MULTI-DIMENSIONAL NITRIC OXIDE EMISSIONS PREDICTOR FOR PRELIMINARY GAS TURBINE COMBUSTOR DESIGN OPTIMIZATION

by

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A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
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This thesis pertains to development of preliminary combustor design tools for prediction of NO\textsubscript{x} emissions from aircraft gas turbine combustors. These tools are developed in the form of chemical reactor models and their objective is to predict the formation of NO\textsubscript{x} based on combustor geometry and engine input parameters such as inlet pressure, inlet temperature, fuel flow and air flow. The construction of the reactor networks follow from cold flow computational fluid dynamics results as it provides a way for allocating volumes to each reactor in the network. The ability of the model to predict NO\textsubscript{x} has been analysed by comparing predictions with measured data and theoretical trends. The model predictions for different combustors satisfy theoretical trends across various thrust levels in that the model correctly captures the effect of various input parameters on NO\textsubscript{x} formation and predicts most power conditions for various combustors within ±15% of the measured value.
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*Variables*

\(A\)  \(\text{Area (m}^2\)\)
\(B_m\)  \(\text{Mass Transfer Number}\)
\(c_p\)  \(\text{Specific Heat (J/kg/K)}\)
\(E\)  \(\text{Energy (cal/gmol)}\)
\(EI\)  \(\text{Emissions Index (g/kg}_{fuel}\)\)
\(FAR\)  \(\text{Fuel/Air Ratio}\)
\(F_{oo}\)  \(\text{Rated Thrust (kN)}\)
\(G\)  \(\text{Gibbs Free Energy (J)}\)
\(H\)  \(\text{Enthalpy (J)}\)
\(h\)  \(\text{Specific Enthalpy (J/kg)}\)
\(K_p\)  \(\text{Equilibrium Constant}\)
\(k\)  \(\text{Thermal Conductivity (W/(m \ast K))}\)
\(MW\)  \(\text{The Molecular Weight (g/mol)}\)
\(\dot{m}\)  \(\text{Mass Flow Rate (kg/s)}\)
\(\dot{m}_a\)  \(\text{Air Mass flow Rate (kg/s)}\)
\(\dot{m}'''\)  \(\text{Volumetric mass production rate (kg/s/m}^3\)\)
\(\dot{m}'''\)  \(\text{Mass Flux (kg/s/m}^2\)\)
\(\pi_{00}\)  \(\text{Takeoff Pressure Ratio}\)
\(P\)  \(\text{Pressure (kPa)}\)
\( P_3 \)  
Inlet Pressure \((kPa)\)

\( \Delta P_3 \)  
Combustor Pressure Drop

\( Pr \)  
Prandtl Number

\( \dot{Q} \)  
Heat Transfer Rate \((W)\)

\( \dot{Q}'' \)  
Heat Flux \((W/m^2)\)

\( Re \)  
Reynolds Number

\( R \)  
Ideal Gas Constant \((8.314J/(kg \cdot K))\)

\( S \)  
Entropy \((J/K)\)

\( SFC \)  
Specific Fuel Consumption \((kg_{fuel}/(hrkN))\)

\( SMD \)  
Sauter Mean Diameter \((\mu m)\)

\( s \)  
Unmixedness Parameter

\( T \)  
Temperature \((K)\)

\( T_3 \)  
Inlet Temperature \((K)\)

\( T_{pz} \)  
Primary Zone Temperature \((K)\)

\( T_{st} \)  
Stoichiometric Temperature \((K)\)

\( TIM \)  
Time in Mode

\( \bar{u} \)  
Velocity \((m/s)\)

\( V_c \)  
Effective Combustion Volume \((m^3)\)

\( V \)  
Volume \((m^3)\)

\( Y \)  
Mass Fraction \((kg/kg)\)

**Greek**

\( \rho \)  
Density \((kg/m^3)\)

\( \sigma \)  
Standard Deviation

\( \lambda \)  
Evaporation Constant \((m^2/s)\)

\( \vec{\nabla} \)  
Del Operator

\( \dot{\omega} \)  
Species Production Rate \((kmol/(s \cdot m^3))\)
\( \phi \)  
Equivalence Ratio

\( \tau \)  
Time (s)

**Abbreviations**

CFD  
Computational Fluid Dynamics

CO  
Carbon Monoxide

CO\(_2\)  
Carbon Dioxide

DZ  
Dilution Zone

FAR  
Fuel Air Ratio

ICAO  
International Civil Aviation Organization

IZ  
Intermediate Zone

NO\(_x\)  
Oxides of Nitrogen (NO and NO\(_2\))

UHC  
Unburned Hydrocarbon

PFR  
Plug Flow Reactor

PSR  
Perfectly Stirred Reactor

PZ  
Primary Zone

**Combustor Nomenclature**

Combustor A  
Can Combustor

Combustor B  
Conventional Single Toroidal Annular Combustor

Combustor C  
Conventional Double Toroidal Annular Combustor

Combustor D  
Modern Single Toroidal Annular Combustor
Chapter 1

Introduction

The increasing trend towards more powerful aircraft engines together with expected future trends of more stringent environmental regulations have led designers to seek for more advanced design tools that can help make the initial design process of gas turbine combustors more efficient. Specifically, a tool that allows designers to predict quantitative relationship between various high level engine parameters and emissions is considered. Current practice in the aviation industry for assessing such relationships is to use engine specific correlations. The main goal of this thesis is to develop a more general method for examining these relationships so that it can be applied to a wide variety of combustors.

1.1 Motivation

Pollutant emissions from gas turbine engines are an important concern for engine manufacturers due to their detrimental effect on the environment. The past few decades have seen a rapid change in emissions regulations for aircraft gas turbine engines [2]. The anticipated increase in air transport around the world in the future and hence its contribution to total emissions has been the primary motivation behind these changes in regulations. Therefore, in order to keep pace with future emissions regulations, it is highly desirable for engine manufacturers to have computational tools that allow them
to study quantitatively the effects of various high level engine parameters such as inlet pressure ($P_3$), inlet temperature ($T_3$), local fuel-air ratio, and local geometry changes on exhaust emission levels. In particular, computational procedures that have shorter run-times would be of great interest at the initial design stage of the engine since it can significantly reduce the time of each concept design iteration.

## 1.2 Major Aircraft Emissions

The major pollutant emissions from an aircraft engine are unburned hydrocarbons (UHC), carbon monoxide (CO), oxides of nitrogen (NO$_x$) and exhaust smoke. The formation of UHC, CO and smoke is intimately related to combustion chemistry and hence the overall combustion efficiency, whereas the NO$_x$ formation rate is directly related to combustion temperature. Over the last 40 years, improvements in fuel burn due to advancements in combustor design as well as increase in engine pressure ratio and combustor temperature have had a significant impact on reduction of smoke, CO and UHC; however, NO$_x$ production has been on a steady increase due to higher combustion temperatures. Although there are four pollutant emissions that have been identified, this thesis only focuses on the prediction methodology for NO$_x$.

### NO$_x$ Emissions

Oxides of nitrogen, commonly referred to as NO$_x$, are generally used to represent the collective quantity of both NO and NO$_2$. Most of the NO that is formed inside the combustor oxidizes to NO$_2$ after leaving the engine by reacting with atmospheric oxygen. The control of NO$_x$ with a simultaneous increase in thermodynamic engine efficiency (and therefore higher combustion temperature) has been one of the main challenges for aircraft manufacturers as these quantities are fundamentally inversely proportional. Although NO$_x$ emission production rates are highest at high power levels such as cruise,
climb-out and takeoff, the contribution of idle to aggregated low altitude NO$_x$ is very significant. The main concern over low altitude NO$_x$ emissions is that of human health; their role in the production of ground level ozone, better known as smog, is of great concern as it can lead to respiratory problems and other health issues.

**CO Emissions**

Carbon monoxide is the intermediate product of combustion of fuel and an oxidizer. Unlike NO$_x$, CO production is highly driven by combustion chemistry. Therefore, any effort aimed at improving combustion efficiency will also lead to lower CO levels. Generally, at high power levels, combustion efficiency is almost 100% and CO production is not a main concern. However, at low power conditions, especially at idle, combustion efficiencies are lower and thus higher levels of CO are produced. This finding holds for all commercial aviation engines, however, the problem of CO formation is more severe for smaller aircraft engines since they operate at very low pressure ratios at idle. Like oxides of nitrogen, carbon monoxide emissions are also a major health concern as they combine with hemoglobin in blood and reduce its oxygen carrying capacity. It should be noted that there are always tradeoffs between CO and NO$_x$ emissions, which need to be addressed during combustor design.

**UHC Emissions**

Unburned hydrocarbons are essentially products of the thermally degraded parent fuel with lower molecular weight species. Like CO, their production is also associated with combustion inefficiency and they tend to be high at low power conditions. In general, the factors that influence UHC emissions are generally found to be similar to those that influence CO emissions, although their formation chemistry is more complex than that of CO [18].
Smoke

Smoke is composed of tiny carbon particles also known as soot. It is formed in fuel rich regions of the combustor which are typically near fuel nozzles. As burnt gases move downstream, a large fraction of soot that is formed upstream is consumed. The amount of smoke in the exhaust therefore depends on how much soot is being produced upstream and subsequently consumed in downstream regions. The primary concern regarding smoke is its visible prominence from the exhaust [18].

1.3 Emission Trends in Aircraft Engines

The nature of pollutant formation is such that a change in thrust level will almost always cause CO and UHC concentrations to change in a direction, which is opposite to that of the change in NO\textsubscript{x} and smoke. This can be seen in figure 1.1. The production of CO and UHC is highest at 7% thrust condition and decreases exponentially as power level goes up with their concentrations being almost insignificant at 85% and 100% thrust conditions. On the other hand, NO\textsubscript{x} and smoke increase with increasing power level and achieve maximum values at 100% thrust. The increase in NO\textsubscript{x} at higher power levels is associated with higher temperature, however, increase in smoke is related to reduced fuel penetration since the higher pressure drop across the nozzle at high power conditions reduces the capability of fuel to penetrate in to surrounding air, thereby leading to local increase in fuel concentration [18].

1.4 ICAO Emission Regulations

The international civil aviation organisation (ICAO) is a specialized agency of the United Nations. Among other policy setting tasks related to air transport, it also outlines standards and regulations for aviation environmental protection. Currently, it has set
Chapter 1. Introduction

Figure 1.1: Typical Emission Trends for Aircraft Engines, adapted from [18]

regulations for civilian aircraft engines with rated thrust levels above 26.7 kN for a defined landing-takeoff cycle (LTO), which is based on an operational cycle around airports [18]. The LTO cycle time includes all operations performed by an aircraft below the altitude of 3000 ft/915 m and is the sum of times in each mode (TIM), i.e., the time that an aircraft spends during each operation. Typically, these operations correspond to four main thrust levels; 7\% (idle), 30\% (approach), 85\% (climb out) and 100\% (takeoff) as shown in figure 1.2. The integrated LTO cycle emissions are calculated in terms of their mass in grams per kilonewton of rated thrust at sea level. It is defined as follows:

$$Emission(\text{g/kN}) = \sum_{i=1}^{4} EI_i \times TIM_i \times Engine\ SFC$$  \hspace{1cm} (1.1)$$

where the sum is over the four ICAO LTO-cycle points. In the above equation, Engine SFC is defined as the fuel flow divided by the rated thrust output. The ICAO emission standards for engines with overall engine pressure ratios of less than 30 are shown in table 1.1. The parameter $\pi_{00}$ in the table represents the engine pressure ratio at takeoff.
and $F_{oo}$ is rated thrust of the engine.

$$
\begin{array}{|c|c|}
\hline
\text{Species} & \text{Subsonic Turbojet/Turbofan Engines Emissions (g/kN)} \\
\hline
\text{HC} & 19.6 \\
\text{CO} & 118.0 \\
\text{NO}_x & 40.052 + 1.5681\pi_{00} - 0.3615F_{oo} - 0.0018\pi_{00}F_{oo} \\
\text{Smoke} & 83.6F_{oo}^{0.274} \\
\hline
\end{array}
$$

Table 1.1: ICAO Gaseous Emissions Standards for Engines Produced on or after 1 January 2014, [2]

Current ICAO regulations are only defined for aircraft operations at low altitudes (below 3000 ft), however, there have been growing concerns about ozone depletion due to greenhouse gases and future regulations may include CO$_2$ emissions at cruise conditions.

### 1.5 Current Emission Prediction Strategies

There are several emissions prediction strategies but generally they can be divided into three broad categories; 1) prediction using correlations 2) prediction using models with reduced order physics and 3) predictions using computational fluid dynamics simulations. Each method has its advantages at a specific design stage and these will be discussed below.
1.5.1 Correlations

These are the simplest of the three methods and are computationally inexpensive in comparison to the other two methods. The inputs to correlations are generally high level global engine parameters such as $P_3$, $T_3$, fuel-air ratio and fuel flow. The use of correlations is extremely simple, however, their predictions are only accurate for a class of combustors for which they are derived. From a fundamental point of view, these correlations are derived from a large number of data set on various conventional combustors, and therefore, the coefficients and exponents that are found in these correlations are only expected to work for similar combustors. Considering their limited prediction capability, correlations may not be feasible for use at the intial design stage of a combustor, especially if its design varies vastly from a conventional combustor design. There are several correlations that are used in practice but they can all be divided in to two main categories. These two types are discussed in the following sections.

**Empirical NO$_x$ Correlations**

Empirical correlations typically only have $P_3$ and $T_3$ as inputs and are highly combustor specific. These correlations are usually developed for specific engines and are tuned to work for the full operating range of the engine. There are several empirical correlations in the open literature with many of them having similar forms. Equation 1.3 shows one such correlation that is used in the NASA Engine Performance Program [8] and has the form

$$EINO_x = 33.2 \left( \frac{P_3}{432.7} \right)^{0.4} \exp \left( \frac{T_3 - 1487.67}{350} \right)$$

(1.2)
where $P_3$ is the inlet pressure in psia, and $T_3$ is the combustor inlet temperature in °R. Another correlation which is used by GasTurb [6] is given by

$$EINO_x = 32 \left( \frac{P_3}{2965} \right)^{0.4} \exp \left( \frac{T_3 - 826}{194} \right)$$  (1.3)

where $P_3$ is in kPa and $T_3$ is in Kelvin.

The use of empirical correlations such as those given above would not be effective for a new combustor design since they do not include other important global parameters such as fuel flow, airflow and overall geometry, all of which significantly affect the emission characteristics of a combustor. Most of the use of current empirical correlations is in engine performance programs since they can be useful in predicting NO$_x$ emissions output at different power levels.

**Semi-empirical NO$_x$ Correlations**

Semi-empirical correlations, compared to empirical correlations, contain few other physical parameters that are very important in the formation of pollutant emissions. Similar to empirical correlations, they have empirically determined coefficients and exponents, but due to the presence of these other input variables, they are able to predict emission trends better than pure empirical correlations. One example of a semi-empirical correlation is

$$EINO_x = \frac{9 \times 10^{-9} P_3^{1.25} V_c \exp(0.01 T_{st})}{\dot{m}_a T_{pz}}$$  (1.4)

where $P_3$ and $T_3$ have the same definition as before, $V_c$ is the effective combustion volume, $T_{st}$ is the stoichiometric temperature of the fuel, $T_{pz}$ is the equilibrium primary zone temperature and $\dot{m}_a$ is the mass flow rate of air. The combination of $\dot{m}_a$, $V_c$, $P_3$ and $T_{pz}$ essentially describe the residence time inside the primary zone of the combustor.

Although the above correlation contains most of the necessary input variables for
Chapter 1. Introduction

NO\textsubscript{x} prediction, namely temperature and residence time, the evaluation of \( V_c \) and \( T_{pz} \) is not very straightforward. This is because the flow field inside the combustor is highly turbulent and the conditions inside the primary zone are not always at equilibrium. For instance, a combustor equipped with an airblast fuel nozzle with a certain set of positions for primary jets, cooling jets and igniter may differ substantially in terms of the flow field inside the primary zone from another combustor that has a pressure fuel nozzle and a different set of air addition sites and igniter positions. Hence, if a combustor design change were to be evaluated using a single global correlation without considering local geometry changes, the prediction results may significantly vary and possibly not even trend properly. On the other hand, if this design change was small and did not involve a drastic variation of the original design, it may perform reasonably well in predicting emissions.

Some publications on emissions prediction in the recent decades have necessitated categorization of semi-empirical correlations into further two categories; a) global Correlations and b) local correlations. Global correlations are the most common types of semi-empirical correlations. In fact, there is no distinction made between semi-empirical correlations and global semi-empirical correlations in most of the publications and the two terms are used synonymously. Global correlations make broad assumptions on the overall conditions within the combustor focusing primarily on the conditions within the primary zone. Equation 1.3 above is an example of a global correlation. Local correlations, on the other hand, divide a combustor into small volumes and, using simple equations within each of these small volumes, attempt to capture emission species concentration in these localized areas of the combustor. An example of a set of local correlations suggested by Rizk and Mongia [27] is given by

\[
\text{EINO}_x = 1 \times 10^{13} \left( \frac{P_3}{1.4 \times 10^6} \right)^{aa} \exp \left( \frac{-71442}{T_c} \right) (7.56\phi^{-7.2} - 1.6)^{0.64} \tau^{0.64} \quad (1.5)
\]
If the equivalence ratio is above 1.08, following equation is used:

$$EINO_x = 1 \times 10^{13} \left( \frac{P_3}{1.4 \times 10^6} \right)^{aa} exp \left( \frac{-71442}{T_c} \right) \left(5.21\phi^{-2.99} - 1.6\right)\tau^{0.64} \quad (1.6)$$

The above two equations are used for volumes in the primary zone. For conditions prevailing in typical intermediate and dilution zones, the following equation was proposed:

$$EINO_x = 1 \times 10^{13} \left( \frac{P_3}{1.4 \times 10^6} \right)^{aa} exp \left( \frac{-71442}{T_c} \right) \left(1.172\phi^{-4.56} - 1.6\right)\tau^{0.876} \quad (1.7)$$

where,

$$aa = 11.95exp \left( \frac{-\phi}{5.76} \right) - 10.0 \quad (1.8)$$

In the above equations, $\phi$ is the local equivalence ratio of a given volume, $T_c$ is defined as the equilibrium reaction temperature of a given volume at the volume’s local equivalence ratio, and $\tau$ is the residence time of gases within that volume. Other variables are defined as before.

The prediction capability of local correlations is highly contingent on the resemblance of a conventional combustor to the combustor under evaluation. In many cases, the predictions can be worse than global correlations due to the presence of a large number of constants and exponents in these equations which can introduce large errors through the over or under estimation of the residence time.

### 1.5.2 Chemical Reactor Models

Unlike empirical and semi-empirical calculations, chemical reactor models do not simplify emissions formation into simple equations. These models divide a combustor into various zones and attempt to simulate them using appropriate ideal chemical reactors. Perfectly stirred and plug flow reactors are the two types of constant pressure reactors that are used for simulation of gas turbine engines. The use of chemical reactors to simulate gas
turbine engines has been made by several researchers in the past although its use in the industry has not been as popular as the use of correlations due to the relative complexity of using these models. Most of the models that are developed in the literature are only verified for a certain class of combustors and this makes it difficult for designers to extend it to other types of combustors. Therefore, models that are developed and verified for a range of different combustors with the ability to capture effects of fuel nozzle, local geometry changes and other physical parameters on emissions would be of great value to the designer as it can significantly reduce the time of each initial design iteration by eliminating use of high fidelity simulations. The details on the application of reactor models to combustors will be discussed in chapter 2.

1.5.3 Computational Fluid Dynamics Simulations

The use of computational fluid dynamics (CFD) simulations for a detailed combustor design is inevitable as they give deep insight into various flow features and performance characteristics of a combustor. Although CFD is capable of predicting performance, emissions and other characteristics of a combustor more accurately than a chemical reactor model or any class of correlations from a fundamental point of view, there remain a few significant problems with its application at the initial design stage. First, CFD requires a detailed knowledge of the geometry and flow splits of the combustor but, as one may expect, these design parameters are generally not well established at a preliminary design stage. In fact, the goal at such an early stage in the design is to obtain these parameters so that they can be used as design constraints for the remaining of the design process. Secondly, if CFD was to be performed, by assuming certain design parameters, it would be very expensive to do so in terms of time and cost. For instance, a full reactive flow simulation of a combustor can take up to days or even weeks. Due to these above reasons, CFD is generally not considered to be a viable tool for preliminary combustor design.
1.6 Scope of Thesis

The main objective of this thesis is to develop a specific methodology to predict NO\textsubscript{x} emissions for each of the generic classes of combustors. The emissions prediction for each of the combustors will involve using two different emissions prediction strategies; correlations and chemical reactor model(s). The results of each of the prediction methods will be evaluated and subsequently, a specific methodology will be selected. The combustors available for this study include can combustor (Combustor A) and single annular combustors. Based on flow fields of single annular combustors, there are three different types available for study; conventional single toroidal combustor (Combustor B), conventional double toroidal combustor (Combustor C) and modern single toroidal combustor (Combustor D).

1.7 Thesis Outline

Chapter 2 provides theoretical background on gas turbine combustion as well as specifics of NO\textsubscript{x} formation and its dependence on various physical parameters. A brief discussion of each of the combustor test cases is done in chapter 3. This chapter also discusses in detail the application of correlations and development of a reactor model for each of the combustors. In chapter 4, results for each case will be presented and evaluated. Finally in chapter 5, some conclusions, based on the results in chapter 4, will be drawn and future work will be discussed.
Chapter 2

Background Information

2.1 Gas Turbine Combustor

The main purpose of the gas turbine combustor in an aircraft engine is to add energy to the flow that is coming from the compressor and direct this hot flow to the turbine with an appropriate temperature distribution. In the early days of combustor development, there was a considerable lack of knowledge of the many physical processes that occur in a combustor and hence it was treated more like a black box that provided energy to the system following reaction of fuel and oxidizer. As time progressed, scientists and engineers developed more understanding of the combustor technology and by around 1950, most of the basic features of conventional gas turbine combustors, as we know them today, were firmly established [18]. Although the specifics of a combustor vary from one design to another, most of them can be characterised by having three distinct combustion zones. They are; primary zone, intermediate zone and dilution zone. The function of each of these zones is independently discussed below.
2.1.1 Primary Zone

The main function of the primary zone is to keep the flame anchored and provide sufficient time for fuel and air to mix and burn to completion. A very common way of achieving this is by the creation of a toroidal flow reversal that recirculates a portion of the hot burnt gases upstream of the flow as shown in figure 2.1. This recirculated flow, in addition to mixing with the upstream flow, acts as an ignition source to the new incoming mixture of fuel and air. There are two ways in which flow recirculation can be created. One is based on the swirl produced by the air swirler while the other method relies on air injected through liner holes.

2.1.2 Intermediate Zone

The intermediate zone serves to complement the function of primary zone by allowing any incomplete reactions upstream to proceed to completion. The role of intermediate zone may vary depending on a particular power condition. For instance, at high power conditions it acts towards lowering the CO$_2$ to CO dissociation losses that result from very high temperatures in the primary zone. On the other hand, at low power conditions, it may act as a reaction completion zone since reaction and mixing rates are slow owing to lower primary zones temperatures. The advancement in aircraft engine technology in the last few decades has led to a substantial reduction in combustor size and an increase in its ability to operate at a higher pressure ratio. For these collective reasons, the size of the intermediate zone has also become much smaller. In fact, many new engines do not even have a prescribed intermediate zone according to its traditional definition.

2.1.3 Dilution Zone

The purpose of dilution air is to bring the temperature of the hot gases coming from primary zone down to a level that is acceptable to turbine as well as to provide the
appropriate temperature distribution for turbine blades. The amount of air entering through dilution holes is a significant percentage of the total combustor air. Most combustion reactions that initiated in the primary zone are largely completed by the time the flow arrives in the dilution zone. The formation of NO\textsubscript{x} essentially comes to a halt as temperatures fall below 1800 K. The oxidation of CO may still be occurring in this zone at high power levels, however, at low power conditions, the rapid cooling of the main stream flow by these large dilution jets may ‘freeze’ the composition of gases at their upstream value leading to higher amounts of CO and unburned hydrocarbons in the exhaust.

![Schematic of a conventional gas turbine combustor](image)

Figure 2.1: Schematic of a conventional gas turbine combustor, adapted from [18]

### 2.2 Combustion Fundamentals

The process of combustion involves rapid oxidation of fuel to produce mainly carbon dioxide, water and heat. The two main modes of combustion are flame and non-flame. The flame mode is characterised by emittance of visible electromagnetic radiation and signifies the region of high intensity chemical reactions whereas the non flame mode does not emit light and is usually attributed to slow chemistry. The flame mode can be further categorized as premixed flame or diffusion flame. In a premixed flame, fuel and air are
fully premixed with a certain ratio of fuel and air before combustion initiates. A diffusion flame, on the other hand, involves the simultaneous process of combustion and diffusion of fuel and air. The fuel and air are preheated as they diffuse into each other around the flame and subsequently react as they approach the flame surface. Most aircraft gas turbine combustors operate on the principle of diffusive combustion.

The design of gas turbine combustors is highly dependent on combustion modelling as it provides insight into various combustion phenomena such as ignition, flame stabilization, burning rates and species concentrations. The modelling of all these combustion phenomena require knowledge of combustion kinetics which comes from the fuel oxidation mechanism. The prediction of species concentrations and pollutant emissions, however, can also be done using equilibrium analysis. A discussion of equilibrium analysis is given below.

2.2.1 Equilibrium Analysis

Equilibrium analysis can only predict species concentrations after the reactants and products have attained thermodynamic equilibrium. These calculations are based on second law of thermodynamics which requires the composition of any reacting isolated system to shift towards the point of maximum entropy. For an isolated system with constant internal energy, volume and mass, the entropy change, \( dS \), can be written as [34]

\[
dS \geq 0 \quad (2.1)
\]

The above argument can be extended to non isolated systems by replacing entropy with Gibbs Free energy, \( G \), as the characteristic thermodynamic property. The Gibbs free energy is defined as

\[
G = H - TS \quad (2.2)
\]
where \( H \) is enthalpy, \( T \) is temperature and \( S \) is entropy of the system. The condition for approaching equilibrium by a fixed mass at a given temperature and pressure then becomes

\[
dG \leq 0 \quad (2.3)
\]

The point at which equilibrium is attained by a fixed mass system at a prescribed temperature and pressure is expressed as

\[
dG = 0 \quad (2.4)
\]

The above relations show the theoretical basis of equilibrium calculations. For details on derivation of the Standard-State Gibbs Function Change \( \Delta G^\circ_T \) and Equilibrium Constant \( K_p \), the reader is referred to Turns [34].

The problem with equilibrium analysis is that it does not provide information about the time evolution of species concentrations (their rate of formation and destruction) during combustion. For reactions occurring in high temperature environments with sufficiently long residence times, it may be reasonable to assume that combustion is essentially completed, but in regions of low temperature with short residence times, it can be quite inaccurate to assume equilibrium species concentrations.

### 2.2.2 Finite-Rate Chemical Kinetics

In many practical situations, combustion process is controlled by chemical reaction rates, and, in most scenarios, chemical rates determine pollutant formation and destruction. The chemical kinetics of the oxidation of fuel are represented by elementary reactions which describe the detailed pathways from which reactants are converted into products. The number of elementary reactions describing the combustion process can include several hundreds of reactions and species depending on the fuel. Generally, larger hydrocarbon fuels have more elementary steps involved than smaller hydrocarbon fuels since
larger hydrocarbon molecules have to go through more intermediate steps than smaller hydrocarbon molecules before finally oxidizing to CO$_2$ and H$_2$O. In some cases, the description of detailed chemical kinetics of the fuel is simplified by reducing the number of elementary reactions in order to bring the computational time of the simulation to a manageable level. Some reactive flow simulations even use global one step reaction mechanism to describe the behavior of fuel oxidation. For more information than is provided here, the reader is referred to [34] and McAllister et al. [21].

### 2.3 Basis for Chemical Reactor Equations

The governing equations for a reactive flow of a gaseous mixture are the mass, momentum, energy and species conservation equations. The most general form of mass conservation for the mixture can be written as

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \tag{2.5}
\]

where $\rho$ is density and $u$ is the flow velocity. The first term in the above equation describes the rate of gain of mass per unit volume whereas the second term describes the net rate of mass flow out per unit volume [34]. The general vector form of the species conservation is expressed as

\[
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot \vec{\dot{m}}_i'' = \dot{m}_i''' \text{ for } i = 1, 2, ..., N, \tag{2.6}
\]

where $Y_i$ is defined as the mass fraction of species $i$, $\dot{m}_i''$ is the mass flux of species $i$, and $\dot{m}_i'''$ is the net rate of production of species $i$. Equation 2.6 states that the sum of the rate of gain of mass of species $i$ per unit volume and the net rate of mass flow of species $i$ out by diffusion and bulk flow per unit volume is equal to the net rate of mass production of species $i$ per unit volume [34]. The vector form of the momentum equation for the
mixture is given by [15]

\[
\frac{\partial (\rho \vec{u})}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \vec{u} + P \vec{I} - \vec{\tau}) = \rho \vec{f}
\]  

(2.7)

where \(P\) is the fluid pressure, \(\vec{I}\) is the identity dyad (matrix) and \(\vec{\tau}\) is the fluid stress dyad. The symbol \(\vec{f}\) on the right represents external body forces. The fluid stress dyad (tensor) in equation 2.7 is related to the fluid strain rate as follows

\[
\vec{\tau} = \mu \left[ (\vec{\nabla} \vec{u} + (\vec{\nabla} \vec{u})^T) - \frac{2}{3} \vec{\delta} (\vec{\nabla} \cdot \vec{u}) \right]
\]  

(2.8)

In the above equation, \(\mu\) is dynamic viscosity and \(\vec{\delta}\) is Kronecker delta. Lastly, the general vector form of the conservation of energy for the mixture is expressed as

\[
\frac{\partial (\rho E)}{\partial t} + \vec{\nabla} \cdot \left[ \rho \vec{u} \left( E + \frac{P}{\rho} \right) - \vec{\tau} \cdot \vec{u} + \vec{q} \right] = \rho \vec{f} \cdot \vec{u}
\]  

(2.9)

where \(E\) is the total specific energy of the fluid (the sum of kinetic energy of bulk motion and internal thermal energy), \(\vec{q}\) is the vector heat flux representing the net flux of heat out of the fluid. The total specific energy is related to fluid enthalpy, \(h\), by equation 2.10 and the heat flux is related to the temperature gradient using Fourier’s law according to equation 2.11.

\[
E = h + \frac{1}{2} \vec{u}^2 - \frac{P}{\rho}
\]  

(2.10)

\[
\vec{q} = -k \vec{\nabla} T
\]  

(2.11)

where \(k\) is the thermal conductivity of the fluid.

The prediction of species concentrations from the simultaneous solution of these four coupled, non-linear, partial differential equations and the chemical kinetics relations can be very expensive in terms of time, even if the computational grid does not contain a
large number of cells. The modelling of unsteady flow phenomena such as turbulence in itself poses a significant challenge, let alone its integration into the combustor model. In addition, such a model would require detailed geometry of the combustor which is generally not available at a preliminary design stage of the engine as was mentioned earlier. Therefore, in an effort to reduce the complexity of a detailed model, a more approximate approach has been adopted which involves either the one dimensional solution of the above equations or the solution of only a reduced set of equations. These simplified equations essentially describe the physics of different types of reactors. The two types of constant pressure reactors that are used in the development of chemical reactor models in this thesis are discussed below.

### 2.3.1 Perfectly Stirred Reactor

The perfectly stirred reactor (PSR) is an ideal reactor in which perfect mixing is assumed inside the control volume, as shown in Fig. 2.2 [34]. The PSR may be suitable for modelling of real combustion processes in which mixing rates are very high and combustion is determined largely by chemical reaction rates. The PSR is a zero dimensional reactor, hence the species concentrations inside the volume do not depend on any spatial coordinate and are only dependent on residence time. The equations that describe the physics of the perfectly stirred reactor are species and energy conservation equations. The overall mass continuity cannot explicitly be used since velocity has no physical definition in a PSR. Similarly, momentum equation is not required as the pressure is constant everywhere in the reactor.

Integrating equation 2.6 over the entire control volume, V, and applying the divergence theorem to the second term on the left hand side, gives the steady state individual species conservation equation for the PSR

\[
\dot{m}_{i,\text{out}} - \dot{m}_{i,\text{in}} = \dot{m}_{i}^{\text{in}}V
\]

(2.12)
The mass generation rate of a species, $\dot{m}_{i}^{m}$, is related to the net species production rate, $\dot{\omega}_{i}$, and species molecular weight, $MW_{i}$ as

$$\dot{m}_{i}^{m} = \dot{\omega}_{i}MW_{i}$$

(2.13)

Considering the transport of species by only bulk fluid motion, the mass flow rate of a particular species is equal to its mass fraction, $Y_{i}$, times the total mass flow rate

$$\dot{m}_{i} = \dot{m}Y_{i}$$

(2.14)

Since all physical and chemical properties of the mixture are the same everywhere in the reactor, the outlet mass fractions should be equal to the mass fractions inside the reactor. After re-arranging and making necessary substitutions, equation 2.12 becomes

$$\dot{\omega}_{i}MW_{i}V + \dot{m}(Y_{i,in} - Y_{i,out}) = 0$$

(2.15)

The application of the conservation of energy equation to a steady-state, steady flow with
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no spatial gradients results in the following simple equation

\[
\dot{Q} = \dot{m}(h_{\text{out}} - h_{\text{in}}) \tag{2.16}
\]

where \( h \) is the specific enthalpy of the mixture. The above equation can be written in terms of the individual species as

\[
\dot{Q} = \dot{m} \left( \sum_{i=1}^{n} Y_{i,\text{out}} h_i(T) - \sum_{i=1}^{n} Y_{i,\text{in}} h_i(T_{\text{in}}) \right) \tag{2.17}
\]

where

\[
h_i(T) = h_{f,i}^{\circ} + \int_{T_{\text{ref}}}^{T} c_{p,i}(T) dT \tag{2.18}
\]

In equation 2.18, \( h_i(T) \) is the specific enthalpy of the \( i^{th} \) species, \( h_{f,i}^{\circ} \) is its enthalpy of formation and \( c_{p,i}(T) \) is its specific heat capacity at constant pressure.

2.3.2 Plug Flow Reactor

A plug flow reactor (PFR), as shown in Fig 2.3, is an ideal reactor whose equations are based on assumptions of steady, inviscid and one-dimensional flow. There is no mixing in the axial direction which implies that the molecular and turbulent mass diffusion is negligible in the flow direction. The physical properties of the flow are assumed to be uniform in the radial direction. Intuitively, a plug flow reactor can be thought of as consisting of a series of PSRs (very thin cylindrical volumes) whose volumes approach zero as the number of PSRs approach infinity. In fact, a plug flow reactor may be approximated by a reasonably large number of PSRs in series, provided that the gradients in temperature and pressure along the length of the PFR are not too significant. The conservation relations for plug flow reactor are written as follows [34]:

**Continuity**

\[
\frac{d(\rho u_x A)}{dx} = 0 \tag{2.19}
\]
Momentum Conservation

\[ \frac{dP}{dx} + \rho u_x \frac{du_x}{dx} = 0 \]  \hspace{1cm} (2.20)

Energy Conservation

\[ \frac{d(h + u_x^2/2)}{dx} + \frac{Q^p}{\dot{m}} = 0 \]  \hspace{1cm} (2.21)

Species Conservation

\[ \frac{dY_i}{dx} - \frac{\dot{\omega}_i MW_i}{\rho u_x} = 0 \]  \hspace{1cm} (2.22)

In the equations above, \( u_x \) represents the axial velocity and \( P \) represents the local perimeter of the reactor. All other variables are defined as before. The solution to the plug flow reactor can be obtained by a numerical scheme that simultaneous solves the coupled set of ordinary differential equations.

2.4 Mechanisms for the Formation of Nitric Oxide

The formation of nitric oxide (NO) during combustion occurs from the reaction of intermediate chemical species with atmospheric Nitrogen. The three main mechanisms through which Nitric Oxide can be formed are: thermal mechanism, fenimore mechanism and N\(_2\)O-intermediate mechanism. Each of these mechanisms are briefly discussed below.
2.4.1 Thermal or Zeldovich Mechanism

Thermal mechanism is the main route for nitric oxide production in aircraft gas turbine engines. Thermal NO is produced by the oxidation of atmospheric nitrogen at high temperatures. The extended Zeldovich mechanism consists of the following three reactions [34]:

\[
\begin{align*}
O + N_2 & \rightleftharpoons NO + N \\
N + O_2 & \rightleftharpoons NO + O \\
N + OH & \rightleftharpoons NO + H
\end{align*}
\]

The activation energy required to break the triple bond of $N_2$ in the first reaction is about an order of magnitude higher than that needed for the second reaction. Once nitrogen is broken into NO and N, the oxidation of nitrogen radical occurs very quickly. Hence, the first reaction is rate limiting and it proceeds at a significant rate only at temperatures above 1800 K. The formation of NO increases at an exponential rate as the temperature is increased beyond this value.

The reaction time for the reaction of equation 2.23 always exceeds the characteristic time of combustion reactions [14] and therefore it may be possible to decouple the kinetics of thermal NO$_x$ from the kinetics of the combustion process. Following this assumption, the concentration of O$_2$, N$_2$, O and OH can be assumed to be at their equilibrium values, the concentration of N can be assumed to be at its steady state value and the concentration of H can be assumed from the partial equilibrium of the following reaction process.

\[
H + O_2 \rightleftharpoons OH + O
\] (2.26)

The above argument may yield reasonable results when residence time of gases in the
combustion chamber are long; however, if the combustion process has not attained equilibrium, the assumption of equilibrium concentrations of O\textsubscript{2}, N\textsubscript{2}, O and OH can lead to erroneous results due to the non equilibrium radical concentrations that exist during the combustion process.

### 2.4.2 N\textsubscript{2}O Intermediate Mechanism

The N\textsubscript{2}O (Nitrous Oxide) mechanism, according to Bowman [14], can be described as follows:

\[
\begin{align*}
\text{NCO} + \text{NO} &\rightleftharpoons \text{N}_2\text{O} + \text{CO} \quad (2.27) \\
\text{NH} + \text{NO} &\rightleftharpoons \text{N}_2\text{O} + \text{H} \quad (2.28)
\end{align*}
\]

The above reactions describe the main route for formation of N\textsubscript{2}O in fossil fuel combustion. In combustion of natural gas with fuel lean mixtures and at low temperatures and elevated pressures, the contribution of the following reaction to N\textsubscript{2}O production is also significant:

\[
\text{O} + \text{N}_2 \rightleftharpoons \text{N}_2\text{O} \quad (2.29)
\]

The removal of N\textsubscript{2}O produced from the combination of the above reactions can occur in the following possible ways:

\[
\begin{align*}
\text{H} + \text{N}_2\text{O} &\rightleftharpoons \text{N}_2 + \text{OH} \quad (2.30) \\
\text{N}_2\text{O} + \text{O} &\rightleftharpoons \text{N}_2 + \text{O}_2 \quad (2.31) \\
\text{N}_2\text{O} + \text{O} &\rightleftharpoons \text{NO} + \text{NO} \quad (2.32)
\end{align*}
\]

with last reaction being the primary one for NO\textsubscript{x} formation. It has been reported in [14] that the lifetimes of N\textsubscript{2}O for combustion processes above 1500 K are very short,
which suggests that, except for very lean fuel-air mixtures, the contribution of NO from N$_2$O intermediate mechanism is relatively insignificant. Since aircraft combustors run on very high temperatures, it is safe to neglect the formation of NO through nitrous oxide mechanism.

### 2.4.3 Fenimore or Prompt Mechanism

According to Fenimore [9], some NO was observed to be formed extremely fast in the flame zone, long before any formation of NO through Zeldovich mechanism would be expected. Fenimore therefore concluded that there must be another mechanism governing such prompt formation of NO in early regions of the flame and that it was closely related to the fuel combustion chemistry. The initiation reactions of this mechanism may be written as follows:

\[
\begin{align*}
\text{CH} + \text{N}_2 & \rightleftharpoons \text{HCN} + \text{N} \\
\text{C} + \text{N}_2 & \rightleftharpoons \text{CN} + \text{N}
\end{align*}
\]

(2.33) \hspace{2cm} (2.34)

where the first reaction is the main path and is rate limiting in the sequence of formation of NO [9]. The oxidation of HCN to NO involves the following reactions:

\[
\begin{align*}
\text{HCN} + \text{O} & \rightleftharpoons \text{NCO} + \text{H} \\
\text{NCO} + \text{H} & \rightleftharpoons \text{NH} + \text{CO} \\
\text{NH} + \text{H} & \rightleftharpoons \text{N} + \text{H}_2 \\
\text{N} + \text{OH} & \rightleftharpoons \text{NO} + \text{H}
\end{align*}
\]

(2.35) \hspace{2cm} (2.36) \hspace{2cm} (2.37) \hspace{2cm} (2.38)

The above four reactions are known to occur in mixtures with equivalence ratios of less than 1.2. For richer mixtures, more reaction pathways open up and the chemistry becomes more complex [34].
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2.5 Factors Affecting Nitric Oxide Formation

2.5.1 Inlet Air Temperature

In aircraft gas turbine combustors where operating temperatures are very high, the primary mode of NO\textsubscript{x} formation is the thermal mechanism. Therefore, a higher inlet air temperature is expected to produce an increase in NO\textsubscript{x} as it increases the combustion temperature. Also, a higher initial mixture temperature increases fuel oxidation rates, which causes the final or maximum flame temperature to be attained earlier and ultimately results in longer residence time of the post flame gases at maximum flame temperature.

2.5.2 Residence Time

Residence time is another very important factor in determining NO\textsubscript{x} concentration following a combustion process. The formation of NO\textsubscript{x} through thermal mechanism is a relatively slow process in comparison to the oxidation of fuel, especially at high temperatures where reaction rates are very high. In processes where NO\textsubscript{x} concentration has not yet attained its equilibrium value, it will continue to rise until it reaches equilibrium. In conventional gas turbine combustors, the flow in the primary zone does not reside long enough to allow NO\textsubscript{x} concentration to reach its equilibrium value and hence the residence time plays a big role in determining the final concentration of NO\textsubscript{x}. Figure 2.4 [18] shows an increase in NO\textsubscript{x} with increasing residence time, except for very lean mixtures where the formation rate is so low that it becomes insensitive to time.

2.5.3 Inlet Air Pressure

The effect of inlet air pressure on NO\textsubscript{x} formation is of great interest to a design engineer due to the growing trend of engines with higher pressure ratio. The experiments carried out by Rink and Lefebvre [26] show that a higher pressure results in higher NO\textsubscript{x} levels.
One such graph is shown in Fig. 2.5. The main reason behind this is that a higher combustion pressure increases chemical reaction rates and decreases dissociation losses and these two effects combined, in turn, result in higher flame temperature. From a perspective of gas turbine engine, a higher inlet air pressure also leads to higher inlet air temperature due to thermodynamic efficiency of a compressor being never equal to 100%.
2.5.4 Equivalence Ratio

The production of NO\textsubscript{x} is highly dependent on equivalence ratio due to its direct impact on combustion temperature. Combustion processes that occur at low equivalence ratios do not produce high quantities of NO\textsubscript{x} since temperatures are low. As mixture equivalence ratio approaches unity the amount of NO\textsubscript{x} produced from a combustion process increases until it reaches an equivalence ratio of slightly lower than unity and then goes back down as equivalence ratio increases past that point. The reason for concentration of NO\textsubscript{x} peaking on the lean side of stoichiometric, although the flame temperature is higher on the slightly rich side, is due to kinetic (non-equilibrium) effects of oxygen concentration which prefers combining with nitrogen than fuel at such equivalence ratios.

2.5.5 Fuel Atomization

The effect of droplet size on NO\textsubscript{x} formation has been observed to be a strong function of equivalence ratio \cite{18}. At low equivalence ratios, the effect of atomization quality on NO\textsubscript{x} is greater than at high equivalence ratios as illustrated in Fig. 2.6. This behaviour can be explained by considering an example of a combustion process which is characterised by low equivalence ratio and poor fuel atomization. The bigger droplet size and lower average flame temperature at lower equivalence ratio slows down the evaporation rate of the liquid fuel, which results in some of the fuel droplets burning around the surface at or near stoichiometric conditions. These small pockets of stoichiometric mixture then result in local regions of high temperature where NO\textsubscript{x} is formed in appreciable quantities. The reason for the diminishing effect of droplet size on NO\textsubscript{x} as the overall mixture equivalence ratio approaches unity is the reduction in the relative contribution of local high temperature regions to overall NO\textsubscript{x} as the average mixture now supports higher quantities of NO\textsubscript{x} in accordance with the thermal mechanism.
In an aircraft engine, the atomization quality of fuel is highly dependent on the type of nozzle the engine is equipped with. There are two main types of fuel atomizers, 1) pressure atomizer and 2) air-blast atomizer. Pressure atomizers achieve their function by forcing the fuel under pressure through a specially designed orifice [18]. These atomizers are typically preferred for low power conditions since their performance is based on fuel pressure which can be optimized to achieve good atomization at these conditions. Air-blast atomizers, on the other hand, work by arranging fuel at low pressure to flow over a lip located in a high-velocity airstream [18]. Air-blast atomizers, unlike pressure atomizers, work better at high power conditions due to high velocity of air through the atomizer at such conditions but do not perform well at low power conditions due to low air velocities through the atomizer. The two different types of pressure atomizers, namely simplex and dual-orifice atomizers, and air-blast atomizer are shown in figure 2.7.
Figure 2.7: Fuel Atomizers: (a) Simplex, (b) Duplex (c) Air-blast, from [18]
Chapter 3

Development of Chemical Reactor Models

3.1 Test Cases

The test cases that were available for reactor model analysis in this thesis consisted of four industry combustors. The categorization of these combustors is as follows.

1. Can Combustor (Combustor A)

2. Annular Combustors
   - Conventional Single Toroidal Annular Combustor (Combustor B)
   - Conventional Double Toroidal Annular Combustor (Combustor C)
   - Modern Single Toroidal Annular Combustor (Combustor D)

Combustor A was the first one to be analysed in this thesis. The relative simplicity of modelling a Can combustor allowed for basic understanding of the capability of Perfectly Stirred and Plug Flow Reactors in predicting emissions from a combustor. Following a positive outcome of the Combustor A model, the annular combustor with double toroidal flow field in the primary zone (Combustor C) was studied since its flow field resembled
somewhat that of Combustor A. Finally, combustors with single toroidal flow field in the primary zone were modelled and the results verified with experimental data.

3.1.1 Description of the Test Cases

Combustor A

In Combustor A, there is one row of combustion jets in the primary zone and one in the dilution zone. There are four cooling louvers which supply cooling air to the inner liner wall. The cooling flow is approximately 38% of the total combustor airflow. The emissions data available for this combustor is for simplex pressure atomizer. Lastly, the available emissions data is for methane fuel. A schematic of the combustor is shown below in figure 3.1.

Combustor B

For Combustor B, the location of combustion jets in the primary zone is such that it forces the creation of a single toroid in the counter clockwise direction. The dilution jets are also located at both the inner and outer annulus, however, their axial locations are not the same. The rest of the inlets provide cooling air to the liner, all of which eventually becomes combustion air as the flow encounters subsequent combustion jets and as it moves downstream. The ICAO measured emissions data available for this combustor is for a duplex pressure atomizer running on jet fuel. Figure 3.2 shows a schematic of Combustor B.
Combustor C

The primary zone flow field of Combustor C is similar to Combustor A’s primary zone flow pattern in that its axisymmetric flow features are somewhat visible in the Combustor C case. The combustion jets in the primary zone are located at both the inner and outer annulus and are approximately at the same axial location as shown in figure 3.3. The air addition sites downstream of the primary zone are similar in structure to that of Combustor B. There is no measured data available for this combustor in the open literature and the model predictions are evaluated based on expected trends of NO\textsubscript{x} formation across various power levels.
Combustor D

Combustor D and Combustor B have very similar primary zone flow pattern, however, Combustor D has an entirely different geometry and air addition locations compared to Combustor B. The direction of the toroid in the primary zone is counter clockwise and it is created by the combination of combustion jets impinged in a particular direction. Combustor D has a bigger primary zone than Combustor B and a very small intermediate zone, followed by a dilution zone. The dilution jet holes in the inner and outer annulus are located at the same axial location. The combustor is fitted with an air-blast fuel nozzle. In addition to ICAO conditions, the measured emissions data is available for a range of different input conditions all of which are used to verify model predictions. A schematic of this combustor is shown in figure 3.4.

Figure 3.4: Schematic of Combustor D

3.2 Model Characteristics

3.2.1 Primary Zone Modelling

The primary zone of all combustors in this thesis is modelled as a parallel and/or serial combination of perfectly stirred reactors. The feasibility of modelling a primary zone with PSRs can be analysed by calculating the Damkohler number, which is defined as
the ratio of a characteristic mixing time \((\tau_{flow})\) to a characteristic chemical time \((\tau_{chem})\) [34].

\[
Da = \frac{\tau_{flow}}{\tau_{chem}}
\]  

(3.1)

For a particular combustion process, a Damkohler number of greater than 1 means that chemical reaction rates are slower in comparison to mixing rates whereas a Damkohler number of less than 1 signifies that a combustion process is controlled mainly by chemical reaction rates. Therefore, the underlying assumption in modelling the primary zone with PSRs is that the high turbulence intensity in the primary zone enhances the mixing rate of the flow to a point where the Damkohler number approaches zero.

### 3.2.2 Intermediate and Dilution Zone Modelling

The intermediate and dilution zones are modelled with plug flow reactors in this thesis. The inherent assumption made in modelling these zones with PFRs is that the mixing of cooling and dilution jets with the main stream flow occurs instantaneously in a plane where these jets are injected in to the liner. The modelling of these zones with PSRs would not be suitable since that would assume that the flow is well mixed in the axial direction beyond the primary zone, which is generally a poor assumption. In all models, the plug flow reactors are simulated as a series of perfectly stirred reactors. The number of PSRs required to simulate a PFR was determined by trial and error in which the number of PSRs was increased until the change in temperature from adding a subsequent reactor was within 1% of the final value. The number that satisfied this limiting criteria was found to be 25 and it corresponded to the maximum length between the two combustion jets and the lowest reaction rate that would be encountered in any of the simulations.
3.2.3 Model Simulation Tools

All model simulations were performed using Cantera version 1.8 with Python interface. For all combustor simulations except for Combustor A simulation, the chemical mechanism that was used to model the oxidation of fuel was the GRI mechanism for propane version 3.0 [5]. For Combustor A simulation, the GRI mechanism for methane was used. The GRI 3.0 mechanism, which includes all three mechanisms of NO\(_x\) formation, consists of 325 elementary reactions and 53 species.

The detailed mechanism for Jet Fuel provided by Westbrook [35] was also examined, however, long computational times and numerical difficulties that are associated with its application did not allow for its practical use in model simulations. In addition, it was found that the difference of flame temperatures between propane and Jet Fuel, for residence times encountered in model simulations, did not exceed by more than 55 degrees and did not significantly affect NO\(_x\) results.

3.2.4 Liquid Fuel Evaporation Modelling

At low power conditions, such as idle and 30%, the performance of the fuel atomizer degrades in quality due to low combustion pressures and inlet air speeds both of which are vital for production of small fuel droplets. The problem of poor atomization at low power is even worse for small aircraft engines because of the extremely low pressures that are encountered in their operation. The eventual result of these bigger droplets, combined with lower turbulent intensities and combustion temperatures, at low power conditions is that a fraction of the fuel in the primary zone remains unburnt until it evaporates and mixes with the flow downstream in intermediate or dilution zone.

Considering the effect of droplet evaporation on primary zone combustion, an attempt to model fuel evaporation in the primary zone was made by developing a procedure which consisted of two steps. In the first step, the mass flow rate of liquid fuel entering the primary zone reactors was decreased to simulate partially reacted fuel in the primary
zone. The amount of liquid fuel reduced was based on the time it took for the fuel to fully evaporate as well as its total residence time in the reactor and is represented by equation 3.2. The unreacted liquid fuel was then added to downstream reactors to achieve mass conservation.

\[ FAR = FAR_o \left( \frac{-0.0295\tau_e}{\tau} + 0.45 \right) \] (3.2)

where \( FAR \) is the effective fuel air ratio in the reactor, \( FAR_o \) is the original fuel air ratio in the reactor, \( \tau \) is the residence time of the fuel air mixture in the reactor and \( \tau_e \) is the evaporation time of the fuel and is given by equation 3.3. The effective fuel mass flow rate is calculated by multiplying \( FAR \) by the mass flow rate of air in the reactor. Equation 3.2 is a modified version of the fuel air ratio correction factor suggested by Rizk and Mongia \[27\] in their model. The constants in equation 3.2 were derived from optimization of predicted and measured emissions results at idle and 30% power conditions.

\[ \tau_e = SMD^2/\lambda_e \] (3.3)

\( SMD \) in the above equation refers to Sauter Mean Diameter of the droplet. The evaporation constant, \( \lambda_e \), is defined as \[27\]

\[ \lambda_e = \frac{8k_g}{\rho_l c_{pg}} ln(1 + B_m)(1 + 0.3Re^{0.5}Pr^{0.33}) \] (3.4)

where \( k_g \) and \( c_{pg} \) represent thermal conductivity and specific heat of the gas, \( \rho_l \) is the fuel density, \( B_m \) is the mass transfer number and Re and Pr are Reynolds and Prandtl numbers based on gas properties at film temperature \[27\].

The second step involved forcing a certain percentage of the primary zone flow to burn at stoichiometric condition. The main reason for this was to simulate burning of droplets around the surface, which, as mentioned in chapter 2, tends to occur at stoichiometric
conditions. The percentage of primary zone flow burning at stoichiometric fuel air ratio was also determined from optimization of measured and predicted emissions results.

### 3.2.5 Development of Chemical Reactor Models

The simulation of gas turbine combustors using chemical reactors relies heavily on the art and craft of an experienced designer because a careful selection of the different proportion of the flows going in to each of the reactors is required to achieve reasonable results. Since perfectly stirred and plug flow reactors are zero and one dimensional, respectively, in nature, it is not possible to predict the direction of flow entering or exiting a reactor mathematically. The estimation of flow distribution in the reactor network in this work has been made by utilizing information from the engine cold flow CFD provided by the industry partner.

### 3.3 Specific Engine Model Analysis

The reactor network specific to each test combustor was developed based on geometry and flow field of a given combustor. An interesting feature of these models is the modelling of zones that lie in a plane between the fuel nozzles. For combustors in which the distance between two subsequent fuel nozzles is fairly large, there may be significant differences in temperature and product composition between zones that lie in the plane of the fuel nozzle and those that lie in a plane between the fuel nozzles. For modelling purposes, it is assumed that very little or no fuel reaches the in-between zone. The flow inputs for most reactors are estimated from cold flow CFD results, however some inputs to reactors in a plane between the fuel nozzles are based on engineering estimates. The volumes of each of the reactors are based on location of jet injection holes as well as visualization of the extent of a particular flow pattern such as recirculation in the primary zone. The reactor networks for each of the annular combustors studied are discussed below.
3.3.1 Combustor A Analysis

Global Correlations

The application of global correlations to Combustor A was crucial in understanding the predictive capability of these correlations to predict emissions from a combustor other than the specific type for which they were derived. Four different global correlations, available in the open literature, were used in the analysis. According to Rizk and Mongia [27],

\[
EINO_x = 15 \times 10^{14} (\tau - 0.5\tau_e)^{0.5} \exp \left( \frac{-71100}{T_{st}} \right) P_3^{-0.05} \left( \frac{\Delta P_3}{P_3} \right)^{-0.5}
\]  

(3.5)

In the above correlation, the characteristic temperature, \( T_{st} \), for NO\(_x\) formation is the stoichiometric temperature of the fuel. \( P_3 \) is the inlet pressure, \( \Delta P_3/P_3 \) is the non-dimensional pressure drop which is used to simulate mixing in the primary zone, \( \tau \) is the residence time in ms of combustion gases in the primary zone and \( \tau_e \) is the fuel evaporation time in ms.

The other three correlations that were used in the analysis are given in the Correlations section of the first chapter and refer to equations 1.2 - 1.4. The equilibrium reaction temperatures in these correlations were obtained from NASA Chemical Equilibrium Program.

Combustor A Reactor Model

The chemical reactor model developed for Combustor A is shown in figure 3.5. The primary zone is modelled with two parallel reactors due to the presence of two recirculation zones that are seen in the cold flow CFD. The inputs to Reactor 1 are fuel air mixture coming from the nozzle, the primary combustion jet and part of its own products that are recirculated back in to it. Reactor 2 inputs consist of products from Reactor 1 and air from the \( \alpha \) inlet. The inputs to reactor 3, a plug flow reactor, are products from
reactor 1 and 2, the cooling flow upstream of this reactor as well as part of the primary combustion jet that doesn’t get entrained in to the primary zone. The plug flow reactor in the dilution zone, reactor 5, derives its inputs from the intermediate zone as well as all the cooling air injected upstream of the dilution zone. In the Combustor A model, there are no reactors in the zone between the fuel nozzles as the flow field is assumed to be axisymmetric.

![Figure 3.5: Combustor A Model](image)

### 3.3.2 Combustor B Model

The model for Combustor B was developed as part of another parallel project on prediction of CO emissions by Marchand [20]. The basics of development of the model are the same, i.e., cold flow CFD and location of liner holes are the main criteria for placing reactors in the network. The model is shown in figure 3.6. The primary zone consists of 16 reactors, 8 in the plane of the nozzle and 8 in a plane between the fuel nozzles. Reactors P1, P2, P3 and P4 in the plane of the nozzle and reactors P5, P6, P7 and P8 (not shown in figure 3.6) in a plane between the nozzles occupy majority of the volume in the primary zone and simulate recirculation of flow. On the other hand, reactors C1, C2, C5 and C6 in the plane of the nozzle and reactors C9, C10, C13 and C14 in a plane between the fuel nozzles simulate near wall effects. The flow from primary zone travels to intermediate zone which is modelled by three plug flow reactors; one around the cen-
Finally, the flow from intermediate zone reactors travels to reactors in the dilution zone.

3.3.3 Combustor C Model

For Combustor C, there is no available cold flow CFD data that could be used in development of the reactor model. Therefore, the flow field in different locations of the combustor is assumed based on experience and location of cooling and dilution jets. The model is developed based on the axisymmetric flow features of the combustor. For simplicity and less parameter estimation, reactors above the centreline are only allowed to receive inputs from other reactors that are also above the centreline. The model consists of five reactors in the primary zone. Reactors 1, 2 and 3 are located in the plane of the nozzle. Inputs to reactor 1 include all the fuel and air coming from the nozzle as well as recirculated products of reactors 2 and 3. Inputs to reactors 2 and 3 consists of air from liner holes that are located in the primary zone and the products of reactor 1. Reactors 4 and 5, as seen in figure 3.8, are located in a plane between the fuel nozzles. The inputs to reactors 4 and 5 include certain proportion of the products leaving reactors 2 and 3 and the flow from liner holes. The intermediate zone consists of 8 reactors. Reactors 6, 7, 8 and 9 receive their inputs from reactors 2, 3, 4 and 5 and liner holes that are located within that zone. Similarly, reactors 10, 11, 12 and 13 acquire their inputs from 6, 7, 8
and 9 respectively, and some air from liner cooling holes in that zone. Reactors closer to the wall have more cooling flow going in to them whereas reactors closer to the centreline are allocated higher proportions of jet flow. The dilution zone reactors inputs are established using similar rules and can be seen in figure 3.7. Note that, in the Combustor C model, there are no reactors in the zone between the fuel nozzles in intermediate and dilution zones as it is assumed that the flow between the two zones mixes as it travels downstream. A schematic of the in between zone reactors in the primary zone is shown in figure 3.8.
3.3.4 Combustor D Model

The model for Combustor D was also developed by Marchand [20]. In this model, the placement of reactors and the distribution of flow into different reactors is similar to Combustor B model due to similarities in their flow field pattern. The model is shown in figure 3.9. In this combustor, the distance between the two adjacent fuel nozzles is very small, therefore, it is assumed that the flow is well mixed between these two zones and that it is sufficient to model the combustor in one plane.

3.3.5 Evaluation of Specific Combustor Models

The analysis of specific combustor models showed that the use of specific reactor networks for prediction of NO\textsubscript{x} at a preliminary design stage may not be feasible since the placement of reactors is dependent on a particular combustor and the results are very sensitive to flow split information in each reactor. Subsequently, a more general approach for establishing a reactor network was analysed and is discussed in the next section.

3.4 General Combustor Model

A general model that could be applied to any type of combustor would be of great importance to a designer as it would eliminate the use of flow splits parameter estimation,
which is cumbersome and heavily dependent on experience. Therefore, an effort was made to develop a single model that could be used to determine NO\textsubscript{x} emissions from any type of combustor given certain rules that would need to be followed during its development.

### 3.4.1 Model Development

The general model is shown in figure 3.10. In this model, the primary zone is simulated as a parallel combination of 10 perfectly stirred reactors with each reactor burning at a certain equivalence ratio. The modelling of primary zone with 10 reactors was based on a reactor density study in which the number of reactors in the primary zone were increased until there was no significant change noticed from addition of the subsequent reactor. For combustors studied in this work, it was found that 10 primary zone reactors were sufficient for NO\textsubscript{x} modelling, however the process of finding the necessary number of reactors in the primary zone can be automated in the code in order to make sure that the primary zone of a given combustor is modelled with appropriate number of reactors. The intermediate and dilution zones are modelled with a serial combination of plug flow reactors. The boundaries of these PFRs are dictated by location of jet injection holes. The starting boundary is in the plane of the current jet injection hole where as the finishing boundary is located in a plane just before the subsequent injection hole.

The technique of modelling a combustor in this manner has been used by several researchers in the past [3, 28]. The idea behind modelling a primary zone with parallel combination of perfectly stirred reactors is to simulate unmixedness in the primary zone since, in a real engine, the mode of combustion is diffusive and the reactions of fuel and air take place at a range of equivalence ratios rather than at a particular value. The unmixedness is modelled by assuming a normal distribution of mixture around a mean primary zone equivalence ratio. The method for determining unmixedness parameter value was thoroughly examined by Allaire [3]. The three methods that were studied in [3] are 1) setting the unmixedness parameter as a single value for all engine power conditions,
2) setting the unmixedness level as a function of primary zone equivalence ratio and using the general curve across all engines, and 3) setting the unmixedness parameter as a function of primary zone equivalence ratio for each individual baseline combustor. The analysis of the three methods by Allaire [3] revealed that setting the unmixedness parameter as a function of primary zone equivalence ratio for each individual baseline combustor produced best results and hence this method of obtaining the unmixedness parameter value has been used in this work.

The full algorithm for construction of this model and achieving results is given below:

- The first step requires creation of boundaries that separates different zones of the combustor from each other. The extent of the primary zone can generally be determined from the size of recirculation region. The reactor boundaries for intermediate and dilution zones are determined based on location of injection jets as mentioned before.
• Air flow to each of the zones is distributed by providing flow from liner holes that lie in that particular zone. All fuel goes in the primary zone.

• Once the overall equivalence ratio in the primary zone, corresponding to a given ICAO condition, has been established, a normal distribution of equivalence ratios for each ICAO power condition is determined based on an assumed value of unmixedness parameter (s) as:

\[ s = \frac{\sigma_{\phi}}{\mu_{\phi}} \]  

(3.6)

where \( \sigma_{\phi} \) is the standard deviation of the distribution and \( \mu_{\phi} \) is the mean equivalence ratio in the primary zone. The unmixedness parameter value is naturally an unknown and therefore the simulations are run for a range of unmixedness parameter values with values ranging from 0 (perfectly mixed primary zone) to 0.3 (the maximum unmixedness that can occur in the primary zone). The unmixedness parameter value is subsequently obtained by optimization of simulation results with measured data for each ICAO power condition.

• Using the four unmixedness parameter values obtained from optimization of four ICAO points, a graph of unmixedness parameter value vs. equivalence ratio is constructed. Once the graph is created for a baseline combustor, the interpolated values of unmixedness parameter (corresponding to a particular value of equivalence ratio) can be used to study the design change on a combustor.

Combustor C is similar to Combustor B in terms of overall geometry and the type of fuel atomizer, both of which are related to unmixedness in the primary zone. Therefore, to evaluate the performance of this general procedure, Combustor C was used as a validation combustor in that the unmixedness parameter values for this combustor were obtained from Combustor B analysis.
Chapter 4

Results and Discussion

This chapter starts with results representing the capability of a single perfectly stirred reactor in predicting NO\textsubscript{x} as a function of various input parameters. Subsequently, NO\textsubscript{x} predictions using specific reactor models are shown and discussed. The last section of this chapter includes results of the application of general reactor model to all of the test combustors of interest and discussion of the corresponding results.

4.1 Influence of Inlet Temperature on PSR NO\textsubscript{x} Prediction

As mentioned earlier, NO\textsubscript{x} in aircraft engines is highly dependent on combustion temperature. Figure 4.1 shows the NO\textsubscript{x} response of PSR to inlet air temperature. Other input variables such as inlet pressure, residence time and equivalence ratio were kept constant. The exponential behaviour of NO\textsubscript{x} around 1800 K is evident in the graph in that it shows that NO\textsubscript{x} concentration is highly dependent on temperatures above 1800 K. This result is also in line with the assumption that NO\textsubscript{x} concentration is primarily dictated by the thermal mechanism at high temperatures, especially considering the relative contributions of the different mechanisms that are known to produce NO\textsubscript{x}. 

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The reason for analysing the response of a single PSR to temperature (and other input parameters in subsequent sections) as opposed to an entire reactor network is to establish understanding of the fundamental elements of a model because the chemical reactor models developed in this work essentially consist of a serial and parallel combination of many perfectly stirred reactors.

### 4.2 Influence of Residence Time on PSR NO$_x$ Prediction

Residence time is another important input parameter that affects NO$_x$ production chemically. Figure 4.2 shows the effect of residence time on PSR prediction of NO$_x$. For residence times shown on the graph, the combustion has essentially reached equilibrium and therefore the temperature stays constant. Note that although combustion is largely finished, the concentration of NO$_x$ is still far from its equilibrium value and it reaches
4.3 Influence of Inlet Pressure on PSR NO\textsubscript{x} Prediction

The influence of pressure on PSR NO\textsubscript{x} prediction is mainly due to the effect of pressure on flame temperature and residence time of gases. An increase in pressure increases flame temperature as there are lower dissociation losses. The increase in residence time due to a pressure increase can be envisioned from the following equation for residence time in a perfectly stirred reactor:

\[
\tau = \frac{PV}{RT\dot{m}}
\]

where \( P \) is combustion pressure, \( V \) is the reactor volume, \( R \) is the ideal gas constant, \( T \) is flame temperature and \( \dot{m} \) is mass flow rate of the fuel air mixture. It can be seen in
Figure 4.3: Influence of Pressure on PSR Flame Temperature and Residence Time Prediction

Figure 4.4: Influence of Pressure on PSR NO\textsubscript{x} Prediction
equation 4.1 that for a given mass flow rate and reactor volume, there are two competing parameters, pressure and temperature, which affect residence time of gases in opposite directions, however, the overall impact on residence time is always such that it increases with the increase in pressure due to its greater relative magnitude. Figure 4.3 shows the impact of pressure on residence time and flame temperature in one graph and it is evident that they both increase with increase in pressure. Figure 4.4 shows impact of pressure on NO\textsubscript{x} and the observed trend agrees well with theoretical argument.

### 4.4 Influence of Equivalence Ratio on PSR NO\textsubscript{x} Prediction

The effect of equivalence ratio on PSR NO\textsubscript{x} prediction is largely due to its effect on temperature and the availability of oxygen to combine with nitrogen. Figure 4.5 shows that NO\textsubscript{x} increases as the value of equivalence ratio approaches unity from either sides.

![Figure 4.5: Influence of Equivalence Ratio on PSR NO\textsubscript{x} Prediction](image-url)
The concentration of NO\textsubscript{x} has its peak on the lean side of stoichiometric although the flame temperature is higher on the slightly rich side. This is because of the greater affinity of fuel than nitrogen to combine with oxygen.

4.5 Predictions for Specific Combustor Models

4.5.1 Combustor A Predictions

Global Approach

The results for Combustor A emissions obtained using global correlations are shown in figure 4.6. The green whiskers on bars of measured values represent ±15% deviation from these values. All correlations predict an increasing trend of NO\textsubscript{x} as power level goes up. This is expected since these correlations are based on global parameters which increase with the increase in power level. For instance, stoichiometric temperature in correlations by Lefebvre [18] and Rizk and Mongia [27] increases as power level goes
up (due to increase in inlet temperature), which would naturally increase NO\textsubscript{x}. The empirical correlations such as equations 1.2 and 1.3, would also predict an increase in NO\textsubscript{x} with power level as both inlet pressure and temperature increase.

**Model Predictions**

The model predictions for Combustor A are shown in figure 4.7. The data in this graph is normalized w.r.t measured EINO\textsubscript{x} value at take-off. The predicted trends for NO\textsubscript{x} agree well with measured data, however, predictions at 7 and 30% do not fall within the 15% boundary. The inaccurate behaviour at low power conditions may be attributed to combustion inefficiency as mixing rates are generally poor at these conditions. Furthermore, at low power conditions, predictions with even a small error can appear outside the 15% boundary since low magnitudes of EINO\textsubscript{x} at these power conditions result in smaller absolute error bounds.

![Figure 4.7: Combustor A Model Predictions - EINO\textsubscript{x}](image)

Since there is no information available for rated thrust for Combustor A, the Dp/Foo cannot be calculated. However, if the information were available the predicted Dp/Foo
would have been over predicted since NO$_x$ at 7% is over estimated by about a 100% and because it contributes a large proportion to the integrated cycle NO$_x$ due to longer time in mode at this condition.

### 4.5.2 Combustor B Model Predictions

As mentioned in chapter 3, the model for Combustor B was developed as part of another parallel project on prediction of CO emissions by Marchand [20]. The model predictions for NO$_x$ for all ICAO power levels are shown in figure 4.8. The model predicts CO emissions for all ICAO conditions reasonably well (the results for CO are not shown here), however, it fails to predict expected NO$_x$ emissions trend, with NO$_x$ peaking at 30% power condition. The high values of NO$_x$ at low power conditions are attributed to high primary zone reactor temperatures, since the equivalence ratio in these reactors is very close to unity; conditions that are prone to high NO$_x$. Several possibilities of flow splits were tested, however, very little success was achieved in getting the correct NO$_x$ trends while preserving the CO prediction capability of the model.

The results for Dp/Foo are shown in figure 4.9. The net effect of over prediction at low power conditions and under prediction at high power conditions is such that it brings the predicted Dp/Foo closer to actual Dp/Foo, although the predicted Dp/Foo is still outside the 15% boundary.

The simulations for which these results are shown include evaporation sub-model with SMD sizes that are shown in table 4.1. These SMD sizes are for a pressure atomizer and the assumptions of their sizes at a particular power condition are based on engineering estimates that are typical of these types of nozzles operating within a range of pressure ratios at which Combustor B is operating. The model predictions made without the application of evaporation sub-model show similar trends but with magnitudes of NO$_x$ at low power conditions being even higher than simulations that include evaporation sub-model.
Figure 4.8: Combustor B Model Predictions - EINO$_x$

Figure 4.9: Combustor B Model Predictions - Dp/Foo
4.5.3 Combustor C Model Predictions

The NO$_x$ emissions predictions for Combustor C are shown in figure 4.10. The simulation results that are shown in the graph does not include application of the evaporation sub-model at idle and therefore the model over predicts NO$_x$ at this condition. Although, there is no ICAO measured emissions data available for this combustor, the assumption that NO$_x$ is over predicted at 7% is based on analysis of the magnitude of NO$_x$ at 30% being lower than 7% power condition, which is known to be false for this combustor. In order to rectify model’s prediction behaviour across all power levels, the evaporation sub-model was included in model simulations and the results for these simulations are shown in figure 4.11.

Figure 4.10: Combustor C Model Predictions without Evaporation Sub-Model - EINO$_x$
The model predictions after including the evaporation sub-model agree with theoretical trends, however, measured data would be required to determine prediction accuracy. It can be seen that magnitudes of EINO$_x$ at 30%, 85% and 100% do not change with the use of evaporation sub-model as it predicts fuel to be fully evaporated for these conditions in early regions of the primary zone.

### 4.5.4 Combustor D Model Predictions

Similar to Combustor B, the Combustor D model was also originally developed for CO prediction by Marchand [20]. The results for each ICAO power condition are shown in figure 4.12. The trends of NO$_x$ formation for Combustor D are also not predicted well and NO$_x$ peaks at 30% power condition for which the reason is similar to what was described for Combustor B. The model simulations for Combustor D, like other engine simulations, incorporate fuel evaporation sub-model with similar SMD sizes that were used for Combustor B and Combustor C. Unlike Combustor B prediction for 85% power condition, which under predicts NO$_x$, the Combustor D model over predicts NO$_x$ at 85%
power condition. The reason for this is that Combustor D has a leaner overall primary zone compared to Combustor B and this results in some of the primary zone reactors in Combustor D model burning closer to stoichiometric and producing more NO\textsubscript{x}.

The Dp/Foo for Combustor D is shown in figure 4.13. Since the model over predicts at most power conditions, it is clear that it will also over predict the integrated cycle NO\textsubscript{x} as is seen in the figure.

![Figure 4.12: Combustor D Model Predictions - EINO\textsubscript{x}](image)

Figure 4.12: Combustor D Model Predictions - EINO\textsubscript{x}
4.6 Predictions with General Combustor Model

For analysis of performance of the general combustor model, Combustor B and Combustor D were treated as baseline combustors. The emissions prediction for Combustor C were made using same model parameters that were established for Combustor B to analyse how well the design change from Combustor B to Combustor C was captured by the model. As for Combustor D, measured data for 33 parametric cases, in addition to ICAO data, was available, and was used to analyse the capability of the model in predicting NO\textsubscript{x} emissions at power levels other than ICAO.

4.6.1 Combustor B Predictions

Using the general model diagram, figure 3.10, that was shown in chapter 3, the model for Combustor B was developed and is shown in figure 4.14. Then, by using the methodology for developing the model, the results for Combustor B were obtained and are shown in figures 4.15 and 4.16. The individual reactor information for all ICAO power conditions
Chapter 4. Results and Discussion

Figure 4.14: Combustor B Model

<table>
<thead>
<tr>
<th>Thrust Level (%)</th>
<th>Unmixedness Parameter Value (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7%</td>
<td>0.08</td>
</tr>
<tr>
<td>30%</td>
<td>0.05</td>
</tr>
<tr>
<td>85%</td>
<td>0.3</td>
</tr>
<tr>
<td>100%</td>
<td>0.28</td>
</tr>
</tbody>
</table>

Table 4.2: Unmixedness Parameter Values for Various Power Levels

are shown in figure 4.17. The equivalence ratios shown in each of the four figures represent calculated values.

The model predictions for all ICAO conditions follow correct trends. In addition, the predictions for EINO_x and Dp/Foo fall within the 15% boundary as the unmixedness parameter value for each ICAO power condition was chosen to minimize the difference between the measured and predicted value. The unmixedness parameter values for each condition are shown in table 4.2.

The third order polynomial connecting these four points is shown in figure 4.18. This is the same polynomial that will be used to predict Combustor C emissions as discussed in the next section.
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Figure 4.15: Combustor B Model Results - EINO$_x$

Figure 4.16: Combustor B Model Results - Dp/Foo
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\[ \phi = 0.558 \]
\[ \phi = 0.625 \]
\[ \phi = 0.794 \]
\[ \phi = 0.828 \]
\[ \phi = 0.862 \]
\[ \phi = 0.760 \]
\[ \phi = 0.727 \]
\[ \phi = 0.693 \]
\[ \phi = 0.659 \]
\[ \phi = 0.591 \]
\[ \phi = 0.427 \]
\[ \phi = 0.222 \]
\[ \phi = 0.154 \]

(a) 7% Thrust

\[ \phi = 0.651 \]
\[ \phi = 0.696 \]
\[ \phi = 0.808 \]
\[ \phi = 0.830 \]
\[ \phi = 0.852 \]
\[ \phi = 0.785 \]
\[ \phi = 0.763 \]
\[ \phi = 0.740 \]
\[ \phi = 0.718 \]
\[ \phi = 0.673 \]
\[ \phi = 0.452 \]
\[ \phi = 0.235 \]
\[ \phi = 0.163 \]

(b) 30% Thrust
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\[ \phi = 0.221 \]
\[ \phi = 0.628 \]
\[ \phi = 1.646 \]
\[ \phi = 1.849 \]
\[ \phi = 2.052 \]
\[ \phi = 1.442 \]
\[ \phi = 1.239 \]
\[ \phi = 1.035 \]
\[ \phi = 0.832 \]
\[ \phi = 0.425 \]
\[ \phi = 0.682 \]
\[ \phi = 0.353 \]
\[ \phi = 0.244 \]
\[ \phi = 0.304 \]
\[ \phi = 0.715 \]
\[ \phi = 1.741 \]
\[ \phi = 1.946 \]
\[ \phi = 2.151 \]
\[ \phi = 1.536 \]
\[ \phi = 1.330 \]
\[ \phi = 1.125 \]
\[ \phi = 0.920 \]
\[ \phi = 0.510 \]
\[ \phi = 0.736 \]
\[ \phi = 0.381 \]
\[ \phi = 0.263 \]

(c) 85% Thrust

(d) 100% Thrust

Figure 4.17: Combustor B Reactor Information for ICAO Thrust Levels
4.6.2 Combustor C Predictions

The model for Combustor C, based on the general model diagram is shown in figure 4.19. The predictions for Combustor C were made based on the unmixedness parameter values that were obtained from Combustor B as can be seen in figure 4.18. The circles in this figure represent unmixedness parameter values that were established for Combustor B whereas the squares represent interpolated unmixedness parameter values for Combustor C. The fact that the primary zone of Combustor C runs richer than Combustor B is evident by the location of squares on the graph, which are always to the right of the corresponding power level of Combustor B. The results for Combustor C, using the unmixedness parameter values dictated by square points, are shown in figure 4.20. The individual reactor information for all ICAO power conditions for this Engine are shown in figure 4.22.

Figure 4.21 shows that predicted NO\textsubscript{x} emissions across all ICAO power levels for Combustor C are lower than Combustor B, which aligns well with theoretical argument.
Two separate regimes, high power level and low power level, need to be considered for explanation of this behaviour. At low power conditions, 7 and 30%, the higher equivalence ratios (towards unity) in the primary zone of Combustor C would lead to higher NO\textsubscript{x} compared to Combustor B, however, the opposite is observed in figure 4.21. This is because the smaller primary zone of Combustor C results in shorter residence times, which in turn directly affects NO\textsubscript{x} production. In addition, the shorter residence times mean that each reactor in the primary zone now has less time to burn (from a chemical kinetics point of view), thereby resulting in lower primary zone temperatures. In fact, the comparison of Combustor B and Combustor C simulations show that both residence time and temperature in each of the primary zone reactors are lower for Combustor C even though the equivalence ratio at low power conditions is closer to unity for Combustor C. The lower NO\textsubscript{x} production of Combustor C compared to Combustor B at high power conditions, 85 and 100%, is trivial since a richer primary zone (above unity equivalence ratio) would naturally result in lower temperatures.
Figure 4.20: Combustor C Model Results - EINO$_x$

The expected trend obtained for Combustor C shows that the general model is able to capture the effect of local geometry changes on NO$_x$ emissions which would not be
Chapter 4. Results and Discussion

\[ \phi = 0.622 \]
\[ \phi = 0.675 \]
\[ \phi = 0.807 \]
\[ \phi = 0.833 \]
\[ \phi = 0.86 \]
\[ \phi = 0.78 \]
\[ \phi = 0.754 \]
\[ \phi = 0.727 \]
\[ \phi = 0.701 \]
\[ \phi = 0.648 \]
\[ \phi = 0.463 \]
\[ \phi = 0.232 \]
\[ \phi = 0.155 \]

(a) 7% Thrust

\[ \phi = 0.701 \]
\[ \phi = 0.738 \]
\[ \phi = 0.831 \]
\[ \phi = 0.85 \]
\[ \phi = 0.869 \]
\[ \phi = 0.813 \]
\[ \phi = 0.794 \]
\[ \phi = 0.775 \]
\[ \phi = 0.757 \]
\[ \phi = 0.719 \]
\[ \phi = 0.491 \]
\[ \phi = 0.246 \]
\[ \phi = 0.164 \]

(b) 30% Thrust
Figure 4.22: Combustor C Reactor Information for ICAO Thrust Levels
possible with empirical or semi-empirical correlations.

### 4.6.3 Combustor D Predictions

The model for Combustor D, derived from the general model, is shown in figure 4.23. The unmixedness parameter values for Combustor D for all ICAO power levels were found to be very close to or exactly 0.25 and therefore, this value is chosen to represent unmixedness across all ICAO power levels. The NO$_x$ prediction results for this engine are shown in figure 4.24 and are compared to ICAO emissions data. The model over predicts NO$_x$ emissions for 30, 85 and 100% thrust levels but the predictions follow the same trend as measured emissions and are within 15% boundary. The Dp/Foo for this engine is also predicted within 15%.

![Combustor D Model](image)

**Figure 4.23: Combustor D Model**
Figure 4.24: Combustor D Model Results - EINO$_x$

Figure 4.25: Combustor D Model Results - Dp/Foo
Chapter 4. Results and Discussion

(a) 7% Thrust

(b) 30% Thrust
Figure 4.26: Combustor D Reactor Information for ICAO Thrust Levels
Combustor D Predictions for Parametric Cases

Similar to how Combustor C predictions were made based on parameters obtained from Combustor B analysis, the predictions for 33 parametric cases were made based on model parameters that were established from ICAO emissions prediction of Combustor D. The measured data for parametric cases was obtained from [31]. Each parametric case consists of a different combination of input parameters, i.e., $T_3$, $P_3$, $\dot{m}_f$ and $\dot{m}_a$. These parametric cases were studied in the original work to analyze effect of altitude on NO$_x$ emissions, and hence they represent input conditions that are typical of altitudes from 0 to 10.7 km above sea level. The results for all 33 parametric cases are shown in figure 4.27 in the form of a scatter plot with measured data on the x-axis and predictions on the y-axis. The dashed lines above and below the line of perfect fit represent the $\pm15\%$ boundary. The model predicts correct sign for changes in NO$_x$ emissions with changing input parameters for most of the cases, as shown in table 4.3, and predicts most conditions within 15% boundary. The percent error values in red in the table represent those cases for which the predictions were more than 15% away from measured values. For those cases in which the sign change of measured and predicted values were different from their previous corresponding conditions, their $\Delta$ arrows are also marked in red.

The power levels whose NO$_x$ predictions are farther away from measured values are generally those that have primary zone equivalence ratios close to unity (similar to 85% and 100% power conditions). This may be related to the use of propane chemical kinetics since jet fuel and propane have slightly different stoichiometry, which could be affecting NO$_x$ formation as it is very sensitive around equivalence ratios of unity. Furthermore, it can be seen in the table that while some input conditions are similar to others, for instance, takeoff and condition 3, condition 32 and 33, but the measured NO$_x$ emissions for these similar conditions vary significantly. This could be due to different levels of turbulence in each case as well as differences in humidity of the air as there is no humidity data available for parametric cases.
Figure 4.27: Combustor D Model Results for Parametric Cases
<table>
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<tr>
<th>Condition</th>
<th>Measured EINO&lt;sub&gt;x&lt;/sub&gt;</th>
<th>Δ&lt;sub&gt;measured&lt;/sub&gt;</th>
<th>Predicted EINO&lt;sub&gt;x&lt;/sub&gt;</th>
<th>Δ&lt;sub&gt;predicted&lt;/sub&gt;</th>
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Δ - Change in NO<sub>x</sub> from Previous Condition

Table 4.3: Measured and Predicted EINO<sub>x</sub> Values for Parametric Cases
Chapter 5

Conclusions and Future Work

5.1 Conclusions

The objective of this thesis was to develop chemical reactor models for prediction of NO$_x$ emissions from conventional and future generation of aircraft gas turbine combustors. The models were developed to help the industry partner in optimizing the preliminary combustor design stage. The primary goal of these models was the ability to use high level combustor input parameters such as $P_3$, $T_3$, $\Delta P_3$, $m_f$, $m_a$, fuel nozzle type and rough estimates of the geometry for predicting emission characteristics of a combustor, so that the effect of design changes on combustor emissions can be evaluated quickly and reliably. The models developed in this work met most of the original objectives but were unable to take in to account the effect of fuel nozzle type on emissions due to fundamental nature of reactors that were used to model a combustor. Overall, the success criteria of the model was to estimate correct NO$_x$ trends across various power levels due to combined effects of combustion temperature, residence time and equivalence ratio and to predict these emissions within 15% of the measured value.
5.1.1 Global Correlations

The use of global correlations to predict Combustor A emissions was not satisfactory since none of the correlations predicted correct NO\textsubscript{x} for all ICAO conditions. In general, it was noticed that most correlations reasonably predicted Combustor A emissions at 85% and 100% thrust conditions with the exception of the correlation by Rizk and Mongia \cite{27}. At low power conditions, the correlations mostly failed to predict emissions within ±15%. This is probably due to the fact that the constants and exponents in these correlations were derived to work for engines with higher pressure ratio where the effect of droplet at low power conditions is not as significant as in smaller engines. The global correlations were also used to predict emissions for Combustor B and Combustor D (the results are not included in this thesis) and the predicted trends varied for each combustor and suffered from poor accuracy. For instance, the NO\textsubscript{x} was significantly over estimated at all thrust conditions for Combustor B whereas NO\textsubscript{x} for Engine D was over-predicted at low power conditions and under-predicted at high power conditions. It is possible for these correlations to predict emissions with accuracy across the full operating range of a combustor if the constants and exponents in these equations can be tuned for a certain family of combustors. Since the intent of this work is not to produce various correlations for different classes of combustors, the prediction capability of global correlations after alteration of their constants and exponents was not analyzed.

Specific Combustor Models

The NO\textsubscript{x} predictions made using the models developed for a specific combustor did not meet the objective of the thesis in all cases. The model for Combustor A worked well in predicting emissions at all ICAO conditions except for idle. The models for Combustor B and Combustor D were primarily developed for prediction of CO emissions by Marchand \cite{20} and when these models were used to predict NO\textsubscript{x} emissions, they failed to predict the trends. The model for Combustor C predicted correct trends of NO\textsubscript{x}, however there was
no ICAO measured data available for this combustor that could confirm the prediction accuracy of this model. In general, it was found that the results obtained from these specific models were too sensitive to flow split information in each of the reactors as well as the geometry of the combustor. In addition, the evaporation model that was developed did not extend well to Combustor B and Combustor D models since it was originally developed to work with Combustor C model. This is likely due to the presence of constants in evaporation correlations which prevent their application as a general liquid fuel evaporation model.

**General Combustor Model**

The idea of a general model was derived from earlier works of Allaire [3] and Rizk and Mongia [28]. The general rules for development of the model helped in locating reactor boundaries and establishing flow splits to each of the reactors in the network. The application of the general model to all annular combustors yielded correct trends and predicted most power levels within ±15% of the measured value. The EINO\(_x\), and hence \(\text{Dp/Foo}\), predictions for Combustor B were all within 15% boundary. The EINO\(_x\) predictions for Combustor C were made based on model parameters obtained from Combustor B and the resulting trends agreed with theoretical trends considering the design changes that were made on Combustor C from Combustor B. As for Combustor D, the predicted EINO\(_x\) values were within 15% of the measured value and so was prediction of \(\text{Dp/Foo}\). The analysis of capability of the model to predict emissions for parametric cases of Combustor D, using the same model parameters that were used for ICAO predictions of Combustor D, resulted in correct sign for changes in NO\(_x\) emissions with changing input parameters for all 33 cases with most predictions falling within the 15% boundary.

Considering the simplicity and flexibility of using the general model across various combustors, it may be used as a viable preliminary design tool for prediction of NO\(_x\) emissions given that the combustor being designed belongs to a combustor of similar
class from which the model parameters are obtained.

5.2 Future Work

There are several aspects of this work that can be further explored in order to increase utility and robustness of the model. The recommendations for further work are as follows:

- The effect of fuel nozzle on NO\textsubscript{x} emissions should be modelled as this can significantly change the mixing characteristics of the flow in the primary zone. The modelling of fuel nozzle effects would also increase the utility of the model in preliminary design studies as this is one of the main parameters that the designers are interested in analysing at such stage.

- Validation of the model on combustors with double toroidal primary zone flow pattern would be required to analyse the reliability of the model. This is important since most modern combustors employ double toroidal flow pattern and if this model is to be used for prediction of emissions from these combustors, it should be verified against these combustors.

- The accurate modeling of chemical kinetics of the combustion process would require use of jet fuel mechanism. This would certainly increase simulation times by a large factor if the detailed chemistry is used, however, if a carefully selected reduced jet fuel mechanism is used, this may not be a big issue.

- The effect of fuel type on NO\textsubscript{x} emissions is another area that may be explored, although this can be very challenging since it requires accurate fuel evaporation modeling in addition to the detailed knowledge of chemical kinetics of the fuel under investigation.

- Currently, the general model can only predict NO\textsubscript{x} emissions with ±15% accuracy. For CO, the model predicts correct trends and does capture the effect of various
input parameters on CO formation, however the predictions are consistently un-
der estimated. This goes to say that the model is correctly capturing some of the underlying phenomena that are important for CO formation but there are refine-
ments that need to be made in the model in order for accurate CO prediction. For instance, the current model can be modified by introducing more reactors in the intermediate and dilution zones to account for quenching reactions which are known to have a significant impact on exhaust CO concentrations.

- The effect of heat transfer through combustor walls may also need to be modeled in order to get more accurate estimates of temperature inside the combustor.

- Finally, models for more advanced combustors such as ultra rich, ultra lean and rich-quench-lean should be developed and verified using the same methodology discussed in this thesis, so that they can be used for development of more futuristic combustor designs.
Bibliography


