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PARAMETERS AFFECTING NITROGEN OXIDES IN A COAL-FIRED FLOW FACILITY SYSTEM

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Prepared by:

Xiaoliang Lu

A Thesis Presented for the Master of Science Degree

The University of Tennessee Space Institute
Energy Conversion Research & Development Programs
Tullahoma, Tennessee 37388-8897

March 1996

For

THE UNITED STATES DEPARTMENT OF ENERGY
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COAL FIRED FLOW FACILITY

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MASTER

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ABSTRACT

The unusually high temperature in the primary combustor of the Coal-Fired Magnetohydrodynamics (MHD) power generation system causes much higher nitrogen oxides (NO_x) to be produced than in a conventional coal fired generation system. In order to lower the NO_x concentration to an acceptable level, it is important to know how parameters of the MHD power generation system affect the NO_x concentration. This thesis investigates those effects in the Coal-Fired Flow Facility (CFFF) at the University of Tennessee Space Institute under the contract of US Department Of Energy (DOE).

With thermodynamic and kinetic computer codes, the theoretical studies were carried out on the parameters of the CFFF system. The results gathered from the computer codes were analyzed and compared with the experimental data collected during the LMF5J test. The thermodynamic and kinetic codes together modeled the NO_x behavior with reasonable accuracy while some inconsistencies happened at the secondary combustor inlet.

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NOMENCLATURE

A	cross section area
a_{ij}	number of kilogram-atoms of element i per kilogram-mole of species j
b_i	number of kilogram-atoms of element i per kilogram of mixture
b_i^*	number of kilogram-atoms of element i per kilogram of total reactant
C_j	radiant heat loss factor
CR	cooling rate
C_w	circumference of bounding tube
g	Gibbs free energy of mixture
h	enthalpy of bulk gas
J_{w_i}	flux of species i at bounding tube wall
M	number of condensed species
m	airleak flow rate
$\dot{m}$	mass rate of gas
N	number of species
n	number of kilogram-mole per kilogram of mixture
n_j	number of kilogram-mole of species j per kilogram of mixture
P	pressure
Q	volumetric heat loss
q_w	heat transport at bounding tube wall
R	gas constant

s	distance along axis
T	temperature
t	gas resident time
T_{DFO}	diffuser outlet temperature
T_{SCI}	secondary combustor inlet temperature
V	specific volume
x_j	mole fraction of species j
y_i	mass fraction of species i
W_i	chemical production rate of species i
μ_j	chemical potential per kilogram-mole of species j
μ_j°	chemical potential of species j in the standard state
λ_i	Lagrangian multiplier for i th constraint
Δp	furnace draft

Abbreviations

BHO	Baghouse Outlet
CFFF	Coal-Fired Flow Facility
DOE	Department Of Energy
DFO	Diffuser Outlet
ESP	Electrostatic Precipitator
LMF	Low-Mass Flow

MHD	Magnetohydrodynamics
NO _x	Nitrogen Oxides
SCI	Secondary Combustor Inlet
SCO	Secondary Combustor Outlet
SHTM	Superheater Test Module
SR	Stoichiometric Ratio
SR1	Primary Stoichiometric Ratio
SR2	Secondary Stoichiometric Ratio
UTSI	University of Tennessee Space Institute

CHAPTER 1

INTRODUCTION

1.1 MHD Background

The biggest advantage of the Magnetohydrodynamics (MHD) power generation system over the conventional one is a higher conversion efficiency of thermal and mechanical energy to electrical energy. This is achieved by adding a seed, an easily ionizable substance such as potassium carbonate into the coal and burning at high temperature and pressure to produce a high temperature plasma working fluid. Then the working fluid is passed through a magnetic field to generate electricity directly. With this technique applied, the overall efficiency of the MHD power plants could be 50% higher than that of conventional one [1].

A typical open cycle coal-fired MHD power plant consists of topping cycle which converts kinetic energy to electrical energy by magnetic field, and bottoming cycle which converts thermal energy to electrical energy by steam turbine. In order to commercialize the MHD power plants, research and development has been carried out on a 28 MWt MHD pilot plant, the Coal-Fired Flow Facility (CFFF), which is located at University of Tennessee Space Institute (UTSI) and operated under contract of US Department Of Energy (DOE). A schematic diagram of the CFFF system is shown in Figure 1.1.1.

Figure 1.1.1 Coal-Fired Low-Mass Flow Facility At UTSI

This system consists of upstream (topping cycle) and downstream (bottoming cycle). The upstream includes vitiation heater, primary combustor, supersonic nozzle, aerodynamic channel and diffuser. The downstream includes radiant furnace, secondary combustor, superheater, air heater, electrostatic precipitator (ESP), baghouse, wet ESP and stack.

1.2 NO_x in the CFFF System

In CFFF primary combustor, a high level of NO_x is produced due to the high temperature (5000°F) and high pressure (6 atm) required by the topping cycle of MHD. It is known that NO_x equilibrium concentration decreases rapidly with decreasing stoichiometry at given temperature while the decomposition rate increases [2] [3]. Also based on the economic optimization of MHD [4], a primary stoichiometry 0.85 has been chosen. With this stoichiometry, first coal and fuel oil burn in the primary combustor at reducing condition, then the reaction gas passes through the radiant furnace to get enough residence time and heat exchange to decompose the NO_x into nitrogen and ammonia [2]. After the reaction gas cools down to about 1400K, it enters the secondary combustor where combustion is completed with excess air. Then it goes through the superheater and air heater to get heat recovery. The typical temperature distribution is about 2400K to 1400K from diffuser outlet (DFO) to secondary combustor inlet (SCI), and about 1800K to 1100K from secondary combustor outlet (SCO) to superheater [5]. Since there

is no significant NO_x that will be generated when the temperature is lower than 1800K [6], in this thesis extensive parametric studies will be focused from DFO to SCO, however some parameters will be investigated after secondary combustor.

1.3 Objective Approach

The temperature distribution of the CFFF upstream, along the diffuser outlet up to the primary combustor, varies from 2400K to much higher. At these temperatures the chemical reactions would be complete and reach equilibrium state quickly. However along the CFFF down stream, from diffuser outlet down to the superheater, the temperature distribution varies from 2400K to 1100K. At these temperatures the chemical reactions, especially for the reactions that involve NO_x , would be dominated by chemical kinetics.

Based on the character of temperature distribution in the CFFF system, an equilibrium computer program, NASA SP-273 code, is chosen to model the NO_x concentration at diffuser outlet and a chemical kinetic program, Premixed One Dimensional Flame (PROF) code is chosen to model the NO_x behavior along the downstream. The results from these two models are then analyzed and compared with those from a CFFF test to get understanding of how parameters affect the NO_x concentrations in CFFF. Reports describing these codes are cited in the next chapter.

CHAPTER 2

THEORETICAL MODELS AND PARAMETERS

DETERMINATION

2.1 NASA SP-273 Equilibrium Code

Chemical equilibrium is usually described by either equilibrium constants or minimization of free energy. Since there are several disadvantages of using the equilibrium constant method [7], Gibbs free energy minimization formulation is used in NASA SP-273 [8].

For a mixture of N species, the Gibbs free energy per kilogram of mixture is given by

$$g = \sum_{j=1}^N n_j \mu_j \quad (2.1-1)$$

where n_j is the number of kilogram-moles of species j per kilogram of mixture. μ_j is the chemical potential per kilogram-mole of species j . The condition for chemical equilibrium is the minimization of Gibbs free energy. This minimization is subject to mass balance constraints

$$\sum_{j=1}^N a_{ij} n_j - b_i^\circ = 0 \quad i=1,2,\dots,L \quad (2.1-2)$$

or

$$b_i - b_i^\circ = 0 \quad i=1,2,\dots,L \quad (2.1-3)$$

where the coefficients a_{ij} are the number of kilogram-atoms of element i per kilogram-mole of species j , b_i° is the assigned number of kilogram-atoms of element i per kilogram of total reactants, and

$$b_i = \sum_{j=1}^N a_{ij} n_j \quad (2.1-4)$$

is the number of kilogram-atoms of element i per kilogram of mixture.

Defining a term G to be

$$G = g + \sum_{i=1}^L \lambda_i (b_i - b_i^\circ) \quad (2.1-5)$$

where λ_i are Lagrangian multipliers, the condition for equilibrium becomes

$$\begin{aligned} \delta G &= \delta g + \sum_{i=1}^L \lambda_i \delta(b_i - b_i^\circ) + \sum_{i=1}^L (b_i - b_i^\circ) \delta \lambda_i \\ &= \sum_{j=1}^N (\mu_j + \sum_{i=1}^L \lambda_i a_{ij}) \delta n_j + \sum_{i=1}^L (b_i - b_i^\circ) \delta \lambda_i \\ &= 0 \end{aligned} \quad (2.1-6)$$

Treating the variations δn_j and $\delta \lambda_i$ as independent variables gives

$$\mu_j + \sum_{i=1}^L \lambda_i a_{ij} = 0 \quad j=1,2,\dots,N \quad (2.1-7)$$

and also the mass balance equation (2.1-3).

Assuming all gases are ideal and the interactions among phases are negligible. The equation of state for the mixture is

$$PV = nRT \quad (2.1-8)$$

where P is pressure (N/m^2), V , specific volume (m^3/kg), n , moles

(kg-mole/kg), T, temperature (K) and R constant (8314.3 J/kg-mole-K). This equation is assumed to be correct even when small amounts of condensed species (up to several percent by weight) are present. In this event, the condensed species are assumed to occupy a negligible volume and exert a negligible pressure compared to the gaseous species.

Base on those assumptions, the chemical potential may be written as

$$\mu_j = \mu_j^\circ + RT \ln(n_j / n) + RT \ln P_{\text{atm}} \quad j=1, \dots, M \quad (2.1-9)$$

and

$$\mu_j = \mu_j^\circ \quad j=M+1, \dots, N \quad (2.1-10)$$

where μ_j° for gases ($j=1$ to M) and for condensed phases ($j > M$) is the chemical potential in the standard state. In above equation, the pressure must be in units of atmosphere, since the μ_j is defined based on 1 atm.

Equation (2.1-3), (2.1-7), (2.1-9), (2.1-10) with given temperature and pressure will determine the composition of the mixture. The output of the NASA SP-273 gives the mole fractions for each species in both condensed phase and gaseous phase. The mole fractions of species are defined as

$$x_j = \frac{n_j}{n} \quad (2.1-11)$$

It should be mentioned that n in equation (2.1-7) is different from that in equation (2.1-11). In equation (2.1-7), only total moles of gas species are included while in equation (2.1-11) total moles of both gas and condensed species are included.

2.2 PROF Chemical Kinetic Code

The Premixed One-dimensional Flame (PROF) code [9] was developed for EPA to predict the detailed chemical kinetics of combustion, well-stirred reactor, plug-flow reactor and fixed mass time-evolution problems. The plug-flow reactor option with nonreactive wall is used to model the chemical reactions of downstream in CFFF system. The governing conservation of mass and energy equations are

$$\dot{m} \frac{dy_i}{ds} = AW_i - C_w J_{w_i} \quad (2.2-1)$$

and

$$\dot{m} \frac{dh}{ds} = AQ - C_w q_w \quad (2.2-2)$$

where $\dot{m}$ is mass rate of gas, y_i , mass fraction of species i , s , distance along axis, A , cross sectional area, W_i , chemical production rate of species i , C_w , circumference of bounding tube, J_{w_i} , flux of species i at bounding tube wall, h , enthalpy of bulk gas, Q volumetric heat loss and q_w heat transport at the bounding tube wall.

The boundary conditions necessary to solve above equations are the initial gas compositions, initial temperature, pressure, heat transfer coefficient and a reaction set. The reaction set collected by Dr. Crawford includes 118 reactions involving 39 species [2] [10] [15].

The output of the PROF includes residence time, enthalpy, temperature,

density, system molecular weight and concentrations of individual species at each specified grid point along the downstream of CFFF.

2.3 Parameter Determination

In the CFFF test, several parameters can be adjusted to control the operation conditions and to get test data related to the objectives. Among these adjustable parameters, stoichiometry, nitrogen to oxygen weight ratio (N/O), air leak, cooling rate and potassium to sulfur molar ratio (K_2/S) are considered relative to their effect on NO_x concentrations. The typical operating conditions of LMF5J test are listed in Table 2.3.1 and Table 2.3.2.

During the LMF5J test (Sep. 21 to Sep. 26 ,1993) Montana Rosebud coal and #2 fuel oil were used. The coal, fuel oil and air analyses are listed in Table 2.3.3, Table 2.3.4 and Table 2.3.5.

2.4 Discussion of Input

The operating conditions listed in Table 2.3.1 and Table 2.3.2 are referred to as base conditions to set up input files for the NASA code and PROF code, first using the upstream operating conditions to set up input for the NASA code and carrying out the calculations to get output of the NASA code that includes the reaction gas compositions at DFO. Then the output of the NASA code and downstream operating conditions are used to set up input of the

Table 2.3.1 Typical Operating Conditions of Upstream

Parameter	Value
Coal Flow (lb/sec)	0.84
Fuel Oil Flow (lb/sec)	0.463
Air Flow (lb/sec)	3.40
Oxygen Flow (lb/sec)	1.83
Stoichiometry	0.85
K ₂ /S Molar Ratio	4.4
Seed Solution Flow (lb/sec)	0.257
Upstream Purge N ₂ (lb/sec)	0.048
Diffuser Outlet Temperature (K)	2438

Seed Solution: 47% K₂CO₃; 53% Water By Mass[11]

Source: LMF5J Test Report [11]

Table 2.3.2 Typical Operating Conditions of Downstream

Parameter	Value
Furnace Draft (inch water column)	-8.36
Stoichiometry	1.05
Secondary Air Flow (lb/sec)	2.66
Secondary Air Temperature (K)	509
SCI Temperature (K)	1256
SCO Temperature (K)	1417
Downstream Purge N ₂ (lb/sec)	0.28

Source: LMF5J Test Report [11]

Table 2.3.3 Coal Analysis For Test LMF5J

Ultimate, Dry Basis	Value
Ash (wt%)	10.47
Sulfur (wt%)	0.71
Carbon (wt%)	66.36
Hydrogen (wt%)	4.51
Nitrogen (wt%)	1.09
Oxygen (wt%)	16.86
Total	100.0
Moisture (wt%)	7.99%
Heating Value (Btu/lb) (Dry)	11445

Source: LMF5J Test Report [11]

Table 2.3.4 Fuel Oil Analysis For Test LMF5J

Component	Value
Carbon (wt%)	87.29
Hydrogen (wt%)	12.42
Nitrogen (wt%)	0.12
Sulfur (wt%)	0.17
Total	100.0
Heating Value (Btu/lb)	19448

Source: LMF5J Test Report [11]

Table 2.3.5 Air Analysis [12]

Major Gas Species	Molecular Weight (kg/kmol)	Fractional Volume (dimensionless)	Fractional Weight (dimensionless)
N ₂	28.0134	0.78084	0.755578
O ₂	31.9988	0.209476	0.2315364
Ar	39.948	0.00934	0.0128882

PROF code and carry out the calculations along the downstream.

In order to investigate how individual parameters affect NO_x distribution behavior in the CFFF, every parameter of stoichiometric ratio, nitrogen to oxygen weight ratio, air leak, cooling rate and potassium to sulfur molar ratio was varied one by one while others were kept at base conditions when the calculations were carried out. It should be mentioned that some parameters are dependent upon each other. For example, increasing primary stoichiometric ratio will cause increasing temperature at DFO. The way to keep the DFO temperature at base condition is that hypothetically we can lower the air inlet temperature or increase the cooling rate to “force” the DFO temperature to be unchanged.

2.4.1 Stoichiometric Ratio (SR)

For combustion, the stoichiometric ratio is defined as the weight ratio of oxygen actually used to oxygen theoretically needed to convert the combustible elements of the fuel into their stable oxides

$$\text{SR} = \frac{(\text{O}_2)_{\text{actual}}}{(\text{O}_2)_{\text{theoretical}}} \quad (2.4-1)$$

The amount of oxygen theoretically needed could be calculated from coal analysis, oil analysis, coal flow rate and oil flow rate with the following stoichiometrically balanced reaction equations.

Once the stoichiometric ratio is specified, the amount of oxygen actually needed can be obtained from equation (2.4-1).

The primary stoichiometric ratio (SR1) is the weight ratio of oxygen actually used to oxygen theoretically needed in the primary combustor. The secondary stoichiometric ratio (SR2) is the weight ratio of oxygen actually used in both primary and secondary combustor to the oxygen theoretically needed.

During the theoretical studies, the SR1 is varied from 0.75 to 1.00 with a step of 0.05 and SR2 is varied from 1.00 to 1.20 with a step of 0.05 also.

2.4.2 Weight Ratio of Nitrogen To Oxygen (N/O)

It can be expected that the amount of nitrogen and oxygen in the primary combustor will affect the NO_x concentration according to the following reaction equation

so N/O ratio may be an important parameter which affects NO_x concentration. The N/O ratio was varied from 0.4 to 1.4 with 0.2 step was selected during the theoretical studies.

2.4.3 Air Leak

In order to avoid leakage of combustible, substoichiometric gases to the atmosphere, the CFFF downstream of the high velocity duct is operated at a negative pressure which is maintained by an induced draft fan [13]. Due to the existence of this negative pressure, air leakage is unavoidable. The air leak flow is given by [10]

$$m = 0.35 \sqrt{\frac{-\Delta p}{7}}$$

where m is air leak flow and Δp is furnace draft. Since air leak will change both overall stoichiometric ratio and N/O ratio, it becomes another important parameter that affects NO_x concentration. During the test, the air leak from the slag rejection outlet which is located near the diffuser outlet is believed to have a strong effect on the formation of NO_x due to the high temperature there. Normal gauge pressure at that place is around -8 inch water column. In the theoretical study, this variable was varied from 0 to -20 inch water column.

2.4.4 Cooling Rate

The cooling rate significantly affects the decomposition of NO_x by decomposition to N_2 and NH_3 [3] [13]. Variation of cooling rate will cause a change of the NO_x concentration distribution profile along the radiant furnace to the secondary combustor outlet. The cooling rate is a parameter

which describes the temperature decrease of reaction gas along the downstream. It is given by

$$CR = \frac{T_{DFO} - T_{SCI}}{t}$$

where CR is cooling rate, T_{DFO} , diffuser outlet temperature, T_{SCI} , secondary combustor inlet temperature and t , gas residence time. In the theoretical studies, furnace cooling rate is affected by a radiant heat loss factor C_j , which is an optional input to the PROF code. Once the DFO temperature and SCI temperature are specified, the C_j factor is obtained. On the other hand, when DFO temperature and C_j factor are specified, the SCI temperature can be calculated. During the theoretical calculations, C_j is varied from 0.0300 to 0.1500 to cover possible operation conditions.

2.4.5 Molar Ratio of Potassium to Sulfur (K_2/S)

K_2/S ratio parameter is important to the SO_2 emission in the CFFF system [5]. But it is not yet clear whether this parameter affects NO_x behavior. So the theoretical studies of K_2/S ratio was also included. K_2/S ratio was 4.4 at base conditions for LMF5J test. The variation of K_2/S in calculations was from 1.5 to 5.5 with step of 1.0.

2.4.6 Modifications of Some Parameters at Base Conditions

During the LMF5J test operating at base conditions, the DFO temperature detected by instrument was 2438K. In calculations this temperature was rounded to 2450K for convenience. At the base conditions of LMF5J test, C_p had the value of 0.0993 which corresponded to cooling down the gas from 2438K at DFO to 1256K at SCI. For the convenience of studies this value is modified to 0.0900 at the base conditions.

CHAPTER 3

THEORETICAL RESULTS AND ANALYSES

3.1 Distribution of NO_x Concentrations From DFO To SCI And NO_x Concentration At SCO

Extensive parametric calculations were carried out from the diffuser outlet to the secondary combustor outlet based on the discussions in Chapter 2. The gas compositions at DFO were assumed to be at equilibrium and were calculated from NASA code first. With this gas composition at DFO, the distribution of gas compositions between DFO and SCI were found by the PROF code when the grid dimensions in the output of the PROF code reached 18.5 m, which corresponded to the distance from DFO to SCI [14]. Then with the SCI gas compositions and secondary stoichiometry, the SCO gas compositions were calculated by the PROF code. It should be mentioned that in the LMF5J test, SCO gas sampling probe and temperature probe were located near the inlet of Superheat Test Module (SHTM). So SCO gas composition data from output of the PROF code came from the grid position which corresponded to the distance of SHTM inlet.

3.1.1 The Effect of SR1 On NO_x Behavior Before SCO

Table 3.1.1.1 lists the molar fraction of nitrogen species at DFO and SCI when SR1 is 0.85. From this table it can be seen that NO, N₂ and NH₃ are the only species for which molar fractions are greater than 10⁻⁶. When SR1 varies from 0.75 to 1.00, the nitrogen species, which molar fractions are greater than 10⁻⁶ along DFO to SCI are plotted in Figure 3.1.1.1, 3.1.1.2, 3.1.1.3 and the corresponding temperature distribution is plotted in Figure 3.1.1.4. It should be mentioned that NO_x is the combination of NO and NO₂.

Figure 3.1.1.1 shows the relationship between NO_x concentration and SR1 along DFO to SCI. It can be seen that SR1 is an important parameter affecting NO_x concentration. Increase of SR1 cause a higher NO_x concentration at all positions in the furnace; In the range of stoichiometries studied, not only is the NO_x concentration higher, but also, the change in NO_x concentration in going from one stoichiometry to another, using equal intervals of stoichiometry, becomes greater at higher stoichiometries. It also can be seen that NO_x concentration is decreasing along the 18.5m pathway of DFO to SCI. The decrease of NO_x before 6m is much faster than that after 6m (roughly). When SR1=0.85, for instance, before 6m the NO_x concentration decreases from 1300ppm at the DFO to 280ppm at 6m position, the decrease of NO_x being more than 1000ppm along 6m distance; After the 6m position, NO_x concentration decreases from 280ppm at the 6m position to 74ppm at the SCI, the decrease of NO_x being only 200ppm along 12.5m distance. While

Table 3.1.1.1 Molar Fraction of Nitrogen Species at DFO and SCI when
SR1=0.85

Nitrogen Species	Molar Fraction At DFO	Molar Fraction At SCI
NO	0.13039E-02	0.74311E-04
N ₂	0.39042E+00	0.39437E+00
CN	0.26250E-10	0.23979E-13
CHN	0.30198E-08	0.37008E-07
HNO	0.91272E-07	0.55212E-08
N	0.11290E-06	0.20990E-10
NCO	0.16490E-09	0.14688E-12
HN	0.10084E-07	0.17306E-09
H ₂ N	0.36110E-07	0.24204E-08
H ₃ N	0.28876E-07	0.10456E-04
NO ₂	0.93735E-07	0.73125E-11
N ₂ O	0.45910E-07	0.33308E-09

(N/O=1.0, Air Leak=0.0, K₂/S=4.4, C_j=0.0900, SR2=1.05)

Figure 3.1.1.1 NO_x Concentration Distribution Along The Pathway From DFO To SCI
(N/O=1.0, Air Leak=0.0, K₂/S=4.4, C_j=0.0900)

Figure 3.1.1.2 N_2 Molar Fraction Distribution Along The Pathway From DFO To SCI
($N/O=1.0$, Air Leak=0.0, $K_2/S=4.4$, $C_f=0.0900$)

Figure 3.1.1.3 NH₃ Concentration Distribution Along The Pathway From DFO To SCI
(N/O=1.0, Air Leak=0.0, K₂/S=4.4, C_f=0.0900)

Figure 3.1.1.4 Temperature Distribution Along The Pathway From DFO To SCI

(N/O=1.0, Air Leak=0.0, $K_2/S=4.4$, $C_i=0.0900$)

checking the temperature distribution of Figure 3.1.1.4, it can be seen that at 6m position the temperature is around 2100-2200K. It also should be mentioned that NO_x concentration is much higher before 6m position than that after 6m position. NO_x decomposition rate is determined by two parameters, which are NO_x concentration level and temperature, and, of course, by stoichiometry. From the above discussion it can be concluded that at fixed temperature, NO_x decomposition rate is from fast to slow while NO_x concentration level from high to low; NO_x decomposition rate decreases quickly when temperature is lower than 2200K.

From Figure 3.1.1.1 it can be concluded that significant decrease of NO_x concentration is achieved in the first $\frac{1}{3}$ of the pathway, however some decrease of NO_x concentration is achieved in the remaining $\frac{2}{3}$ of pathway.

Comparing Figure 3.1.1.1 with Figure 3.1.1.2 and Figure 3.1.1.3, it can be seen that NO_x decomposes quickly via N_2 at high NO_x concentration level, slowly via N_2 at medium NO_x concentration level and more slowly via both N_2 and NH_3 at low NO_x concentration level and low temperature and stoichiometry. This can be seen clearly from the individual distribution lines of Figure 3.1.1.1, 3.1.1.2 and 3.1.1.3. For example, when $\text{SR1}=1.00$, NO_x concentration is higher than 1400ppm before 6m, at this region NO_x concentration decreases quickly while N_2 concentration increases proportionally. After this region NO_x decomposition slows down while N_2

formation slows down also. Because the stoichiometry is high, there is almost no formation of NH_3 . When $\text{SR}=0.85$, before 6m position the NO_x concentration decreases quickly while N_2 concentration increases proportionally. After this region the NO_x decomposition slows down and N_2 formation slows down also. As NO_x decomposes to lower than about 500ppm, the formation of NH_3 begins, however the NH_3 concentration reaches no more than 12ppm at SCI.

NO_x decomposition to N_2 and NH_3 also can be seen clearly from Table 3.1.1.2. Table 3.1.1.2 shows the normalized atomic fraction of nitrogen species along DFO to SCI when SR1 is 0.85. From this table it can be seen that NO_x atomic fraction decreases along the distance while the total atomic fraction of N_2 and NH_3 increases at the same amount. However the increasing of NH_3 is negligible.

The chemical mechanism of NO decomposition has been described by Dr. Crawford[2] [15]. A brief description of the NO decomposition mechanism is presented in the Appendix.

Table 3.1.1.3 shows the relationship of NO_x concentration at DFO, SCI and SCO with the SR1 . From this table, it can be seen that NO_x concentration increases at DFO, SCI and SCO while SR1 increases. Actually at fixed SR2 , NO_x concentration at SCO is decided by both SCI NO_x concentration and SCI temperature. Increasing SCI NO_x concentration or SCI temperature will cause increasing SCO NO_x concentration. Since increase of SR1 causes increase of

Table 3.1.1.2 Normalized Atomic Distribution of N Among NO_x, N₂ and NH₃

Along DFO to SCI When SR1=0.85

Distance From DFO To SCI (m)	NO _x Atomic Fraction (%)	N ₂ Atomic Fraction (%)	NH ₃ Atomic Fraction(%)
0	0.167	99.833	0.000
2	0.096	99.904	0.000
4	0.052	99.948	0.000
6	0.032	99.968	0.000
8	0.023	99.977	0.000
10	0.018	99.982	0.000
12	0.015	99.985	0.000
14	0.012	99.987	0.001
16	0.011	99.988	0.001
18	0.010	99.989	0.001
18.5	0.009	99.990	0.001

(N/O=1.0, Air Leak=0.0, K₂/S=4.4, C_j=0.0900, SR2=1.05)

Table 3.1.1.3 The Effect of SR1 On NO_x At DFO, SCI And SCO

SR1	NO _x At DFO (ppm)	NO _x At SCI (ppm)	T _{sci} (K)	NO _x At SCO (ppm)
0.75	654	16	1541	25
0.80	919	34	1515	38
0.85	1303	74	1497	71
0.90	1873	164	1490	129
0.95	2710	363	1501	267
1.00	3829	803	1541	582

(N/O=1.0, Air Leak=0.0, K₂/S=4.4, C_i=0.0900, SR2=1.05)

SCI NO_x concentration and small variations of SCI temperature, the net effect of NO_x and temperature variations at SCI causes increase of NO_x concentration at SCO. When SR1 increases the entire NO_x concentration level increases from DFO to SCO.

3.1.2 The Effect of N/O On NO_x Behavior Before SCO

N/O was varied at the ratios 0.4, 0.6, 0.8, 1.0, 1.2 and 1.4, while keeping other parameters at base conditions. The result from the calculations are shown in Figure 3.1.2.1, 3.1.2.2, 3.1.2.3 and listed in Table 3.1.2.1.

Figure 3.1.2.1 shows the relationship between NO_x concentration and N/O ratio from DFO to SCI. It can be seen that increasing N/O ratio causes increasing NO_x concentration. However, the change from one ratio to the next is not large, and is not very dependent on N/O ratio. The NO_x concentration is not as sensitive to N/O as to SR1, since increasing SR1 causes an increase both in NO_x concentration and in the change from one stoichiometry to another.

From Figure 3.1.2.1 it also can be seen that the distribution of NO_x concentration along DFO to SCI is similar to that in Figure 3.1.1.1. Before 6m position, within the 6m distance NO_x decomposition is very fast. For instance, NO_x concentration decreases from 960ppm to 140ppm for N/O=0.4 line and from 1420ppm to 360ppm for N/O=1.4 line. After the 6m position, within the 12.5m distance NO_x decomposition is quite slow. For instance, it

Figure 3.1.2.1 NO_x Concentration Distribution Along The Pathway From DFO To SCI
(SR1=0.85, Air Leak=0.0, $K_2/S=4.4$, $C_f=0.0900$)

Figure 3.1.2.2.2 N_2 Molar Fraction Distribution Along The Pathway From DFO To SCI
(SR1=0.85, Air Leak=0.0, $K_p/S=4.4$, $C_p=0.0900$)

Figure 3.1.2.3 NH₃ Concentration Distribution Along The Pathway From DFO To SCI
(SR1=0.8, Air Leak=0.0, K₂/S=4.4, C_i=0.0900)

Table 3.1.2.1 The Effect of N/O Ratio On NO_x At DFO, SCI And SCO

N/O Ratio	NO _x At DFO (ppm)	NO _x At SCI (ppm)	T _{sci} (K)	NO _x At SCO (ppm)
0.4	958	54	1119	50
0.6	1111	60	1258	55
0.8	1220	67	1385	61
1.0	1303	74	1497	71
1.2	1369	84	1596	91
1.4	1421	95	1683	127

(SR1=0.85, Air Leak=0.0, K₂/S=4.4, C_j=0.0900, SR2=1.05)

decreases from 140ppm to 50ppm for N/O=0.4 line and from 360ppm to 90ppm for N/O=1.4 line. Most of the NO_x decomposition is achieved in the first $\frac{1}{3}$ of the pathway.

Comparing Figure 3.1.2.1 with Figure 3.1.2.2 and 3.1.2.3, it can be concluded that NO_x decomposition rate is from fast to slow while NO_x concentration level is from high to low and temperature is high. When NO_x concentration is lower than about 500ppm and temperature is low the formation of NH₃ occurs, though the concentration of NH₃ never reaches 25ppm.

Table 3.1.2.1 shows the relationship of NO_x concentration at DFO, SCI and SCO with N/O ratio. From the table it can be seen that NO_x concentration increases at DFO, SCI and SCO while N/O ratio increases. So increasing of N/O ratio will cause increasing of entire NO_x concentration level from DFO to SCO. There is a temperature effect of N/O ratio. It is noted in Table 3.1.2.1 that temperatures are higher at the SCI for higher N/O. This is an artifact having higher mass flow, for higher N/O, and of having mass dilute radiating gases such as H₂O and CO₂. If the total mass flow had been kept constant, it is possible that different effects would be seen.

Comparing the effect of increasing SR1 with the effect of increasing N/O ratio on NO_x behavior, it can be seen that they have similar apparent effects on NO_x behavior, except that the NO_x concentration is more sensitive to

stoichiometry at high stoichiometry, while sensitivity to N/O ratio does not change much with the N/O ratio.

3.1.3 The Effect of Air Leak On NO_x Behavior Before SCO

Table 3.1.3.1 shows the relationship of furnace draft with air leak, SR1 and N/O ratio. From this table it can be seen that increase of furnace draft causes increase of air leak, eventually increasing both SR1 and N/O ratio in the CFFF system. It can be anticipated that the effect of air leak on NO_x behavior will be the combined effects of SR1 and N/O ratio on NO_x behavior.

Furnace draft was varied through the values 0, -4, -8, -12, -16 and -20 inch water while keeping other parameters at base conditions. The results from calculations are shown in Figure 3.1.3.1, 3.1.3.2, 3.1.3.3 and listed in Table 3.1.3.2.

Figure 3.1.3.1, which is similar to Figure 3.1.1.1 and Figure 3.1.2.1, shows before the 6m position NO_x decomposition rate is fast and after the 6m position NO_x decomposition rate is rather slower.

Comparing Figure 3.1.3.1 with Figure 3.1.3.2 and 3.1.3.3, it can be concluded that NO_x decomposition rate is from fast to slow by decomposition to N₂ while NO_x concentration level from high to low. When NO_x concentration is lower than about 500ppm and temperature is lower, the formation of NH₃ occurs, however the concentration of NH₃ never reaches 12ppm.

Table 3.1.3.1 Effect of Air Leak On SR1 and N/O

Furnace Draft (Inch H ₂ O)	Air Leak (lb/sec)	SR1	N/O Ratio
0	0	0.850	1.00
-4	0.2656	0.870	1.05
-8	0.3742	0.878	1.07
-12	0.4583	0.884	1.09
-16	0.5292	0.890	1.10
-20	0.5916	0.894	1.11

Table 3.1.3.2 The Effect of Air Leak On NO_x At DFO, SCI And SCO

Furnace Draft (Inch H ₂ O)	Air Leak (lb/sec)	NO _x At DFO (ppm)	NO _x At SCI (ppm)	T _{sci} (K)	NO _x At SCO (ppm)
0	0	1304	74	1497	71
-4	0.2656	1524	104	1520	95
-8	0.3742	1625	120	1530	106
-12	0.4583	1708	133	1537	114
-16	0.5292	1781	146	1544	122
-20	0.5916	1848	158	1550	129

(SR1=0.85, N/O=1.0, K₂/S=4.4, C_j=0.0900, SR2=1.05)

Figure 3.1.3.1 NO_x Concentration Distribution Along The Pathway From DFO To SCI
(SR1=0.85, N/O=1.0, K₂/S=4.4, C_j=0.0900)

Figure 3.1.3.2 N_2 Molar Fraction Distribution Along The Pathway From DFO To SCI
(SR1=0.85, N/O=1.0, $K_2/S=4.4$, $C_f=0.0900$)

Figure 3.1.3.3 NH_3 Concentration Distribution Along The Pathway From DFO To SCI
($\text{SR}_1=0.85$, $\text{N/O}=1.0$, $\text{K}_2/\text{S}=4.4$, $\text{C}_1=0.0900$)

Table 3.1.3.2 shows the relationship of NO_x concentration at DFO, SCI and SCO with air leak. From this table it can be seen that NO_x concentration increases at DFO, SCI and SCO while air leak increases. So increase of air leak will cause increase of entire NO_x concentration level from DFO to SCO.

Since the effect of air leak on NO_x behavior is the combined effects of SR1 and N/O ratio on NO_x behavior and effect of SR1 is more sensitive on NO_x than that of N/O ratio on NO_x , it can be concluded that the sensitivity of air leak on NO_x should be less than that of SR1 and greater than that of N/O ratio.

3.1.4 The Effect of K_2/S Ratio On NO_x Behavior Before SCO

K_2/S ratio was varied at the values 1.5, 2.5, 3.5, 4.5 and 5.5 while keeping other parameters at base conditions. The results of the calculations were shown in Figure 3.1.4.1, 3.1.4.2, 3.1.4.3 and listed in Table 3.1.4.1.

From Figure 3.1.4.1 it can be seen that increasing of K_2/S only causes a slight increase of NO_x concentration at DFO and almost no change of NO_x concentration at SCI.

Table 3.1.4.1 shows when K_2/S increases from 1.5 to 5.5 with a step 1.0, NO_x concentration at DFO just increases about 7ppm for every step and almost has no change at SCI and SCO. The effect of K_2/S ratio on NO_x can be neglected, according to the calculations, and assuming of other parameters

Figure 3.1.4.1 NO_x Concentration Distribution Along The Pathway From DFO To SCI
(SR1=0.85, N/O=1.0, Air Leak=0.0, C_f=0.0900)

Figure 3.1.4.2 N_2 Molar Fraction Distribution Along The Pathway From DFO To SCI
($SR_1=0.85$, $N/O=1.0$, Air Leak=0.0, $C_f=0.0900$)

Figure 3.1.4.3 NH₃ Concentration Distribution Along The Pathway From DFO To SCI
(SR1=0.85, N/O=1.0, Air Leak=0.0, C_f=0.0900)

Table 3.1.4.1 The Effect of K_2/S Ratio On NO_x At DFO, SCI And SCO

K_2/S Ratio	NO_x At DFO (ppm)	NO_x At SCI (ppm)	T_{sci} (K)	NO_x At SCO (ppm)
1.5	1284	72	1490	73
2.5	1291	73	1492	72
3.5	1298	74	1495	71
4.5	1305	74	1497	71
5.5	1312	75	1499	71

(SR1=0.85, N/O=1.0, Air Leak=0.0, C_j =0.0900, SR2=1.05)

are constant.

Comparing Figure 3.1.4.1 with Figure 3.1.4.2 and 3.1.4.3, the same NO_x decomposition characteristics as those in section 3.1.1, 3.1.2 and 3.1.3 can be seen, in which NO_x decomposition rate is from fast to slow by decomposition to N_2 while NO_x concentration level changes from high to low and temperature is high, while formation of NH_3 occurs after NO_x concentration lower than about 500ppm and temperature is relatively low. Most of the NO_x decomposition is achieved in the first $\frac{1}{3}$ of the path.

3.1.5 The Effect of Cooling Rate On NO_x Behavior Before SCO

In the calculations, C_f factor was varied from 0.03 to 0.15 while keeping other parameters at base conditions. The results are plotted in Figure 3.1.5.1, 3.1.5.2, 3.1.5.3 and listed in Table 3.1.5.1.

Figure 3.1.5.1 shows the relationship between C_f factor and distribution of NO_x concentration along DFO to SCI. It can be seen that increasing cooling rate causes increase of NO_x decomposition rate before the 6m position and decrease of NO_x decomposition rate after the 6m position. Since the overall NO_x decomposition rate is the combination of NO_x decomposition rate on entire region, there should exist an optimum cooling rate to get the maximum decomposition of NO_x .

Table 3.1.5.1 shows the effects of cooling rate on NO_x concentration at SCI

Figure 3.1.5.1 NO_x Concentration Distribution Along The Pathway From DFO To SCI
(SR1=0.85, N/O=1.0, Air Leak=0.0, K₂/S=4.4)

Figure 3.1.5.2 N_2 Molar Fraction Distribution Along The Pathway From DFO To SCI
(SR1=0.85, N/O=1.0, Air Leak=0.0, $K_2/S=4.4$)

Figure 3.1.5.3 NH₃ Concentration Distribution Along The Pathway From DFO To SCI
(SR1=0.85, N/O=1.0, Air Leak=0.0, K₂/S=4.4)

Table 3.1.5.1 The Effect of Cooling Rate On NO_x At DFO, SCI And SCO

(C_j From 0.030 To 0.120)

C _j	CR (K/sec)	NO _x At SCI (ppm)	T _{sci} (K)	Peak Temperature In Secondary Combustor(K)	T _{sc0} (K)	NO _x At SCO (ppm)
0.0300	250	142	2101	2269	2170	1636
0.0600	451	73	1772	2102	1579	235
0.0700	509	70	1673	2047	1529	124
0.0800	551	70	1582	1993	1483	83
0.0900	587	74	1497	1939	1440	71
0.1000	617	81	1417	1888	1403	71
0.1100	641	88	1343	1840	1369	75
0.1200	661	96	1274	1804	1338	81

(SR1=0.85, N/O=1.0, Air Leak=0.0, K₂/S=4.4, SR2=1.05)

and SCO, on temperature at SCI and SCO , and on peak reaction temperature in the secondary combustor. The peak reaction temperature of secondary combustor is defined as the highest temperature between SCI and SCO (probe location). It can be seen that increasing of C_j factor from 0.03 to 0.07 will cause decrease of NO_x concentration from 142ppm to 70ppm at SCI, but further increasing of C_j factor from 0.07 to 0.12 will cause increase of NO_x concentration from 70ppm to 96ppm. Thus $C_j=0.07$ minimizes the NO_x concentration at the SCI, but it does not minimize NO_x concentration at SCO, since NO_x concentration at SCO is decided by both NO_x concentration and temperature at SCI. When $C_j=0.07$, the 1673K SCI temperature will bring the peak reaction temperature up to 2047K in the secondary combustor region. This quite high reaction temperature will cause NO_x production. From Table 3.1.5.1 it can be seen when C_j has a value between 0.09 and 0.10, NO_x concentration at SCO has a minimum value. Further calculations of C_j between 0.09 to 0.10 were carried out and the results were listed in Table 3.1.5.2.

Table 3.1.5.2 gives when $C_j=0.094$, NO_x concentration is at a minimum value of 70ppm. However, when C_j varies from 0.09 to 0.10, the variation of NO_x concentration is less than 2ppm, which can be neglected safely. For engineering purposes, the optimal C_j factor can be any value in the range of 0.09 to 0.10. This corresponds to SCI temperature in the range of 1417K to 1497K and SCO temperature in the range of 1403K to 1440K.

Table 3.1.5.2 The Effect of Cooling Rate On NO_x At DFO, SCI And SCO

(C_j From 0.090 To 0.100)

C _j	CR (K/sec)	NO _x At SCI (ppm)	T _{sci} (K)	Peak Temperature In Secondary Combustor(K)	T _{SCO} (K)	NO _x At SCO (ppm)
0.0900	587	74	1497	1939	1440	71
0.0920	593	75	1480	1929	1433	71
0.0940	600	77	1464	1918	1425	70
0.0960	606	78	1448	1908	1418	70
0.0980	612	79	1432	1898	1410	71
0.1000	617	81	1417	1888	1403	71

(SR1=0.85, N/O=1.0, Air Leak=0.0, K₂/S=4.4, SR2=1.05)

Comparing Figure 3.1.5.1, 3.1.5.2 and 3.1.5.3, with similar figures in previous sections, it can be concluded the same characteristics of NO_x decomposition occur, in that NO_x decomposition rate is from fast to slow by decomposition to N_2 while NO_x concentration level varies from high to low and temperature varies from high to low.

3.1.6 The Effect of SR2 On NO_x Concentration At SCO

The secondary stoichiometry, SR2, was varied from 1.00 to 1.20 with step 0.05 while keeping other parameters at base conditions. The calculation results are listed in Table 3.1.6.1.

From Table 3.1.6.1 it can be seen that NO_x concentration at SCO increases while SR2 increases from 1.00 to 1.15, then decreases while SR2 increases from 1.15 to 1.20. From the temperature data in Table 3.1.6.1, it seems that temperature greater than 1900K favors the formation of NO_x . However, the purpose of the secondary combustor is let the gas flow be burned completely. When $\text{SR2}=1.05$ the secondary combustor has a peak temperature of 1939K, which is the highest temperature among the temperature data. It indicates that gas is burned completely. So $\text{SR2}=1.05$ is recommended according to this theoretical study. A calculation of NO_x Emission Index is included in Table 3.1.6.1. While the NO_x concentration could be decreased by adding more and more air, the Emission Index is a measure of amount of NO_x produced per

Table 3.1.6.1 The Effect of SR2 On NO_x Concentration At SCO

SR2	Peak Temperature In Secondary Combustor (K)	NO _x At SCO (ppm)	NO _x At SCO (lb/10 ⁶ Btu)
1.00	1823	60	0.044
1.05	1939	71	0.056
1.10	1934	92	0.077
1.15	1912	97	0.086
1.20	1880	89	0.085

(SR1=0.85, N/O=1.0, Air Leak=0.0, K₂/S=4.4, C_j=0.0900)

unit thermal input. It is Emission Index rather than NO_x concentration which is specified in recent US government regulations.

3.2 NO_x Behavior After SCO

After the SCO, the gas flow passes through the superheater and airheater to get heat recovery. So the only operating parameter which may affect NO_x concentration along the pathway is the cooling rate. In order to cover the possible operating temperature at SCO, 1500K has been chosen since SCO temperature is always less than 1500K when CFFF system operates under the normal conditions. With 1500K of SCO and SCO gas composition of base conditions, the C_i factor was varied from 0.03 to 0.15 with step 0.03 while carrying out calculations. The results are listed in Table 3.2.1.

Table 3.2.1 shows that NO_x concentration has no change while varying the C_i from 0.03 to 0.15. It can be concluded that after temperature lower than 1500K no NO_x decomposition occurs. So NO_x concentration at SCO can be considered as the emission NO_x concentration in CFFF system.

Table 3.2.1 The Effect of Cooling Rate On NO_x After SCO

C_j	Temperature (K) (20m after SCO)	NO_x Concentration (ppm) (20m after SCO)
0.0300	1260	71
0.0600	1124	71
0.0900	1076	71
0.1200	910	71
0.1500	830	71

(SCO Temperature=1500K, SCO NO_x =71ppm)

CHAPTER 4

COMPARISON OF ANALYTICAL RESULTS WITH EXPERIMENTAL DATA

4.1 NO_x Measurement In CFFF

In CFFF system, a gas sampling system has been established to monitor the gas compositions along the system. Among the gas sampling system, there are six sampling positions which located at DFO, RFI, SCI, SCO, baghouse and stack. At these six positions NO (nitrogen monoxide) concentrations were measured at DFO, RFI and SCI, NO_x (Nitrogen monoxide and nitrogen dioxide) were measured at SCO, baghouse and stack and data were stored in computer tape and disk.

The recent test, LMF5J test, was run about 150 hours (9:30am Sep 20, 1993 to 9:30am Sep 26, 1993), 50 hours on coal and the NO/NO_x concentrations were measured about 5 hours (11:30am to 4:30pm Sep 25, 1993. The measurement at the stack did not work during LMF5J). In this 5 hour period, five test with various objectives were carried out, three for variation of primary stoichiometry, one for seed off and one for increasing air leak. The test data of NO_x concentrations in LMF5J were used to evaluate the theoretical models of NASA SP-273 and PROF code.

4.2 Comparison of Theoretical Results with Experimental Data

In order to evaluate theoretical calculations, real operating parameters should be used as the input of theoretical models when NO_x concentrations were being measured. The operating conditions of five test with various objectives of LMF5J are listed in Table 4.2.1 to 4.2.5.

4.2.1 Theoretical and Experimental Results For Changing of SR1 Before SCO

Table 4.2.1.1 shows the calculated and measured data with three different SR1. It can be seen that at three sampling positions all the calculated data are greater than the measured data and the differences between the calculated data and measured data increase as SR1 increases.

The inconsistency between calculation and experiment may be due to the further NO_x decomposition in the sampling probe[15] [16] and the deviation of measurement. The standard deviation of NO_x measurement at DFO, SCI and SCO is about 500ppm, 30ppm and 30ppm respectively. The calculated data seem much closer to the measured data at DFO than those at SCI and SCO. The reason is that the internal diameter of probe used at DFO is smaller than those used at SCI and SCO. Gas residence time in probe of DFO is less than that in probe of SCI and SCO, and the relative amount of NO_x decomposition in probe of DFO may be less than that in probe of SCI and SCO.

Table 4.2.1 Operating Conditions of SR1=0.80

Parameter	Value
Coal Flow (lb/sec)	0.835
Oil Flow (lb/sec)	0.514
Air Flow (lb/sec)	2.423
Pure O ₂ Flow (lb/sec)	2.077
Seed Flow (lb/sec)	0.120
Up Stream N ₂ (lb/sec)	0.048
Down Stream N ₂ (lb/sec)	0.281
Furnace Draft (Inch water)	-7.89
Secondary Air (lb/sec)	3.141
DFO Temperature (K)	2408
SCI Temperature (K)	1258
SCO Temperature (K)	1467

Source: LMF5J Test Report [11]

Table 4.2.2 Operating Conditions of SR1=0.85

Parameter	Value
Coal Flow (lb/sec)	0.835
Oil Flow (lb/sec)	0.462
Air Flow (lb/sec)	2.428
Pure O ₂ Flow (lb/sec)	2.075
Seed Flow (lb/sec)	0.132
Up Stream N ₂ (lb/sec)	0.048
Down Stream N ₂ (lb/sec)	0.280
Furnace Draft (Inch water)	-8.37
Secondary Air (lb/sec)	2.111
DFO Temperature (K)	2428
SCI Temperature (K)	1256
SCO Temperature (K)	1418

Source: LMF5J Test Report [11]

Table 4.2.3 Operating Conditions of SR1=0.90

Parameter	Value
Coal Flow (lb/sec)	0.834
Oil Flow (lb/sec)	0.411
Air Flow (lb/sec)	2.423
Pure O ₂ Flow (lb/sec)	2.077
Seed Flow (lb/sec)	0.145
UpStream N ₂ (lb/sec)	0.048
DownStream N ₂ (lb/sec)	0.281
Furnace Draft (Inch water)	-7.92
Secondary Air (lb/sec)	1.840
DFO Temperature (K)	2464
SCI Temperature (K)	1264
SCO Temperature (K)	1323

Source: LMF5J Test Report [11]

Table 4.2.4 Operating Conditions of Double Furnace Pressure

Parameter	Value
Coal Flow (lb/sec)	0.835
Oil Flow (lb/sec)	0.462
Air Flow (lb/sec)	2.422
Pure O ₂ Flow (lb/sec)	2.075
Seed Flow (lb/sec)	0.133
Up Stream N ₂ (lb/sec)	0.049
Down Stream N ₂ (lb/sec)	0.280
Furnace Draft (Inch water)	-15.91
Secondary Air (lb/sec)	2.269
DFO Temperature (K)	2437
SCI Temperature (K)	1275
SCO Temperature (K)	1383

Source: LMF5J Test Report [11]

Table 4.2.5 Operating Conditions at Seed Off Condition

Parameter	Value
Coal Flow (lb/sec)	0.838
Oil Flow (lb/sec)	0.462
Air Flow (lb/sec)	2.430
Pure O ₂ Flow (lb/sec)	2.077
Seed Flow (lb/sec)	0.000
Up Stream N ₂ (lb/sec)	0.045
Down Stream N ₂ (lb/sec)	0.278
Furnace Draft (Inch water)	-8.46
Secondary Air (lb/sec)	2.130
DFO Temperature (K)	2463
SCI Temperature (K)	1263
SCO Temperature (K)	1410

Source: LMF5J Test Report [11]

Table 4.2.1.1 The Relationship Between NO_x Concentration And SR1 AT DFO, SCI And SCO

SR1	NO _x At DFO (ppm)		NO _x At SCI (ppm)		NO _x At SCO (ppm)	
	Calculated	Measured	Calculated	Measured	Calculated	Measured
0.80	1291	1170	141	77	214	194
0.85	2197	2041	426	146	319	273
0.90	4134	3500	1115	414	817	578

Despite of the inconsistency between calculation and experiment, calculated data and measured data from Table 4.2.1.1 support the theoretical studies of Sec 3.1.1, in which the NO_x concentration increases significantly at DFO, SCI and SCO while SR1 increases.

From theoretical studies of Chapter 3, NO_x decomposition rate is faster at high NO_x concentration level than at low NO_x concentration level. Since SR1 increase causes NO_x concentration level increase, so the decomposition of NO_x in sampling probe increases while SR1 increases. This is why from Table 4.2.1.1 the difference between calculated data and measured data increases while SR1 increases.

4.2.2 Theoretical and Experimental Results For Variation of Furnace Draft

Before SCO

Table 4.2.2.1 shows the calculated and measured data with two different furnace draft conditions: From this table it can be seen that the calculated data are greater than the measured data, possibly due to the further NO_x decomposition in sampling probes and the deviation of NO_x measurement. However, the calculated data and measured data do prove the theoretical results of Sec 3.1.3, which NO_x concentration increases while air leak increases.

Table 4.2.2.1 The Relationship Between NO_x Concentration And Air Leak AT DFO, SCI And SCO

Furnace Draft (Inch-H ₂ O)	Air Leak (lb/sec)	NO _x At DFO (ppm)		NO _x At SCI (ppm)		NO _x At SCO (ppm)	
		Calculated	Measured	Calculated	Measured	Calculated	Measured
-8.37	0.3827	2197	2041	426	146	319	273
-15.91	0.5277	2469	2388	525	216	382	323

4.2.3 Theoretical and Experimental Results for Seed Off Before SCO

Table 4.2.3.1 shows the measured NO_x concentration and temperature data when seed is turned on and off.

Because seed off will cause the temperature of the primary combustor to be high enough possibly to damage the Busek Generator, in LMF5J test the seed off condition lasted less than 6 minutes. Within 6 minutes the effect of seed off on temperature might be detected at DFO but hardly be measured accurately at SCI and SCO due to the delay in system. This is why in Table 4.2.3.1 there is 70K temperature increasing at DFO and almost no temperature changes at SCI and SCO.

From theoretical studies of Sec 3.1.4 it has been concluded that seed does not affect NO_x concentration in CFFF. But from Table 4.2.3.1 it can be seen that NO_x concentrations increase when seed turns off. The reason is that turning seed off causes temperature increase in the system and it is the increased temperature which causes NO_x concentrations to increase. It is believed that seed alone does not affect NO_x concentration in CFFF system.

4.2.4 Theoretical and Experimental Results After SCO

Table 4.2.4.1 shows the measured data of NO_x concentration at SCO and BHO. From theoretical studies in Sec 3.2 it has been concluded that there is no NO_x decomposition occurs after SCO. But from this table it looks as if the NO_x still decomposes after SCO since the NO_x concentration becomes much

Table 4.2.3.1 The Experimental Data of Seed On And Seed Off AT DFO, SCI And SCO

	NO _x At DFO (ppm)	Temperature At DFO (K)	NO _x At SCI (ppm)	Temperature At SCI (K)	NO _x At SCO (ppm)	Temperature At SCO (K)
Seed On	2448	2429	144	1256	161	1417
Seed Off	2710	2499	200	1263	197	1411

Table 4.2.4.1 Experimental Data After SCO

	NO _x At SCO (ppm)	NO _x At BHO (ppm)
SR1=0.80	194	121
SR1=0.85	273	172
SR1=0.90	578	361
Double Furnace Draft	323	188

lower at BHO. Actually the NO_x concentration decrease after SCO is not caused by decomposition but by additional air leakage [10], since the air leakage dilutes NO_x concentration all the way along SCO to BHO. It is not surprising that measured data at BHO are much lower than those at SCO. CO_2 concentrations also decrease, while O_2 concentrations increase.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

From theoretical calculations and CFFF experimental data presented in previous chapter the following conclusions can be made:

- 1) NASA SP-273 code and PROF code together can predict NO_x behavior in CFFF system reasonably well.
- 2) Increasing of SR1, N/O and air leak will cause increasing of NO_x concentration level in CFFF system.
- 3) Seed alone does not affect NO_x concentration distribution in CFFF system.
- 4) From DFO to SCI most NO_x decomposition is achieved in the first $\frac{1}{3}$ of path way, while some NO_x decomposition continues in the remaining $\frac{2}{3}$ of path way.
- 5) NO_x decomposition does not occur after SCO.

5.2 Recommendations

Future experiment concerning effect of cooling rate on NO_x behavior is recommended. The optimum operating SCI temperature range and SCO

temperature range theoretically concluded from this thesis is waiting a proof in a future CFFF test.

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APPENDIX

APPENDIX

NO DECOMPOSITION CHEMICAL MECHANISM [2] [15]

At high temperature, the Zeldovich reactions are dominant.

At lower temperature, the first and second reactions are very slow, and other reactions become important at low stoichiometry, such as

and

etc.