STUDIES OF PARAMETRIC EMISSIONS MONITORING AND DLN COMBUSTION NOX FORMATION

by

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B.S., Kansas State University, 2002

A THESIS

submitted in partial fulfillment of the requirements for the degree

MASTER OF SCIENCE

Department of Mechanical and Nuclear Engineering
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KANSAS STATE UNIVERSITY
Manhattan, Kansas

2011

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2011
Abstract

The increased emissions monitoring requirements of industrial gas turbines have created a demand for less expensive emissions monitoring systems. Typically, emissions monitoring is performed with a Continuous Emissions Monitoring System (CEMS), which monitors emissions by direct sampling of the exhaust gas. An alternative to a CEMS is a system which predicts emissions using easily measured operating parameters. This system is referred to as a Parametric Emissions Monitoring System (PEMS). A review of the literature indicates there is no globally applicable PEMS. Because of this, a PEMS that is applicable to a variety of gas turbine manufacturers and models is desired.

The research presented herein includes a literature review of NO$_x$ reduction techniques, NO$_x$ production mechanisms, current PEMS research, and combustor modeling. Based on this preliminary research, a combustor model based on first-engineering principles was developed to describe the NO$_x$ formation process and relate NO$_x$ emissions to combustion turbine operating parameters. A review of available literature indicates that lean-premixed combustion is the most widely-used NO$_x$ reduction design strategy, so the model is based on this type of combustion system. A review of the NO$_x$ formation processes revealed four well-recognized NO$_x$ formation mechanisms: the Zeldovich, prompt, nitrous oxide, and fuel-bound nitrogen mechanisms. In lean-premixed combustion, the Zeldovich and nitrous oxide mechanisms dominate the NO$_x$ formation.

This research focuses on combustion modeling including the Zeldovich mechanism for NO$_x$ formation. The combustor model is based on the Siemens SGT-200 combustion turbine and consists of a series of well-stirred reactors. Results show that the calculated NO$_x$ is on the same order of magnitude, but less than the NO$_x$ measured in field tests. These results are expected because the NO$_x$ calculation was based only on the Zeldovich mechanism, and the literature shows that significant NO$_x$ is formed through the nitrous oxide mechanism. The model also shows appropriate trends of NO$_x$ with respect to various operating parameters including equivalence ratio, ambient temperature, humidity, and atmospheric pressure. Model refinements are suggested with the ultimate goal being integration of the model into a PEMS.
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# Nomenclature

## Variables

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<th>Symbol</th>
<th>Description</th>
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</tr>
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</tr>
<tr>
<td>d</td>
<td>Diameter</td>
<td>m</td>
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## Greek Symbols

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CHAPTER 1 - Introduction

Oxides of Nitrogen (NOx), including nitrogen monoxide (NO) and nitrogen dioxide (NO2), have long been identified as harmful atmospheric pollutants. These compounds, which are formed during the combustion of fossil fuels, are detrimental to the atmosphere in numerous ways, including:

- Environmental acidification – NOx mixes with rain water and acidifies it, creating nitric acid (HNO3). This acid rain can kill vegetation and fish as it falls onto plants and into streams. In addition, acid rain accelerates the decay of man-made outdoor structures such as buildings and statues. (Environmental Protection Agency, 2011)

- Stratospheric ozone depletion – NOx reacts with ozone and free oxygen in the atmosphere to destroy upper-level ozone, which is an ultraviolet light-blocking compound. This chemical mechanism is depicted in Figure 1.1.

- Respiratory problems - NOx is harmful to the respiratory system in three ways. Firstly, it can react with ammonia, moisture, and other compounds to form small particles. These small particles can get into the lungs and create or worsen respiratory complications

![Figure 1.1 NOx Ozone Depletion Chemical Mechanism (National Institute of Environmental Health Sciences, 2011)]
including airway inflammation in healthy people or increased symptoms in people with asthma, emphysema, and bronchitis. Secondly, NO\textsubscript{x} reacts with atmospheric oxygen to produce ground level ozone that contributes to respiratory problems through the oxidation of lung tissue. Thirdly, \( \text{NO}_2 \) itself has been deemed toxic from indoor exposure studies (Environmental Protection Agency, 2011).

Because of these harmful effects, various government agencies place restrictions on NO\textsubscript{x} emissions. These restrictions are enforced through the Clean Air Act Amendments (CAAA) of 1990, which established upper-limit standards for a number of atmospheric pollutants, including NO\textsubscript{x}. In order to prove compliance with these standards, combustion turbine operators must implement continuous NO\textsubscript{x} monitoring (Hung, 1995). The restriction on NO\textsubscript{x} emissions has led to combustion turbine technology enhancements for NO\textsubscript{x} control, while the associated requirement for continuous monitoring has lead to the demand for less expensive, more efficient emissions monitoring technologies.

Monitoring NO\textsubscript{x} from gas turbines is typically done with a complex and costly Continuous Emissions Monitoring System (CEMS). This system monitors NO\textsubscript{x} and other emissions through direct sampling of the exhaust gas. In addition to the initial cost of a CEMS, there are significant annual costs for calibration and maintenance. The typical interior of a CEMS cabinet is shown in Figure 1.2.
A less expensive and thus more desirable approach is to calculate NO\textsubscript{x} using easily measured parameters. These parameters can include ambient conditions, combustion pressure, fuel-air ratio, and gas-generator turbine exit temperature. A package consisting of the appropriate sensors, hardware, and incorporated algorithms used to calculate emissions is referred to as a Parametric Emissions Monitoring System (PEMS). A PEMS is less complex, does not require periodic calibration using costly calibration gases, and can be incorporated into existing gas turbine monitoring systems which already measure most of the appropriate parameters. Significant work has been done to develop a PEMS. However, a review of the literature indicates that the PEMS previously developed are primarily statistical based and specific to particular combustion turbine models. PEMS which are more broadly applicable do not exist.

The goal of the present research was to develop a combustion turbine model which could be used to generate correlations between NO\textsubscript{x} and appropriate operating parameters. Such a model could be applied to develop a broadly-applicable PEMS for use on a wide range of gas turbine models from multiple manufacturers. The combustor modeling techniques were based on first-engineering principles, with model inputs from a gas turbine manufacturer. The model was validated by comparing its outputs to gathered field data including gas turbine operating
parameters and NO\textsubscript{x} emissions. The development of this model required a detailed understanding of NO\textsubscript{x} formation and gas turbine combustion processes.

A thorough literature review was performed to gain an understanding of PEMS technology, NO\textsubscript{x} reduction techniques, NO\textsubscript{x} formation processes, and combustor modeling techniques. This knowledge base was necessary to establish the necessity of this research and to develop an appropriate path forward for the combustor modeling. This thesis will present a description of the work done including a description of the combustor model, a presentation of the model capabilities, and suggestions for future refinements.
CHAPTER 2 - Literature Review

The primary goal of the present research is to develop a combustor model based on first-engineering principles for calculating NO\textsubscript{x} emissions based on combustion turbine operating parameters. This type of model could ultimately be used in a PEMS. To begin this journey, an investigation of the available literature was performed to review the current PEMS technology and to develop an appropriate path for the combustor modeling.

Current PEMS Technology

The literature review of current PEMS technologies revealed a significant amount of work that has been done to develop gas-turbine PEMS. The bulk of this work was done by W.S.Y. Hung for Solar. The previously developed PEMS were primarily based on statistical analysis of CEMS data, not fundamental engineering principles.

PEMS Development by W.S.Y. Hung

Most of the work published on NO\textsubscript{x} prediction technology is by W.S.Y. Hung. In 1975, he first published a description of an analytical model used to determine NO\textsubscript{x} emissions for a specific family of conventional gas turbine combustors (Hung, 1975). Shortly after, he published a description of modifications made to the model to include the effects of water injection, operation at reduced air/fuel ratio, primary air leaning, fuel with low flame temperatures, and fuel/air premixing (Hung, 1975). Because the main feature of this model was the way in which the diffusion process was modeled, it was later referred to as the diffusion-limited mixing model. The model showed good agreement with laboratory and field data, but at that time it was only used as a design tool for NO\textsubscript{x} reduction in combustors.

Beginning in 1991, Hung published work on a PEMS in which the diffusion-limited mixing model was referenced, but not directly used (Hung, 1991). Instead, the PEMS was based on a performance and emissions program that was developed for various gas turbine models using field data on NO\textsubscript{x} emissions. The program was basically developed by gathering NO\textsubscript{x} data, correcting it to ISO (e.g. 20°F, 14.73 psia) conditions (using either EPA correlations or special expressions developed by Hung), and establishing the ISO corrected NO\textsubscript{x} as functions of fuel/air ratio and water/fuel ratio (if applicable) (Hung, 1995). User inputs of fuel type, duct
losses, elevation, combustion system, humidity, and water injection schedule are used to calculate the ISO corrected NO\textsubscript{x} as a function of ambient temperature and either power turbine inlet temperature ($T_5$) or gas producer speed. These two functions are stored in the PEMS and used to calculate NO\textsubscript{x} based on inputs of those two parameters from the gas turbine control system. The calculated NO\textsubscript{x} is corrected to ambient pressure and humidity using the same correlations used in the development of the performance and emissions program. The diffusion-limited mixing model was used to verify the performance and emissions program, but no results of this verification were provided (Hung, 1995).

At the end of 1994, Hung reported that 36 PEMS were installed on various Solar gas turbines using conventional combustion, water injection, and “SoLoNO\textsubscript{x}” (Solar’s version of lean-premixed) combustion. The relative accuracy ranged from about 2 to 12% when compared to CEMS measurements (Hung, 1995). However, because of problems with the correlations, the end-users removed most, if not all, of these PEMS.

**Other PEMS Development**

A paper on PEMS development was published by Marshall and Bautista (1997). The goal of their project was to develop CO and NO\textsubscript{x} emission algorithms for small (<20 MW) stationary gas turbines used in natural gas pipeline compression stations. The general forms of the NO\textsubscript{x} and CO predictive algorithms were said to be based on first engineering principles, but the forms of these algorithms were said to be proprietary and no details of how these algorithms were developed were described in the paper. The coefficients for these algorithms were determined based on regression analysis of data gathered with a CEMS.

The analysis was completed on data from GE Frame 3 and Rolls Royce Avon turbines so that the technique employed could be validated on engines representing old (Frame 3) and recent (Avon) technologies. The data was taken over a wide range of operating conditions and divided into a development subset and a validation subset. The coefficients and applicable operating parameters for the predictive algorithms were determined by using regression analysis on the development subset. The algorithms used parameters such as humidity, ambient temperature, exhaust gas temperature, and gas generator speed, which are all routinely monitored for process control. These applicable operating parameters were then used from the development subset to
generate NO\textsubscript{x} and CO data to be compared to the validation subset. Relative accuracy for the NO\textsubscript{x} data varied between 3 and 5%.

While the results of this work are promising, neither additional publications referencing the continued development of this technique, nor publications describing the application of these algorithms to a field-installed PEMS could be found.

A pure statistical based PEMS was developed by CMC Solutions and the result of their work was published in 2003. Their PEMS uses historical CEMS data to generate predicted emission rates. The PEMS was installed on two GE Frame 7 gas turbines which are operated in a power plant. One of the turbines was a peaking unit burning natural gas and utilizing a DLN (dry low-NO\textsubscript{x}) combustor, while the other was a base-load unit firing natural gas and/or fuel oil and utilizing steam injection for NO\textsubscript{x} reduction. The PEMS algorithm was generated using an initial 40 or 60 hours of data gathered by a CEMS. Details of the algorithm development were not provided. The final PEMS algorithm was based on an additional 720 hours of data that was gathered during the demonstration period. This type of PEMS differs from the work presented in this report in that the models are not based on the fundamental physical processes controlling NO\textsubscript{x} production.

In addition to the direct PEMS development, a number of semi-analytical expressions have been developed to determine NO\textsubscript{x} emissions from gas turbines. In 1981, Lewis published the following expression for NO\textsubscript{x} prediction from experimental flame data published by NASA:

$$\text{NO}_x = 7.50 \times 10^{-6} e^{8.28 \times 10^{-7} T}$$

This expression is a function of only flame temperature, but there are accompanying expressions for correcting this temperature based on humidity, fuel type, power, and water injection. Lewis notes that these correlations are only useful as a design tool (Lewis, 1981).

In 1994, Becker and Perkavec published a summary of four equations for NO\textsubscript{x} emission prediction. All of these equations make use of a different set of parameters and constants that were found by fitting curves to experimental or field data. The parameters include fuel/air ratio (or equivalence ratio), combustion pressure, combustion temperature, humidity, and air mass flow rate. The authors state that the four equations are limited to the gas turbine model, operating conditions, and type of fuel used at the time of the equation development. Because of these limitations, a new semi-analytical equation was developed with a minimum number of constants that need to be determined for each combustor and environment it is applicable to. The
expression is semi-analytical because it is based on a combustor energy balance used to calculate the flame temperature, but the dependence on NOx is still found by statistically analyzing the test data. The published comparison between the expression and experimental data is very good for some combustors and fuels, while not so good for others. Although it was concluded that the developed expression is effective, there are no published results of an actual PEMS installation using the correlation.

A similar paper was published in 1995 by Bakken and Skogly. Two previously developed correlations are presented, along with the following new correlation:

\[ \text{NO}_x = 62 p_3^{0.5} f^{1.4} \exp\left(-635/T_4\right) \]  

(2)

In this equation, \( T_4 \) is the combustor discharge temperature, \( f \) is the fuel-air ratio, and \( p_3 \) is the compressor discharge pressure. The new correlation was developed to include the effects of component degradation. Based on their statistical analysis, the effects of component degradation can be captured by measuring only the compressor discharge pressure, fuel/air ratio, and combustor discharge temperature. The correlation presented was implemented in the condition monitoring system of a Sleipner A installation, but the results of this effort were never published.

**NOx Reduction Techniques**

There are many widely-differing techniques for NOx reduction, all of which employ various types of combustion. Because the combustor designs involved with these various types of combustion vary greatly, the literature was reviewed to select the most common technique to be employed in the combustor model used in the present research.

A conventional combustion turbine combustor burns fuel using a diffusion flame. In this type of flame, the pure fuel and pure air combust stoichiometrically through the flame boundary. Stoichiometric combustion creates the highest peak combustion temperatures. Because NOx emissions increase exponentially with temperature, stoichiometric combustion also produces the highest concentrations of NOx (Lewis, 1981). The primary method for NOx reduction in gas turbines is to reduce peak temperatures within the combustor. Gas turbine manufacturers have developed a number of methods for doing this. The primary methods are water injection, rich burn – quick quench – lean burn (RQL) combustion, catalytic combustion, and lean-premixed combustion. Additional methods, selective catalytic combustion (SCR) and selective non-
catalytic reduction (SNCR), use chemical reactions in the post-turbine exhaust gas to convert the NO\textsubscript{x} into less-harmful compounds.

**Water Injection**

The concept behind water injection is simple: Liquid water or steam is injected into the combustor to act as a heat sink, drawing heat away from the hottest combustion products to lower their temperature and mitigate NO\textsubscript{x} formation. This procedure is very effective, offering NO\textsubscript{x} reductions up to 60 percent in natural gas burning combustors (Hilt, 1984). However, water injection has significant drawbacks. There are increased capital costs from the water injection equipment which usually includes a water treatment facility to produce the required demineralized water. The operating costs can also increase due to the additional fuel consumption necessary to heat the water to combustion temperatures, the water treatment maintenance requirements, and the additional combustion turbine maintenance requirements due to the accelerated combustor corrosion. Water injection has also been shown to increase CO (carbon monoxide) emissions, UHC (unburned hydrocarbon) emissions, and combustion pressure pulsations (Lefebvre, 1999).

**Rich Burn – Quick Quench – Lean Burn (RQL) Combustion**

RQL combustors rely on the principal that combustion temperatures, and therefore NO\textsubscript{x} production, are lower at rich and lean conditions than at stoichiometric conditions. Combustion begins in a fuel-rich primary zone followed by quenching with dilution air and further burning in a lean zone. The effectiveness of this complex process is limited by the rate at which the dilution air can quench the rich combustion products (Correa, 1991). During the transition from rich to lean combustion, the complete avoidance of brief stoichiometric conditions, and therefore high NO\textsubscript{x} production rates, is not possible.

**Catalytic Combustion**

Catalytic combustion employs various catalysts inside the combustion chamber to allow the fuel to be oxidized at temperatures and equivalence ratios below the normal lean flammability limit of the fuel-air mixture. Combustion at such low temperatures dramatically reduces NO\textsubscript{x} emissions. However, the temperatures are still high enough to approach the stability limits of most catalyst substrate materials. This shortens the catalyst life and makes the
combustor unreliable. The effectiveness of the system (NO\textsubscript{x} concentrations <5 ppm) provides incentive for researchers to overcome the durability issues of the catalytic combustor, but it has yet to become widely-used technology (Lefebvre, 1999).

**Lean-Premixed Combustion**

In a conventional diffusion-flame combustor, the hot combustion products are diluted and cooled to meet the material-limited temperature requirements of the compressor-drive turbine inlet temperature. The dilution is accomplished using excess air from the gas turbine compressor. In lean-premixed combustion, the excess air available for dilution is instead used to premix the air and fuel at a low equivalence ratio (fuel-lean) prior to combustion. This lean mixture burns at a lower temperature, thus reducing NO\textsubscript{x} emissions. Because the theoretical cycle efficiency depends only on the compressor-drive turbine inlet temperature, the point of dilution with excess air should not affect efficiency when compared to an equivalent diffusion-flame combustor.

NO\textsubscript{x} emission levels below 10 ppm have been demonstrated with lean-premixed combustion (Correa, 1991). Gas turbines using this type of combustion have difficulty operating at partial loads, but this is often overcome by operating the combustor in a diffusion flame mode during these periods, thus creating a high temperature – high NO\textsubscript{x} environment. Since partial loads in industrial gas turbines are typically only experienced during startups and transients, lean-premixed combustion is overall a highly effective NO\textsubscript{x} reduction strategy.

The concept of lean-premixed combustion (also called dry low-NO\textsubscript{x} combustion because low NO\textsubscript{x} is achieved without water injection), is used in some form by nearly every gas turbine manufacturer (Lefebvre, 1999). It is currently the most widely-used combustor design method for reducing NO\textsubscript{x} emissions from gas turbines.

**Selective Catalytic Reduction (SCR) and Selective Non-Catalytic Reduction (SNCR)**

In the SCR and SNCR technologies, NO\textsubscript{x} is converted to nitrogen and water by injecting a nitrogen-containing additive (usually ammonia) into the exhaust gas. The SCR system uses a catalyst to aid the reaction, while SNCR does not. The process is effective over a limited temperature range, so it is restricted to gas turbines that exhaust to a heat recovery device. The catalytic process has been shown to reduce NO\textsubscript{x} emissions to concentrations below 10 ppm when
combined with water injection. Major drawbacks of SCR and SNCR are the size and cost of the equipment, the performance degradation associated with the additional turbine exhaust pressure losses from the catalyst, and the complex control system with continuous monitoring required to adjust the ammonia flow based on load as excess unreacted ammonia which passes to the atmosphere is undesirable. In large-scale applications such as combined-cycle power plants, the effectiveness of these systems typically outweighs the drawbacks, making them viable NOx reduction methods. However, for smaller gas turbine applications with no heat recovery device, other methods are typically used.

**NOx Formation Processes**

“NOx” refers to the sum of NO (nitric oxide) and NO2 (nitrogen dioxide). The formation of NO2 results only from the subsequent oxidation of NO, so the total NOx (NO + NO2) is not affected by the amount of NO2 formed (Turns, 2000). Therefore, the calculation of NO is sufficient for determining total NOx and the literature review of NOx formation processes focused only on NO formation.

There are four well-recognized chemical mechanisms for NO formation. These include the Zeldovich, prompt, nitrous oxide, and fuel-bound nitrogen mechanism. The following sections provide a description of these four NO-producing chemical pathways.

**Zeldovich Mechanism**

The Zeldovich Mechanism produces NO by the reaction of atmospheric oxygen and nitrogen at elevated temperatures. The mechanism consists of two chain reactions:

\[
O + N_2 \rightleftharpoons NO + N \tag{3}
\]

\[
N + O_2 \rightleftharpoons NO + O \tag{4}
\]

These reactions can be further extended by adding the reaction:

\[
N + OH \rightleftharpoons NO + H \tag{5}
\]

This three-reaction set is known as the Extended Zeldovich Mechanism. The NO formed through the Zeldovich mechanism is commonly referred to as thermal NO because the formation rates are only significant at high temperatures (~1800+ K). This set of reactions is a widely-used and recognized mechanism for NO formation (Turns, 2000).
Prompt Mechanism

The prompt, or Fenimore mechanism, was first proposed by Fenimore in 1971 to account for NO formation that occurred very quickly in the primary reaction zone of the combustor (Fenimore, 1971). It was later found that the NO is formed from the reaction of hydrocarbon radicals present during the combustion process reacting with atmospheric nitrogen (Nicol, 1995). The primary initiating reaction is:

\[ \text{N}_2 + \text{CH} \rightleftharpoons \text{HCN} + \text{N} \]  \hspace{1cm} (6)

The N atom becomes NO through the last two reactions in the Zeldovich mechanism. The HCN route to NO is complex, but the main path is through NCO, NH, N, and then finally to NO through the same Zeldovich N atom reactions.

Nitrous Oxide Mechanism

The nitrous oxide (N\(_2\)O) mechanism was recognized by Malte and Pratt in 1974 as an important NO pathway (Corr, 1991). It is regarded as being most important in fuel-lean (\(\phi < 0.8\)), low-temperature conditions, such as those experienced in lean-premixed combustion (Turns, 2000). The three main steps of this mechanism are:

\[ \text{O} + \text{N}_2 + \text{M} \rightleftharpoons \text{N}_2\text{O} + \text{M} \]  \hspace{1cm} (7)

\[ \text{H} + \text{N}_2\text{O} \rightleftharpoons \text{NO} + \text{NH} \]  \hspace{1cm} (8)

\[ \text{O} + \text{N}_2\text{O} \rightleftharpoons \text{NO} + \text{NO} \]  \hspace{1cm} (9)

Fuel-Bound Nitrogen Mechanism

Combustors burning fuel which contains nitrogen show an increase in NO production (Toof, 1985). This increase in NO results from the conversion of the organically-bound nitrogen in the fuel to NO. The mechanism begins with the pyrolysis of the nitrogen containing fuel to HCN. The HCN then follows the same pathway to NO as the prompt mechanism. Because of this, the fuel and prompt NO are considered linked processes (Toof, 1985). This mechanism is obviously unimportant in fuels containing no nitrogen, such as natural gas, but contributes significantly when burning nitrogen containing fuels such as coal. Because the present research
focuses on gas turbine combustion with fuels containing negligible nitrogen, this mechanism is not further considered.

**Relative Contributions of Each Mechanism**

There are several publications by various authors that analyze the relative contribution of each NO$_x$ mechanism for different fuels, conditions, and combustion types. Many of these studies involve the analysis of lean-premixed combustion because of its popularity as a NO$_x$ reduction strategy.

Correa and Smooke (1990) performed a number of experiments and numerical simulations to determine the relative contributions of the thermal, nitrous oxide, and prompt NO mechanisms. An early study used experimental NO$_x$ data taken from turbulent, premixed methane-air flames using a perforated-plate burner and compared this data to results from a numerical modeling study which used a well-stirred reactor (WSR) followed by a plug flow reactor (PFR) combined with a kinetic scheme including the Zeldovich and prompt mechanisms. The results of the study showed that the prompt mechanism dominates below a flame temperature of about 1800K (Leonard, 1990). The study also concluded that NO varies as the square-root of pressure in near-stoichiometric premixed flames, but is independent of pressure in flames below an equivalence ratio of about 0.75. Another pure numerical study was performed for premixed laminar methane-air flames under various conditions (Correa, 1990). This study used the Miller-Bowman mechanism for methane combustion and NO formation, which includes the Zeldovich, prompt, and now also the nitrous oxide NO mechanisms (Miller, 1989). The study also concluded that thermal NO$_x$ dominated in the near-stoichiometric flames, but that the nitrous oxide mechanism is predominant in lean-premixed, laminar flames. The absence of pressure dependence in very lean flames was also confirmed.

Corr et al. (1991) presented results from experiments conducted at the University of Washington using a jet-stirred reactor operating at atmospheric pressure that was fired with ethylene and methane using premixed and non-premixed flames. Both NO and NO$_2$ were measured, and the contribution of each mechanism was deduced from the calculated free radical concentration that would be required to produce the measured NO$_x$. Both the Zeldovich and nitrous oxide mechanisms rely on the O atom radical for initiation of the reactions, while the prompt mechanism requires the CH radical. The study concluded that unreasonable O atom
concentrations would be necessary for the NO\textsubscript{x} to be formed by either the Zeldovich or nitrous oxide mechanisms, but that the CH concentrations were reasonable based on an accompanying numerical study which used select reactions from the Miller-Bowman mechanism. Because of these findings, it was concluded that the prompt NO mechanism was dominant (Corr, 1991).

Later work done by Nicol et al. (1995), also at the University of Washington, indicates that the nitrous oxide and Zeldovich mechanisms are equally important in high-pressure lean-premixed methane combustion, while the prompt mechanism is practically negligible. Modeling was performed using a WSR to represent the flame zone and a PFR for the post-flame zone. Three different kinetic mechanisms were used, including the previously mentioned Miller-Bowman scheme, and all showed similar trends. The modeling efforts were verified from porous-plate burner experiments. The result also indicates that for temperatures, pressures, and equivalence ratios capable of producing NO less than 10 ppmv, the relative contribution of the nitrous oxide mechanism increases steeply and approaches 100 percent. However, for atmospheric combustion, all three pathways contribute similar amounts, and none can be dismissed.

These conclusions differ from the earlier ones of Corr et al. (1991) which determined that the prompt mechanism was most dominant. The discrepancy was likely because the Corr study used only select reactions from the Miller-Bowman mechanism which caused the scheme to neglect the super-equilibrium concentration possibilities for the O and OH atoms. These super-equilibrium concentrations can exist at up to 1000 times the equilibrium concentrations in flame regions, and this high concentration possibility could perhaps accommodate the high O atom requirement calculated in their study to produce the measured NO\textsubscript{x} from the Zeldovich or nitrous oxide mechanisms. This type of NO formation is sometimes linked to the prompt mechanism because it takes place early in the flame front, but the pathway is still that of the Zeldovich mechanism (Turns, 2000).

**Conclusion of Literature Review**

Based on this review of the current PEMS technology it is clear that the objective of the present research is warranted. There have been sporadic PEMS developments but none have become accepted in the gas turbine industry. Industry feedback indicates that the few PEMS predictive algorithms developed are not reliable. The premise for the research presented herein
is that the failure of the existing algorithms is because they were developed primarily using statistical CEMS and operating data, not fundamental principles. The fundamental-principle based correlations should be more reliable as they would account for unforeseen variations in operating parameters and/or turbine degradation that could not be captured during the relatively brief operating periods when the statistical-based PEMS correlations were developed.

Based on the literature review of NO\textsubscript{x} reduction techniques, lean-premixed combustion is the most widely used combustor-based technology. Because of this, the combustion model developed as part of this research was based on lean-premixed combustion. Although selective catalytic reduction is also used, it is applied external to the combustion process making it irrelevant to this research.

The conclusion drawn from the review of the studies to determine the relative contributions of the NO\textsubscript{x} chemical mechanisms is that the Zeldovich and nitrous oxide mechanisms are the most important for lean-premixed combustion at gas turbine operating conditions, while the prompt mechanism makes insignificant contributions. These results are largely based on combustor modeling using the most accepted chemical kinetic mechanisms available. In addition, the most accurate method for NO calculation should use a complete kinetic scheme that models both the combustion process and nitric oxide formation. The lean-premixed combustor model selected will employ the Zeldovich mechanism for NO prediction. The remainder of this thesis focuses on the development of a combustor model, the validation of this model using field test data, and parametric studies of data generated from the model.
CHAPTER 3 - Combustor Model Development

Based on the literature review of NO\textsubscript{x} reduction technology and NO formation processes, the combustor process modeled was lean-premixed combustion with NO formation modeled by the extended Zeldovich mechanism. This chapter focuses on describing the detailed design of the combustor model including all engineering principles used.

**Combustor Model Arrangements**

The previously discussed study by Nicol et al. (1995) at the University of Washington described modeling combustion with a WSR for flame stabilization, followed by a PFR. A WSR (well-stirred reactor, sometimes called PSR or perfectly stirred reactor) is a one-dimensional control volume in which perfect instantaneous mixing of all species is assumed. The control volume is also assumed to have uniform temperature and pressure, and the gaseous species are assumed to behave as ideal gases. A PFR (plug-flow reactor) represents an ideal reactor in steady-state, with steady-flow. It is also assumed that there is no mixing in the axial (or flow) direction, and that the mixture properties are uniform in the radial direction. Ideal frictionless flow, and ideal gas behavior is also assumed.

The modeling method used by Nicol et al. is one of many potential ideal-reactor schemes for modeling an axial-flow combustor. Some other arrangements are shown in Figure 3.1.

![Figure 3.1 Ideal Reactor Arrangement Examples for Combustor Modeling](image)

(1a) 

(1b) 

(1c) 

(1d)
Arrangement 1a shows the simplest combustor model, which is a lone WSR. This model is very limited in that only one temperature, pressure, and species concentration can be calculated. Because of the temperature gradients, a single WSR is not conducive for representing the conditions of a real combustor. Arrangement 1b shows the combination of reactors that were previously mentioned, the WSR followed by a PFR. This combination better represents the actual combustion, in that combustion takes place in the WSR followed by a PFR for modeling the kinetics of the combustion products, which is where much of the NO is formed. A temperature profile to better match actual combustor conditions can be achieved with this arrangement, since a result of the PFR model is the distribution of temperature with respect to axial distance. An even better arrangement is shown in Arrangement 1c. This model has a second WSR to model the secondary combustion zone, and a recycle path on the first WSR to model the recirculation flow path that occurs in combustors for flame stabilization. The last possibility shown in Arrangement 1d is a series of WSR’s. This arrangement is very flexible because the number, size, flow paths, and properties of the WSR’s can be adjusted to fit various combustor types. More complex arrangements of parallel reactors are proposed by Rizk and Mongia (1993) to include radial effects within the combustion zone.

**Description of Developed Combustor Model**

The present research focuses on modeling the Siemens SGT-200 (formerly known as the Tornado DLE) gas-turbine combustor. This combustor uses a lean-premixed combustion system burning natural gas. Siemens refers to their lean-premixed combustion system as “dry-low emission” (DLE). The turbine is a single-shaft industrial gas turbine which uses twelve (12) of the DLE combustors in a can arrangement. The unit is capable of 7.7 MW of power when used as a mechanical drive (Siemens, 2011). Sketches of the SGT-200 and a typical combustor can arrangement are shown in Figure 3.2 and Figure 3.3.
Although the can arrangement consists of multiple combustors per engine, only one combustor was modeled in the program. This is acceptable for NO calculations, because each combustor can should produce the same emissions concentration. If an emissions mass flow calculation was performed then the calculated number would need to be multiplied by the number of combustor cans.

Figure 3.4 illustrates a model of a single can that is developed with a series of WSR’s to represent the combustion zone. Outside and concentric to this is another series of WSR’s that represent the combustion liner cooling air. The modeling is done with the aid of information from Siemens regarding the ratio of combustion air to cooling air, velocities through the
The series of WSR’s method of combustor modeling was chosen for its previously mentioned flexibility and the ease of calculation when compared to PFR’s. The additional capability of velocity calculation that is provided from a PFR calculation is not necessary since this information is already known. The solution of the mathematics representing the physics of the combustion process is accomplished using a developed FORTRAN program. A graphical representation of the model is shown in Figure 3.4.

Figure 3.4 Combustor Model Diagram
Air/Fuel Chemistry Calculations

The turbine inlet air is assumed to be composed of oxygen, nitrogen, and water vapor. The amount of water vapor initially present is based on the user input of relative humidity. The fuel, which is pure methane, is allowed to partially react in each zone. This leads to the following stoichiometric chemical relationship for each combustion zone:

$$z_r CH_4 + a_1 O_2 + a_2 N_2 + a_3 H_2 O + a_4 CO_2 \rightarrow b CO_2 + c H_2 O + d N_2 + e O_2 + z_p CH_4$$  \hspace{1cm} (10)

The coefficient $z_r$, which varies between 0 and 1, represents the fraction of the total amount of reactant fuel that is oxidized in the given zone. These fractions are an input to the combustor model for each region. The corresponding value of $z_p$ is the remaining fuel fraction in the combustion zone products. The initial value of $a$ is found from the equivalence ratio by:

$$a = \frac{\text{MW}_f}{4.76 \phi f_{\text{sto}}, \text{MW}_a}$$ \hspace{1cm} (11)

The initial $a_1$ is found from the known molar concentration of air by:

$$a_1 = 3.76a$$ \hspace{1cm} (12)

Now $a_2$ is found using the ambient relative humidity and corresponding water vapor pressure:

$$a_2 = a \left\{ 1.608 \times \frac{0.622 P_{\text{sat}} \text{RH}}{P_{\text{atm}}} \right\}$$ \hspace{1cm} (13)

The carbon dioxide coefficient, $a_3$, is initially zero. The coefficients $z_r$, $a$, $a_2$, and $a_3$ vary throughout the downstream combustor zones as the fuel and oxygen is consumed and converted to carbon dioxide and water. With $z_p$ known from user input, the remaining product coefficients are found by balancing the C, O, H, and N atoms. The results of this are as follows:
\[ b = z_r + a_z - z_p \]  
\[ c = 2z_r + a_z - 2z_p \]  
\[ d = a_z \]  
\[ e = \frac{2a + a_z + 2a_z - 2b - c}{2} \]  

Since all product coefficients are known, the mole fractions of all five product species (CO₂, H₂O, N₂, O₂, and CH₄) can be calculated for each zone. These values are used for later temperature and NOₓ formation calculations. Finally, the products are carried over as reactants to the subsequent zone so the atom balancing and mole fraction determinations can be repeated until the values are known for all reactor zones.

**Temperature and Pressure Calculations**

Figure 3.5 represents the standard gas turbine numbering convention which will be used to designate conditions at the corresponding locations.

**Compressor Discharge**

Region 3 represents the compressor discharge conditions. The pressure and temperature for region 3 are calculated based on the ambient conditions, compressor pressure ratio, and compressor isentropic efficiency. The compressor discharge pressure is given by:

\[ p_3 = PR(p_2) \]

To calculate the compressor discharge temperature, the isentropic temperature \( T_{3s} \) is first calculated:

\[ T_{3s} = T_2 \left( PR \right)^{\frac{k-1}{k}} \]

The actual temperature \( T_3 \) is determined from the isentropic efficiency relationship:
\[ T_3 = \frac{T_{3x} - T_1}{\eta_{comp}} + T_1 \]  

(20)

**Combustor Discharge**

The combustor is assumed to incur no pressure loss, so the combustor discharge pressure equals the compressor discharge pressure.

\[ p_4 = p_3 \]  

(21)

To determine the temperature of the combustor discharge, the temperatures of the combustion and cooling air zones must be solved iteratively along the entire length of combustor. The temperatures of the combustion and cooling air zones are designated in Figure 3.4. To solve for these temperatures, an energy balance is applied to each zone. For each zone (cooling air or combustion), the energy balance is:

\[ \frac{q_{\text{conv,rad}}}{n_f} = \bar{h}_p - \bar{h}_r \]  

(22)

In this equation, \( q_{\text{conv,rad}} \) represents the heat transfer from the combustion zone as shown in Figure 3.4. The molar fuel flowrate is based on the fuel-air ratio and the mass flow rate of air. This term can be solved explicitly based on known parameters and is given by:

\[ \dot{n}_f = \left( \frac{P_c MW_a}{R_u T} \right) V A f_{act} \frac{MW_f}{MW_f} \]  

(23)

The right hand side of equation (22) represents the energy entering and leaving a zone, while the left hand side represents the heat transfer to or from the zone. More specifically, the right hand side is the reactant (incoming) and product (exiting) specific molar enthalpies. For a cooling air zone, the reactant and product enthalpies simply represent the inlet and outlet conditions of a cooling air region, since there are no chemical reactions taking place. For a combustion zone, the absolute enthalpies of the incoming reactants and outgoing products are calculated from the enthalpy of formation and sensible enthalpy of each chemical species:

\[ \bar{h} = \bar{h}_f^0 + \Delta \bar{h}_i(T_i) \]  

(24)

The sensible enthalpy is calculated by integrating the specific heat over the temperature range between the reference temperature, and the actual temperature:
\[ \Delta \bar{H}_f(T_r) = \int_{T_{ro}}^{T_r} \bar{C}_p dT \quad (25) \]

The relationship for \( \bar{C}_p \), from Moran and Shapiro (1999), is generically given as:
\[ \bar{C}_p = R(\alpha + \beta T + \gamma T^2 + \delta T^3 + \varepsilon T^4) \quad (26) \]

The values of the Greek constants are available for various chemical species.

Summing the absolute enthalpies for all products and reactants completes the right side of equation (22). However, as noted in equation (24), the enthalpy of formation is dependent on a known reference temperature, while the sensible enthalpy is a function of the species temperature. The reactant species temperature is assumed to be that of the preceding zone (or \( T_3 \) for the initial zones), while the product species temperature (which is also assumed to be the temperature of the current zone) is unknown. To solve for this unknown temperature, the heat transfer to and from the zone, which is also a function of the product species temperature, must be analyzed.

The heat transfer term on the left hand side of equation (22) designates the radiative and convective heat transfers from a combustion zone. This term can be broken down further as the separate radiative and convective fluxes multiplied by the segmental area over which the heat transfer takes place:
\[ q_{\text{conv,rad}} = A \left( q_{\text{conv}} + q_{\text{rad}} \right) \quad (27) \]

The area, \( A \), is the area of the combustion chamber liner section for a given combustion zone. These areas are calculated based on the user-chosen segmentation of the overall combustor and the manufacturer-provided combustor diameter. Because the heat transfer from a combustion zone flows into a cooling air zone, the entire thermal resistance from the combustion zone, through the liner wall, and into the cooling air zone must be considered to get an accurate temperature for the combustion zone. In addition, heat transfer from the cooling air zone to the ambient is considered to ensure that the temperature of the cooling air zone remains accurate as the cooling air flows down the length of the combustor. The following sections will describe the analysis of these heat transfer modes through the combustor.
Heat Transfer from Combustion Gases to Cooling Air

Heat transfer from a combustion zone to a cooling air zone is modeled in three parts (see Figure 3.6):

1. Heat transfer from combustion products to combustor liner inner wall
   - Radiation ($q_{rad,1}$)
   - Convection ($q_{conv,1}$)

2. Heat transfer through liner wall ($q_{cond,12}$)

3. Heat transfer from combustion liner outer wall to cooling air
   - Radiation ($q_{rad,2}$)
   - Convection ($q_{conv,2}$)

Figure 3.6 Combustor Heat Transfer Arrangement

Heat Transfer from Combustion Gases to Combustor Liner Inner Wall, Radiation

The radiation from the combustion products to the combustor liner wall is calculated using the method outlined in Lefebvre’s *Gas Turbine Combustion* book, which considers the combustion products as non-luminous gases (Lefebvre, 1999). The radiative flux is calculated as:
\[ q_{\text{rad},1} = 0.5\sigma (1 + \varepsilon_w) \varepsilon_g T_i^{1.5} \left( T_i^{2.5} - T_{w1}^{2.5} \right) \]  

The parameter \( \sigma \) is the Stefan-Boltzman constant, \( \varepsilon_w \) is the emissivity of the wall, \( \varepsilon_g \) is the emissivity of the gas, \( T_i \) is the temperature of the gas in the zone being considered, and \( T_{w1} \) is the inner liner-wall temperature.

An expression for the emissivity of the gas is also provided:

\[ \varepsilon_g = 1 - \exp \left[ -290 p \left( l_b f \right)^{0.5} T_i^{-1.5} L \right] \]  

(29)

Where \( p \) is the gas pressure in kPa, \( l_b \) is the average beam length in meters, \( f \) is the fuel/air ratio by mass, and \( L \) is a unitless luminosity factor to account for the luminosity of the soot particles formed during hydrocarbon fuel combustion. Many different expressions exist for the luminosity factor, but Lefebvre recommends the following expression:

\[ L = \frac{336}{H^2} \]  

(30)

In this expression, \( H \) is the percentage of hydrogen by mass in the fuel. Lastly, the average beam length for tubular systems is given by:

\[ l_b = 3.4 \times \frac{V}{A} \]  

(31)

**Heat Transfer from Combustion Gases to Combustor Liner Wall, Convection**

For the purposes of calculating the convective heat flux, the combustor liner is treated as a straight pipe. There are many expressions used to calculate convective heat transfer within a cylindrical pipe, but Lefebvre recommends the following expression, which is based on a turbulent Reynolds number:

\[ q_{\text{conv},1} = 0.020 \frac{k_g}{d_h^{0.2}} \left( \frac{\dot{m}_g}{A_L \mu_g} \right)^{0.8} (T_i - T_{w1}) \]  

(32)

In this expression, \( \dot{m}_g \) is the mass flow rate of the combustion gases, \( A_L \) is the cross-sectional area of the liner, \( k_g \) is the thermal conductivity of the combustion gases given by:

\[ k = \frac{2.495 \times 10^{-3} T^{1.5}}{T + 194} \]  

(33)

The dynamic viscosity of the gas, \( \mu_g \), in units of Pa-s, is given by:
The temperature used in this equation is again in Kelvin. The final parameter, \( d_h \), is the hydraulic diameter given by:

\[
d_h = 4 \frac{A_l}{P_{wetted}}
\]

The constant in equation (32) is lowered from 0.020 to 0.017 in the first zone calculations to account for the gas flow reversal (to stabilize the flame) and the greatly reduced gas temperature near the liner wall.

### Heat Transfer Through Liner Wall

Heat transfer through the liner wall is modeled as one-dimensional conduction and is given by:

\[
q_{\text{cond},12} = \frac{k_w}{t_w}(T_{w1} - T_{w2})
\]

The thermal conductivity of the liner wall material is given by \( k_w \) with \( t_w \) as the wall thickness.

### Heat Transfer from Combustion Liner Outer Wall to Cooling Air, Radiation

The heat transfer from the combustion liner outer wall to the cooling air can be expressed as:

\[
q_{\text{rad},2} = 0.6\sigma(T_{w2}^4 - T_{ci}^4)
\]

Here, \( T_{ci} \) is the cooling air zone temperature. This equation assumes the following:

- Cooling air temperature equals temperature of outer casing.
- Radiative shape factor equal to unity.
- Ratio of liner wall area to casing surface area equals 0.8.
Heat Transfer from Combustion Liner Outer Wall to Cooling Air, Convection

Convection between the hot liner outer wall and the cooling air in the annulus air space between the liner and the casing is modeled assuming fully turbulent flow. The equation is:

\[ q_{\text{conv,2}} = 0.020 \frac{k}{d_h^{0.2}} \left( \frac{m_c}{A_f \mu_r} \right)^{0.8} (T_{ci} - T_{w2}) \]  

(38)

Overall Heat Transfer

All parameters in the energy balance, equation (22), are known except for \( T_i \) and \( \bar{h}_p \), which is a function of \( T_i, T_{ci}, T_{w1}, \) and \( T_{w2} \). Rewriting equation (22) to show the temperature dependencies gives:

\[ \frac{q_{\text{conv,rad}}(T_i, T_{ci}, T_{w1}, T_{w2})}{\dot{n}_f} = \bar{h}_p(T_i) - \bar{h}_r \]  

(39)

Equation (39) represents the four unknowns in a specific zone, while Table 3.1 outlines these unknowns and the sets of equations solved to calculate them.

Table 3.1 Combustor Model Unknowns and Equations

<table>
<thead>
<tr>
<th>UNKNOWNS</th>
<th>PRIMARY EQUATIONS</th>
<th>DESCRIPTION</th>
</tr>
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<tbody>
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<td>( T_i )</td>
<td>(22), (28), (32)</td>
<td>COMBUSTION ZONE ENERGY BALANCE</td>
</tr>
<tr>
<td>( T_{ci} )</td>
<td>(22), (37), (38)</td>
<td>COOLING AIR ZONE ENERGY BALANCE</td>
</tr>
<tr>
<td>( T_{w1} )</td>
<td>(10)</td>
<td>COMBUSTION CHEMISTRY</td>
</tr>
<tr>
<td>( T_{w2} )</td>
<td>(36)</td>
<td>COMBUSTION AND COOLING AIR ZONE INTERFACE</td>
</tr>
</tbody>
</table>
These primary equations and the relevant secondary equations are solved numerically for the four unknown temperatures. The previous section outlined how to calculate a single set of temperatures for one pair of combustion/cooling air zones. The following section describes how the combustion and cooling air zones are iterated in the calculation scheme to find all of the unknown temperatures along the entire length of the combustor.

**Combustion and Cooling Air Zone Temperature Calculation Scheme**

The first cooling air zone and the reactant temperatures in the first combustion zone are assumed to be the same temperature as the compressor discharge, $T_3$ (see Figure 3.4). This is the starting point for the combustion and cooling air zone temperature calculations.

The combustion zone reactant enthalpies ($h_r$ term, equation (22)) for the first zone are calculated using the compressor discharge temperature, $T_3$. The product temperatures are solved iteratively using the equations for the dissipated heat transfer through the liner wall to the cooling air zone, as well as the product enthalpy term in the energy balance ($h_p$ term, equation (22)).

The heat transfer calculated from the combustion zone is assumed to be transferred to the subsequent cooling air zone. The incoming “reactant” enthalpy in a cooling air zone is calculated using the temperature of the previous cooling air zone. Using this heat transfer, the ambient heat transfer and “product” enthalpy is solved iteratively to find the temperature of the cooling air zone. The temperature is iterated in increments which can be specified by the user, with a default of 0.1 deg. K.

The calculation scheme progresses to the next combustion zone using the most recently calculated cooling air zone temperature as the heat transfer medium. This is continued through the length of the combustor until all zone temperatures are calculated. The calculation sequence described above is indicated by the numbered circles on Figure 3.4.

**Combustor Discharge Temperature Calculation**

The previous section described the temperature calculations for the individual combustion and cooling air zones. After exiting the combustion chamber, the combustion gases are mixed with the cooling air. The temperature of this mixture is $T_4$, the combustor discharge temperature. This temperature is calculated from an energy balance on the combustor exit including the cooling air and combustion air:
\[ \dot{m}_e h_4 = \dot{m}_{e,i} h_{e,i} + \dot{m}_{\text{combp}} h_{\text{combp}} \]  

(40)

A parameter \( r \), which is provided from the combustor manufacturer, is defined as the ratio of combustion air to cooling air:

\[ r \equiv \frac{\dot{m}_{\text{comba}}}{\dot{m}_{e,i}} \]  

(41)

Substituting this expression, along with \( \dot{m}_{e,i} = \dot{m}_{e,j} \), gives the result:

\[ rh_{\text{combp}} + h_c = (r + 1)h_4 \]  

(42)

The combustor exit enthalpy, \( h_4 \), is a function of the temperature \( T_4 \). This equation can also be solved iteratively using Newton’s method until the converged \( T_4 \) is determined.

**Gas Generator Turbine Discharge**

The temperature \( T_5 \) (gas-generator turbine outlet temperature) is determined based on using a coupled compressor-turbine such that the compressor work equals the gas-generator turbine work. If the gas-generator turbine operates isentropically, the energy balance expression for this coupled arrangement reduces to:

\[ h_5 - h_2 = (1 + f)(h_4 - h_{5s}) \]  

(43)

In this expression, the only unknown is \( h_{5s} \). This is the enthalpy that would occur if the gas-generator turbine operated isentropically. To find the actual enthalpy, \( h_5 \), the gas-generator turbine isentropic efficiency is used:

\[ h_5 = h_4 - \eta_{\text{turb}} (h_4 - h_{5s}) \]  

(44)

The temperature \( T_5 \) can now be calculated from the known \( h_5 \).

**NOx Concentration Calculation**

The equations to calculate the temperature profile of the gas turbine, including the segmented combustor, have now been developed. However, in order to calculate the NO concentration, a relationship between the combustion temperature and species concentrations must be used.
**NO Relationship**

In Chapter 2 it was concluded that the Extended Zeldovich Mechanism is the dominant chemical process for NO formation in lean-premixed combustion. Again, this chemical mechanism consists of three reactions; equations (3), (4), and (5).

With certain assumptions, the first two reactions (generally considered the most important) can be used to create a simple expression for the rate of NO formation. Reaction 2 has a much faster reaction rate than reaction 1, so the N atom can be assumed to be in steady state. In addition, the NO formation process is assumed to be much slower than the combustion process; this allows the assumption that the elements affecting the formation of NO are in their equilibrium concentrations during the NO formation process (Turns, 2000). With these assumptions, the rate of NO formation can be expressed by (Heywood, 1988):

\[
\frac{d[NO]}{dt} = \frac{2R_1 \left\{1-\left([NO]/[NO]_e\right)^2\right\}}{1+\left([NO]/[NO]_e\right)R_1/(R_2 + R_3)}
\]  

(45)

The \( R \) parameters are based on the forward kinetic reaction rate constants for the three reactions in the Extended Zeldovich Mechanism and the equilibrium concentrations of the applicable species:

\[
R_1 = k_{f,1}^+ [O]_e [N_2]_e
\]  

(46)

\[
R_2 = k_{f,2}^+ [N]_e [O_2]_e
\]  

(47)

\[
R_3 = k_{f,3}^+ [N]_e [OH]_e
\]  

(48)

The kinetic rate constants are based on the temperature of the reacting mixture and are readily available for each reaction.

**Determination of Equilibrium Subspecies**

Because the equilibrium concentrations of the combustion sub-species are not part of the global combustion reaction (equation (10)) used to calculate zone temperatures, a separate combustion equilibrium subroutine is necessary to calculate these concentrations. This subroutine was extracted from software that was provided with the textbook *An Introduction to Combustion* (Turns, 2000). The software calculates the equilibrium products of combustion for a
fuel composed of C, H, O, and N atoms using the method of equilibrium constants, along with
six gas-phase equilibrium reactions. Eleven species are considered in the products of
combustion: H, O, N, H₂, OH, CO, NO, O₂, H₂O, CO₂, and N₂. Included in these species are
those necessary for the determination of the NO formation rate in equation (45). The routine
requires an input of fuel composition (model input), temperature (previously calculated),
pressure (assumed constant from compressor), gas enthalpy (calculated from known temperature
and bulk species composition), and equivalence ratio (model input).

The subroutine just described is written assuming complete combustion. As described
previously, the combustor model is divided into a series of WSR’s with partial combustion
taking place in the initial zones until all fuel is consumed. The method of calculating
combustion equilibrium with equilibrium constants is not conducive to this type of arrangement.
However, based on preliminary model runs in comparison to Siemens’ CFD analysis of the SGT-
200 combustor (See Figure 3.7), it was determined that most (> 90%) of the fuel must be
consumed in the first zone. This allows for the assumption that the mole fractions of the species
affecting NO formation are constant through the remaining zones. The concentrations are still
allowed to vary based on temperature differences.
Implementation of the NO Relationship

Equation (45) is a relatively simple expression that can be used to calculate the NO formation rate when the temperature and equilibrium concentrations of the applicable species are known. Using this formation rate, concentration of NO can be determined in each zone.

To translate from a NO formation rate to a NO concentration, a residence time is calculated for each zone based on the gas velocity and cross-sectional area:

$$\tau = \frac{A_s}{V}$$

(49)

This residence time allows for the calculation of the change in NO concentration for each zone:
\[
\Delta [\text{NO}] = \frac{2R_t \left( 1 - \left[ \frac{[\text{NO}]}{[\text{NO}_e]} \right]^2 \right)}{1 + \left[ \frac{[\text{NO}]}{[\text{NO}_e]} \right] R_t / \left( R_2 + R_3 \right)} \tau \tag{50}
\]

Again, this calculation assumes that the combustion process is not coupled with the NO formation process. Summing the changes in NO concentration for each zone results in a total NO concentration in the final combustion zone.

**NO Mole Fraction Calculation**

Using equation (50) the NO concentration is calculated in a mole per volume basis. To convert this to a mole fraction, the following equation based on the ideal gas law is used.

\[
\chi_{\text{NO,comb}} = \frac{[\text{NO}] R T_{\text{comb}}}{p} \tag{51}
\]

This mole fraction of NO is typically multiplied by \(10^6\) and denoted as “ppmvw”. This is meant to indicate “parts per million by volume, wet”. Using parts per million allows the emissions to be reported in easily communicable numbers, while the “by volume” notation is typical for gaseous concentrations, and is equivalent to mole fractions. In addition, the concentrations may be expressed on a wet or dry basis depending on whether water is accounted for in the combustion products. The natural combustion process produces water vapor in the combustion products, thus the NO concentration in the exhaust stream is a wet basis by default. However, CEMS analyzers require dry samples, so they typically report emission concentrations with a dry basis.

Equation (51) gives the NO concentration in the final combustion zone. To calculate the NO concentration at the combustor discharge, the dilution of the cooling air must be accounted for. The total NO concentration, after dilution of cooling air, can be written as:

\[
\chi_{\text{NO,tot}} = \frac{\dot{n}_{\text{NO,comb}} + \dot{n}_{\text{NO,c}}}{\dot{n}_{\text{comb}} + \dot{n}_c + \dot{n}_f} \tag{52}
\]

Using the defined ratio of combustion air to cooling air (equation (41)), the fuel-air ratio, and the fact that there is zero NO in the cooling air, equation (52) becomes:
The NO concentration in the combustion products, equation (51), can also be defined as:

\[ \chi_{\text{NO,combp}} = \frac{n_{\text{NO,combp}}}{n_{\text{combp}}} \]  

(54)

Substituting into equation (53) yields:

\[ \chi_{\text{NO,tot}} = \frac{\chi_{\text{NO,combp}}}{1 + \frac{1}{r} + \frac{MW_{\text{fuel}}}{MW_{\text{air,f}}}} \]

(55)

Equation (55) allows the conversion from NO concentration in the combustion products to the overall NO concentration after dilution by the cooling air.

**NO Concentration Conversion to Reference Values**

To provide a consistent reference point to account for varying dilution and pressures, NO\(_x\) concentrations are typically corrected to specific oxygen levels. The general equation for this conversion from one oxygen level to another is as follows:

\[ \chi_{\text{NO,O}_2,2} = \chi_{\text{NO,O}_2,1} \frac{N_{\text{mix,O}_2,1}}{N_{\text{mix,O}_2,2}} \]

(56)

Where \(N\), the total number of moles in the combustion product mixture, can be calculated by:

\[ N_{\text{mix}} = 4.76 \left[ \frac{b + (1 + \chi_{\text{O}_2})}{1 - 4.76 \chi_{\text{O}_2}} \right] + 1 \]

(57)

The “\(b\)” term is the CO\(_2\) molar product coefficient from the combustion reaction equation (10). The O\(_2\) mole fraction is calculated using the coefficients from this same equation and can be calculated on a wet or dry basis:
\[ \chi_{O_2,\text{wet}} = \frac{e^{\text{tot}}}{b^{\text{tot}} + c^{\text{tot}} + d^{\text{tot}} + e^{\text{tot}}} \]  

(58)

\[ \chi_{O_2,\text{dry}} = \frac{e^{\text{tot}}}{b^{\text{tot}} + d^{\text{tot}} + e^{\text{tot}}} \]  

(59)

The “tot” subscripts are necessary because the combustion product coefficients must be reevaluated for this analysis to account for the cooling air dilution. This is done by calculating a total fuel-air ratio:

\[ f^{\text{tot}} = f (1 + r) \]  

(60)

Equation (11), the reacting oxygen molar coefficient, can now be rewritten as:

\[ a^{\text{tot}} = \frac{MW_f}{4.76 f^{\text{tot}} MW_a} \]  

(61)

The subsequent reactant and product coefficients can be calculated using the method described by equations (12) through (17). Finally, to convert between wet and dry concentrations:

\[ \chi_{O_2,\text{dry}} = \chi_{O_2,\text{wet}} \frac{N_{\text{m}a,\text{wet}}}{N_{\text{m}a,\text{dry}}} \]  

(62)

This set of equations allows the NO calculations performed in the combustion modeling program to be converted to industry-standard measurement references.

**Modeling Program Description**

The subsequent sections outlined the equations and methods used to develop the combustor model. Implementing these equations and methods into an executable computer program was done concurrently in steps of increasing complexity. The combustor modeling computer program was named Kombust. Table 3.2 summarizes the revision notes for the Kombust program.
## Table 3.2 Kombust Revision Notes

<table>
<thead>
<tr>
<th>Kombust Version</th>
<th>Revision Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>Original</td>
</tr>
<tr>
<td>1.1</td>
<td>Used Cp functions from Van Wylen and Sonntag (valid to 3500K) instead of Moran and Shapiro (valid to 1000K).</td>
</tr>
<tr>
<td>1.2</td>
<td>Added ambient humidity into combustion chemical reaction.</td>
</tr>
<tr>
<td>2.0</td>
<td>Incorporated specific component enthalpy change functions.</td>
</tr>
<tr>
<td>2.1</td>
<td>Developed multi-zone combustion.</td>
</tr>
<tr>
<td>2.2</td>
<td>Added heat transfer effects between combustion and cooling zones.</td>
</tr>
<tr>
<td>2.3</td>
<td>Added Carvalho NOₓ Model.</td>
</tr>
<tr>
<td>3.0</td>
<td>Integrated TPEQUIL, equilibrium combustion routine from combustion book by Turns, replaced Carvalho NOₓ model with Heywood NOₓ model using equilibrium concentrations from TPEQUIL.</td>
</tr>
<tr>
<td>3.1</td>
<td>Use TPEQUIL equilibrium routine assuming cumulative radical concentrations in combusting zones and constant concentrations in non-combusting zones.</td>
</tr>
<tr>
<td>3.2</td>
<td>Added $T_5$ calculation.</td>
</tr>
<tr>
<td>3.3</td>
<td>Integrate heat transfer calculation from Lefebvre to include radiative heat transfer. Correct $T_5$ calc to include isentropic turbine efficiency. Correct $T_5$ calc to use proper specific enthalpy (per mole vs. per mass). Fix area calc error in adflame subroutine. Update adflame Newton solving iteration scheme so loops exit when positive/negative increments stop.</td>
</tr>
<tr>
<td>4.0</td>
<td>Include external heat transfer with ambient. Update $T_4$ and $T_5$ Newton solving iteration schemes so loops exit when positive/negative increments stop. Calculate NOₓ at 15% O₂, wet and dry basis.</td>
</tr>
<tr>
<td>4.1</td>
<td>Update NOₓ calc to account for cooling air dilution.</td>
</tr>
<tr>
<td>4.2</td>
<td>Incorporate external program loop for parametric studies.</td>
</tr>
</tbody>
</table>
Kombust was written in the FORTRAN programming language and consists of a main module which calls multiple subroutines and functions. In addition, there is an input file specifying ambient conditions, equivalence ratio, number of combustion regions, combustor geometry, gas velocity, fuel fraction oxidized in each region, compressor pressure ratio and isentropic efficiency, gas-generator turbine isentropic efficiency, mass flow ratio between the combustion and cooling air, and other various parameters. The code outputs a file containing NOx concentration in ppmv (uncorrected and corrected to 15% O2), temperature of each combustion and cooling air region, concentrations of species in each region, \( T_3, T_4, \) and \( T_5 \). The program subroutine logic flow diagram is shown in Figure 3.8, while Table 3.3 outlines a brief description for each subroutine. The complete program can be found in Appendix A, including the input file “komin.inp” which lists the complete set of program inputs.
Figure 3.8 Kombust Program Subroutine Logic Flow Diagram
<table>
<thead>
<tr>
<th>INPUT</th>
<th>Reads the input file and writes corresponding inputs to the command prompt window.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHEMSETUP</td>
<td>Calculates the combustion chemistry properties for the combustor model including reactant/product molar coefficients and mole fractions.</td>
</tr>
<tr>
<td>PSAT</td>
<td>This is a single subroutine which is part of the larger set of subroutines, steam.f90 (Iowa State University, 2011). PSAT calculates the saturation pressure of air.</td>
</tr>
<tr>
<td>ADFLAME</td>
<td>This is the primary subroutine which calculates effects of the turbine compressor and iteratively solves for the combustion zone and cooling air zone temperatures,</td>
</tr>
<tr>
<td>EXTERN_HEATXFER</td>
<td>Determines the external convective heat transfer coefficient (from the casing to the ambient air).</td>
</tr>
<tr>
<td>HEAT XFER</td>
<td>Calculates the convective, conductive, and radiative heat transfer properties from the combustion zones to the cooling air zones. Also calculates the cooling air liner inner and outer wall temperatures.</td>
</tr>
<tr>
<td>TPEQUIL</td>
<td>This subroutine calculates the H, O, N, NO and OH, equilibrium concentrations for use in equation (50). This program accompanies the textbook <em>An Introduction to Combustion</em> (Turns, 2000).</td>
</tr>
<tr>
<td>SPECIES_ENTH</td>
<td>This is a set of functions written for enthalpy calculation calls from the ADFLAME subroutine. Allows enthalpy calculations for CH₄, O₂, N₂, H₂O, CO₂ and air.</td>
</tr>
<tr>
<td>EQ_NOX</td>
<td>A subroutine to calculate the NO concentration and corresponding dry and wet correct mole fractions.</td>
</tr>
<tr>
<td>T4CALC</td>
<td>$T_4$ (combustor exit) temperature calculation after mixing of cooling air.</td>
</tr>
<tr>
<td>T5CALC</td>
<td>$T_5$ (gas generator turbine) temperature calculation using calculated compressor power.</td>
</tr>
<tr>
<td>OUTPUT</td>
<td>The final subroutine writes pertinent data to an output file, komout.out.</td>
</tr>
</tbody>
</table>
After the development of the theory, equations, methods, and computer program of the combustor model, the next step was to review the validity of the model and develop parametric studies that could be the basis for implementation into a PEMS.
CHAPTER 4 - Combustor Model Validation

As previously discussed, the combustor model was based on a Siemens SGT-200 industrial gas turbine. This engine was selected primarily because of the field data gathered and provided by a corporate partner for this research, Advanced Engine Technologies Corporation (AETC), on this same engine. This field data was used for comparison to the model outputs to validate the Kombust program. Before this was done, however, a qualitative trend evaluation was performed and the optimal number of combustion regions to be analyzed was determined. This chapter discusses a review of the trend evaluation, the combustion region analysis, a general review of the AETC field data, and a comparison study of some Kombust output data to the field data.

General Combustor Model Trend Analysis

Before quantitative test data comparisons could be made, the model was first used to examine the trend of NO$_x$, $T_4$, and $T_5$ vs. equivalence ratio to qualitatively determine its validity. Ambient conditions were input as 25°C, 50% relative humidity, and barometric pressure of 101.325 kPa. Five combustion zones were used in the analysis.

It is expected that an increase in equivalence ratio will increase NO$_x$ production exponentially, because temperature is increased with an increase in equivalence ratio (under lean conditions) and NO$_x$ production increases exponentially with temperature (Turns, 2000). Figure 4.1 demonstrates this relationship:
To validate this relationship, multiple runs of the Kombust program were executed with the equivalence ratio ranging from 0.6 to 1.0 in 0.05 increments. This represents an increase in the fuel flow rate to the engine with a constant air flow rate, i.e. an increase to the fuel-air ratio. Figure 4.2 shows the results of these calculations:
Figure 4.2 Kombust NO\textsubscript{x} vs. Equivalence Ratio

Based on a general shape comparison of Figure 4.1 to Figure 4.2, the Kombust program combustor model correctly predicts the trend that is expected for the temperature-dependant Zeldovich NO\textsubscript{x} mechanism.

Because the computational path through the Kombust program that is required to relate NO\textsubscript{x} to equivalence ratio encompasses most of the program routines, this sensitivity analysis provides a general validation of most of the calculations performed, with the exception of the NO\textsubscript{x} concentration adjustment calculations and downstream temperature calculations, including $T_4$ and $T_5$. The latter can be easily plotted from the same program outputs used on the initial analysis:
There are two things that can be highlighted from these results. Firstly, there is a nearly constant differential between $T_4$ and $T_5$. This temperature differential represents the power supplied by the gas-generator turbine to the compressor. The engine is modeled with a constant pressure ratio, and these Kombust program runs were performed with constant ambient conditions, so this constant differential between $T_4$ and $T_5$ is justified. Secondly, the relationship between equivalence ratio and both $T_4$ and $T_5$ is approximately linear. Increasing the equivalence ratio is the same as increasing the fuel-to-air ratio, or increasing the mass flow rate of fuel into the engine. By increasing the mass flow of fuel to the engine, the amount of energy supplied is increased by:

$$\Delta \dot{E} = \Delta \dot{m}_f (LHV)$$

(63)

Since the heating value is constant, the mass flow rate of fuel is directly and linearly related to the change in energy, so the linear relationship shown in Figure 4.3 is appropriate.
These two preliminary sensitivity studies indicate that the Kombust program is producing reasonable qualitative results, and thus the fundamental equations and methods used in the program are acceptable. The next step in the development of the model was to determine the proper number of combustion zones to be used in subsequent analyses.

**Formulation of Proper Number of Combustor Zones**

Before any useful data could be generated with the combustor modeling program, it had to be set up with an appropriate number of combustion regions and their corresponding dimensions.

In its simplest form, the combustor can be modeled in two regions:

![2-Combustion Region Model](image)

**Figure 4.4 2-Combustion Region Model**

The dimensions shown are typical for the SGT-200 DLN combustor, and were provided by Siemens. Running the Kombust program with this model arrangement produced the combustor zone temperature profile shown in Figure 4.5, with a $T_z$ of 625°C and a NO$_x$ concentration of 165 ppmvw @ 15% O$_2$ at an equivalence ratio of 0.8.
It was anticipated that the discretization effect from the increase in combustion zone regions would refine the model to a more realistic scenario, similar to the techniques employed by finite element analysis (FEA) and computational fluid dynamics (CFD). To test this, the number of combustion zones was increased systematically by breaking the pre-chamber and combustor sections into multiple zones:
Figure 4.6 Multi-Combustion Region Model
Using 29 zones had the following effect on the combustor temperature profile:

![Combustor Temperature Profile, 29 Zone](image)

**Figure 4.7 Combustor Temperature Profile, 29 Zone**

This appears a valid trend as the combustion products to the cooling air temperature delta is reduced along the combustion chamber by the heat transfer. For this arrangement, \( T_5 \) was 460°C with a NO\(_x\) concentration of 26 ppmv \( @ \) 15% O\(_2\). Both of these parameters were decreased from the 2-zone run, and they continued to decrease asymptotically as the number of zones increased:
The asymptotic nature of this change can be seen more clearly if the data is plotted as a change in dependant variable per zone number increase:
As Figure 4.9 illustrates, the change in $T_5$ and NO$_x$ per unit increase in the number of combustion regions approaches zero. The last data point was 104 zones which resulted in a variable change of 0.09°C/zone for $T_5$ and 0.06 ppm/zone for NO$_x$. These small variable changes per zone number increase were deemed insignificant enough to conclude that a further increase in the number of zones would not justify the increased computational demand required to converge the more complex simulation. Because of this, 104 zones were selected henceforth as the proper quantity to use in subsequent calculations.

With the number of combustion zones selected, the primary work of this chapter, which was to compare Kombust program outputs to the field-gathered operating data provided by AETC, could proceed. The first step in doing this was to review said data and determine the appropriate trends for comparison.
Combustion Turbine Operating Reference Data

The data used for comparison to the combustor model was from an SGT-200 test run and data collection by AETC on March 9, 2004. The combustion turbine is installed as a compressor drive on the Trans Canada Pipeline, station 148. Eighteen (18) test runs were performed over a two-day period. The data collected was extensive, with the primary parameters of interest for this research being NOx concentration, $T_1$, $T_3$, $T_5$, and $T_7$. AETC also did extensive analysis on the data to develop trends and examine variable relationships. They showed that many parameters strongly correlated, including fuel flow and torque vs. power, as shown in Figure 4.10, as well as $T_5$ (gas generator turbine exit temperature) and $T_7$ (exhaust temperature) vs. power, as shown in Figure 4.11.

![Fuel Flow and Torque vs. Power](image)

**Figure 4.10 AETC Field Data Fuel Flow and Torque Curves**

$R^2 = 0.9913$

$R^2 = 0.9979$
Figure 4.11 AETC Field Data $T_5$ and $T_7$ Curves

These relationships are expected as these parameters should relate almost directly to power with no additional strongly-correlating variables that would not be accounted for on these plots. Contrary to this, Figure 4.12 shows that NO$_x$, does not correlate well with power. This difference in parameter correlation alludes to the complexity of the NO$_x$ formation process.
To find variable dependency with $\text{NO}_x$, more complex relationships must be investigated. AETC accomplished this by correlating various temperature differences with $\text{NO}_x$. These temperature differences were also grouped by load ranges to find dependencies. Figure 4.13 shows one such instance of this investigation, in which $\text{NO}_x$ was correlated to $T_5$ minus $T_3$. 

Figure 4.12 AETC Field Data $\text{NO}_x$ vs. Power Plot
The data was grouped by load ranges for low, mid, and max loads. The general trend for all three of these load ranges is that NO\textsubscript{x} directly correlates with an increase in the $T_5$ minus $T_3$ temperature difference. For the max load points, this correlation can be well-represented by an exponential curve fit.

Fundamentally speaking, $T_4$ minus $T_3$ should represent the heat input into the combustor. However, the high temperatures associated with $T_4$ are very difficult to measure. In addition, as discussed in the previous section and shown on Figure 4.3, the temperature difference across the gas-generator turbine, $T_3$ minus $T_4$, is constant. Therefore, using $T_3$ minus $T_3$ instead of $T_4$ minus $T_3$ is appropriate and should not affect the trend. The combustor model validation will focus on recreating this dependency as accurately as possible.
**Kombust Model Comparison to Field Data**

As previously mentioned, the goal of the model validation was to recreate the $T_5$ minus $T_3$ NO$_x$ relationship for the max load conditions shown in the AETC field data and plotted in Figure 4.13. To recreate this relationship, values of equivalence ratio were selected that correspond to an equal range of NO$_x$ outputs that were seen in the AETC field data points, about 9 to 22 ppmvw. This corresponds to a Kombust program equivalence ratio of 0.73 to 0.79. Note that this is slightly less than the values that would be selected from Figure 4.2 because the field data is absolute NO$_x$ while the data plotted in Figure 4.2 is corrected to 15% O$_2$. The Kombust program was rerun through this range of equivalence ratio in 0.01 increments. The data from these runs were reconciled and plotted on Figure 4.14 below, along with the AETC field data.

![Field Data/Kombust Comparison 1, NO$_x$ vs. $T_5$-$T_3$](image)

**Figure 4.14 AETC Field Data/Kombust Comparison 1**
The results show that the Kombust-generated values of $T_5$ minus $T_3$ are approximately 20°C to 50°C than less the AETC field data, for a given concentration of NO$_x$. The range of the temperature offset is because the slopes, ppmv/°C, are also different.

The previous analysis assumes that the equivalence ratio range used to match the NO$_x$ output of the field data is appropriate, i.e. the Kombust model will calculate all the NO$_x$ measured in the field data. However, there are three items which may contribute to this being an incorrect assumption:

1. It is anticipated that the modeled NO$_x$ will be less than the actual NO$_x$ because the model is only calculating the thermal NO$_x$ contributed from the Zeldovich chemical mechanism, while the literature review deemed that the nitrous oxide mechanism is also prevalent for lean-premixed combustion.

2. The SGT-200 DLE combustion system uses a pilot flame configuration that would operate with a diffusion flame at a near-stoichiometric fuel-air ratio. This would produce a maximum temperature combustion region thus producing additional thermal NO$_x$ not accounted for in this analysis.

3. In discussions with Siemens it was also determined that the SGT-200 typically operates at an equivalence ratio of about 0.67.

The slopes of the trend lines fit to the modeled and tested NO$_x$ vs. $T_5-T_3$ are 0.54 ppmv/°C and 0.21 ppmv/°C respectively. Because the NO$_x$ vs. equivalence ratio relationship presented in Figure 4.2 is an exponential one, the slope, or derivative, decreases with decreasing equivalence ratio. Thus in order to produce data more resembling the slope of the field data it is necessary to decrease the range of equivalence ratios analyzed, which would also decrease the NO$_x$ range of the outputs. This methodology agrees with the three items above.

To determine the proper range of equivalence ratios necessary to reproduce the slope of the field data, a plot of the NO$_x$ vs. $T_5-T_3$ derivative vs. equivalence ratio was created and the vertical axis ranged for the slope values seen on Figure 4.14.
This plot shows the 0.73 beginning range of equivalence ratio used in the previous analysis corresponding to 0.54 ppmvw/°C slope. To reach the 0.21 ppmvw/°C slope of the field data, the Kombust model equivalence ratio should be reduced to about 0.69. This value was straddled in the next set of Kombust model runs, ranging from 0.66 to 0.72.
This set of Kombust runs demonstrates that the model creates a nearly equal slope of the AETC field data for NO\textsubscript{x} vs. $T_5-T_3$, albeit with lesser values of NO\textsubscript{x} and $T_5-T_3$. The lesser values of NO\textsubscript{x} are expected per the above three discussion points, but the lower $T_5-T_3$ values are a different story. There are a number of factors that may contribute to this discrepancy including:

- Inaccurate modeling of the heat transfer – Obviously the heat transfer involved in a combustion turbine is a very complex process, especially due to the extremely high temperatures and temperature gradients which make the complex radiative heat transfer process so important. While the goal of this research was to model the heat transfer process as accurately as possible by accounting for all modes of heat transfer including conductive, convective, and radiative mechanisms, in judging Figure 4.16 it would appear that the calculated heat transfer was excessive.
• Fuel – The Kombust model uses pure methane as the fuel, while the field turbine was burning natural gas with an unknown heating value.

• Compressor and turbine efficiencies – The compressor and gas-generator turbine efficiencies used in the Kombust model were typical values of 0.85. Differences in the actual efficiencies will affect the accuracy of the calculated temperatures.

While the model validation exercise revealed potential for future enhancements, the model comparison to the field data was deemed sufficient for the purpose of this research. The following chapter will focus on creating additional sensitivity studies and a review of the potential incorporation of the Kombust program into a PEMS.
CHAPTER 5 - Parametric Studies and PEMS Implementation

The preceding chapters reviewed the necessity of this research, determined the appropriate path forward including the general type of combustor model to be developed, reviewed the development of the model through fundamental chemistry, thermodynamic, and heat transfer principles, and validated the model both qualitatively and quantitatively. The present chapter will focus on additional sensitivity studies.

Parametric Studies

The goal of this chapter is to review some additional parametric studies to further validate the Kombust program and gain an understanding of some of the variable dependencies. The parameter studies reviewed are as follows:

1. NO\textsubscript{x} vs. Ambient Temperature
2. NO\textsubscript{x} vs. Ambient Relative Humidity
3. NO\textsubscript{x} vs. Ambient Atmospheric Pressure
4. NO\textsubscript{x} vs. Combustion to Cooling Air Ratio
5. NO\textsubscript{x} vs. Compressor Pressure Ratio

To review the effects of changing these parameters on combustion temperature, all plots will also include $T_5$. In addition, to review the relative contribution of a change in combustion temperature vs. other effects to the change in NO\textsubscript{x} concentration, a new parameter, $dT_5/d[NO\textsubscript{x}]$, will be calculated and reviewed for each study.

*NO\textsubscript{x} vs. Ambient Temperature*

The first parametric study reviewed was NO\textsubscript{x} vs. ambient temperature. For this study, all program input parameters were held constant while the ambient temperature (dry bulb) was adjusted from -30°C to 50°C in 10 degree increments. The relative humidity was 50% with an equivalence ratio of 0.7. The results of this are shown in Figure 5.1.
Figure 5.1 Kombust NO\textsubscript{x} vs. Ambient Temperature

The plot shows a direct relationship between the ambient temperature change and NO\textsubscript{x} output, with an increase of about six-fold in the NO\textsubscript{x} output over the analyzed temperature range. If $T_5$ is added to this same plot it alludes to the reason for this increase in NO\textsubscript{x}. Because thermal NO\textsubscript{x} is modeled with the Kombust program, the increase in NO\textsubscript{x} should be a direct result of the increase in combustion temperature. This is represented by a similar rise in $T_5$ relative to NO\textsubscript{x} shown in Figure 5.2.
The next parameter reviewed was the ambient relative humidity vs. NO\textsubscript{x}. For this curve, the ambient temperature was held at 25°C with the relative humidity varying from 20% to 100% in 10% increments with an equivalence ratio of 0.7. The results of this are shown in Figure 5.3 along with a plot of $T_5$. 

\textbf{NO\textsubscript{x} vs. Ambient Relative Humidity}

Figure 5.2 Kombust NO\textsubscript{x} and $T_5$ vs. Ambient Temperature
The plot shows a rather strong inverse linear correlation for NOx while $T_5$ remains nearly constant. This difference in correlation is not expected, because as discussed for the ambient temperature graph, the thermal NOx model should only be affected by combustion temperatures. After reviewing the calculations it was revealed that the decrease in NOx concentration is actually a result of the dilution effects of the increased humidity, meaning the humidity has little effect on the combustion temperatures but a larger effect on the mass flow through the engine.

Referring again to equation (45), the NOx formation rate equation, and the associated equations of its parameters, it is apparent that a change in the equilibrium concentration of the combustion species will affect the rate of NOx formation. To confirm the downward trend in NOx with increasing relative humidity, two points were checked manually (by debugging the program) to prove the reduced NOx formation rate. The results of this are shown in Table 5.1 which shows the slight difference in the rate of NOx formation, assuming an initial NO concentration of 1.
Table 5.1 Relative Humidity Effect on NO\textsubscript{x} Formation Rate Parameters

<table>
<thead>
<tr>
<th>Relative Humidity 0.5</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>R\textsubscript{1}</td>
<td>1.86x10^{-4}</td>
<td></td>
</tr>
<tr>
<td>R\textsubscript{2}</td>
<td>1.54x10^{-7}</td>
<td></td>
</tr>
<tr>
<td>R\textsubscript{3}</td>
<td>7.37x10^{-5}</td>
<td></td>
</tr>
<tr>
<td>[NO]\textsubscript{e}</td>
<td>3.22x10^{-4}</td>
<td></td>
</tr>
<tr>
<td>d[NO]/dt</td>
<td>0.459</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Relative Humidity 0.9</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>R\textsubscript{1}</td>
<td>1.84x10^{-4}</td>
<td></td>
</tr>
<tr>
<td>R\textsubscript{2}</td>
<td>1.52x10^{-7}</td>
<td></td>
</tr>
<tr>
<td>R\textsubscript{3}</td>
<td>7.29x10^{-5}</td>
<td></td>
</tr>
<tr>
<td>[NO]\textsubscript{e}</td>
<td>3.21x10^{-4}</td>
<td></td>
</tr>
<tr>
<td>d[NO]/dt</td>
<td>0.454</td>
<td></td>
</tr>
</tbody>
</table>

The results show that there is a lower NO formation rate for a higher humidity. This indicates that the NO\textsubscript{x} concentration change is due to the increase in water vapor concentration diluting the remaining exhaust gas constituents.

**NO\textsubscript{x} vs. Ambient Atmospheric Pressure**

The NO\textsubscript{x} vs. ambient atmospheric pressure chart is shown in Figure 5.4. This chart shows a similar increase in NO\textsubscript{x} as the ambient pressure is increased from 91 kPa up to 102 kPa (sea level = 101.3 kPa).
The NO\textsubscript{x} effect over this studied range is less than that of the previous analyses. However, because the variables adjusted are mutually exclusive, comparing the absolute change in NO\textsubscript{x} over the parameter range is not beneficial. To review the relative contribution a change in combustion temperature has on the change in NO\textsubscript{x}, it was determined that a change in $T_5$ relative to the change in NO\textsubscript{x} would be a more useful comparison. A summary of this comparison is presented in Table 5.2.
Table 5.2 NO\textsubscript{x} Concentration Change per Change in $T_5$

<table>
<thead>
<tr>
<th>PARAMETER STUDY</th>
<th>$dT_5/d[NO_x]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO\textsubscript{x} vs. Ambient Temperature</td>
<td>8.3 kmol/m\textsuperscript{3}-C</td>
</tr>
<tr>
<td>NO\textsubscript{x} vs. Ambient Relative Humidity</td>
<td>N/A</td>
</tr>
<tr>
<td>NO\textsubscript{x} vs. Ambient Atmospheric Pressure</td>
<td>33.0 kmol/m\textsuperscript{3}-C</td>
</tr>
<tr>
<td>NO\textsubscript{x} vs. Combustion to Cooling Air Ratio</td>
<td>68.6 kmol/m\textsuperscript{3}-C</td>
</tr>
<tr>
<td>NO\textsubscript{x} vs. Compressor Pressure Ratio</td>
<td>8.7 kmol/m\textsuperscript{4}-C</td>
</tr>
</tbody>
</table>

The variable $dT_5/d[NO_x]$ represents the change in gas-generator turbine exit temperature relative to a change in NO\textsubscript{x} as the parameter in question is varied. As this variable decreases, the relative amount of thermal NO\textsubscript{x} change contributing to the overall NO\textsubscript{x} change increases, thus the contribution from other sources decreases. In other words, when a greater change in $T_5$ is required for a given change in NO\textsubscript{x} concentration, other sources besides thermal NO\textsubscript{x} must be contributing to the NO\textsubscript{x} concentration change.

Of the three parametric studies reviewed thus far, the atmospheric pressure analysis has a lesser influence by change in thermal NO\textsubscript{x} than does the ambient temperature analysis. The ambient relative humidity term is not applicable because $T_5$ was constant throughout. This difference is partly because of the constant compressor pressure ratio used, which results in combustion air density changes corresponding to the density changes of the incoming atmospheric air. This causes subsequent concentration changes of the species used in the NO\textsubscript{x} concentration calculation.

The parameters studied thus far are ambient conditions, thus they are independent of engine’s design. The remaining parameters studied are design and/or operating parameters.

**NO\textsubscript{x} vs. Combustion Air to Cooling Air Ratio**

As defined by equation (39), the combustion air to cooling air ratio, $r$, represents the split of the incoming compressor air. This variable was changed from 0.85 to 1.15 and plotted against NO\textsubscript{x} and $T_5$.  

66
Figure 5.5 Kombust NO\textsubscript{x} and T\textsubscript{5} vs. Combustion to Cooling Air Ratio

The design value for $r$ is 0.94. The plot shows another near-linear influence with a very high $dT_5/d[NO_x]$ per Table 5.2. Because the cooling air acts to absorb heat from the combustion process, as more cooling air is used the average combustion air temperature decreases. However, adjusting this ratio does not affect the combustion process immediately. Only the lower temperature downstream NO\textsubscript{x} formation is affected, hence the very high $dT_5/d[NO_x]$. It is also important to note that the equivalence ratio, and thus the fuel-air ratio, remains constant as $r$ is adjusted, so the only effect is from differences in cooling air.

The final parameter reviewed is also engine-specific.

**NO\textsubscript{x} vs. Compressor Pressure Ratio**

The design compressor pressure ratio is 11.7, so the parameter was ranged from 10 to 12 with more margin on the low-end in anticipation of compressor degradation. Figure 5.6 plots NO\textsubscript{x}, $T_5$, and $T_3$ vs. $PR$. 

67
Figure 5.6 Kombust NO\textsubscript{x} and $T_5$ vs. Compressor Pressure Ratio

An increase in the compressor pressure ratio results directly in an increase in combustion temperature, as the more compression done on the air creates a larger temperature increase across the compressor. This is shown directly by the $T_3$ line, with the parallel $T_5$ line indicating that all the temperature increase through the engine is a direct result of an increase in compressor exit temperature.

These studies show that the Kombust program is capable of accounting for a number of ambient and design parameters corresponding to the overall operating conditions of the combustion turbine.
CHAPTER 6 - Conclusion

The premise for this research was to investigate methods for less expensive NO\textsubscript{x} emission monitoring that could be used on a wide-variety of combustion turbines. Specifically, the goal was to use first-principle engineering to calculate emissions from operating parameters. The expansion of this simple idea was necessitated by the complexity of the engineering principles involved with the NO\textsubscript{x} formation and control process, as well as the significant preceding work involving similar topics.

It was ultimately determined that a mathematical combustor model based on lean-premixed combustion would be used to facilitate these goals. The modeling equations and principles were developed and transcribed into a FORTRAN computer program deemed Kombust.

The Kombust program showed valid trends and reasonable accuracy compared to the field test data when considering its limitations. There are a number of refinement opportunities suggested beyond the scope of the present research, including:

- Modeling of the pilot flame system.
- Including the chemical process for the nitrous-oxide NO\textsubscript{x} mechanism.
- Adding the ability to model additional fuels beyond methane.
- Validation and/or modification of the heat transfer model through laboratory testing.
- Refinement of the airflow calculations to allow for part-load modeling.
- Refinement of the reactor scheme to represent recirculation.

The goal of these model refinements would be to approach an appropriate accuracy, when compared to a CEMS, such that the program could be integrated a PEMS. Further field test data and program comparisons would be necessary to establish confidence in the program; first on a specific gas turbine model, and ultimately on a family of models with similar design characteristics.

The integration of the model into a PEMS has also been briefly reviewed. As discussed in Chapter 2, the prior PEMS development was focused on primarily statistical techniques to
map the emissions over operating parameters for future prediction. The fundamental problem with this is that the emission-mapping process takes place at a certain condition of the engine that will change over time and affect its operation, including emissions. The best way to account for this is to model the turbine using first-principle concepts that will capture the effects of degradation; this was precisely the goal of this research, and the Kombust program.

The basis for potential integration of the Kombust program into a PEMS is to separate the “base” operating parameters from the “adjusting” operating parameters. The base operating parameters can initially be used to calculate a “new and clean” NOx concentration. This “new and clean” concentration represents the NOx produced by the engine shortly after commissioning. However, as run hours progress on the turbine, the remaining parameters may indicate deviation from the new and clean condition, and thus the calculated NOx should be adjusted accordingly.

A potential scheme for integrating Kombust into a PEMS is shown in Figure 6.1.

Figure 6.1 Kombust-PEMS Integration Flowchart

The input boxes labeled 1A through 3A represent ambient conditions while boxes labeled 1B through 3B represent operating parameters. The diagram represents calculating a “new and clean” NOx value based on the ambient conditions and load. This calculation would be corrected by the $T_5-T_3$ and PR variables to account for component degradation and give a final, corrected
concentration of NOx. It is in such a manner as this that the NOx calculated by a PEMS could closely match the actual NOx and/or that analyzed by a CEMS.
References


Boyns, M. (Siemens), 2004, Personal Correspondence, Kansas State University, Manhattan, KS.


Appendix A - Kombust Combustion Modeling Program

The following pages present the input file, primary subroutines, and output file of the Kombust program.
0.5   equivrat  equivalence ratio
25    tamb    ambient temperature (°C)
101.325 patm    atmospheric pressure (kPa)
0.5    rh      relative humidity
11.66  pratio  compressor pressure ratio (pout/pin)
0.837  comp_eff  isentropic compressor efficiency
0.850  turb_eff  isentropic turbine efficiency
0.938  r        ratio of combustion air to cooling air
2000  tguess  temperature guess (K)
0.1    tinc    temperature increment used in iterations (K)
1.0e-4  timestp  timestep (s)
5    nmrg    number of combustion regions
1.0    comfrac  fuel fraction burnt in each region (must add to 1)
0
0
0
0
0
0
0
0.086  dia    diameter of each region (m)
0.086
0.165
0.165
0.165
0.13    lnth    length of each region (m)
0.13
0.1
0.1
0.0869
0.0012  t_w    liner wall thickness of each region (m)
0.0012
0.0012
0.0012
0.0012
35    vel    average air velocity in each region (m/s)
35
12
12
12
0.7    e_w    emissivity of liner wall
0.4    e_c    emissivity of casing
26    k_w    thermal conductivity of liner (W/m*K)
8.33    h_perc  hydrogen content of fuel (%-mass)
0.03    an_gap  annulus air gap between liner and casing
1.0    dia_case  casing diameter
program main
include 'var.i'

call input
call chemsetup
call adflame
call t4calc
call eq_nox
call t5calc
call output

dend
subroutine input
include 'var.i'

open(10, file='komin.inp')

! READ STATEMENTS
read(10,*) equivrat
read(10,*) tamb
read(10,*) patm
read(10,*) rh
read(10,*) pratio
read(10,*) comp_eff
read(10,*) turb_eff
read(10,*) r
read(10,*) tguess
read(10,*) tinc
read(10,*) timestep
read(10,*) nmrg

do j=1, nmrg
read(10,*) comfrac(j)
enddo

do j=1, nmrg
read(10,*) dia(j)
enddo

do j=1, nmrg
read(10,*) lnth(j)
enddo

do j=1, nmrg
read(10,*) t_w(j)
enddo

do j=1, nmrg
read(10,*) vel(j)
enddo

read(10,*) e_w
read(10,*) e_c
read(10,*) k_w
read(10,*) h_perc
read(10,*) an_gap
read(10,*) dia_case

! WRITE STATEMENTS
write(*,*) equivrat,
1 'equivrat, Equivalence ratio'
write(*,*) tamb,
1 'tamb, Ambient temperature, C'
write(*,*) patm,
1 'patm, Ambient pressure, kPa'
write(*,*) rh,
1 'rh, Ambient relative humidity'
write(*,*) pratio,
1 'pratio, Compressor pressure ratio'
write(*,*) comp_eff,
1 'comp_eff, Isentropic compressor efficiency'
write(*,*) turb_eff,
write(*,*) turb_eff, 'Isentropic turbine efficiency'
write(*,*) r, 'r, Combustion air to cooling air ratio'
write(*,*) tguess, 'tguess, Initial adiabatic flame temperature guess, K'
write(*,*) tinc, 'tinc, Temperature increment for temp calcs'
write(*,*) timestep, 'timestep, Timestep for NOx calculation, s'
write(*,100) nmrg
100   format(i5, t26, 'numreg, Number of modeling regions')
write(*,*) comfrac, 'comb frac, Combustion fraction in each zone'
do j=1, nmrg
write(*,*) j, comfrac(j)
enddo
write(*,*) dia, 'Combustion zone diameter'
do j=1, nmrg
write(*,*) j, dia(j)
enddo
write(*,*) lnth, 'lnth, Combustion zone length'
do j=1, nmrg
write(*,*) j, lnth(j)
enddo
write(*,*) t_w, 't_w, Liner wall thickness'
do j=1, nmrg
write(*,*) j, t_w(j)
enddo
write(*,*) vel, 'vel, Air velocity in each zone'
do j=1, nmrg
write(*,*) j, vel(j)
enddo
write(*,*) e_w, 'e_w, Liner emissivity'
write(*,*) e_c, 'e_c, Casing emissivity'
write(*,*) k_w, 'k_w, Liner thermal conductivity, W/m*k'
write(*,*) h_perc, 'h_perc, Hydrogen content of fuel, %-mass'
write(*,*) an_gap, 'an_gap, Annulus air gap, m'
write(*,*) dia_case, 'dia_case, Casing diameter, m'
return
end
subroutine chemsetup
!CHEMSETUP DETERMINES CHEMICAL EQUATION COEFFICIENTS BASED ON COMBUSTION
!WITH MOIST AIR AND EQUIVALENCE RATIO
include 'var.i'

!zr*FUEL + a*O2 + a3*N2 + a1*H2O + a2*CO2 -> b*CO2 + c*H2O + d*N2 + e*O2 + zp*FUEL
zr(1) = 1
zp(nmrg)=0

do i=1, nmrg-1
zp(i)=zr(i) - comfrac(i)
zr(i+1)=zp(i)
enddo

!CONVERT AMBIENT TEMPERATURE TO KELVIN
tamb=tamb + 273.15

!DETERMINE SATURATION PRESSURE, CONVERT TO kPa
call psat(tamb, psatu, rhol, rhov)
psatu=psatu*1000

!HUMIDITY MOLE RATIO AND AIR MOLE FRACTION FROM REL. HUMIDITY AND SAT. PRESSURE
humr=1.608*(0.622/((patm/(rh*psatu)) - 1))
xa=1.0/(1.0 + humr)

!FUEL MOLECULAR WEIGHT (METHANE FUEL ONLY (CH4))
fuelmw=ch4mw

!STOICHIOMETRIC AIR COEFFICIENT (METHANE FUEL ONLY)
a_st=2

!STOICHIOMETRIC FUEL-AIR RATIO
fstoi=(1.0*fuelmw)/(4.76*a_st*airmw)

!ACTUAL FUEL-AIR RATIO BASED ON EQUIVALENCE RATIO
fact=equivrat*fstoi

!ACTUAL AIR COEFFICIENTS FOR INITIAL ZONE
a(1)=(1.0*fuelmw)/(fact*4.76*airmw)
a1(1)=a(1)/xa - a(1)
a2(1)=0
a3(1)=3.76*a(1)

!CALCULATE ACTUAL COEFFICIENTS OF PRODUCTS (METHANE FUEL ONLY)

do i=1, nmrg
b(i)=zr(i) + a2(i) - zp(i) !CARBON BALANCE
c(i)=2*zr(i) + a1(i) - 2*zp(i) !HYDROGEN BALANCE
d(i)=a3(i) !NITROGEN BALANCE
e(i)=(2*a(i) + a1(i) + 2*a2(i) - 2*b(i) - c(i))/2 !OXYGEN BALANCE
if(i .lt. nmrg)then
!PRODUCTS CARRIED OVER AS REACTANTS TO NEXT ZONE
a(i+1)=e(i)
a3(i+1)=d(i)
a1(i+1)=c(i)
a2(i+1)=b(i)
endif
enddo
!NUMBER OF MOLES OF MOIST COOLING AIR BASED ON r
a_coola=a(1)/r
a1_coola=a_coola/xa - a_coola

do i=1, nmrg
!MOLE FRACTIONS IN COMBUSTION ZONES
co2frac(i)=b(i)/(b(i) + c(i) + d(i) + e(i) + zp(i))
h2ofrac(i)=c(i)/(b(i) + c(i) + d(i) + e(i) + zp(i))
n2frac(i)  =d(i)/(b(i) + c(i) + d(i) + e(i) + zp(i))
o2frac(i) =e(i)/(b(i) + c(i) + d(i) + e(i) + zp(i))
endo

!AIR MOLE FRACTIONS
  o2frac_a= a_coola/(a_coola + 3.76*a_coola + a1_coola)
n2frac_a=3.76*a_coola/(a_coola + 3.76*a_coola + a1_coola)
h2ofrac_a= al_coola/(a_coola + 3.76*a_coola + al_coola)

return
end
subroutine adflame
include 'var.i'

! GET CONVECTIVE HEAT TRANSFER COEFFICIENT FROM CASING TO AMBIENT FROM extern_heatxfer SUBROUTINE
call extern_heatxfer

! CALCULATE COMBUSTOR INLET TEMPERATURE BASED ON COMPRESSOR PRESSURE RATIO,
! ISENTROPIC IDEAL GAS RELATIONSHIP, AND COMPRESSOR EFFICIENCY ASSUMING
! CONSTANT Cp
p=pratio*patm
tin(1)=tamb*(((air_k - 1)/air_k))
tca(1)=tin(1)

! COMBUSTION AIR MASS FLOW RATE
mcomba=((p*airmw)/(rbar*tin(1)))*vel(1)*0.25*pi*dia(1)**2

! COOLING AIR MASS FLOW RATE
do i=1, nmrg
mca(i)=mcomba/r
enddo

! FUEL MOLAR FLOW RATE
nf=(mcomba*fact)/fuelmw

!========================================================================
do 1000 i=1, nmrg
zz1 = 0
zz2 = 0
xx1 = 0
xx2 = 0

if(i .gt. 1) tin(i) = t(i-1)
area(i) = lnth(i)*pi*dia(i)

! H_RHS = DELTAH(REACTANTS) + ENT_FORMATION(REACTANTS) - ENT_FORMATION(PRODUCTS)
! LHS = DELTAH(PRODUCTS)
h_rhs(i) = zr(i)*delh_ch4(tin(i)) + a(i)*delh_o2(tin(i)) +
1 a3(i)*delh_n2(tin(i)) + a1(i)*delh_h2o(tin(i)) +
2 a2(i)*delh_co2(tin(i)) + zr(i)*hf_ch4 + a1(i)*hf_h2o +
3 a2(i)*hf_co2 - b(i)*hf_co2 - c(i)*hf_h2o - zp(i)*hf_ch4

if(i .eq. 1) then
   t(i)=tguess
else
   t(i) = t(i-1)
endif

!----------------------------------------------------------------------
do 500 j=1, maxit
if(j .eq. maxit) then
   write(*,*) 'Combustion temp calc not converged'
   write(15,*) 'Combustion temp calc not converged'
call exit(0)
endif
if(i .gt. 1 .and. j .eq. 1) tca(i) = tca(i-1)
if(i .eq. 1) then
   qn(i) = 0
   goto 400
endif
if(b(i)*delh_co2(t(i)) + c(i)*delh_h2o(t(i)) +
1 d(i)*delh_n2(t(i)) + e(i)*delh_o2(t(i)) +
2 zp(i)*delh_ch4(t(i)) = qn(i)
3 .gt. h_rhs(i))
then
   t(i)=t(i) - tinc
   zz1=zz1+1
endif

!----------------------------------------------------------------------
call heatxfer
!qn(i) = (((r_1(i) + c_1(i))*area(i)) /nf ) /8
qn(i) = 0
400

else
  t(i)=t(i) + tinc
  zz2=zz2+1
endif
if(zz1 .gt. 0 .and. zz2 .gt. 0) exit

500       continue

!------------------------------------------------------------------------
if(i.eq.1)then
  call TPEQUIL(equivrat,t(i),p,h_mofc(i),o_mofc(i),n_mofc(i),h2_mofc(i),
  loh_mofc(i),co_mofc(i),no_mofc(i),o2_mofc(i),h2o_mofc(i),co2_mofc(i),
  2n2_mofc(i),zr(i),zp(i),a1(i),a(i),i)
endif

!COOLING AIR ZONES TEMPERATURE CALCULATION
if(i .gt. 1)then

!------------------------------------------------------------------------
do 600 j=1, maxit
  if(j .eq. maxit)then
    write(*,*) 'Cooling air temp calc not converged'
    call exit(0)
  endif
q_amb(i) = h_amb*pi*dia_case*lnth(i)*((tca(i)-0.6*tca(i)) - tamb)
if( (mca(i-1)*(delh_air(tca(i-1))/airmw) -
1    qn(i-1)*nf - q_amb(i)) / mca(i) >
2   delh_air(tca(i))/airmw)
  then
    tca(i)=tca(i) + tinc
    xx1=xx1 + 1
  else
    tca(i)=tca(i) - tinc
    xx2=xx2 + 1
  endif
if(xx1 .gt. 0 .and. xx2 .gt. 0) exit

600       continue

!------------------------------------------------------------------------
endif

write(*,*) i, t(i), tca(i)

1000       continue

!------------------------------------------------------------------------
return

end
subroutine extern_heatxfer
include 'var.i'
double precision k_atm, nud

!EXTERNAL HEAT TRANSFER CALC

Pr = 0.71       !PRANDTL NUMBER
v = 3           !ASSUME AIR SPEED OF 3 m/s
u_atm = (2.27e-8*( (1.8*(tamb))**1.5/(1.8*(tamb)+198.6) ) )*47.88
k_atm = 2.495e-3*tamb**1.5/(tamb+194)

!REYNOLDS NUMBER
Red = ( ((patm*airmw)/(rbar*(tamb)))*v*dia_case ) / u_atm

!EXPERIMENTAL NUSSELT NUMBER CORRELATION FOR A SINGLE CYLINDER WITH FORCED CONVECTION
!FROM WELTY, "FUNDAMENTALS OF MOMENTUM, HEAT, AND MASS TRANSFER, 4TH ED, PP. 328
nud = 0.3+((0.62*Red**0.5*Pr**(1/3))/(1 + (0.4/Pr)**(2/3))**0.25)*
(1 + (Red/282000)**(5/8))**(4/5)

h_amb = (nud*k_atm)/dia_case

return
end
subroutine heatxfer
include 'var.i'

k=1

! LUMINOSITY, BEAM LENGTH, AND COMBUSTION GAS EMISSIVITY
lum = 336/h_perc**2
l_b = 0.8*dia(1)
e_g(i) = 1 - exp(-290*p*lum*(fact*1_b)**0.5*t(i)**-1.5)

! DYNAMIC VISCOSITY OF AIR FROM SUTHERLAND'S FORMULA
! THERMAL CONDUCTIVITY OF AIR FROM:

u_g = ( 2.27e-8*( (1.8*t(i))**1.5/(1.8*t(i)+198.6) ) )*47.88
k_g = 2.495e-3*t(i)**1.5/(t(i)+194) !0.157
u_a = ( 2.27e-8*( (1.8*tca(i))**1.5/(1.8*tca(i)+198.6) ) )*47.88
k_a = 2.495e-3*tca(i)**1.5/(tca(i)+194)!0.053

! RADIATION BETWEEN COMBUSTION GASES AND LINER WALL
r1 = r1c1 - r1c2*tw1**2.5
r1c2 = 0.5*sig*(1 + e_w)*e_g(i)*t(i)**1.5
r1c1 = r1c2*t(i)**2.5

! RADIATION BETWEEN LINER WALL AND CASING
r2 = r2c1*tw2**4 - r2c2
r2c1 = 0.5*sig
r2c2 = r2c1*tca(i)**4

! CONVECTION BETWEEN COMBUSTION GASES AND LINER WALL
c1 = c1c1 - c1c2*tw1

! CONVECTION BETWEEN LINER WALL AND COOLING AIR
! ASSUME LINER AND CASING ARE CONCENTRIC CYLINDERS
ca_dia = dia(i) + 2*an_gap !CASING DIAMETER
a_an = 0.25*pi*(ca_dia**2 - dia(i)**2) !ANNULUS AREA

! INITIAL GUESS FOR Tw2
tw2(i) = t(i) - 500

! LOOP TO SOLVE FOR Tw1 and Tw2
do 100 k=1, maxit
  if (k .eq. maxit) then
    write(*,*) 'Heat transfer calc not converged'
    write(17,*) k, 'Heat transfer calc not converged'
    call exit(0)
  endif

  r_2(i) = r2c1*tw2(i)**4 - r2c2
  c_2(i) = c2c1*tw2(i) - c2c2
  tw1(i) = (t_w(i)/k_w)*(r_2(i) + c_2(i)) + tw2(i)

enddo

! CALCULATE R2 and C2 based on Tw2 guess

! CALCULATE Tw1
tw1(i) = (t_w(i)/k_w)*(r_2(i) + c_2(i)) + tw2(i)
! CALCULATE R1 and C1 based on Tw1
r_1(i) = r1c1 - r1c2*tw1(i)**2.5
c_1(i) = c1c2 - c1c1*tw1(i)

zz1 = r_1(i) + c_1(i)
zz2 = r_2(i) + c_2(i)

if(r_1(i) + c_1(i) .gt. r_2(i) + c_2(i)) then
tw2(i) = tw2(i) + tinc
zx1 = zx1 + 1
endif
if(r_1(i) + c_1(i) .lt. r_2(i) + c_2(i)) then
tw2(i) = tw2(i) - tinc
zx2 = zx2 + 1
endif

if(zx1 .gt. 0 .and. zx2 .gt. 0) exit

100 continue

!---------------------------------------------------------------------------
return
end
double precision function delh_ch4(tmpfc)
include 'var.i'
double precision tta,ttaref,tmpfc
tta=tmpfc/100
ttaref=tref/100
delh_ch4=100*
    alp_ch4*(tta - ttaref) +
( bet_ch4/(betx_ch4 + 1))*
( tta**(betx_ch4 + 1) - ttaref**(betx_ch4 + 1)) +
( gam_ch4/(gamx_ch4 + 1))*
( tta**(gamx_ch4 + 1) - ttaref**(gamx_ch4 + 1)) +
( del_ch4/(delx_ch4 + 1))*
( tta**(delx_ch4 + 1) - ttaref**(delx_ch4 + 1))
end

!--------------------------------------------------------------------------------------!
double precision function delh_o2(tmpfc)
include 'var.i'
double precision tta,ttaref,tmpfc
tta=tmpfc/100
ttaref=tref/100
delh_o2=100*
    alp_o2 *(tta - ttaref) +
( bet_o2 /(betx_o2 + 1))*
( tta**(betx_o2 + 1) - ttaref**(betx_o2 + 1)) +
( gam_o2 /(gamx_o2 + 1))*
( tta**(gamx_o2 + 1) - ttaref**(gamx_o2 + 1)) +
( del_o2 /(delx_o2 + 1))*
( tta**(delx_o2 + 1) - ttaref**(delx_o2 + 1))
end

!--------------------------------------------------------------------------------------!
double precision function delh_n2(tmpfc)
include 'var.i'
double precision tta,ttaref,tmpfc
tta=tmpfc/100
ttaref=tref/100
delh_n2=100*
    alp_n2 *(tta - ttaref) +
( bet_n2 /(betx_n2 + 1))*
( tta**(betx_n2 + 1) - ttaref**(betx_n2 + 1)) +
( gam_n2 /(gamx_n2 + 1))*
( tta**(gamx_n2 + 1) - ttaref**(gamx_n2 + 1)) +
( del_n2 /(delx_n2 + 1))*
( tta**(delx_n2 + 1) - ttaref**(delx_n2 + 1))
end

!--------------------------------------------------------------------------------------!
double precision function delh_h2o(tmpfc)
include 'var.i'

double precision tta,ttaref,tmpfc

tta=tmpfc/100

ttaref=tref/100

delh_h2o=100*(
alp_h2o *(tta - ttaref) +
(bet_h2o / (betx_h2o + 1)) *
(tta**((betx_h2o + 1)) - ttaref**((betx_h2o + 1))) +
(gam_h2o / (gamx_h2o + 1)) *
(tta**((gamx_h2o + 1)) - ttaref**((gamx_h2o + 1))) +
(del_h2o / (delx_h2o + 1)) *
(tta**((delx_h2o + 1)) - ttaref**((delx_h2o + 1)))
)

end

!--------------------------------------------------------------------------------------!

double precision function delh_co2(tmpfc)

include 'var.i'

double precision tta,ttaref,tmpfc

tta=tmpfc/100

ttaref=tref/100

delh_co2=100*(
alp_co2 *(tta - ttaref) +
(bet_co2 / (betx_co2 + 1)) *
(tta**((betx_co2 + 1)) - ttaref**((betx_co2 + 1))) +
(gam_co2 / (gamx_co2 + 1)) *
(tta**((gamx_co2 + 1)) - ttaref**((gamx_co2 + 1))) +
(del_co2 / (delx_co2 + 1)) *
(tta**((delx_co2 + 1)) - ttaref**((delx_co2 + 1)))
)

end

!--------------------------------------------------------------------------------------!

double precision function delh_air(tmpfc)

include 'var.i'

double precision tta,ttaref,tmpfc

tta=tmpfc/100

ttaref=tref/100

delh_air=o2frac_a*100*(
alp_o2 *(tta - ttaref) +
(bet_o2 / (betx_o2 + 1)) *
(tta**((betx_o2 + 1)) - ttaref**((betx_o2 + 1))) +
(gam_co2 / (gamx_co2 + 1)) *
(tta**((gamx_co2 + 1)) - ttaref**((gamx_co2 + 1))) +
(n2frac_a*100*(
alp_n2 *(tta - ttaref) +
(bet_n2 / (betx_n2 + 1)) *
(tta**((betx_n2 + 1)) - ttaref**((betx_n2 + 1))) +
(gam_n2 / (gamx_n2 + 1)) *
(tta**((gamx_n2 + 1)) - ttaref**((gamx_n2 + 1))) +
(del_n2 / (delx_n2 + 1)) *
)
+

88
(tta**(delx_n2 + 1) - ttaref**(delx_n2 + 1))

end

!--------------------------------------------------------------------------------------!
subroutine eq_nox

include 'var.i'

double precision r1, r2, r3, k1_f, k2_f, k3_f, nmixwet_15,
lmixdry_15, fraco2_wet, fraco2_dry, nmixwet_act, nmixdry_act, tmp
dimension r1(mxrg), r2(mxrg), r3(mxrg)

do i=1, nmrg

k1_f=1.8e11*exp(-38370/t(i))
k2_f=1.8e7*exp(-4680/t(i))
k3_f=7.1e10*exp(-450/t(i))

timetot(i)=lnth(i)/vel(i)
umit(i)=int(timetot(i)/timestep)

!MOLAR CONCENTRATIONS IN COMBUSTION ZONE BASED ON TURNS EQUILIBRIUM CODE (kmol/m^3)
o_con(i)  =((o_mofc(1)*p)/(rbar*t(i)))
n_con(i)  =((n_mofc(1)*p)/(rbar*t(i)))
h2_con(i) =((h2_mofc(1)*p)/(rbar*t(i)))
oh_con(i) =((oh_mofc(1)*p)/(rbar*t(i)))
co_con(i) =((co_mofc(1)*p)/(rbar*t(i)))
no_con(i) =((no_mofc(1)*p)/(rbar*t(i)))
o2_con(i) =((o2_mofc(1)*p)/(rbar*t(i)))
h2o_con(i)=((h2o_mofc(1)*p)/(rbar*t(i)))
co2_con(i)=((co2_mofc(1)*p)/(rbar*t(i)))
n2_con(i) =((n2_mofc(1)*p)/(rbar*t(i)))

r1(i)=k1_f*o_con(i)*n2_con(i)
r2(i)=k2_f*n_con(i)*o2_con(i)
r3(i)=k3_f*n_con(i)*oh_con(i)

   do j=1, numit(i)
   
   !HEYWOOD NOX CORRELATION PG. 574
   nocon=nocon+
1      ( 2      (2*r1(i)*(1 - (nocon/no_con(i))**2)) /
2      (1 + ((nocon/no_con(i))*r1(i))/(r2(i)+r3(i)))
3      ) * timestep
4   
   enddo
   
endo

!NOX CONCENTRATION IN COMBUSTION ZONE (ppmv = noxfrac * 10^6)
noxppmv_cma_wt = ( (nocon)*rbar*t(nmrg))/p ) * 10**6
noxppmv_tot_wt = noxppmv_cma_wt/(1+(1/r)+(airmw*fact)/fuelmw)

!RECALCULATE COMPLETE COMBUSTION COEFFICIENTS TO ACCOUNT FOR COOLING AIR DILUTION
!zr*FUEL + a*O2 + a3*N2 + a1*H2O + a2*CO2 -> b*CO2 + c*H2O + d*N2 + e*O2 + zp*FUEL
ftot = fact + r*fact
atot = (1.0*fuelmw)/(ftot*4.76*airmw)
a1tot = atot/xa - atot
a2tot = 0
a3tot = 3.76*atot

90
btot = 1  
ctot = a1tot + 2  
dtot = a3tot  
etot = atot - 1  

!CORRECT NOX TO 15% O2  
!SEE TURNS, PG. 556  

!ACTUAL O2 FRACTIONS, WET AND DRY BASIS  
fraco2_wet = etot / (btot+ctot+dtot+etot)  
fraco2_dry = etot / (btot+dtot+etot)  

!TOTAL NUMBER OF MOLES AT 15% O2, WET AND DRY BASIS  
nmixwet_15 = 4.76* ((btot + (1+0.15))/(1 - 4.76*0.15) ) + 1  
nmixdry_15 = 4.76* ((btot + (1-0.15))/(1 - 4.76*0.15) ) - 1  

!ACTUAL TOTAL NUMBER OF MOLES, WET AND DRY BASIS  
nmixwet_act = 4.76*  
1  
2 + 1  
nmixdry_act = 4.76*  
1  
2 - 1  

!CORRECT ACTUAL NOX TO DRY BASIS  
noxppmvact_dry = noxppmv_tot_wt * (nmixwet_act/nmixdry_act)  

!NOX CONCENTRATION CORRECTED TO 15% O2, WET AND DRY BASIS  
noxppmv15_wet = noxppmv_tot_wt*(nmixwet_act/nmixwet_15)  
noxppmv15_dry = noxppmvact_dry*(nmixdry_act/nmixdry_15)  

end
subroutine t4calc
include 'var.i'

! ENERGY BALANCE AT COMBUSTOR EXIT (ENTHALPYS ARE PER UNIT MASS)
!(1 + fact) hcombp_m + (1/r) ha_m = (1 + 1/r + fact) he_m
! r = comba/coola
! ENTHALPY PER MASS IS ENTHALPY PER MOLE DIVIDED BY MOLEULAR WEIGHT
! h = h_/M

! ADD MOLES OF MOIST COOLING AIR TO COMBUSTION PRODUCTS
! c_tot = c(nmrg) + a1_coola
! d_tot = d(nmrg) + 3.76*a_coola
! e_tot = e(nmrg) + a_coola

! ADDITIONAL MOLE FRACTIONS
! co2frac_e = b(nmrg)/(b(nmrg) + c_tot + d_tot + e_tot)
! h2ofrac_e = c_tot/(b(nmrg) + c_tot + d_tot + e_tot)
! n2frac_e = d_tot/(b(nmrg) + c_tot + d_tot + e_tot)
! o2frac_e = e_tot/(b(nmrg) + c_tot + d_tot + e_tot)

! MOLECULAR WEIGHT OF MIXES
! mw_combp = co2frac(nmrg)*co2mw + h2ofrac(nmrg)*h2omw +
! 2 n2frac(nmrg)*n2mw + o2frac(nmrg)*o2mw
! mw_e = co2frac_e*co2mw + h2ofrac_e*h2omw + n2frac_e*n2mw +
! 1 o2frac_e*o2mw

! ENTHALPY CALCULATIONS
! ha = o2frac_a*delh_o2(tca(nmrg)) + n2frac_a*delh_n2(tca(nmrg)) +
! 1 h2ofrac_a*delh_h2o(tca(nmrg)) + h2ofrac_a*hf_h2o
! hcombp = co2frac(nmrg)*delh_co2(t(nmrg)) +
! 1 h2ofrac(nmrg)*delh_h2o(t(nmrg)) +
! 2 n2frac(nmrg)*delh_n2(t(nmrg)) +
! 3 o2frac(nmrg)*delh_o2(t(nmrg)) +
! 4 h2ofrac(nmrg)*hf_h2o + co2frac(nmrg)*hf_co2
! he = (((1.0 + fact)*(hcombp/mw_combp) + (1.0/r)*(ha/airmw))*mw_e)/
! 1 (1 + 1.0/r + fact)
! he_i = he - h2ofrac_e*hf_h2o - co2frac_e*hf_co2

! t4 = tguess
! xxy1 = 0
! xxy2 = 0

! do j = 1, maxit
! if (co2frac_e*delh_co2(t4) + h2ofrac_e*delh_h2o(t4) +
! 1 n2frac_e*delh_n2(t4) + o2frac_e*delh_o2(t4) .gt. he_i)
! then
! t4 = t4 - tinc
! xxy1 = xxy1 + 1
! else
! t4 = t4 + tinc
! xxy2 = xxy2 + 1
! endif
! if (xxy1 .gt. 0 .and. xxy2 .gt. 0) exit
! enddo

return
end
subroutine t5calc
include 'var.i'

! WORK OF COMPRESSOR = WORK OF GAS GENERATOR TURBINE
! n(t3-h2) = (1+f)(h4-h5), h4=he from t4calc
! ENTHALPY PER MASS IS ENTHALPY PER MOLE DIVIDED BY MOLEULAR WEIGHT
! h = h_/M
! h2, h3, and h5 all enthalpy per mole
! h2 = o2frac_a*delh_o2(tamb) + n2frac_a*delh_n2(tamb) +
! 1   h2ofrac_a*delh_h2o(tamb) + h2ofrac_a*hf_h2o
! h3 = o2frac_a*delh_o2(tin(1)) + n2frac_a*delh_n2(tin(1)) +
! 1   h2ofrac_a*delh_h2o(tin(1)) + h2ofrac_a*hf_h2o
! h5 = (he/mw_e - (turb_eff*((h3/airmw) - (h2/airmw))/(1+fact)))*mw_e

h5_i = h5 - h2ofrac_e*hf_h2o - co2frac_e*hf_co2

end
subroutine output
include 'var.i'

open(11,file='komout.out')

write(11,100) equivrat
write(11,101) tamb-273.15
write(11,102) patm
write(11,103) rh
write(11,104) pratio
write(11,105) comp_eff
write(11,106) turb_eff
write(11,107) tguess
write(11,109) tinc
write(11,110) timestep
write(11,111) nmrg

do j=1, nmrg
  write(11,112) j, comfrac(j)
enddo

do j=1, nmrg
  write(11,113) j, dia(j)
enddo

do j=1, nmrg
  write(11,114) j, lnth(j)
enddo

do j=1, nmrg
  write(11,156) j, t_w(j)
enddo

do j=1, nmrg
  write(11,115) j, vel(j)
enddo

write(11,118) e_w
write(11,119) e_c
write(11,157) k_w
write(11,158) h_perc
write(11,159) an_gap
write(11,161) dia_case

write(11,117)
write(11,150) fact
write(11,151) tin(1)-273.15
write(11,152) t4-273.15
write(11,153) t5-273.15
write(11,154) t5-tin(1)
write(11,162) t5-tamb
write(11,155) noxppmv_tot_wt
write(11,163) noxppmvact_dry
write(11,164) noxppmv15_wet
write(11,165) noxppmv15_dry

do j=1, nmrg
  write(11,200) j, t(j)
enddo
Equivalence Ratio                          = ',F12.4
Ambient Temperature                    (C) = ',F12.4
Ambient Pressure                     (kPa) = ',F12.4
Relative Humidity                      (%) = ',F12.4
Compressor Pressure Ratio                  = ',F12.4
Compressor Efficiency                      = ',F12.4
Turbine Efficiency = ',F12.4
Initial Temperature Guess              (K) = ',F12.4
Max Error for Enthalpy Iteration           = ',F12.4
Temp. Increment for Iteration              = ',F12.4
Timestep for NO Calc = ',F12.4
Number of Combustion Regions               = ',I7)
Combustion Fraction in Region ',I2,'            = ',F12.4)
Diameter of Region ',I2,'                  (m) = ',F12.4)
Length of Region ',I2,'                    (m) = ',F12.4)
Gas Velocity in Region ',I2,'            (m/s) = ',F12.4)
Emissivity of liner                        = ',F12.4)
Emissivity of casing                       = ',F12.4)
Fuel/air Ratio                             = ',F 12.4)
T3                                     (C) = ',F12.4)
T4                                     (C) = ',F12.4)
T5                                     (C) = ',F12.4)
T5-T3                                  (C) = ',F12.4)
Actual NOx concentration, wet       (ppmv) = ',F12.4)
Liner wall thickness of region ',I2,'      (m) = ',F12.4)
Thermal conductivity of liner      (W/m*K) = ',F12.4)
Hydrogen content of fuel          (%-mass) = ',F12.4)
Annulus air gap                        (m) = ',F12.4)
Max Error for Temp. Iteration              = ',F12.4)
Casing Diameter                        (m) = ',F12.4)
T5-T1                                  (C) = ',F12.4)
Actual NOx concentration, dry       (ppmv) = ',F12.4)
NOx concentration @ 15% O2, wet       (ppmv) = ',F12.4)
NOx concentration @ 15% O2, dry       (ppmv) = ',F12.4)
Temperature of region ',I2,'               (K) = ',F12.4)
return
end
Equivalence Ratio = 0.5000
Ambient Temperature (°C) = 25.0000
Ambient Pressure (kPa) = 101.3250
Relative Humidity (%) = 0.5000
Compressor Pressure Ratio = 11.6600
Compressor Efficiency = 0.8370
Turbine Efficiency = 0.8500
Initial Temperature Guess (K) = 2000.0000
Temp. Increment for Iteration = 0.1000
Timestep for NO Calc = 0.0001
Number of Combustion Regions = 5
Combustion Fraction in Region 1 = 1.0000
Combustion Fraction in Region 2 = 0.0000
Combustion Fraction in Region 3 = 0.0000
Combustion Fraction in Region 4 = 0.0000
Combustion Fraction in Region 5 = 0.0000
Diameter of Region 1 (m) = 0.0860
Diameter of Region 2 (m) = 0.0860
Diameter of Region 3 (m) = 0.1650
Diameter of Region 4 (m) = 0.1650
Diameter of Region 5 (m) = 0.1650
Length of Region 1 (m) = 0.1300
Length of Region 2 (m) = 0.1300
Length of Region 3 (m) = 0.1100
Length of Region 4 (m) = 0.1100
Length of Region 5 (m) = 0.0869
Liner wall thickness of region 1 (m) = 0.0012
Liner wall thickness of region 2 (m) = 0.0012
Liner wall thickness of region 3 (m) = 0.0012
Liner wall thickness of region 4 (m) = 0.0012
Liner wall thickness of region 5 (m) = 0.0012
Gas Velocity in Region 1 (m/s) = 35.0000
Gas Velocity in Region 2 (m/s) = 35.0000
Gas Velocity in Region 3 (m/s) = 12.0000
Gas Velocity in Region 4 (m/s) = 12.0000
Gas Velocity in Region 5 (m/s) = 12.0000
Emissivity of liner = 0.7000
Emissivity of casing = 0.4000
Thermal conductivity of liner (W/m*K) = 26.0000
Hydrogen content of fuel (%-mass) = 8.3300
Annulus air gap (m) = 0.0300
Casing Diameter (m) = 1.0000

***KOMBUST OUTPUT***

Fuel/air Ratio = 0.0291
T3 (°C) = 387.3760
T4 (°C) = 1004.0500
T5 (°C) = 751.3500
T5-T3 (°C) = 363.9740
T5-T1 (°C) = 726.3500
Actual NOx concentration, wet (ppmv) = 1.0263
Actual NOx concentration, dry (ppmv) = 1.0718
NOx concentration @ 15% O2, wet (ppmv) = 0.5124
NOx concentration @ 15% O2, dry (ppmv) = 0.6327
Temperature of region 1 (K) = 1770.6000
Temperature of region 2 (K) = 1770.6000
Temperature of region 3 (K) = 1770.6000
Temperature of region 4 (K) = 1770.6000
Temperature of region 5 (K) = 1770.6000