach No. = .9, $\gamma = 1.18$.

Figure 1.2-6 Overall Efficiency vs. Primary Stoichiometry 36% Oxygen Enrichment by Volume (1000 MWe)

Figure 1.2-7 NO_x at Cyclone Exit Vs. Oxidant Ratio

CHAPTER 2

THE NO_x EXPERIMENTS

2.0 The Experimental Apparatus

2.1 The Low Mass Flow (LMF) Train

The LMF flow train was originally conceived and proposed as a simulation of the Coal Fired MHD Steam Power Plant concept. The Low Mass Flow designation was to distinguish the size at a nominal 20 MW_t as opposed to the planned High Mass Flow (HMF) train which was to be at a nominal 50 MW_t thermal input. The LMF test train was installed in Bay 1 and the HMF train was to be in Bay 2 of the CFFF test building. The HMF was never built at the CFFF although the superconducting magnet was completed and remains in storage at Argonne National Laboratory. In addition, the primary emphasis for the CFFF test program was shifted to the steam bottoming plant development in 1982 when the MHD development program was reduced in size.

The LMF flow train was fabricated and erected in stages as indicated in Table 2.1-1. The design philosophy for NO_x control was to burn sub-stoichiometrically in the primary combustor and design the radiant furnace to have sufficient heat transfer to cool the gas and sufficient residence time for the NO to decompose to near equilibrium at the reduced temperature.

TABLE 2.1-1
CFFF LMF TEST TRAIN CONFIGURATIONS

Test Configurations

COMPONENT	LMF0	LMF1	LMF2	LMF3	LMF4	LMF5
Vitiation Heater	X	X	X	X	X	X
Coal Combustor	X	X	X	X	X	X
Nozzle	X	X	X	X	X	X
MHD Generator*	- -	- -	X	- -	X	- -
Diagnostic Channel*	- -	X	- -	- -	- -	- -
Replacement Channel*	X	X	X	X	X	X
Diffuser	X	X	X	X	X	X
Radiant Slagging Furnace	X	X	X	X	X	X
Secondary Combustor	X	X	X	X	X	X
ITAH Materials Test Module	- -	X	- -	- -	- -	- -
Superheater Test Module	- -	- -	X	X	X	X
Dry ESP	- -	- -	- -	- -	X	X
Wet ESP	- -	- -	- -	- -	- -	X
Baghouse	- -	- -	- -	X	X	X

*MHD Generator, Diagnostic Channel and Aerodynamic Replacement duct were used interchangeably.

2.2 Measurement Methodology

NO_x measurements were made by inserting a probe into the gas stream and inducting a sample. The probe must be water cooled in most locations due to the high gas temperature. The extracted sample is cooled by the water cooled probe to quench the chemical reactions. It is then filtered to remove particulate from the sample. Next the gases enter a sample conditioner which provides additional particulate removal, acid gas removal and a dryer to remove water vapor. The sample is then applied to a commercial NO/NO_x meter such as a Thermo Electron Model 10AR. The equipment to extract and process the sample was improved with experience over time as the testing progressed and modified for the specific location to optimize its performance. Detailed descriptions of this equipment and its operation are contained in Reference 6-7.

2.3 NO_x Sampling Locations

2.3.1 The LMF0 Test

LMF0 sampling locations are shown on Figure 2.3.1-1⁶. The sample locations as shown on the Figure are T225:Radiant Furnace, T273:Secondary Combustor Inlet, T315:Secondary Combustor Outlet and the Stack. Typical results from these early tests are shown in Figures 2.3.1-2 and 2.3.1-3. Note that these results confirm that lower stoichiometry produces lower NO_x levels both at the radiant furnace and at the stack. The lower NO_x with N/O ratio and with increased mass flow are indicative of the fact that higher temperatures produce more NO decomposition, even at the radiant furnace sampling location. These early tests were conducted with a slag screen in the radiant furnace, installed so that the diffuser exhaust impinged on it and flowed down past the slag screen, then back up in the radiant furnace. The result of this circuitous route through the lower furnace was a large temperature drop and a large decay in the NO concentration in the gas. (This effect led the DOE on-site representative to describe the slag screen as a "NO_x disintegrator" during these early tests). Note, however, in Figure 2.3.1-3 that the stack NO_x values are high due to this rapid cooling in the lower radiant furnace plus the water quench immediately following the secondary combustor.

2.3.2 LMF1 Tests

The LMF1-A&C sampling locations are shown in Figure 2.3.2-1.⁷ This test series had as a major objective the characterization of NO_x emissions. A total of eight NO_x sampling locations were used for these tests, including a sample port in the diffuser outlet and in the lower radiant furnace.

During this test series, systematic variations were made in primary stoichiometry, nitrogen-to-oxygen ratio and thermal input. Only the stoichiometry presents a clear "cause and effect" relationship with NO_x and even that also has some impact on gas temperature. A scatter plot showing much of the test data from the stack port versus stoichiometry as shown in Figure 2.3.2-2 perhaps best illustrates the relationship. Table 2.3.2-1 gives representative NO_x test data for each of the sample ports for the various conditions cited. Figure 2.3.2-3 shows this data for the radiant furnace inlet and the secondary combustor outlet for a number of different conditions. From this plot, one can see clearly the more rapid decomposition of NO in the fuel rich zone with lower stoichiometry.

LMF-O TEST TRAIN CONFIGURATION

Figure 2.3.1-1

Figure 2.3.1-2

Figure 2.3.1-3

Measurement	Location / Nomenclature							
	1/DF5	2/RF0	3/RF1	4/RF2	5/RF3	6/SCI	7/SCO	8/STK
NO / NO _x	X	X	X	X	X	X	X	X
CO			X			X	X	X
CO ₂							X	X
O ₂							X	X
SO ₂							X	X
GC*			X					

* At the end of the test series, the Gas Chromatograph was set up to measure H₂, CO, CO₂, CH₄, O₂, and N₂; CO and CH₄ were not measured in early tests.

Figure 2.3.2-1 Summary of Gas Analysis Operation in LMF1

Figure 2.3.2-2

TABLE 2.3.2-1

GAS ANALYSIS - LMF1-C TESTS

***** GAS ANALYSIS *****												
	THERMAL	STOICH. %		N2/O2	***** NO, ppm *****							NO _x , ppm
	INPUT	AVG. RANGE		Wt.	***** NO, ppm *****							SCO
	MW				DF5	RFO	RF1	RF2	RF3	SCI		STK
LMF1-C1												
STEP												
5	23.2	84.5	74/91	0.4	---	---	---	173	---	---	109	---
6	23.2	84.8	79/92	0.7	---	---	236	208	---	---	101	---
LMF1-C2												
STEP												
5	23.2	78.0	66/99	0.4	1490	---	---	---	---	416	113	118
6	23.2	79.0	67/89	0.4	1460	---	---	---	---	---	118	---
LMF1-C3												
STEP												
5	23.2	82.9	79/90	0.4	3885	548	258	---	---	---	146	---
6	23.2	92.6	89/96	0.4	7165	2195	965	---	---	---	709	---
7	23.2	92.0	89/96	0.7	7326	---	1358	---	---	---	---	---
8	23.2	89.4	83/93	1.0	---	2269	1519	---	876	---	856	---
9	23.2	83.2	80/87	1.0	4138	703	505	---	---	---	148	---
LMF1-C4												
STEP												
5	23.2	83.5	81/87	1.0	5070	1437	1114	635	---	---	195	177
6	23.2	93.6	87/95	1.0	7568	2528	2273	1665	1273	---	1087	925
7	27.9	85.5	80/114	0.7	2172	889	---	427	---	---	145	166
8	27.9	94.6	90/111	0.7	4747	4317	2859	2226	2072	---	2049	1920
LMF1-C5(1)												
STEP												
5	15.5	86.1	80/100	0.4	3329	---	---	1401	---	1218	677	424
6	15.8	84.0	78/97	0.4	3270	522	249	---	---	---	176	127
7	23.0	93.9	89/99	0.7	7395	---	2430	1950	1993	1871	1994	---
8	23.2	91.7	87/116	0.4	5587	1281	788	561	---	---	403	---
LMF1-C6(1)												
STEP												
4A	27.9	87.0	83/91	0.5	6179	---	---	1429	299	262	237	---
4B	27.9	83.0	81/85	0.5	---	---	---	740	78	---	118	76
5A	27.9	80.1	78/81	0.7	---	275	---	253	---	---	95	60
5B	27.9	77.6	75/81	0.7	---	338	---	167	---	---	96	59
6A	27.9	95.8	94/98	0.5	6909	2490	---	2144	1588	---	1011	663
6B	27.9	90.5	88/92	0.5	4848	1166	---	887	435	530	373	257
7	27.9	87.1	77/84	0.7	3051	874	---	622	96	97	138	85
8	27.9	81.7	77/84	1.0	1821	710	---	281	---	---	109	56
9	27.9	94.6	92/97	0.7	5066	3180	---	---	1629	---	1605	765
10	27.9	87.5	86/89	1.0	3793	1372	---	597	244	---	269	124
11	27.9	93.3	92/94	1.0	9386	5837	4500+	4068	4932	---	3472	3160
12	23.2	82.6	80/85	1.5	2888	1115	---	420	---	---	162	84
14	23.2	82.3	80/106	0.4	2999	447	194	160	---	---	127	62

(1) STACK NO_x VALUES LOW DUE TO AIR LEAK.

CFFF TEST LMF1C NO_x DATA

Figure 3.2-3 NO₂ and N₂O (Equivalent) Levels at Radiant Furnace Inlet and Secondary Combustor Outlet Probes vs. Primary Stoichiometry.

Because it is not feasible to change the furnace size and heat transfer characteristics to simulate everything about a commercial size plant, it was rapidly concluded that the value of this test series lies primarily in calibrating a computational model for NO_x decomposition.

The variables that affect NO_x control are the fuel, oxidant, gas temperature (especially that entering the radiant furnace), gas cooling rate in the furnace, temperature at which secondary combustion is completed, primary stoichiometry and the secondary combustion stoichiometry (overall stoichiometry). These issues are treated by use of the validated chemical kinetic model as described in the next section on modeling.

The probe used in the LMF diffuser was subject to high heat flux conditions. It was installed in a gas at high velocity and at temperatures in the 2200-2400K (3500°F to 3860°F) range. As a result, some burnouts occurred during testing. In later tests, this measurement was normally not made because it jeopardized the reliability of tests with other primary objectives. It was also learned that within this high temperature range and at stoichiometries around 85%, the final NO_x emission was almost independent of the diffuser NO_x level. This is not true, of course, for lower temperatures or higher stoichiometries.

Another problem experienced with extractive gas sampling in the high temperature zones was continued chemical reaction in the probe. That is, it was not possible to cool the gas rapidly enough to freeze the NO decomposition immediately upon the gas entering the probe for very high temperatures. A study⁸ of this effect showed that readings from the diffuser may be low by as much as 30% due to this effect.

2.3.3 LMF2 & 4 Tests

The LMF2 test was conducted as a special configuration (including the 45° DCW MHD generator and the 3.2 Tesla magnet) of the LMF4 test series. The LMF3 test series was the first configuration that included the Superheater Test Module (SHTM). Components past the secondary combustor had little effect on the NO_x emissions so this and the later LMF4 series was largely a repeat of LMF1 tests insofar as NO_x emissions are concerned. The variations in primary stoichiometry, thermal input and N/O were repeated for all configurations, however. The NO_x sampling ports for LMF3 are shown in Figure 2.3.3-1 and for early LMF4 in Figure 2.3.3-2. Later LMF4 tests used a redesigned SHTM, but there was negligible effects on NO_x emissions.

2.3.4 LMF5 Tests

The LMF5 tests included NO_x sampling ports identical to the later LMF4, but the fuel used was Montana Rosebud Coal. There were two major impacts on the NO_x emission levels, however. One relevant difference was that there was more heat loss to the walls in the upstream portion of the test train (combustor, nozzle, aerodynamic replacement duct and diffuser), which led to about 100K (180°F) lower temperatures entering the radiant furnace. This difference in heat loss was attributed to the lower viscosity of the slag in the Western coal, thus a thinner slag layer on the walls. The other significant difference is that the Western coal has a sulfur content around 1% whereas the Eastern Coal (Illinois No. 6 Seam) typically had around 3% sulfur. This is due to the reactions for decomposition of NO that utilize sulfur. This is

Figure 2.3.3-1 Gas Analysis Instrumentation Locations for the LMF3 Series

IL-0108 2/96

LMF4 Test Train Configuration

Figure 2.3.3-2 LMF4 Test Train Configuration

discussed more fully in Chapter 3, Modeling. Figure 2.3.4-1 provides an aggregate view of the difference between Western and Eastern coal NO_x emissions. Note that in the LMF5-B test, sulfur was added to the Western coal and the NO_x emissions were similar to that of the high sulfur Eastern coal.

NO_x vs Primary Stoichiometry

Figure 2.3.4-1 CFFF NO_x Data

CHAPTER 3

NUMERICAL MODELING OF NITROGEN OXIDE DECOMPOSITION

Chemical kinetic calculations have been carried out on the homogeneous reactions occurring in the radiant furnace. The calculations are performed from the CFFF diffuser exit through the upward pass of the radiant furnace into the secondary combustor. The computer program used has been adapted (most modifications involving input-output operations) from the "Premixed One-Dimensional Flame" (PROF) code developed for EPA.¹¹ In the chemical kinetics calculations for the radiant furnace, the particular PROF option used has been that involving specification of an inlet composition together with temperature and pressure as a function of time. The time-temperature-pressure data are obtained from a furnace heat transfer calculation.

The numerical code requires a list of species with inlet concentrations, and a reaction set. For conditions which do not include sulfur, a total of 63 reactions are used involving 22 species containing the elements C, H, N, and O.¹² For mixtures including sulfur, an additional 31 reactions involving some of the above 22 species and 8 more species containing H, N, O, and S are included.

Many reactions involving the C-H-N-O species were obtained from a compilation presented by Hahn and Wendt¹³ which was derived from a set described by Levy et al.¹⁴ In particular, the set presented in ref. 12 was decreased by excluding all C-H and C-H-O compounds, leaving 49 reactions. Reactions involving the formyl radical, CHO, were obtained from Levy et al.¹⁵ which cites a pending publication by Corley and Bowman.¹⁶ Eight other reactions were included. The recommended list is in Table 3.1. Twenty-three of the reactions involving sulfur species were obtained from Wendt et al.¹⁷, four from other sources. The last four were postulated, using plausible parameters for the reaction rate coefficients.

The NO decomposition results for test LMF1C5, Step 5 (a low-stoichiometry oil run) were modeled using the set derived from Hahn and Wendt.¹³ (Species aside from NO were considered to be in equilibrium at the inlet, except that H₂, H₂O, CO, CO₂, and N₂, were adjusted to account for the measured inlet value of NO). It was found that the calculation led to too rapid a decomposition rate for NO, compared with experiment. One particular reaction, the reduction of HNO to HN by CO, was found to lead to the over-prediction. On the other hand, complete exclusion of this particular reaction caused a very significant under-prediction of NO decomposition rate for the test in question. (Wendt et al.¹⁷ also found that this reaction over-predicted NO decomposition in a CO flame experiment, using the original estimated reaction rate coefficient). A number of alternatives were tested, but no other reaction was found which could cause the appropriate NO decomposition rate. For this reason, the reaction rate coefficient for the reaction $\text{CO} + \text{HNO} \rightarrow \text{CO}_2 + \text{HN}$ was adjusted to give the proper results for test LMF1C5, Step 5, in conjunction with the remainder of the reaction set. In the adjustment, the activation energy was modified rather than the pre-exponential factor. It is important that the reaction set as a whole be considered, since, for example, modification of some of the other reaction rate coefficients, especially for other reactions involving CO being oxidized to CO₂, and formation of HNO, could lead to a poor prediction for NO decomposition using the adjusted activation energy mentioned above.

HN may react with NO to form N₂O, which decomposes by a variety of paths to N₂, or HN

TABLE 3.1 KINETIC REACTION DATA

REACTION (a)				Pre-exponential Factor, A (b)	Temp. Exp.	Activation Energy, E (c)
CO2		M	CO O	.38000E+31	-4.	134.021
CO	HO		CO2 H	.15000E+08	1.3	-.765
CO	O2		CO2 O	.32000E+13	0.	50.
H2		M	H H	.21000E+16	.07	103.83
HO	O	M	HO2	.16000E+21	-1.5	0.
H	O2	M	HO2	.30000E+16	0.	-1.
H2O		M	HO H	.23000E+25	-2.	122.6
H	HO		H2 O	.27000E+18	-.94	14.69
H	HO2		HO HO	.25000E+15	0.	1.9
HO	H2		H H2O	.25000E+14	0.	5.2
HO	HO		H2O O	.60000E+13	0.	1.
HO	O		H O2	.63000E+12	.5	0.
HO2	H		O2 H2	.25000E+14	0.	.7
HO2	O		HO O2	.50000E+14	0.	1.
CHN	HO		CN H2O	.20000E+12	.6	5.
CN	CO2		NCO CO	.37000E+13	0.	0.
CN	HO		NCO H	.62000E+14	0.	0.
CN	H2		CHN H	.62000E+13	0.	5.3
CN	O		CO N	.63000E+12	.5	0.
NCO	H		HN CO	.50000E+12	.5	6.87
CO	HNO		CO2 HN	.10000E+12	.5	21.0
H	NO	M	HNO	.20000E+17	0.	0.
NO	O	M	NO2	.14000E+22	-1.82	0.
N2O		M	N2 O	.40000E+15	0.	51.4
H	HNO		H2 NO	.10000E+14	0.	2.5
H	N2O		HO N2	.80000E+14	0.	15.
HN	NO		H N2O	.90000E+10	.75	00.
H	NO2		HO NO	.32000E+15	0.	1.5
HNO	HO		H2O NO	.36000E+14	0.	0.
HNO	O		HO NO	.50000E+12	.5	0.
HNO	O		HN O2	.10000E+12	.5	7.
HO	N2O		HO2 N2	.32000E+14	0.	15.
N2	O		NO N	1.84+14	0.	76.25
O	NO		N O2	2.36+09	1.0	38.65
NO	H		N HO	2.22+14	0.	50.5
HN	H		N H2	.63000E+12	.5	8.
HN	HO		H2O N	.50000E+12	.5	2.
HN	HO		NO H2	.50000E+12	.5	2.
HN	O		NO H	.63000E+12	.5	0.
H2N	H		HN H2	.14000E+12	.67	4.3
H2N	HO		HN H2O	.30000E+11	.68	1.3
H2N	O		HN HO	.92000E+12	.5	0.
H2N	H2N		H3N HN	.17000E+12	.63	3.6
H3N	HO		H2N H2O	.17600E+13	0.	1.7
H3N	H		H2N H2	.24600E+14	0.	17.07
H2N	NO		N2 H2O	.50000E+13	0.	0.
H3N	O		H2N HO	.15000E+13	0.	6.
H3N	O2		H2N HO2	.50000E+12	.5	56.
NO	HO2		NO2 HO	.50000E+12	.5	3.52

Table 3.1 Kinetic Reaction Data Continued

HN	HO		HNO	H	5.00+11	.5	5.62
CO	N2O		CO2	N2	3.00+11	0.	17.2
CHO		M	H	CO	1.55E+14	0.	14.7
CHO	H		CO	H2	2.00E+14	0.	0.
CHO	O		CO	HO	5.50E+12	0.5	0.
CHO	O		CO2	H	5.50E+12	0.5	0.
CHO	HO		CO	H2O	3.00E+12	1.0	0.
CHO	O2		CO	HO2	5.00E+11	0.5	0.83
H2N	O		H	HNO	2.10E+12	0.0	0.00
CO2	N		NO	CO	2.00E+11	-.5	8.00
NO	NO		N2O	O	1.29E+12	0.0	63.8
HNO	HNO		N2O	H2O	.300E+12	0.0	3.5
NO	HNO		N2O	HO	2.00E+12	0.0	26.
NO	NO		N2	O2	3.10E+13	0.0	63.1
K	H2O		HKO	H	6.02+13	0.	39.7
K	HO	M	HKO		2.18+20	-1.	0.
KO	HO		HKO	O	2.00+11	0.5	8.
KO	H		HO	K	2.00+11	0.5	8.
HS	S		H	S2	6.31+11	.5	.000
HS	H		S	H2	6.31+11	.5	0.000
H2S	H		HS	H2	9.03+12	.0	1.700
HS	HS		H2S	S	1.00+14	.0	1.420
HO	H2S		H2O	HS	1.40+13	.0	.894
OS	HO		H	O2S	6.46+14	.0	2.10
S	HO		OS	H	6.31+11	.5	.000
HS	O		OS	H	6.31+11	.5	.000
O	H2S		HS	HO	4.40+12	.0	3.298
HS	O		S	HO	6.31+11	.5	8.00
OS	O2		O2S	O	1.81+11	.0	5.600
S	O2		OS	O	6.31+11	.5	0.
O	S2		OS	S	6.31+11	.5	.0
OS	OS		O2S	S	4.10+11	.0	3.23
S	H2O		HS	HO	4.40+12	.0	28.
S	S	M	S2		1.00+18	-1.	0.
S	O	M	OS		5.50+13	.0	1.788
S	H	M	HS		7.20+15	.0	0.
H2S		M	HS	H	2.00+14	.0	74.
OS	O	M	O2S		1.22+22	-1.84	0.
O2S	O	M	O3S		4.00+20	-4.	5.3
O3S	O		O2S	O2	2.80+14	0.	12.0
N	OS		NO	S	6.31+11	.5	2.
NO	S		NS	O	1.00+12	.5	34.8
NS	O		OS	N	6.31+11	.5	8.
N	NS		N2	S	6.31+11	.5	0.
N	HS		NS	H	6.31+11	.5	8.
OS	HNO		O2S	HN	6.31+11	.5	8.
NO	NS		N2O	S	6.31+11	.5	8.
N	O2S		NO	OS	2.00+11	.5	8.0
H2N	HS		H2S	HN	6.31+11	.5	0.0
CS2	O		CS	OS	.50000E+14	0.	1.9
CS2	O		COS	S	.17000E+13	0.	1.2

Table 3.1 Kinetic Reaction Data Continued

CS2	O		CO	S2	.32000E+13	0.	1.0
COS	O		CO	OS	.60000E+14	0.	5.5
COS	O		CO2	S	.12000E+15	0.	11.
CS	O		CO	S	.11000E+14	0.	41.
CS2	S		CS	S2	.15000E+14	0.	00.
COS	S		CO	S2	.90000E+12	0.	2.5
COS	OS		CO2	S2	.10000E+09	0.	0.
CS	O2		CO	OS	.55000E+08	0.	2.
CS	O2		COS	O	.31000E+10	0.	9.5
CS	OS		CO	S2	.10000E+14	0.	00.
CS	S	M	CS2		.51000E+25	-3.	00.
CO	S	M	COS		.29000E+26	-3.6	00.
O	KS		KO	S	6.31+11	.5	8.
KO	HS		KS	HO	6.31+11	.5	8.
HO	KS		HKO	S	6.31+11	.5	8.
H	KS		K	HS	6.31+11	.5	8.
KO	NS		KS	NO	6.31+11	.5	8.
CO	KS		COS	K	6.31+11	.5	8.

NOTES:

(a) Species M, any gaseous species, exchanges energy but does not react.
M also participates in the reverse direction.

(b) Units are Mole-cm-sec. Forward rate coefficient, in direction shown, is given in Arrhenius form $A(T^n) \exp(-E/RT)$, T in K. Reverse rate coefficient is obtained from (forward coefficient)/(concentration equilibrium constant).

(c) Units are KCAL/MOLE

may accept an atom of H to form H_2N , which can react with NO to form N_2 . It is important to note that ammonia, NH_3 , may form to a level of several ppm, but is not added in the tests conducted or calculations in this report.

The result of the calculations for test LMF1C5, Step 5 is shown in Figure 3-1 together with a result obtained omitting the reduction of HNO to HN. It is evident that the conventional decomposition mechanism through N atoms (the modified Zeldovich mechanism) is inadequate to predict the NO decomposition.

As a particular example of NO decomposition involving coal as fuel, the result from CFFF test LMF1C4, Step 5 is illustrated in Figure 3-2. This was also a low stoichiometry test, with a somewhat higher mass flow and thermal input, hence a higher furnace inlet temperature, than the previous oil test analyzed. It is apparent from the calculated results that decomposition through the Zeldovich mechanism is greater in this case, but even with HN formation from HNO, the experimental NO decomposition rate is more rapid than the predicted rate. Incorporation of the reactions involving sulfur species significantly improves the agreement between numerical analysis and experiment.

Figure 3-3 shows NO decomposition for test LMF1C6, Step 9 (a test at higher stoichiometry than the above), together with calculated results (i) excluding sulfur reactions and HN formation from HNO, (ii) including HN formation, and (iii) including HN formation and sulfur reactions. It is apparent from these results that the reverse Zeldovich mechanism accounts for most of the decomposition.

The question naturally arises as to whether, in the coal-fired tests, there could be some residual unburned carbon which could reduce NO heterogeneously. The retention time in the high-pressure combustor of the CFFF is relatively short, generally 50 milliseconds or less, depending on conditions. Some additional time for carbon burning, if required, is available in the diffuser before the combustion products enter the furnace. For at least two reasons, the effect of heterogeneous reduction of NO is thought to be minimal. First, examination of furnace deposits (post-test) in the CFFF tests has never shown any significant carbon content in deposits. The second reason is related to a completely independent research effort by Glass and Wendt.¹⁸ In that study, a Utah bituminous coal was burned in a laboratory combustor with air at a stoichiometry of 0.8. Careful measurements after the major part of combustion had occurred showed up to 10 percent unburned carbon at temperatures in the range 1600-1800K with a retention time of about 1 sec., time-temperature conditions similar to those in the CFFF radiant furnace. However, a heterogeneous mechanism, which, according to Glass and Wendt, yielded higher rates than any previously used, still failed to predict the observed decomposition rate of NO. Glass and Wendt observed decomposition of NO from 1000 ppmv to 500 ppmv, while they predicted an exit value as a result of the heterogeneous reduction reaction, of 9000 ppmv. A crude approximation, assuming complete carbon combustion, yielded an exit value of about 600 ppmv, using the homogeneous reaction set in Table 3.1.

A point which has not been addressed above is the question of how nitric oxide is formed in the CFFF, as opposed to how it decomposes. It is usually assumed that, at the high temperature and pressure of the primary combustor, NO will approach equilibrium in the gas phase very rapidly. Kalfadelis et al.¹⁹ carried out a numerical experiment which showed that, in the primary MHD combustor, NO would reach within 90 percent of the equilibrium value in 1 ms at 2830K, and in 2 ms at 2700K for the conditions they chose.

Figure 3.1 Calculated and Experimental NO Levels in CFFF Flow Train.

Calculated and Experimental NO Levels in the CFFF Flow Train

Figure 3.2 Calculated and Experimental NO Levels in the CFFF Flow Train.

Calculated and Experimental NO Levels in the CFFF Flow Train.

Figure 3.3 Calculated and Experimental NO Levels in the CFFF Flow Train.

This numerical experiment has been repeated by the writers for the combustor conditions of test LMF1-C4 Step 5. At the measured pressure of 0.634 MPa (6.26 atm) and the computed combustor exit temperature of 2817K, an equilibrium of the gas phase species was calculated assuming complete combustion. The NO level was set to be near zero, while N₂ and O₂ concentrations were correspondingly increased, for input to chemical kinetics calculation at constant temperature and pressure. The NO content reached 50 percent of equilibrium in 0.3 ms, 95 percent in 1 ms, and over 99 percent in 2 ms. Since MHD combustor retention times are much greater than 2 ms, the usual equilibrium assumption appears to be justified. It would be anticipated that equilibration time in the combustor would be inversely proportional to the pressure, for moderate pressure changes at the same temperature and stoichiometry. It would also be anticipated that equilibration would be much slower at much lower temperatures. However, the combustor temperature used was typical to the CFFF and those projected for large MHD plants.

The PROF kinetic calculational model with the reaction set listed in Table 3.1 were validated in the cases cited above and in many subsequent tests. The model should provide a good prediction for the design of coal fired MHD steam power plants.

CHAPTER 4

NITROGEN OXIDE EMISSION ISSUES FOR PLANT DESIGN

The previous chapter discussed the methodology for kinetic calculations of NO decomposition in the radiant furnace. When the NO has decomposed to a suitable low level, the remaining combustibles in the gas need to be oxidized. If this is done at conditions which result in a high temperature in the secondary combustor, additional NO_x^* will be generated. There are two design choices that can avoid significant additional NO_x production in the secondary combustor. The first of these is to allow the gases to cool to a sufficiently low temperature that the combustor equilibrium NO_x level will be below desired emission level. The second method is to design the secondary combustor so that little or no temperature rise occurs. This may be done by staging the air addition over space and time while simultaneously removing energy from the gas. It may also be done by recirculating and injecting cooler flue gas from downstream so that no temperature rise occurs. Any of these techniques have a tendency to reduce the combustion efficiency of the secondary combustor and thus tend to increase the emission of carbon monoxide. In addition, if one assumes, as normally done, that all the heat transfer surface from the diffuser outlet to the secondary combustor inlet is refractory covered boiling surface and all the metallic tubes (ITAH, SH, RH, etc.) are downstream of the secondary combustor, there are plant heat balance implications, to the choice of secondary combustor inlet temperature.

4.1 Parametric Studies²⁰

It was not possible, in the CFFF, to assign all process variables to have specified values. The furnace is of a fixed size. Changes in stoichiometry affect flow rates and retention times, with changes, for example, in the furnace inlet temperature and the secondary combustor inlet (SCI) temperature. Changes in total thermal input also change retention times and cooling rate, and temperature levels at various places in the whole flow train.

The chemical kinetic calculations mentioned above are carried out in a parametric fashion. (The computer procedure used is described previously.) In the calculations, it was assumed that an MHD facility using Illinois #6 coal could be operated at a furnace inlet temperature of 3950°F (2450K), and that one using Montana Rosebud coal would have a furnace inlet temperature of 3750°F (2339K). Furnace operation, was considered to be at 1 atm (1.013 bar, 101.3 kPa). In the program used, a radiation parameter was used to affect the cooling rate, which was not constant, but decreased as temperature decreased. Experience with the chemical kinetic program has shown that at such inlet temperatures, the mixture is very close to equilibrium, hence equilibrium values were used as starting concentrations. At various

*Nitrogen Oxide (NO) is formed almost exclusively in the reducing zone prior to the secondary combustor. After secondary combustion, the NO may be converted to nitrogen dioxide (NO_2) with very small quantities of Nitrous Oxide (N_2O). The standards for emission of nitrogen oxides are stated in weight of NO_2 /unit of fuel input, pounds mass/million BTU of fuel input or nanograms of NO_2 /Joule of fuel input. The molecular weight of NO_2 is used in the calculation, in effect assuming that all the oxides are converted to NO_2 . We have called this the emission index in this and other reports.

radiation parameters, the reacting mixture at two different secondary combustor inlet temperatures was considered to be mixed with sufficient secondary air to achieve an overall stoichiometry of 105 percent, and the mixture was allowed to react while radiation heat transfer occurred. The main part of the oxidation of fuel constituents, such as CO, H₂, and H₂S, occurred in one or two computational steps, whereupon the secondary combustor outlet (SCO) mixture also started to cool. Some NO could be generated by thermal processes.

Table 4.1-1 shows some of the most significant results. Coal is considered to be burned with an oxidizer containing 38 volume percent O₂ (believed to be representative of early retrofit scenarios). Potassium was included as K₂CO₃, with 1 mass percent K in the primary mixture. Various primary stoichiometries were considered, as indicated in the table. A representative Illinois #6 coal, at 3.4 percent S, was considered to be the fuel for one part of the study, while a Montana Rosebud coal at 0.8 percent S was considered for the other part. In the table, SR1 refers to the primary stoichiometry, SR2 to the secondary stoichiometry. CR refers to an average cooling rate between furnace inlet and secondary combustor inlet, for a secondary combustor inlet (SCI) temperature of 2000°F (1366K).

At a given cooling rate for a given sulfur content, primary stoichiometry has a pronounced effect on NO_x emissions, emissions being higher at higher primary stoichiometry. At a given primary stoichiometry, for a given sulfur content, cooling rate has a significant effect on NO_x emissions, emissions being higher at higher cooling rate. Finally, in the table, there is a predicted difference in the NO_x emissions, which are ascribed mainly to the difference in sulfur contents in the flow. These differences are in line with the differences observed in the LMF5 tests described previously, although conditions in the tests are somewhat different, in particular the cooling rate, which is about 900-1300°F/sec in the CFFF, depending on flow rate and primary stoichiometry.

Another issue which has a significant effect on NO_x emissions is the secondary combustor inlet (SCI) temperature. Two factors are involved. The first factor is that by causing mixing at a higher temperature, not as much NO has decomposed as when decomposition is allowed to proceed to a lower temperature. The second factor is that the maximum temperature reached during secondary combustion is higher, since the starting point is higher, hence more NO will be produced thermally for a higher SCI temperature. These points are illustrated by Figures 4.1-1, 4.1-2 and 4.1-3. In Figure 4.1-1 the temperatures are shown for cooling rates of about 800°F/S over the temperature range from furnace inlet to an SCI temperature of 2000°F, for combustion products of the two coals at a primary stoichiometry of 80 percent. The cooling rate for an SCI temperature of 2300°F would be slightly higher, since cooling rate decreases as temperature decreases. There is a dip in each temperature as secondary air is mixed (secondary air is considered to be at 600°F). (By the calculation procedure used, which is one dimensional, mixing is considered to be non-reaction.) As reaction is allowed to continue, the temperature rises abruptly, then drops off when the secondary combustion reaction is essentially complete, and radiation to the walls cools the mixture. Figure 4.1-2 shows calculated NO contents for the process described (there is negligible NO₂ at these conditions). Figure 4.1-3 shows the NO_x emission index for the various flows considered. Because of the assumptions involved, for each coal combustion product, the NO content and NO_x emission index are identical in the high temperature range, prior to secondary combustion for the case of SCI temperature at 2300°F.

TABLE 4.1-1

PARAMETRIC STUDY OF EXIT COOLING RATES IN THE RADIANT FURNACE ON NO_x EMISSIONS

NO_x Illinois #6 Coal (3.4% Sulfur)

SR₁	SR₂	CR °F/Sec	NO_x #/MMBtu
.80	1.05	800	.050
.80	1.05	600	.035
.80	1.05	400	.028
.85	1.05	800	.105
.85	1.05	600	.068
.85	1.05	400	.042
.90	1.05	800	.240
.90	1.05	600	.160
.90	1.05	400	.095

Conditions

3950°F - Exit Temperature Diffuser

2000°F - Inlet Temperature Secondary Combustor

NO_x Rosebud Coal (0.8% Sulfur)

SR₁	SR₂	CR °F/Sec	NO_x #/MMBtu
.80	1.05	800	.067
.80	1.05	600	.049
.80	1.05	400	.038
.85	1.05	800	.130
.85	1.05	600	.092
.85	1.05	400	.060
.90	1.05	800	.300
.90	1.05	600	.220
.90	1.05	400	.140

Conditions

3750°F - Exit Temperature Diffuser

2000°F - Inlet Temperature Secondary Combustor

NOTE: It is mentioned here that similar effects occur at other stoichiometries and cooling rates. At higher primary stoichiometries, NO generated during secondary combustion is lower than at 80 percent, but the SCI NO content is higher. It turns out that more NO remains in the gas, after secondary combustion, for higher stoichiometries.

CG-2513

Figure 4.1-1 Parametric Study, NO_x Emissions, Illinois #6 and Rosebud Coal Fuels at 85 Percent Stoichiometry, Cooling Rate Approx. 600°F/S - Temperature Profiles.

Figure 4.1-2 Parametric Study, NO_x Emissions, Illinois #6 and Rosebud Coal Fuels at 85% Primary Stoichiometry, Cooling Rate Approx. 600°F/S - NO Contents.

Figure 4.1-3 Parametric Study, NO_x Emissions, Illinois #6 and Rosebud Coal Fuels at 85 Percent Primary Stoichiometry, Cooling Rate Approx. 600°F/S - Emission Index.

While SCI temperature has a significant effect on NO_x emissions, the furnace inlet (or diffuser outlet) temperature does not have much of an effect, as long as the furnace inlet temperature is above about 2300K (3680°F). At such temperatures, for cooling rates considered here, the NO content is very close to equilibrium.

4.2 Minimization Study

As can be noted from Table 4.1-1 and the previous figures, all reasonable design conditions for the MHD Steam Power Plant easily meet the New Source Performance Standards (NSPS) that were in effect during the MHD development program, 0.6 lbm/MMBtu. The Clean Air Act Amendments of 1990 tasks EPA to promulgate more stringent standards and they have suggested that standards as low as 0.15 lbm/MMBtu may be imposed by the year 2003.²¹ In addition, some state governments have already proposed limits for new facilities as low as 0.10 lbm/MMBTU. With this in mind, calculations were performed to find conditions which minimize the NO_x emissions for Rosebud Coal. (The emissions would be somewhat less with a high sulfur coal.) The results for reasonable average cooling rates and secondary combustor inlet conditions are shown in Figure 4.2-1. The 600°F/sec (average cooling rate implies residence times of 2.4 seconds to get to an SCI temperature of 2300°F and 2.9 seconds to get to 2000°F, but both could be used to meet a 0.1 lbm/MMBTU standard. If one were willing to build a larger radiant furnace having residence times of 3.6 seconds to get to a SCI of 2300°F or 4.4 seconds for a SCI of 2000°F, the plant could operate at a higher stoichiometry and thus a higher efficiency and still meet the 0.1 lbm/MMBTU emission criterion. Obviously, this is an economic choice between higher capital costs for a larger furnace and the higher efficiency possible with a higher primary stoichiometry. This argument assumes that given control of the size and shape of a radiant furnace that cooling rates as low as 400°F/sec can be realized. In the concept for an advanced technology MHD steam power plant, in which a ceramic tube high temperature air heater extracts energy from the gas in this temperature zone, additional difficulty and/or capital costs may be encountered in designing for these very low gas cooling rates.

4.3 Multi-Dimensional Modeling

All of the calculations previously presented are based on one-dimensional flow and heat temperature calculations to get the time-temperature history of the gases for input to the chemical kinetic calculation. In reality, of course, these are both velocity and temperature boundary layers that influence the NO decomposition, especially in the vicinity of the walls when the gas cooling rate is normally higher than in the center of the furnace. A methodology was developed and demonstrated to take these multi-dimensional effects into account.²² The procedure is to make a multi-dimensional calculation, then run the chemical kinetic calculation along streamlines. A typical result for a case calculated in the LMF radiant furnace is shown in Figure 4.3-1. It should be noted that this furnace is very small (4 ft. by 4 ft.) in cross section. The effects of the walls will decrease significantly for larger furnaces, eg. a 40 ft. x 40 ft. cross section would be the approximate size for a 1000 MW_e plant.

5.0 Conclusions

The experimental program conducted by UTSI during the MHD POC program, coupled with a validated chemical kinetic calculational methodology provides the tools needed for design of MHD Steam Power plants for prescribed levels of NO_x emissions.

Figure 4.2-1 Effects of Cooling Rate and SCI Temperature on NO_x Emissions at Various Primary Stoichiometry.

Figure 4.3-1 Spatial Character of Computed CFFF
Radiant Furnace NO Decomposition -
Lines of Constant NO.

The MHD Steam Power plant can be designed for NO_x emissions of NO more than .05 lbm/MMBTU (22 ng/Joule) without auxiliary NO_x control systems.

Design for NO_x emissions below this level will likely require catalytic reduction.

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