MULTI-DIMENSIONAL CARBON MONOXIDE EMISSIONS PREDICTOR FOR PRELIMINARY GAS TURBINE COMBUSTOR DESIGN OPTIMIZATION

by

Michael David Marchand

A thesis submitted in conformity with the requirements for the degree of Master’s of Applied Science Graduate Department of Aerospace Studies University of Toronto

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Abstract

Multi-Dimensional Carbon Monoxide Emissions Predictor for Preliminary Gas Turbine Combustor Design Optimization

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Master’s of Applied Science
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The objective of this thesis was to compare the predictive capabilities of a new proposed reactor network methodology, to past methods in an attempt to determine which best predicts Carbon Monoxide (CO) emissions from aviation combustors. The proposed methodology focused on three key characteristics affecting CO emissions; the internal combustor flow field, combustion chemistry and liquid fuel evaporation. The proposed model was able to capture these characteristics using cold flow computational fluid dynamics, ideal reactors and correlations for evaporation and droplet size. The predictive capabilities of the models were tested by comparing calculated CO emissions against measured data from four aviation industry combustors. The proposed methodology performed better than past methods at predicting CO emissions and trends associated with increased thrust and alterations in droplet size. Additional testing is needed on variations in chemical mechanisms, combustor geometries and internal flow fields to further verify the application of this tool.
Dedication

This thesis is dedicated to my grandmother,
Mary Leonie Marchand,
she may be gone but she will always
be with me in spirit
Acknowledgements

I would like to acknowledge the large number of people that provided technical, literary and moral support throughout the completion of this thesis. First and foremost I would like to thank my supervisor Professor Sam Sampath; his guidance and technical support were critical in the completion of this thesis. For academic guidance I would like to thank the University of Toronto Institute for Aerospace Studies Combustion Research Assessment Committee (RAC) including Professor Clinton Groth, Professor Omer Gulder and Professor David Zingg for overseeing the progress and final approval of this thesis. In addition, I would like to thank the project industrial partner, specifically employees Dr. Hayley Ozem, Dr. John Hu, Jian-Ming Zhou and Kian McCaldon for providing support for the project, including emissions and computational fluid dynamics information. I would also like to thank my girlfriend Kaylee Sarah Shannon for her continuous moral and literary support during the progress of this thesis. Finally, I would like to thank the rest of my family and friends for their continuing support during the completion of the project.
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<th>Description</th>
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<tbody>
<tr>
<td>$A$</td>
<td>Area ($m^2$)</td>
</tr>
<tr>
<td>$AFR$</td>
<td>Air/Fuel Ratio</td>
</tr>
<tr>
<td>$a$</td>
<td>Constant ($gmol/cm^3s$)</td>
</tr>
<tr>
<td>$a_1$</td>
<td>Constant</td>
</tr>
<tr>
<td>$a_2$</td>
<td>Constant</td>
</tr>
<tr>
<td>$a_3$</td>
<td>Constant</td>
</tr>
<tr>
<td>$a_4$</td>
<td>Constant</td>
</tr>
<tr>
<td>$b$</td>
<td>Constant</td>
</tr>
<tr>
<td>$B$</td>
<td>Mass Transfer Number</td>
</tr>
<tr>
<td>$C_{ph}$</td>
<td>Constant</td>
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<tr>
<td>$CE$</td>
<td>Constant</td>
</tr>
<tr>
<td>$d$</td>
<td>Diameter ($m$)</td>
</tr>
<tr>
<td>$E$</td>
<td>Energy ($cal/gmol$)</td>
</tr>
<tr>
<td>$EI$</td>
<td>Emissions Index ($g/kg_{fuel}$)</td>
</tr>
<tr>
<td>$EICO$</td>
<td>Emissions Index for CO ($g/kg_{fuel}$)</td>
</tr>
<tr>
<td>$F$</td>
<td>Thrust Level ($kN$)</td>
</tr>
<tr>
<td>$FAR$</td>
<td>Fuel/Air Ratio</td>
</tr>
<tr>
<td>$FN$</td>
<td>Flow Number ($m^2$)</td>
</tr>
<tr>
<td>$FT$</td>
<td>Film Thickness ($m$)</td>
</tr>
</tbody>
</table>
\begin{align*}
g & \quad \text{Gravity (}m/s^2) \\
H & \quad \text{Heat of Vaporization (}kJ/kg) \\
HHV & \quad \text{Higher heating value (}kJ/kg) \\
h & \quad \text{Enthalpy (}J/gmol) \\
K & \quad \text{Equilibrium Constant} \\
k & \quad \text{Thermal Conductivity (}W/(m \cdot K)) \\
l & \quad \text{Length (}m) \\
MW & \quad \text{The Molecular Weight (}g/mol) \\
m & \quad \text{Mass (}kg) \\
\dot{m} & \quad \text{Mass flow rate (}kg/s) \\
\dot{m}'' & \quad \text{Volumetric mass production rate (}kg/(s \cdot m^3)) \\
Oh & \quad \text{Stability Number} \\
\pi & \quad \text{Takeoff Pressure Ratio} \\
P & \quad \text{Pressure (}MPa) \\
\Delta P & \quad \text{Change in Pressure (}MPa) \\
\Delta P/P & \quad \text{Combustor Pressure Drop} \\
Pr & \quad \text{Prandtl Number} \\
\dot{Q} & \quad \text{Heat-Transfer Rate (}W) \\
\dot{Q}'' & \quad \text{Heat Flux (}W/m^2) \\
\bar{R} & \quad \text{Universal Gas Constant (}8.314J/(kg \cdot K)) \\
Re & \quad \text{Reynolds Number} \\
R & \quad \text{Ideal Gas Constant, }\bar{R}/MW \\
SFC & \quad \text{Specific Fuel Consumption (}kg_{fuel}/(hr \cdot kN)) \\
SMD & \quad \text{Mean Droplet Size (}\mu m) \\
s & \quad \text{Unmixedness Parameter} \\
T & \quad \text{Temperature (}K) \\
t & \quad \text{Time (}s) \\
\end{align*}
<table>
<thead>
<tr>
<th>Symbol</th>
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<tr>
<td>$U$</td>
<td>Velocity (m/s)</td>
</tr>
<tr>
<td>$V$</td>
<td>Volume (m$^3$)</td>
</tr>
<tr>
<td>$v$</td>
<td>Velocity (m/s)</td>
</tr>
<tr>
<td>$We$</td>
<td>Weber Number</td>
</tr>
<tr>
<td>$\dot{W}$</td>
<td>Power (W)</td>
</tr>
<tr>
<td>$X$</td>
<td>Ratio of Air Core to Discharge Surface Area (m$^2$/m$^2$)</td>
</tr>
<tr>
<td>$x$</td>
<td>Distance in x-Direction (m)</td>
</tr>
<tr>
<td>$\bar{x}$</td>
<td>Mean</td>
</tr>
<tr>
<td>$Y$</td>
<td>Mass Fraction (kg/kg)</td>
</tr>
<tr>
<td>$z$</td>
<td>Distance in z-Direction (m)</td>
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**Greek**

<table>
<thead>
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<th>Symbol</th>
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<tbody>
<tr>
<td>$\rho$</td>
<td>Density (kg/m$^3$)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Surface Tension (kg/s$^2$)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Standard Deviation</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Evaporation Constant (m$^2$/s)</td>
</tr>
<tr>
<td>$\dot{\omega}$</td>
<td>Species Production Rate (kmol/(s * m$^3$))</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Equivalence Ratio</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>Local Reactor Perimeter</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Spray Cone Angle (deg)</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Time (s)</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Kinematic Viscosity (m$^2$/s)</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic Viscosity (kg/(s * m))</td>
</tr>
</tbody>
</table>

**Subscripts**

<table>
<thead>
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<th>Subscript</th>
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<tbody>
<tr>
<td>0</td>
<td>Initial Condition</td>
</tr>
<tr>
<td>3</td>
<td>Combustor Inlet Condition</td>
</tr>
</tbody>
</table>
Combustor Exit Condition / Turbine Inlet Condition

Ambient

Actual Conditions

Air

Activation

Carbon Monoxide

Combustor

Chemical Characteristics

Constant Volume

Evaporation

Effective

Fuel

Flow Characteristics

Gas

Gaseous fuel

ith Species/Reactor

Inlet Condition

Jet Fuel

Liquid Fuel

Mass

nth Reactor

Nozzle Orifice

Rated

Atmosphere

Outlet Condition

Equivalence Ratio

Propane Fuel
\(pz\) Primary Zone Condition
\(q\) Quench
\(ref\) Reference Parameter
\(Stoich\) Stoichiometric Conditions
\(s\) Surface
\(sl, CO\) Flame Stability Shear Layer
\(T\) Thermal
\(x\) x-Direction

**Acronyms**

- CFD Computational Fluid Dynamics
- CO Carbon Monoxide
- \(CO_2\) Carbon Dioxide
- DZ Dilution Zone
- EPA Environmental Protection Agency
- FAR Fuel Air Ratio
- ICAO International Civil Aviation Organization
- IPCC Intergovernmental Panel on Climate Change
- 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
Chapter 1

Introduction

Invented by John Barber in 1791, the Brayton cycle is a thermodynamic cycle that contains a compressor, combustion chamber and turbine to help convert thermal energy to mechanical energy as seen in Figure 1.1 [10]. The Brayton cycle, most commonly known as a gas turbine engine, is currently used for both aircraft propulsion and power generation applications. Gas turbine engines have been used since the 1700’s because of their efficient use of power. The compressor performs work on the inlet air, increasing the air pressure as the air transfers to the combustion chamber. In the combustion chamber, the high pressure air mixes with a fuel and is ignited, adding heat to the fuel/air mixture. The high temperature fuel/air mixture then travels to turbines where the fuel/air mixture performs work on the turbines, reducing the pressure. In aircraft engines, the work
extracted by the turbines powers an external fan to propel the aircraft. For power generation applications, the turbine supplies power to a generator which converts the mechanical energy to electrical energy. Power that is not transferred to an external source goes to the compressor, making the cycle more efficient. Once air travels through the turbine disks, it is expelled from the engine through an exhaust nozzle. The effects of gas turbine steps on the temperature and pressure throughout an ideal engine cycle can be seen in Figure 1.2.

1.1 Environmentally Hazardous Emissions

Gas turbine engine cycles are mostly powered using hydrocarbon based fuels. As a result, gas turbine engines can produce environmentally hazardous emissions. Reports from the Intergovernmental Panel on Climate Change (IPCC) have determined that aircraft engines account for 3.5% of the total anthropogenic radiative force caused by all human activity [4]. Furthermore, a recent study from the Federal Aviation Administration (FAA), reveals that in the next 20 years, more than 400 million more people will be flying [6]. This increase in traffic will result in an increase in emissions production worldwide. Consequently, research focusing on engine performance and emissions reduction are becoming increasingly important.

Aircraft engine emissions not only affect climate change but can also have toxic effects
on humans. The most abundant environmentally hazardous emissions produced in the combustion process of an aircraft engine include:

- Carbon Monoxide (CO)
- Nitrogen Oxides (NO\textsubscript{x})
- Unburned Hydrocarbons (UHC)
- Particulates

### 1.1.1 Carbon Monoxide

CO is a colorless odourless gas that, reduces that amount of oxygen that can be absorbed by blood cells. If inhaled with restricted oxygen levels, humans exposed to moderate concentrations of CO can suffer from angina, impaired vision, reduced brain function and even death \[1\]. The greatest source of CO emissions comes from incomplete and inefficient combustion in engines, boilers and even outdoor fires. CO emissions from aircraft engines are predominately a concern at ground level as CO is relatively resistant to oxidation \[16\] and can accumulate to dangerous concentrations. On the other hand, CO emissions produced at high altitudes can oxidise over time to create Carbon Dioxide (CO\textsubscript{2}), which contribute to global warming.

### 1.1.2 Nitrogen Oxides

Nitrogen oxides (NO\textsubscript{x}) represent both nitrogen monoxide (NO) and nitrogen dioxide (NO\textsubscript{2}) gases. NO\textsubscript{x} molecules have many negative effects on the environment. The most common effect of nitrogen oxide emissions is the contribution to global warming. Nitrogen oxides contributes to global warming by radiating heat through the production of ozone (O\textsubscript{3}) a ground levels \[5\]. In addition, the ozone that is produced can be toxic to humans and other organisms \[5\].
1.1.3 Unburned Hydrocarbons

Similar to CO, unburned hydrocarbons (UHC) are produced through inefficiency in the combustion process. UHC’s are toxic to biological life, especially to the respiratory systems of humans [27]. Since most UHCs’ are much heavier than air, UHCs’ from aircraft engines have the potential to contaminate biological ecosystems including ponds and lakes.

1.1.4 Particulates

Particulates account for all of the various compounds and elements that continue through the exhaust after the combustion process. Particulate matter can include nitrates, sulphates, organic compounds and a variety of metals [1]. The volatility of particulate matter is based on the size of carbon and other particulate molecules. Fine particles pose a much higher risk to humans as they can easily enter a persons respiratory system. As a result, these particles can cause many respiratory and cardiovascular diseases [7].

1.2 International Civil Aviation Organization Emission Regulations

To develop regulations for each of these environmentally hazardous emissions, the International Civil Aviation Organization (ICAO) requires emissions on an aircraft over a landing and take-off (LTO) cycle. As seen in Figure 1.3, the LTO cycle consists of four conditions, take-off, climb, approach and taxi conditions. the first condition is take-off where the airplane is running at 100% thrust for approximately 0.7 minutes. While the airplane climbs to an altitude of 3000 ft, the airplane reduces thrust to 85% maximum power for approximately 2.2 minutes. Once the airplane completes a specific flight path the airplane will take approximately 4 minutes to descend from 3000 ft at 30% thrust.
The final LTO condition, also known as taxi or idle, represents the time the airplane is on the ground running at 7% thrust; the airplane operates at this condition for approximately 26 minutes.

Using the LTO cycle, ICAO regulates emission standards for aircraft engines. The ICAO emission standards for engines manufactured after January 1st 2014 having a maximum thrust rating at or higher than 26.7 kN can be seen in Table 1.1 where $\pi_{oo}$ represents the engines pressure ratio at takeoff and $F_{oo}$ represents the rated thrust level [12]. These standards represent the limits of emission products for an aviation gas turbine engine.

<table>
<thead>
<tr>
<th>Emission ($g/kN$)</th>
<th>Subsonic Turbojet/Turbofan Regulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>UHC</td>
<td>19.6</td>
</tr>
<tr>
<td>CO</td>
<td>118.0</td>
</tr>
<tr>
<td>$NO_x$</td>
<td>$40.052 + 1.5681\pi_{oo}$</td>
</tr>
<tr>
<td></td>
<td>$-0.3615F_{oo} - 0.0018\pi_{oo}F_{oo}$</td>
</tr>
</tbody>
</table>

Table 1.1: ICAO gaseous emission standards for engines with a maximum thrust rating at or higher than 26.7 kN, manufactured after January 1st 2014 [12]
ICAO determines emission production for a given engine during the LTO cycle using the expression

\[
\text{Emissions} \left( \frac{g}{kN} \right) = EI \left( \frac{g}{kg fuel} \right) \ast SFC \left( \frac{kg fuel}{hr \ast kN} \right) \ast \text{CycleTime}(hr), \tag{1.1}
\]

which relates the total cycle time to the emissions index (EI) for a given amount of fuel and the specific fuel consumption (SFC) of the engine. The overall emission rating given by ICAO to an engine is averaged based on multiple test cases [12].

Emissions are strictly regulated and ICAO continues to encourage companies to generate more environmentally friendly engines. As a result, companies are focusing on predicting emissions at the preliminary design phase as it is imperative to future engine design.

### 1.3 Predicting Emissions

In the past, several techniques have been used for predicting the emission production of a gas turbine engine during the design phase. These techniques include using correlations, chemical kinetics and computational fluid dynamic (CFD).

#### 1.3.1 Correlations

Correlations are equations that are derived from gas turbine engine emissions data. There are two categories of correlations, empirical and semi-empirical. Empirical correlations are based solely on experimental and observational data from gas turbine engines running and multiple conditions [24]. Semi-empirical correlations are more common due to the fact that the equations contain key theoretical characteristics that drastically affect emission production. Semi-empirical correlations for CO and NO\(_x\) emissions are commonly expressed as [16]
\[ \text{CO} = f \left[ (\text{dilution term}) (\text{chemical residence time})^{-1} (\text{reaction rate}) (\text{mixing rate}) \right], \]  
(1.2)

\[ \text{NO}_x = f \left[ (\text{dilution term}) (\text{thermal residence time}) (\text{reaction rate}) (\text{mixing rate}) \right]. \]  
(1.3)

Similar to empirical equations, semi-empirical equation coefficients are tuned to replicate specific emissions data.

Correlations are beneficial in determining emissions because they are simple and require negligible computational time. As a result, designers can test a number of theoretical combustion chambers during the preliminary combustion chamber design phase. Unfortunately, there is uncertainty in using these correlations because they are derived from past gas turbine engine emissions data. Although semi-empirical correlations include first principles of combustion, the coefficients that control these equations can be drastically affected by different emissions data. Therefore, unless the correlation is used on theoretical combustion chambers that are similar to the engine in which the correlation was derived from, the correlation may not function correctly. In addition, many scholars are apprehensive to use such a simple method in determining emissions due to the complexity of the combustion process. Therefore, many emissions predictors utilize chemical kinetic based calculations.

### 1.3.2 Reactor Networks

Reactor network models use a simplified mesh of reactors to determine localized conditions throughout a combustion chamber. To calculate conditions within each reactor, chemical kinetics is used to determine the concentration of chemical species throughout the combustion chamber. Chemical kinetic methods use detailed or reduced chemical mechanisms for the combustion of jet fuel. In using chemical kinetics, detailed chemistry
that is related to combustion is captured within a multi-staged calculation. From a mechanism that would include many chemical reactions and chemical species, the Arrhenius equation, expressed as

\[ K = aT^b e^{-E_{\text{act}}/RT}, \]  

is used to determine the forward rate coefficient of a given reaction \((K)\) [27].

Identifying the forward rate coefficient for each reaction will give the rate at which each reaction is occurring and the overall rate of change of each chemical species. The Arrhenius equation depends on the localized temperature \((T)\), activation energy \((E_{\text{act}})\) and constants \((a, b)\) which depend on the given reaction. As a result, chemical kinetic models can monitor the concentration of chemical species throughout the combustor process.

The benefit of using a reactor network based models over correlations is the additional user control. Unlike correlations which assume conditions over the entire combustor geometry, reactor network models break a combustor into finite volumes. Within each of these volumes, chemical mechanisms calculate the concentration of emissions and the average temperature. Unfortunately, due to the additional calculations, computational time of reactor network models is much longer than that of correlations. A concern of using reactor network models is that computational times may rival Computational Fluid Dynamic (CFD) software.

### 1.3.3 Computational Fluid Dynamics

Currently, companies use CFD based simulations to determine combustor emissions. CFD simulations not only uses chemical kinetic reactions in determining emissions but also calculate an accurate representation of air and fuel flow through the combustor with the use of turbulence models. A CFD simulation separates a known combustor geometry into a mesh containing millions of nodes, each representing a finite volume. An example
of these finite volume can be seen in Figure 1.4 where Kalla separated a can combustor into millions of nodes to replicate conditions within the combustor.

![Figure 1.4: Computational fluid dynamic mesh of a can combustor, courtesy of Kalla](image)

Unfortunately, due to the complexity of using chemical kinetics and turbulence models over millions of nodes, CFD stimulations require a lot of setup, computational energy and process times. Setting up the proper mesh to calculate properties throughout a given combustor geometry can take weeks with multiple mesh iterations. Once an appropriate mesh is obtained, equations for chemical reactions and flow characteristics within each of the millions of nodes are applied throughout the combustor. A single iteration of a CFD simulation can take multiple days to complete. Prolonged setup and computational times make CFD simulations impractical for determining emissions at the conceptual and preliminary design phase of a combustor.

## 1.4 Scope of Thesis

CFD simulations are imperative to determining accurate emissions data without experimental testing. However, due to the long computational times, CFD is not ideal for testing a variety of combustor designs over a short period of time. Therefore, during the preliminary design phase of a gas turbine engine, a correlation or reactor network would be beneficial in quickly determining emissions under different engine conditions. The
scope of this thesis will be to compare CO emission results from correlations and chem-
ical kinetic models to determine the most accurate method in predicting CO emissions
during the preliminary design phase of gas turbine combustor. The objective will be
to validate past approaches in calculating CO emissions while producing a new physics
based model. Each approach will be validated using data from gas turbine engines with
varying geometries and flow fields.

1.5 Thesis Outline

The thesis begins with background information on combustion chamber design, char-
acteristics effecting CO formation and types of combustion chamber atomizers. With
an understanding of combustion chambers and CO formation, Chapter 3 goes over past
methods for predicting CO emissions. Chapter 4 summarizes the different combustors
that will be analysed and available CO emissions data. Chapter 5 then outlines the
new proposed methodology used to calculate CO emissions. Chapters 6, 7, 8 and 9 goes
through the analysis of each test case, comparing measured CO emissions to the predicted
emissions calculated using the new proposed methodology and past methodologies. The
results from each analyses are discussed in Chapter 10 where a conclusion is made on
which methodology best predicts CO emissions for the given test cases. The thesis ends
in Chapter 11 with future work to be done.
Chapter 2

Background Information

Before examining past correlations and models, one must understand what correlations and models should be considered when predicting Carbon Monoxide (CO) emissions. Not only is it important for models to consider what drives the formation of CO when making assumptions but also the geometry of the combustion chamber. As a result, Chapter 2 looks at combustion chamber design, the main factors affecting CO formation within conventional gas turbine engines and the different types of atomizers chosen to inject fuel into the combustion chamber.

2.1 Combustion Chamber

The fundamental goal in the design of a gas turbine combustion chamber is to generate thermal energy through the combustion of fuel and air. Thermal energy created in the combustion chamber is then converted to mechanical energy to propel the aircraft. Unfortunately, there are limiting factors in the design of a combustion chamber which can limit the maximum amount of thermal energy from reaching an engine's turbine blades.

One of the limiting factors is the maximum allowable temperature of the turbine blades. The high temperatures produced through the combustion process cause the turbine blades to ex-
pand and deflect. In conjunction with a high angular velocity and tight tolerances within a gas turbine engine, any deflection or expansion of turbine blades can result in engine failure. As a result, the fuel/air mixture must be cooled before leaving the combustion chamber to prevent damage to turbine blades.

Another limiting factor in combustion chamber design is the maximum allowable temperature of the combustion chamber walls. High temperatures from the combustion process require additional cooling air at the walls of a combustor. As a result, considerable inlet air from the compressor is allocated to the walls of the combustor through small inlets called louvres.

Each limiting factor can have an affect on a combustors’ flow field, allocation of cooling air and overall geometry. In order to control internal temperatures while maintaining combustion efficiency, conventional combustors are separated into three sections, each with their own purpose. These areas include the primary, intermediate and dilution zones as illustrated in Figure 2.1.

![Figure 2.1: Conventional Combustion Chamber Layout, adapted from [16]](image)

### 2.1.1 Primary Zone

The primary zone of a combustion chamber contains the combustion of fuel and air. The purpose of the primary zone is to sustain a diffusion flame and replicate complete combustion within a highly turbulent environment [16]. To achieve these goals while
upholding the limitations of the combustor walls, the flow field of the fuel/air mixture and the allocation of air within the primary zone is important and maybe unique to a specific combustor.

A combustion chamber flow field depends on many parameters. These parameters include an appropriate type of fuel atomizer, addition of air and fuel swirlers, position of cooling louvres and penetration of mixing air. Both fuel atomizers and swirlers control the flow and evaporation of liquid fuel within the primary zone; these parameters affect the efficiency of combustion. The position and penetration of cooling louvres and jets within the combustion chamber, direct flow to different areas of the combustor. Cooling louvres near the wall of the combustor directs hot gases away from the wall while providing enough air to prevent any thermal deformation. A common flow field produced from penetrating cooling jets in the primary zone is recirculating flow as seen in Figure 2.2.

Figure 2.2: Primary zone recirculation flow, from [16]

Recirculating flow improves the combustion efficiency and stability by keeping the fuel within the domain of the primary zone. The highly turbulent environment of the primary zone allows the recirculated unburned fuel to be further atomized and burned; thus improving the overall combustion efficiency. Local temperatures and residence times also affect UHC and NO\textsubscript{x} emissions, which will not be considered in this thesis.
To accurately predict CO emissions within a gas turbine combustion chamber it will be imperative that the complex flow within the primary zone is understood as most of the CO emissions are primarily a result of combustion inefficiencies. Furthermore, as primary zone conditions affect downstream characteristics, flow transitions to the intermediate zone will require some knowledge of a mixtures’ flow pattern.

\subsection*{2.1.2 Intermediate Zone}

The purpose of the intermediate zone of a combustion chamber is to assist in burning fuel and CO that may have escaped from the primary zone of the combustor \[16\]. Moderate amounts of cooling air are added to the intermediate zone to reduce the temperature of the fuel/air mixture, complete combustion and protect the walls of the combustor. However, the temperature of the fuel/air mixture stays at a high temperature to rapidly oxidise CO. A high residence time in the intermediate zone will reduce CO emissions but can cause an increase in NO\textsubscript{x} emissions. In more modern combustion chambers, the intermediate zone is being reduced in size to save money on materials and improve fuel efficiency by reducing the overall weight of the gas turbine engine \[16\].

\subsection*{2.1.3 Dilution Zone}

The purpose of the the combustion chamber dilution zone is to reduce the temperature of the fuel/air mixture before reaching the turbine stage downstream of the combustor. To reduce the temperature of the fuel/air mixture, large cooling jets are positioned at the beginning of the dilution zone to quench the fuel/air mixture. Approximately 20\%-40\% of the total inlet air flow is used to quench the fuel/air mixture \[16\] to gain the required temperature distribution for the turbine blades.
Dilution Jets

Dilution jets are designed to penetrate deep into the combustor to mix with hot gases from the intermediate zone. The high velocity jet creates a downstream pressure reduction and an upstream increase in pressure, resulting in a force that deforms the jet \[16\]. By quenching the mixture, reactions that effect the concentration of CO and NO\textsubscript{x} are suppressed due to the reduction in temperature of the fuel/air mixture.

2.1.4 Combustor Types

Although the primary, intermediate and dilution zones are common among most gas turbine combustion chambers, there have been multiple combustion chamber designs. This report will focus on two commonly used combustors, the can and annular combustion chambers.

Can Combustors

The can combustor, as seen in Figure 2.3, is a simple cylindrical tube. Within the gas turbine engine, can combustors are mounted concentrically \[16\]. The main advantage of the can combustor is the ease of maintenance and design. Unfortunately, multiple combustion chambers within a gas turbine engine increases the weight of the engine, making can combustors less fuel efficient for aviation applications \[16\].

Figure 2.3: Multi-can combustor arrangement, from \[16\]
Annular Combustors

The annular combustor is most commonly used in aircraft engines [16]. One annular combustor consists of a single interconnected, concentric combustion chamber with fuel injectors positioned periodically throughout, as seen in Figure 2.4 [16]. The reason why annular combustors are so common is due to the efficient use of materials and aerodynamic shape. As engines get larger, annular combustors provide a lighter weight alternative to can combustors. Consequently, the annular combustor is more fuel efficient and cost effective. The aerodynamic shape of the combustor allows for minimal pressure losses [16].

![Figure 2.4: RB211 Annular Combustor, from [16]](image)

2.2 Carbon Monoxide Formation

When designing a combustor, an important parameter to consider is emission production. In the combustion process, several hundreds of chemical reactions and species are generated within milliseconds. Based on the ICAO conditions discussed in section 1.2, CO emissions are produced in abundance during idle and approach conditions as seen in
Figure 2.5: Emissions characteristics during ICAO engine conditions, adapted from [16]

Figure 2.5: With an increase in power, the amount of CO being produced is exponentially reduced for both take off and climb. Therefore, when predicting CO emissions it will be important to focus on emissions at idle and approach as they produce the majority of CO emissions during the entire ICAO cycle.
In general CO emissions are governed by inefficiencies in the combustion process; however, there are many specific conditions that can have affects on CO formation. These conditions include the oxidation of CO to carbon dioxide (CO\(_2\)), combustor inlet pressure, combustor inlet temperatures, equivalence ratio, fuel droplet size and wall quenching, as seen in Figure 2.6.

### 2.2.1 Carbon Monoxide Oxidation / Carbon Dioxide Dissociation

The most important characteristic that affects CO emissions within a combustion chamber is the oxidation of CO to CO\(_2\) and dissociation of CO\(_2\) to CO. During the combustion process, CO and CO\(_2\) continually react through the following secondary reactions [27]:

\[
\begin{align*}
    \text{CO} + \text{O}_2 & \rightleftharpoons \text{CO}_2 + \text{O}, \\
    \text{CO} + \text{OH} & \rightleftharpoons \text{CO}_2 + \text{H}, \\
    \text{CO} + \text{HO}_2 & \rightleftharpoons \text{CO}_2 + \text{OH}, \\
    \text{CO} + \text{H}_2\text{O} & \rightleftharpoons \text{CO}_2 + \text{H}_2. 
\end{align*}
\] (2.1) (2.2) (2.3) (2.4)

These reactions continue to occur until an equilibrium is met between all species. The most prominent oxidation reaction occurs between OH and CO; this is due to the fact that OH radicals are rapidly consumed whereas HO\(_2\), H\(_2\)O and O\(_2\) require chain branching before these reactions can continue [27].

The rate of these reactions are based on the surrounding pressure and temperature within a localized region of the combustion chamber. As the temperature and pressure increase, CO oxidation occurs more rapidly, thus obtaining a more complete combustion and lower CO emission. If the temperature and pressure decreases, CO oxidation occurs much slower, reducing the efficiency of combustion and increasing CO emissions. As a
result, the amount of CO produced is limited by the rate of oxidation and dissociation reactions. With high efficiency combustion occurring at takeoff conditions, the amount of CO emissions will be determined by the dissociation of CO$_2$. Therefore, being able to replicate the rate of oxidation within localized areas of the combustor will be important for predicting CO emissions.

### 2.2.2 Combustor Inlet Pressure ($P_3$)

The inlet pressure of the combustion chamber affects CO emissions through the process of fuel and air mixing. High pressure combustion chambers have better mixing of liquid fuel, assisting in fuel evaporation and improving combustion efficiency [16]. Due to the improvement in combustion efficiency, many current engines contain pressure ratios well above 20:1 pressure ratios [16]. The increase in combustion efficiency creates more hydrogen containing species from the dissociation of fuel [27]. As a result, CO emissions will decrease due to the promotion of CO oxidation; experimental results supporting this conclusion can be seen in Figure 2.7.

![Figure 2.7: Effects of Pressure on CO concentration, developed by Lefebvre using an in-house tubular gas turbine combustor, from 22](image)

Figure 2.7: Effects of Pressure on CO concentration, developed by Lefebvre using an in-house tubular gas turbine combustor, from [22]
The experimental results were developed by Lefebvre while measuring CO emissions produced from varying the internal pressure of a combustion chamber [22]. Lefebvre performed the experiment using an in house tubular gas turbine combustor comprised of an airblast atomizer running on diesel oil (DF2); the gas turbine combustor configuration was developed at Purdue University [22]. With a constant inlet temperature, fuel and mean droplet size, the results show that increasing the combustor pressure from 0.76 MPa to 1.27 MPa decreases CO emissions [22].

### 2.2.3 Combustor Inlet Temperature ($T_3$)

The inlet temperature of air and fuel entering the combustion chamber affects CO production by altering the temperature of the flame. In an ideal cycle, when the ambient air temperature increases, the fuel’s adiabatic flame temperature will increase accordingly [27]. As a result, the higher temperature flame will promote CO oxidation, decreasing CO emissions. As seen in Figure 2.8, a study done by Hung and Agan has proven such a relationship between a combustors’ inlet temperature and resulting CO emissions in a non-ideal cycle. Using a 7-MW industrial gas turbine engine burning natural gas at

![Figure 2.8: Ambient temperature effect on CO emissions from a 7-MW industrial gas turbine running on natural gas, from [11]](image)
a constant fuel flow, Hung results show a linearly decreasing CO concentration as the ambient air temperature increases [11]. Although aviation gas turbine engines use liquid based fuels and complex combustor systems, a similar trend in CO concentration will be produced.

2.2.4 Equivalence Ratio

Similar to the affects of inlet temperature, the equivalence ratio of the fuel and air within the primary zone of a combustion chamber affects CO production by altering the flame temperature. A localized equivalence ratio ($\phi$) is determined by dividing the actual fuel/air ratio (FAR) by the stoichiometric or ideal FAR, yielding

$$\phi = \frac{FAR_{Actual}}{FAR_{Stoich}}.$$  \hspace{1cm} (2.5)

The flame temperature produced in the combustion process is at a maximum near a fuel stoichiometric FAR ($\phi = 1$) resulting in minimum CO production. When the equivalence ratio is less than one ($\phi < 1$), combustion is characterized as lean due to an excess amount of air in the system. As a result, the flame temperature decreases thus hindering CO oxidation. When the equivalence ratio is greater than one ($\phi > 1$), combustion is characterized as rich due to the excess amount of fuel in the system. As a result, the flame is saturated with fuel, lowering the flame temperature and reducing the rate of CO oxidation [27]. The parabolic function reveals the relationship between primary zone equivalence ratio and flame temperature can be seen in Figure 2.9.

Figure 2.9 was produced through a numerical simulation previously performed by Turns [27]. The simulation reproduces the combustion between propane and air within a constant volume reactor and at a pressure of 1 atm. Although this graph only shows the results of reactions between propane and air, all fuels produce a similar parabolic relationship between flame temperature and equivalence ratio.
Figure 2.9: The simulated effect of equivalence ratio on adiabatic flame temperature for propane burning in air at 1 atm, replicated from [27]

### 2.2.5 Wall Quenching

A phenomena that affects CO formation within a combustion chamber is wall quenching. Wall quenching occurs when the hot gas of the combustion process reach a cool region of air near the wall of the combustor as seen in Figure [2.10]. Most combustors are fitted with film cooling to help protect the walls of the combustion chamber. When hot gases reach the cold air, the mixture quenches, reducing the temperature of the mixture dramatically at the localized region near the wall. The reduction in temperature of the mixture significantly reduces the rate of CO oxidation, essentially keeping the concentration constant or ‘freezing’ the CO molecules within localized volume of the combustor [16]. Improving cooling methods can reduce CO emissions by reducing quenching near the wall of the combustor.

![Figure 2.10: Conventional film cooling, adapted from [16]](image-url)
2.2.6 Droplet Size

The final factor that affects CO formation within gas turbine engines is fuel droplet size. Droplet size depends on two key characteristics. The first is atomization of the fuel as it enters the combustion chamber. The second factor is how the droplets evaporate throughout the combustor.

Atomization

In most conventional gas turbine engines, two different kinds of atomizers are used to break up the liquid fuel into small droplets. The two kinds of atomizers include pressure and airblast based atomizers. Droplets produced from these atomizers are affected by many different parameters.

In a pressure atomizer, fuel pressure is a key variable in determining mean droplet size, specifically the pressure drop across the nozzle of the atomizer. The pressure drop dictates the momentum at which fuel enters the combustor [15]. As the pressure drop over the nozzle increases, the fuel becomes finer; this affect can be seen in Figure 2.11 [15].

For airblast based atomizers, the rate and density of air passing through the atom-
izer is important to droplet size [15]. An increase in kinetic energy from the air-stream will improve fuel ligament separation while entering the atomizer [16]. Unlike pressure atomizers, airblast atomizers do not require high-pressure fuel pumps. As a result, the mean droplet size from airblast atomizers is not as dependent on the pressure drop at the point where fuel enters the atomizer as a pressure atomizer.

A key variable affecting both pressure and airblast atomizers is the properties of the fuel being used. Three of the more important fuel properties are, surface tension, density and viscosity of the fuel [15]. Each of these fuel properties determine how easily the fuel can break apart from the original ligament into smaller fuel droplets as seen in Figure 2.12.

![Figure 2.12: Fuel Ligaments Evolution, from [9]](image)

Finally, another factor that can affect mean droplet size from both pressure and airblast atomizers is the amount of fuel passing through the atomizer. As the mass flow rate of fuel increases, more fuel is flowing through the atomizer, increasing the mean droplet size as fuel ligaments become more dense [15].

**Evaporation**

Depending on the atomizer used to break up the liquid fuel, the mean droplet size can be effected by both pressure and the contents of air through the nozzle. Once atomized, the liquid fuel must evaporate before the fuel is able to burn and produce CO molecules.
As a result, the process of evaporation is the second most important characteristic in CO formation due to the fuel droplet. To evaporate, liquid fuel droplets go through five stages before evaporating into a gaseous fuel that can be burned; these stages include [20]:

- Stage #1 - Initial Heating and Evaporation
- Stage #2 - Quasi-equilibrium Evaporation
- Stage #3 - Crust Formation and Growth
- Stage #4 - Boiling
- Stage #5 - Particle Drying

When fuel is burned, the outer layer of the droplet evaporates. Once the fuel burns around the surface of the droplet, the crust will thicken towards the center of the droplet [20]. As a result, more fuel will be burned with smaller droplet diameters, thus improving combustion efficiency. Improving mixing will also prevent the droplets from forming crust allowing for more fuel to be evaporated [20]. In addition, as the temperature at the core of the droplet begins to increase, more fuel will evaporate at the surface of the droplet.

![Figure 2.13: Affect of Mean Droplet Diameter on CO concentration, developed by Lefebvre using diesel oil (DF2) fuel, from [22]](image-url)
as long as the temperature is above the boiling point of the fuel. The improvement to combustion efficiency as a result of smaller droplets will generate more hydrogen containing species from the dissociation of fuel. Experimental results showing the relationship between mean droplet size and CO emission can be seen in Figure 2.13 [22].

Figure 2.13 was developed by Lefebvre using an in house tubular gas turbine engine at Purdue University. Lefebvre was able to show, using a constant pressure and diesel oil (DF2) fuel, that increasing the mean droplet diameter from 30 microns to 110 microns reduced CO emissions for a variety of equivalence ratios [22].

2.3 Types of Atomizers

In previous sections, the effect of different atomizers on CO emissions were discussed. Although the overall conditions affecting the size of droplets produced by different atomizers is consistent, there have been many different atomizers constructed to improve fuel atomization. In this section, the types of atomizers used in this thesis will be discussed.

2.3.1 Pressure Atomizers

A pressure atomizer uses high pressure flow to propel the fuel through a fuel nozzle. The high velocity of the flow increases the turbulence of the fuel within the air and allows for better mixing, shearing the fuel into a fine spray [15]. There are many different kinds of pressure atomizers. For the purpose of this thesis only the simplex and duplex pressure atomizers will be considered. Examples of both pressure atomizer can be seen in Figure 2.14 [15].

The simplex pressure atomizer has a single orifice including an internal swirl chamber within the core of the atomizer. In the swirler chamber, fuel flows tangentially creating a
Chapter 2. Background Information

2.3.2 Airblast Atomizers

Airblast atomizers, also known as two-flow atomizers, use inlet air from the front face of the nozzle to shear fuel ligaments into small fuel droplets as the mixture enters the combustor. The high velocity inlet air is able to impinge upon the fuel flow internally or externally from the atomizer. For the purposes of this thesis, only internal and external air-assist airblast atomizers were be considered. Examples of these atomizers can be seen in Figure 2.15 [15].
Figure 2.15: AirBlast Atomizers, from [15]

An internal air-assist airblast atomizer mixes the fuel and air within the atomizer before the mixture enters the combustion chamber. The benefit of using this type of atomizer is that it can atomize high viscosity fuels [15].

An external air-assist airblast atomizer on the other hand mixes the fuel and air within the combustion chamber. Like the internal air-assist atomizer, the external air-assist atomizer performs quite well at atomizing high viscosity flows [15]. Unfortunately, the external air-assist airblast atomizer is less efficient and requires more air flow to achieve the same results as the internal air-assist airblast atomizer [15]. The benefit of using the external over the internal air-assist airblast atomizer is that the internal air-assist atomizer can have issues with back pressure, where as the external air-assist atomizer does not have that problem [15].

2.4 Summary of Background Information

From the literature review, gas turbine combustion chambers can be defined by three distinct areas, the primary, intermediate and dilution zones. The primary zone is a highly turbulent zone where liquid fuel evaporates to generate combustion. The intermediate zone is used to burn any additional fuel and promote CO oxidation. The dilution zone is used to reduce the temperature of the fuel/air mixture as it passes out of the combustion chamber. These zones can be seen in different types of combustion chambers such as annular and can type combustors.
CO is formed within each of these zones based on six characteristics. These characteristics include CO oxidation, pressure, inlet temperature, equivalence ratio, wall quenching and droplet size. Based on ICAO conditions, CO is formed in abundance at lower power levels such as idle and approach.

Based on the characteristics of CO formation discussed, droplet size is affected by the type of atomizer used. As a result, two types of atomizers were investigated including pressure and airblast atomizers. Although there are many different types of atomizers, the atomizers chosen were based on the available test cases and correlations.

With an understanding of combustion chamber design, CO formation and atomizer functionality, methods can be developed to predict CO emissions. In the next chapter, previous methods for predicting CO emissions will be analysed to determine the most affect methodology.
Chapter 3

Past Modelling Methodologies

In the past, there have been many attempts to predict CO emission production for conventional combustion chambers. Each methodology focuses on different characteristics of CO production; ultimately comparing data with experimental results. There have been two different approaches to determining CO emissions; global approaches and localized approaches.

3.1 Global Approach

The global approach to determining CO emission production is based on the overall combustor geometry and conditions within the primary zone of the combustion chamber. The global approach uses one dimensional equations known as global correlations. Global correlations account for CO forming characteristics by including variables in the equations and altering coefficients based on experimental data. As a result of their simplicity, global correlations have a negligible computational time. Three correlations have been investigated in this thesis; they include:

- Mellor Correlation
- Lefebvre Correlation
- Rizk Correlation
3.1.1 Mellor Correlation

The Mellor correlation, developed by Mellor and Leonard at Purdue University, primarily focuses on the idea of CO quenching. Mellor postulated that the atomization process has little effect on the formation of CO emissions \[17\]. Since most gas turbines operate at a high efficiency combustion process, Mellor assumed that within the primary zone, the combustion process operated at near perfect conditions \[17\]. Using the expression

$$l_{CO} = (l_q^{-1} + d^{-1})^{-1},$$  \hspace{1cm} (3.1)

Mellor calculated an equivalent mixture quenching length \(l_{CO}\) which is dependent on the diameter \(d\) of the combustor and the axial length before the mixture is quenched \(l_q\) \[17\].

Using the velocity \(v_3\) of air in the annulus as calculated in the expression

$$v_3 = \frac{\dot{m}_aRT_3}{P_3A_{ref}},$$  \hspace{1cm} (3.2)

Mellor then calculates the time step before CO is quenched, represented by a variable known as the flame stabilizing shear layer \(\tau_{sl,CO}\). The flame stabilizing shear layer is calculated based on the expression

$$\tau_{sl,CO} = \frac{l_{CO}}{v_3}.$$  \hspace{1cm} (3.3)

In addition, the Mellor correlation captures the affects of varying inlet temperature \(T_3\) and pressure \(P_3\) within the equation for the velocity \(v_3\) of air.

Finally, the flame stabilizing shear layer variable can then be compared to the rate of production of CO \(\tau_{CO}\) from \[17\]

$$\tau_{CO} = 10^{-3} \exp \left( \frac{10760}{R(0.5T_3 + 0.5T_{pz})} \right).$$  \hspace{1cm} (3.4)
The rate of production of CO is mainly dependent on the average temperature between the inlet temperature \( T_3 \) and the primary zone temperature \( T_{pz} \) \([19]\).

Mellor was able to generate an estimation of CO production based on the following correlation \([17]\):

\[
EICO = 35 \frac{\tau_{CO}}{\tau_{st,CO}}.
\]  

(3.5)

This correlation shows that all CO is produced prior to quenching, thus by estimating the approximate time scale before quenching and comparing that to the formation rate of CO at specific temperatures, an approximate CO emission index can be calculated.

The coefficients from each equation in the Mellor global correlation were developed based on experimental results generated from an in house combustion chamber apparatus seen in Figure 3.1 \([3]\). The apparatus mimics the conditions where the combusted material is quenched before entering the turbines of the gas turbine engine. As a result, it can be hypothesized that CO emissions from a combustor with a single quench cooling jet should be predicted using the Mellor correlation.

Figure 3.1: Mellor model experimental apparatus, from \([3]\)

The main issue with the Mellor correlation is that it is based on the idea that mean droplet size has little affect on the production of CO emissions. From investigations done in Section 2.2.6 it is easy to see that this assumption is untrue. However, under high
temperature and pressure conditions, when atomization is at its most optimal, the Mellor correlation could produce a reasonable estimation of CO emissions.

3.1.2 Lefebvre Correlation

The second and more commonly used correlation for determining CO emissions is the Lefebvre correlation developed by Lefebvre in 1984. The Lefebvre correlation takes into account more variables that affect CO compared to the Mellor correlation. The Lefebvre correlation, expressed as

\[
EICO = \frac{86\dot{m}_a T_{pz} \exp(-0.00345 T_{pz})}{(V_c - V_e) \sqrt{\frac{\Delta P_3}{P_3} P_3^{1.5}}},
\]

contains many common variables that effect CO levels include inlet pressure \(P_3\), pressure drop \(\Delta P_3\) and primary zone temperature \(T_{pz}\) \[14\].

One of the biggest differences between the Lefebvre correlation and the Mellor correlation is the addition of a ratio between the volume of combustion \(V_c\) and the volume needed for fuel to evaporate \(V_e\) \[14\]. In using the volume of evaporation, the Lefebvre correlation is able to account for the atomization within the primary zone. From the expression

\[
V_e = 0.55 \frac{\dot{m}_a SMD^2}{\rho_{pz} \lambda_{eff}},
\]

the volume required for evaporation is dependent on both the mean droplet diameter \(SMD\) and the evaporation constant \(\lambda_{eff}\) of the fuel. Both mean droplet size and evaporation rate are affected by the method of atomization and the geometry of the atomizer \[14\].

Lefebvre developed the correlation through first grouping variables that influence CO
emissions together and setting coefficients such as constants and exponents that would allow the correlation to replicated experimental data. The coefficients that are contained within both Equations (3.6) and (3.7) were determined based on experimental data developed at the Wright Patterson Aero Propulsion Laboratory [14]. The data includes information on commercial and military engines in operation.

### 3.1.3 Rizk Correlation

The last global correlation looked at was developed by Rizk and Mongia in 1994. The Rizk correlation is similar to the Lefebvre correlation and is expressed as [23]

\[
EICO = \frac{0.179 \times 10^9 \exp \left( \frac{7600}{T_{pz}} \right)}{(t_c - t_e) \sqrt{\frac{dP_3}{P_3} P_3^2}}.
\]

(3.8)

Both correlations include variables representing primary zone temperature, inlet pressure and combustor pressure drop. Furthermore, the Rizk correlation also includes aspects of evaporation within the time of evaporation variables. From the expression

\[
t_e = \frac{SMD^2}{\lambda_{eff}},
\]

(3.9)

the time of evaporation \( t_e \) is dependent on the mean droplet size \( SMD \) and evaporation rate \( \lambda_{eff} \) [23]; similar to the volume of evaporation in the Lefebvre correlation. It is however not a coincidence that the Rizk and Lefebvre correlations are similar as the Rizk correlation was derived from the Lefebvre correlation. Rizk and Mongia attempted to improve upon the past results of the Lefebvre correlation, discussed in Section 3.1.2 by assuming that CO emissions are much more dependent on pressure [23].

Although these equations are computationally attractive, these simplification can break down due to the complex internal flow field of the combustor. With the introduction of turbulence into the flow field, especially near the wall of the combustor, CO emissions can be significantly affected.
3.2 Local Approach

Where the global approach analyses a gas turbine combustor in a generalized way, focusing only on the inlet and primary zone conditions, local approaches divide a combustor into finite volumes to determine conditions throughout the combustor. Therefore, local approaches use a reactor network based model to mimic the geometry within a gas turbine combustor.

3.2.1 Rizk Model

Another model developed by Rizk and Mongia in the 90’s included a localized approach to predicting CO and NO\textsubscript{x} emissions. As seen in Figure 3.2, Rizk and Mongia divided a conventional annular combustor into seven reactors based on the geometry of the combustor. Once divided, Rizk and Mongia attempted to generate equations that would quickly predict CO emissions for combustors using liquid jet fuel. Due to the changes in CO formation in different areas of the combustor, Rizk and Mongia developed equations based on the area of the combustor and the localized reactor temperatures. Since CO is formed through the combustion process, the production of CO within primary zone reactors is calculated using the expression

\[
EICO = \exp\left(\frac{-CE}{T_{pz}}\right) C_{ph} \left(\frac{P_3}{1.4E6}\right)^{a_1} \left(\frac{\tau}{0.5}\right)^{a_2}.
\]  

(3.10)
As the fuel/air mixture travels into the intermediate zone and dilution zone of the combustor, CO levels are controlled by dissociation. As a result, Rizk developed three equations depending on the localized temperature of the reactor. For localized temperatures above 2000 K, the expression

$$EICO = 2.52 \exp\left(-\frac{5000}{T_c}\right) \left(0.00017 \exp\left(\frac{\phi}{1.26}\right) + 0.05\right) CO_i \left(\frac{P_3}{1.4E6}\right)^{a_3} \tau^{a_4}, \quad (3.11)$$

is used, for temperatures between 2000 K and 1370 K, the expression

$$EICO = 0.122T_c^{-0.2} \phi^{-2.45} CO_i \left(\frac{P_3}{4.35E5}\right)^{0.62}, \quad (3.12)$$

is used and for temperatures below 1370 K, the following expression is used:

$$EICO = (7^{-15} \exp T_l + 140) \left(\frac{P_3}{4.34E5}\right)^{0.62}. \quad (3.13)$$

Each of these equations require assumptions about the temperature within different areas of the combustor. To determine the temperature within each of these reactors, Rizk and Mongia assumed these temperatures based on the chemical kinetics of propane gas [23]. The equations would serve as a correction to the amount of CO being produced by the propane gas. To relate the propane gas to the liquid based fuel within the primary zone of the combustor, an additional equation was used to correct the fuel air ratio within the reactors with the amount of liquid fuel that would be evaporated. Using the pressure drop at the atomizer, mean droplet size and evaporation rate of the fuel, the fuel air ratio within a reactor is altered in the chemical kinetic calculations, using the expression

$$FAR_{eff} = FAR \left(0.015 \left(\frac{\lambda_{ev}}{SMD^2}\right) \left(\frac{\delta P_3}{P_3}\right)^{0.5}\right)^{0.1}. \quad (3.14)$$

As a result the Rizk model could also have the potential to predict combustor blow out conditions [23].
3.2.2 MIT Model

The MIT Model, created by Allaire at the Massachusetts Institute of Technology, continued to develop on that of the Rizk model by focusing on the combustion chemistry and flow within the primary zone of the combustor. The purpose of the MIT model was to develop a method for predicting the ‘unmixedness’ within the primary zone of the combustor by creating a large number of colinear reactors with varying equivalence ratios [2], as seen in Figure 3.3. The reactor network methodology assumes that the set localized equivalence ratios will occur somewhere within the primary zone volume. Since the primary zone of a combustion chamber can have a large variance of localized equivalence ratios, the MIT model used statistical analysis to generate a normalized distribution of localized equivalence ratios. The model user first chooses an unmixedness parameter ($s$) and calculates the mean equivalence ratio ($\bar{\phi}$) of fuel and air within the primary zone of the combustor [2]. Finally, a standard deviation ($\sigma_\phi$) is calculated using the expression

![MIT reactor network methodology, from [2]](image-url)
\[
\sigma_\phi = s \bar{x}_\phi,
\]

(3.15)

to determine the localized equivalence ratios within the primary zone reactors [2].

The resulting standard deviation is used to determine the localized equivalence ratios within the primary zones. Using the cumulative distribution function, a normalized distribution of mass flow was calculated for a set number of reactors within the primary zone. An example calculation performed by Allure using ten reactors within the primary zone and a mean equivalence ratio of 1.0 can be seen in Figure 3.4 [2].

![Figure 3.4: Example of equivalence ratio normalized distribution using unmixedness parameter, from [2]](image)

The MIT model used an innovative reactor network methodology to determine emissions for modern engines. Unfortunately, there are a few concerns with the MIT methodology which can significantly affect the calculated CO emissions. The most prominent concern with the MIT model is that the assumed value of the unmixedness parameter must account for important parameters such as droplet evaporation [2]. In addition, there is no set relationship between the unmixedness parameter and droplet evaporation; therefore
the MIT model cannot track variations in mean droplet size.

Another concern with the MIT model is that due to the co-linear structure of the reactors and the calculation of the localized equivalence ratios, the MIT model does not adapt to different flow fields. The creator, Douglas Allaire, recommended that a similar unmixedness parameter be used for a combustion chamber with similar flow fields [2]. Therefore, when predicting CO emissions, the engine must have a similar flow field to accurately predict CO emissions.

### 3.2.3 Laval Model

The Laval model developed by Kalla focused on gaseous fuels, specifically propane. Kalla used simplified chemical kinetics for the chemical reaction of propane with air, expressed as

$$ aC_3H_8 + bO_2 + cN_2 \rightarrow dH_2O + eCO + fH_2 + gO_2 + hN_2, $$

(3.16)

and two secondary reactions

$$ CO + \frac{1}{2}O_2 \rightleftharpoons CO_2 $$

(3.17)

and

$$ H_2O \rightleftharpoons H_2 + \frac{1}{2}O_2, $$

(3.18)

to efficiently solve for the CO emissions produced in the combustion of propane gas within a can combustor known as GHOST [13]. To balance the chemical equations, Kalla used a correlation to solve for the concentration of each species within a given reactor. In addition to simplifying the chemical kinetics of a propane reaction, Kalla also created the idea of using cold flow CFD to generate a simplified reactor network. Both the can combustor CFD and corresponding reactor network can be seen in Figure 3.5 [13].
One of the most important aspects of creating a CO model is producing an accurate representation of air flow throughout the interior of the combustor. The concept of using cold flow CFD to generate assumptions about the flow splits throughout the combustor gives a more accurate representation of localized equivalence ratios within finite volumes of the combustor. Kalla has only performed validation testing on a can combustor using gaseous fuel and did not examine annular combustors using liquid fuel.

### 3.2.4 Aerospace Industry Developed Models

During this chapter, simplistic methodologies developed by institutions for predicting CO emissions have been examined. Industries have also attempted to develop models for predicting CO emissions using similar methodologies. Aviation gas turbine engine companies have developed models in the past and continue to investigate methods for predicting CO emissions. The models developed by each of these companies has produced a similar trend. Each model contains three aspects; a method for dividing the combustor into a reactor network, tracking combustion chemistry and evaporation. These three characteristics not only affect CO production but are important to capture within any model attempting to accurately predict CO emissions and trends.
3.3 Impact of Liquid Fuel

Past approaches that have accounted for a liquid based fuel have all used submodels that solve for the evaporation of fuel within the combustion chamber; one of the most difficult aspects of predicting carbon monoxide emissions. From information gathered in Section 2.2.6, CO emissions are directly correlated with combustion efficiency; therefore, it is important to keep track of the liquid fuels droplet size and rate of evaporation throughout different areas of the combustor. In this section, past correlations for calculating mean droplet size and droplet evaporation were investigated.

3.3.1 Mean Droplet Size Correlations

Since each atomizer has different flow characteristics and overall geometries, it is difficult to predict the mean droplet size of fuel exiting a given atomizer using a single correlation. From the literature survey, multiple correlations were found that have been developed focus on key characteristics for both pressure and airblast atomizers.

Pressure Atomizer

As discussed in Section 2.2.6, a pressure atomizer depends highly upon the fuel pressure drop \( (dP_f) \), mass flow rate of fuel \( (\dot{m}_f) \) and fuel properties. Each of these parameters have been used to develop many empirical correlations to solve for a fuel’s mean droplet size. Equations developed by Radcliffe and Jasuja utilized each of these parameters, however, exponential coefficients used in each equation are different based on the experimental data that they have been derived from. The Radcliffe and Jasuja formulas are expressed as

\[
SMD = 7.3(\sigma_f)^{0.6}(\nu_f)^{0.2}(\dot{m}_f)^{0.25}(dP_f)^{-0.4} 
\]

and

\[
SMD = 4.4(\sigma_f)^{0.6}(\nu_f)^{0.16}(\dot{m}_f)^{0.22}(dP_f)^{-0.43}. 
\]
Using a similar methodology, Lefebvre uncovered that the properties of the air around the nozzle can have an affect on the overall mean droplet size. If the fuel is entering a combustion chamber with dense air, the air will reduce the velocity of the fuel, preventing the ligaments from breaking apart. Therefore, Lefebvre altered the previous equations not only to include the density of air \((\rho_a)\), but to also make the equation, dimensionally correct [10]. The formula developed by Lefebvre is expressed as [15]

\[
SMD = 2.25(\sigma_f)^{0.25}(\mu_f)^{0.25}(m_f)^{0.25}(dP_f)^{-0.5}(\rho_f)^{-0.25}. \tag{3.21}
\]

After learning the importance of air around the nozzle for the calculation of mean droplet size, Lefebvre developed another correlation to determine mean droplet size that focused on the conditions of the fuel and air mixture around the nozzle. The equation represents two stages that fuel ligaments go through as they break down into smaller droplets. The first stage represents the surface instabilities due to internal hydrodynamics and external aerodynamic forces [15]. The second stage represents the transition from ligaments into spherical droplets. The formula developed by Lefebvre and Wang is stated as [15]

\[
SMD = 4.52 \left( \frac{\sigma_f \mu_f^2}{\rho_a dP_f^2} \right)^{0.25} (FT \cos \theta)^{0.25} + 0.39 \left( \frac{\sigma_f \rho_f}{\rho_a dP_f} \right)^{0.25} (FT \cos \theta)^{0.75}. \tag{3.22}
\]

In addition to the previous parameters discussed in the chapter, Lefebvre and Wang also take into account the spray cone angle \((\theta)\) and the film thickness \((FT)\). The film thickness of the spray is found using an iterative process between expressions [16]

\[
FT^2 = \frac{1560 m_f \mu_f}{\rho_f d_o dP_f} * \frac{(1 + X)}{(1 - X)^2} \tag{3.23}
\]

and

\[
X = \frac{(d_o - 2FT)^2}{(d_o)^2}. \tag{3.24}
\]
Airblast Atomizers

Also discussed in Section 2.2.6 were the properties that affected air-blast atomizers. Unlike pressure atomizers which are predominately affected by pressure drop over the nozzle, airblast atomizer performance is dependent on fuel and air properties. Both fuel and air properties can be seen in many airblast based atomizer correlations. The first correlation was developed by Rink and Lefebvre and is expressed as [22]

\[
SMD = 0.00365 \left( \frac{\rho_L \sigma}{\rho_A \sigma R} \right)^{0.5} \left( 1 + \frac{1}{AFR} \right)^{0.7}.
\] (3.25)

Another correlation found for external air-assist airblast atomizers was developed by Inamura and Nagai. The main difference between the Inamura correlation and Rink’s correlation was that it included a variable for the geometry of the atomizer. The Inamura correlation included a variable for the film thickness of the fuel (\(FT\)). In addition, the correlation classified the relationship between the fuel flow and air flow in numbers known as the stability number and the Weber number, expressed as [15]

\[
Oh = \left( \frac{\mu_f^2}{\rho_f FT \sigma} \right)^{0.5}
\] (3.26)

and

\[
We = \frac{\rho_a U_a^2 FT}{\sigma}.
\] (3.27)

As a result the final correlation yields [15]

\[
SMD = FT \left[ 1 + \frac{16850 Oh^{0.5}}{We \left( \frac{\rho_f}{\rho_a} \right)} \right] \left[ 1 + \frac{0.065}{\left( \frac{\dot{m}_f}{\dot{m}_a} \right)^2} \right].
\] (3.28)

The last correlation analysed was developed by Elkotb. Elkotb attempted to use the concept of calculating turbulence to determine the mean droplet of an air-assist airblast atomizer by determining the Reynolds number (\(Re\)) at the fuel nozzle, expressed as [15]
\[ Re = \frac{\rho_f U_r d_o}{\mu_f}. \] (3.29)

In addition, like the Inamura correlation, Elkotb included a variable to represent the geometry of the fuel atomizer; this variable is known as the discharge orifice diameter \((d_o)\). The Elkotb correlation is expressed as \[15]\
\[ SMD = 51d_o Re^{-0.39} We^{-0.18} \left( \frac{\dot{m}_f}{\dot{m}_a} \right)^{0.29}. \] (3.30)

### 3.3.2 Fuel Droplet Evaporation

After using a correlation to determine the mean droplet diameter leaving the atomizer, an evaporation model must then be used to determine how fuel evaporates throughout the combustor.

In order to simplify the evaporation model, previous models have assumed a steady state evaporation of a perfectly spherical droplet. In using these assumptions the rate of evaporation of a droplet was then defined by a single linear function known as the \(d^2\) law \[9\]. The \(d^2\) law is defined as
\[ d^2(t) = d^2 - \lambda t, \] (3.31)
where the diameter is changing based on an evaporation constant \((\lambda)\) \[9\].

**Evaporation Constant**

The evaporation constant \((\lambda)\) is highly dependent on the localized temperature. As a result, the evaporation constant will change depending on the droplet’s location within the combustor.
The evaporation constant ($\lambda_{eff}$) is important because it describes the evaporation rate of fuel droplets [15]. Assuming the droplet of fuel is stationary, the evaporation constant can be solved using fuel properties such as thermal conductivity ($k_{fg}$), density ($\rho_f$), specific heat ($C_{pg}$) and the mass transfer rate ($B_m$) at the surface of the droplet, yielding [15]

$$\lambda_{eff} = 8 \frac{k_{fg}}{C_{pg}\rho_f} \ln (1 + B_m).$$

(3.32)

The evaporation constants’ dependence on localized temperature is found within the equation for mass transfer. Assuming steady state conditions, the mass transfer number is equal to that of the heat transfer number ($B_m = B_T$), as heat transfer becomes dominant within a gas turbine combustor [15]. The heat transfer number represents the transition of liquid fuel to gaseous fuel at the surface of the droplet. As a result, the heat transfer number includes variables such as the latent heat of fuel vaporization between the fuel and the atmospheric medium ($H_{fg}$), the surface temperature of the fuel ($T_s$), the average localized temperature ($T_\infty$) and the specific heat of the medium ($C_{pg}$), yielding

$$B_T = \frac{C_{pg}(T_\infty - T_s)}{H_{fg}}.$$  

(3.33)

When the temperature within the reactor is much higher than the boiling point of the fuel, the heat transfer number can be simplified further by assuming that the temperature at the surface of the gas is the boiling point of the fuel ($T_b$) [15].

**Convective Correction**

In a gas turbine engine, fuel is mixed within a turbulent primary zone. Therefore, it would not be effective to assume that the fuel is stationary when calculating the change in droplet size. In previous models, a correction factor was used when calculating the effective evaporation rates. Although academics have used many different convective correction factors, all of the factors have included similar variables. These variables
include Reynolds Number of the droplet \((Re_D)\) and the Prandtl number \((Pr)\) \[15\]. For this thesis, the convective correction that is used is expressed as \[15\]

\[
1 + 0.3Re_D^{0.5}Pr^{0.33}.
\] (3.34)

The equation for the Reynolds number of a droplet can be seen in Equation (3.29) \[15\]. The Reynolds number of the droplet is dependent on its relative velocity to the gas within the combustion chamber. Therefore allowing the droplet to evaporate faster for counter facing flows. On the other hand, the Prandtl number captures the ratio of viscous diffusivity to the diffusivity related to heat transfer, yielding \[15\]

\[
Pr = \frac{C_p\mu}{k}.
\] (3.35)

Combining the convective correction in Equation (3.34) with the calculation of the evaporation constant in Equation (3.32) yields

\[
\lambda_{eff} = 8\frac{k_fg}{C_p\rho_f} \ln (1 + B_m) \ast (1 + 0.3Re_D^{0.5}Pr^{0.33}).
\] (3.36)

### 3.4 Summary of Past Modelling Methodologies

After investigating past methodologies for calculating CO emissions, many different models have been developed with relative success. Many of the models that were investigated such as the global correlations and MIT model can be tested against against additional combustors to test their validity. On the other hand, the industrial models, Laval and Rizk model, have been developed for specific combustors and can be further developed into a new methodology. In later chapters, a new physics based model will attempt to combine the Rizk, Laval and Industrial methodologies into a single idea.

In addition to investigating CO emission predictors, the use of liquid fuel based correlations is important to not only capture the affects of mean droplet size on CO emissions
but the trends resulting from varying combustor conditions parameters. Although only a few correlations are being looked at in this thesis, there are many correlations for a variety of different atomizers. As a result, when producing a model to predict CO emissions, it will be important to determine what atomizer is being used and how it will affect the conditions within the combustor.
Chapter 4

Thesis Test Cases

To validate computational models in the prediction of CO emissions, multiple combustors were chosen based on variations in combustor geometry and flow fields. For the scope of this thesis, combustors from the following engines will be analysed in later chapters:

- Engine A
- Engine B
- Engine C
- Engine D

Combustor selection was made under the recommendation by the project industrial partner. In this chapter, combustors from each engine will be summarized.

4.1 Engine A Combustor

Engine A contains a simple can combustor. A can combustor geometry was chosen for this analysis because of its' simplicity and for the large amount of available information. The information chosen for this analysis can be seen in reference [29].

In this analysis, three different engines using various fuel and atomizers to determine
their effects on engine performance, efficiency and emissions \[29\]. Engines were chosen based on varying geometries and differing combustor flow fields. The first engine tested from the alternative fuels report and the focus for this thesis was Engine A, the can combustor system. A cross section of the Engine A combustor can be seen in Figure 4.1.

![Figure 4.1: Engine A combustor cross section, from \[29\]](image)

The Engine A combustor was tested using fifteen different fuels, four different nozzle types and under varying inlet conditions \[29\]. Emissions data was taken for Engine A using both methane gas and Jet-A1 fuel, a simplex type atomizer and inlet conditions based on ICAO thrust levels. Methane was chosen to test the reactor methodology without the need for an evaporation sub-model. Jet-A1 fuel was chosen due to its’ regular use in commercial aircraft engines and the simplex nozzle due to its’ simplicity. All combustor test data and inlet conditions can be seen in reference \[29\].

### 4.2 Engine B Combustor

The next test case is an annular combustor containing 12 pressure atomizers with a single toroidal flow field in the primary zone. The Engine B combustor was chosen as it is an annular combustor and contains a simplistic geometry as seen in Figure 4.2. The single toroid encompasses the entire primary zone of the combustor and is initiated by a single
cooling jet located at the inner diameter of combustion chamber.

Figure 4.2: Engine B combustor cross section, from [30]

4.3 Engine C Combustor

The third combustor to be analysed is an annular combustor containing 12 pressure atomizers and a double toroidal flow field within the primary zone. The Engine C combustor contains a similar geometry and operating conditions to Engine B’s combustor because they are the same. The difference between the combustors from Engine B and Engine C is the position of cooling louvres and jets were altered to produce a double toroidal flow field within the primary zone. As seen in Figure 4.3, the flow field within the combustor of Engine C shows two distinct areas of rotating fuel/air mixture within the primary zone. These zones of rotation are caused by high velocity jets located at the edge of the primary zone. The benefit of using a double toroidal flow field is that Engine C produces less CO emissions than Engine B. Lower CO emissions are achieved from the increase in recirculating flow from the double toroidal flow field compared to a single toroidal flow field. Additional recirculating flow decreases the amount of unburned hydrocarbon allowing for more complete combustion. Finally, the inlet conditions for the Engine C combustor can be seen in reference [30].
Chapter 4. Thesis Test Cases

4.4 Engine D Combustor

The final combustor that will be analysed for CO emissions is a modern annular combustor. To reduce emissions and save weight, the combustor from Engine D uses a much more complex and compact geometry compared to combustors from Engine B and C; the complex cross section of the Engine D combustor can be seen in Figure 4.4. The combustor utilizes a single toroidal based flow field with 24 airblast based atomizers.

Information used to verify the predicted emissions data from the Engine D combustor was available by the European Union in a report entitled *AeroNOx: Impact of NO*\textsubscript{x} *Emissions from Aircraft Upon the Atmosphere at Flight Altitudes 8-15km*. In August of
1995 the European Union conducted tests on multiple engines in hopes that the results would be used to develop a model that would determine emissions over an entire ICAO cycle [25]. The entire bank of information includes aircraft engine data at different inlet conditions and altitudes and can be seen in reference [25].

4.5 Summary of Thesis Test Cases

Before testing past models and producing new model methodologies, a variety of test cases were gathered. In producing a model that will be used to predict emissions for experimental engines, the test cases were chosen based on varying geometries, flow fields and combustor types. In addition to focusing on the ICAO cycle, the use of additional engine data will provide model to test the effects of key parameters on CO emissions. Engine A contains a can combustor which allows the models to be tested under a very simple geometry. The Engine B combustor is used as a second test to transition the model to a simplistic annular combustor. The Engine C combustor is used to determine if the models can capture multiple flow fields within a given annular combustor. Finally, the Engine D combustor allows the models to predict emissions for a complex modern annular combustion chamber. Each combustor is chosen to slowly increase the complexity of the developed reactor models. In the next chapter, a new methodology used to analyse CO emissions within each of the test cases will be explained.
In creating a physics based model that will assist in predicting carbon monoxide (CO) emissions for each of the test cases discussed in the previous chapter, elements from the Laval, Rizk and industry models were combined to develop a complete physics based model. To accurately predict CO emissions the model would need to capture three key characteristics. These characteristics include a reactor network development methodology, combustion chemistry and liquid fuel evaporation.

5.1 Reactor Network Development Methodology

The new reactor network development methodology is designed to accommodate all different types of combustors and consists of two step. The first step is to determine the cross sectional reactor network configuration based on the combustion geometry and understanding of the combustors’ internal flow field. The second is to determine the tangential reactor network based on the fuel spray trajectory. This section will outline assumptions and procedures used in creating a reactor model for a given combustor.
5.1.1 Cross Sectional Reactor Network

In the development of a cross sectional reactor network, elements of the Laval model were used as it allows the model to conform to changing flow fields for different engine configurations. The methodology states that in order to understand the flow of fuel and air throughout an experimental combustion, a cold flow CFD calculation is required [13]. The cold flow CFD generates velocity contours for the fuel/air mixture throughout the combustion chamber. The cold flow CFD example in Figure 7.1 shows the velocity contours of the single toroidal flow field found in the combustor of Engine B.

![Figure 5.1: Cold flow CFD of the Engine B combustor produced by the project industrial partner in the plane of the nozzle](image)

The cold flow CFD is a relatively quick calculation to determine an assumed flow field for the fuel/air mixture. Since the localized equivalence ratios of fuel and air can have a significant affect on CO formation, determining where the fuel and air is travelling within the combustion chamber is important [13]. From the calculated velocity contours, a reactor model can be generated around areas that are prone to changes in CO concentrations. Key areas of the combustion chamber to focus reactor development include the primary zone of the combustion chamber, downstream mixing within the intermediate
zone of the combustion chamber and the near wall regions of the combustor. These areas are highlighted in Figure 5.2.

![Figure 5.2: Key zones within the cold flow CFD of the Engine B combustor where CO concentrations are prone to change](image)

The first zone on Figure 5.2 is important as it is where CO is produced through the process of incomplete combustion. Furthermore, the combustion within the primary zone is dependent on the evaporation of liquid fuel. Reactors within the first region will be important as they will track the evaporation of fuel throughout the primary zone. The second zone in Figure 5.2 represents the intermediate zone of the combustion chamber. This area is important for two reasons as it allows for CO to oxidise and it can also host quenching between material within the plan of the nozzle and between adjacent nozzles. Finally, the third zone is the near wall region of the combustion chamber. This zone is important because the hot contents of the primary zone can quench near the walls of the combustion chamber. The near wall at the inner diameter is important as the contents is not recirculated back into the primary zone or the center of the intermediate zone. As a result, the contents is pushed further downstream preventing the CO within the mixture from oxidizing as the region will continue to operate at a low temperature.
In addition to developing the reactor network, the cold flow CFD can give estimation on the percentage of flow from one reactor to another, air entering the reactor network and fuel entering the reactor network. These percentages are paramount in determining accurate localized equivalence ratios within a given combustor model. For example, as seen in Figure 5.3, a percentage of the contents exiting a primary zone reactor enters the near wall reactor while the remaining contents is sent further downstream to the intermediate zone, thus conserving mass at the exit of the reactor. Alterations to these flow splits allow the user full control over conditions throughout the combustor. With an understanding of the flow and reactor definition within the plane of the nozzle, the next step is to investigate the tangential area that is affected by the fuel spray.

![Diagram](image)

Figure 5.3: Example of percent being transferred from reactor to reactor within a reactor network

### 5.1.2 Tangential Reactor Network

A new idea in the development of reactor networks is to consider the region of the combustion chamber which is between adjacent combustor nozzles. The region in question is where the fuel spray cannot be reached by the atomizers’ assumed fuel spray trajectory. A graphical representation of this region can be seen in Figure 5.4.

The importance of this region is the dependence on the amount of fuel nozzles used in
Figure 5.4: Tangential reactor development based on the estimated trajectory of the fuel spray

a given combustion chamber. With an increase in fuel nozzles, the area becomes much smaller as the fuel spray produced from a given atomizer overlaps within the region between the nozzles. On the other hand, when reducing the amount of nozzle being used, the atomizer fuel sprays no longer overlap and a region with cold air is produced. As a result, quenching can occur when the high temperature region of the combustion chamber mixes with the low temperature region downstream of the primary zone. As quenching zones can produce high levels of CO emissions, the use of a tangential reactors to predict CO emissions will be important in the development of a reactor model.

5.1.3 Methodology Limitations

An evident limitation of this methodology is the use of cold flow CFD to make assumptions about the flow. Although cold flow CFD calculations can take less than a day to complete, if a solid model is not developed for the experimental combustor, the time taken to predict CO emissions can increase to well over a day. Without cold flow CFD the user would have to make assumptions about the internal flow field based similar combustor geometries and flow fields.
Another limitation of the reactor network development methodology is the use of tangential reactors representing the fuel/air mixture travelling in between two adjacent fuel nozzles. If the conical fuel spray from two adjacent nozzles do not overlap, a rectangular reactor is generated receiving little to no direct fuel from the fuel nozzles. Unfortunately, the area which receives no direct fuel from the fuel nozzles is not limited to reactors in between adjacent nozzles. To better track the flow of fuel from the nozzles to areas within the combustion chamber, additional reactors would be required to capturing backwards flowing fuel.

5.2 Chemical Reactors

From investigating past models and how CO is formed throughout a combustor, one of the most important aspects of any CO model must be the use of chemical reactors. Chemical reactors not only allow the user full customization of inputs but also provides the localized concentration of different chemical species. There are two types of reactors that are typically used in combustion analysis to provide a simplistic method of calculating chemical reactions while conforming to the laws of conservation of mass, energy, momentum and species. They include perfectly stirred reactors (PSR) and plug flow reactors (PFR).

5.2.1 Perfectly Stirred Reactors (PSR)

A PSR reactor is an ideal reactor which assumes that a mixture within the reactor is perfectly distributed throughout \[27\]. The effect that this assumption has on the combustion process can be described using the Damkohler number \((Da)\). The Damkohler number represents the relationship between the characteristic flow time \((\tau_{flow})\) which is controlled by the mixing rate and the characteristic chemical time \((\tau_{chem})\) which is controlled by the rate of reactions; the resulting equation can be seen below \[27\]:
Chapter 5. New Proposed Model

\[ Da = \frac{\tau_{\text{flow}}}{\tau_{\text{chem}}} \]  \hspace{1cm} (5.1)

In cases where the characteristic flow time is larger than that of the characteristic chemical time \((\tau_{\text{flow}} \gg \tau_{\text{chem}})\), combustion is dependent on the mixing rate of the fluid throughout the reactor. By assuming that the contents is perfectly mixed at the instant it enters the reactor, the characteristic flow time will approach a value of zero \((\tau_{\text{flow}} \rightarrow 0)\). Consequently, the combustion process in a PSR based reactor is solely driven by the rate of chemical reactions within the constant volume.

Laws of Conservation

In addition to assuming that the contents is perfectly mixed, a PSR assumes steady-state and steady flow. With both of these assumptions the laws of conservation can be simplified from ordinary differential equations, to coupled, non-linear, algebraic equations \[27\]. From the diagram representing a PSR reactor, seen in Figure 5.5 the conservation of mass equation for a given species \(i\) is as follows:

\[
\frac{dm_{i,cv}}{dt} = \dot{m}^{\prime\prime\prime} V + \dot{m}_{i,in} - \dot{m}_{i,out}.
\]  \hspace{1cm} (5.2)
Chapter 5. New Proposed Model

Within this equation, the amount of mass accumulated within the reactor over time \( \left( \frac{dm_{i,cv}}{dt} \right) \) is equal to the rate at which mass is generated \( (\dot{m}'')V) \) within the reactor and the difference between mass entering and exiting the reactor \( (\dot{m}_{i,in} - \dot{m}_{out}) \). Under steady-state conditions, calculations are no longer dependent on time; therefore the rate at which a species accumulates within a reactor is assumed to be zero \([27]\). The production rate of species within a reactor can be related to the net production rate \( (\omega_i) \) as seen in the equation below \([27]\):

\[
\dot{m}'' = \omega_i MW_i. \tag{5.3}
\]

The mass of a given species entering and exiting the PSR is calculated based on a species mass fraction \( (Y_i) \). Using the mass flow rate of the mixture, the mass flow rate of a given species is obtained using the expression

\[
\dot{m}_i = \dot{m}Y_i. \tag{5.4}
\]

The result of combining the Equations \([5.4]\) and \([5.3]\) with the assumed steady-state and steady flow of the PSR simplifies the conservation of mass equation, yielding \([27]\):

\[
\dot{\omega} MW_i V + \dot{m}(Y_{i,in} - Y_{i,out}) = 0. \tag{5.5}
\]

Similar to the conservation of mass, the conservation of energy, initially expressed as

\[
\dot{Q}_{cv} - \dot{W}_{cv} = \dot{m}[(h_{out} - h_{in}) + 0.5(v_{out}^2 - v_{in}^2) + g(z_{out} - z_{in})], \tag{5.6}
\]

can be simplified from the assumptions of the PSR. From the conservation equation, the total energy produced \( (\dot{Q}_{cv} - \dot{W}_{cv}) \) is equal to the internal energy \( (\dot{m}(h_{out} - h_{in})) \), the kinetic energy \( (0.5\dot{m}(v_{out}^2 - v_{in}^2)) \) and the potential energy \( (\dot{m}g(z_{out} - z_{in})) \). Since the PSR is not doing any work, the potential energy is negligible and the steady flow means there is no transfer of kinetic energy; therefore the conservation of energy equation is simplified to the following \([27]\):

\[
\dot{Q} = \dot{m}(h_{out} - h_{in}). \tag{5.7}
\]

Finally, as a result of the steady-state assumption and instantaneous mixing, the conservation of momentum is not applicable to a PSR.
Application

Due to the instantaneous mixing and dependence on chemical reaction rates, a PSR reactor would be more suited for calculating the conditions within the primary zone of the combustion chamber. The assumption of instantaneous flow assumes that the turbulence intensity within the region of the PSR is high. With the primary zone being a highly turbulent environment a PSR would be ideal. In addition, the low time characteristic of flow will produce an environment that is driven by chemical reactions.

Unfortunately, it would be unwise to use a single PSR reactor for the primary zone as mixing and flow throughout the primary zone of the combustion chamber can have a large effect on CO emissions. As fuel evaporation is affected by mixing within the primary zone and localized equivalence ratios affect the formation of CO, multiple PSR’s would be required to capture combustion within the primary zone. Therefore, the ideal application for PSR reactors within the primary zone is to use a network of PSR reactors with a corresponding sub-models to track fuel evaporation.

5.2.2 Plug Flow Reactors (PFR)

A PFR is also an ideal reactor that is similar to a PSR. The PFR assumes steady-state flow, no mixing in the axial direction and ideal frictionless flow [27]. What makes a PFR unique is that it allows one-dimensional flow. As a result, properties at different positions along a given axis can be determined. A diagram representing a plug flow reactor can be seen in Figure 5.6.

![Diagram of Plug Flow Reactor](image-url)
From Figure 5.6 the conservation of mass through a PFR is represented as [27]

\[
\frac{d(\rho v_x A)}{dx} = 0. \tag{5.8}
\]

The equation simply states that the mass flow rate in the axial direction \((\rho v_x A)\) does not change as the fuel/air mixture travels axially through the PFR.

Unlike a PSR, the PFR has an equation for the conservation of momentum due to the application of one-dimensional flow. The conservation of momentum equation in the dimension of flow simplifies to [27]

\[
\frac{dP}{dx} + \rho v_x \frac{v_x}{x} = 0. \tag{5.9}
\]

From the equation, if a pressure change occurs along the PFR, the acceleration \((\frac{v_x}{x})\) or transport flux \((\rho v_x)\) of the fuel/air mixture will be affected.

With the addition of one-dimensional flow, the law of conservation of energy can no longer ignore the presence of kinetic energy. As a result the conservation of energy equation is simplified to [27]

\[
\frac{d(h + \frac{v_x^2}{2})}{dx} + \frac{\dot{Q}' \Phi}{\dot{m}} = 0. \tag{5.10}
\]

From the equation, any change in kinetic or internal energy \((\frac{d(h + \frac{v_x^2}{2})}{dx})\) will be assumed to be released as heat into the atmosphere. The exchange of heat from the PFR to the atmosphere is represented by the local perimeter of the reactor \((\Phi)\).

The final conservation law is the conservation of species, which is expressed [27]

\[
\frac{dY_i}{dx} - \frac{\dot{\omega} MW_i}{\rho v_x} = 0. \tag{5.11}
\]
The equation states that any change is species \( \frac{dY_i}{dx} \) along the one-dimensional flow is a result of a change in the species generation (\( \dot{\omega}MW_i \)) or transport flux (\( \rho v_x \)) of the flow through the PFR.

**Application**

Due to the similarity of the PFR to a PSR, a PFR can be represented as a set number of PSR’s placed in succession; the more PSR’s used, the more information will be known throughout the combustor. The areas of the combustor which benefit from the use of PFR’s is the intermediate and dilution zones.

After combustion has occurred within the primary zone of the combustor, the fuel/air mixture moves to the intermediate zone where the concentration of species begin to change. As the length of the intermediate zone increases, more CO oxidation can occur as a result of the longer exposure to high temperatures. A PFR would be the best way to track emissions through the intermediate and dilution zones as changes in CO within these regions are primarily based on oxidation of CO molecules.

**5.2.3 Cantera**

To calculate chemical reactions while conforming to the laws of conservation within both PSR and PFR’s, a program known as Cantera was used. Cantera is an object oriented software developed by Goodwin at the California Institute of Technology [8]. The software focuses primarily on chemical kinetic, thermodynamics and transport process based calculations [8]. For applications within the scope of this thesis, Cantera will be used to complete chemical kinetic calculations within a reactor network.

Within the proposed model, each reactor is represented as a PSR in Cantera. The PSR requires inputs such as a constant volume and initial content set by the user. For
all cases the initial contents is assumed to be air at standard temperature and pressure. Once the PSR is created in Cantera, reservoirs are generated for all flows leading to a given PSR. Each reservoir requires a given temperature, pressure and contents set by the user. Once the mass flow rate from each reservoir to the PSR is set, the PSR object will simulate the mixing of each material over the entire volume of the PSR. To replicate a combustion chamber at steady state conditions, the simulation advances the reactor in time by one second. Since hundreds of reactions take seconds to complete and the contents of the reactors only stays within the PSR for milliseconds, a one second simulation time was deemed sufficient. Alterations to the time step was done with no improvements to computational time. Material mixed within the PSR is then exhausted out of the PSR into a reservoir where the contents’ pressure, temperature and species concentrations are measured, recorded and used as inputs for downstream reactors. By setting an input to a downstream reactor as the contents of the exhaust, a reactor network can be created representing volumes throughout the combustor. The calculation process of a PSR is graphically represented in Figure 5.7.

Each PSR within a combustion chamber goes through the above computational process. For PFR based reactors a similar methodology is used, however the reservoir containing the exhaust of the initial PSR object is then passed down to another PSR reactor to replicate that of a PFR based reactor. This process is graphically represented in Figure 5.8. Since increasing the number of PSR reactors within a PFR can increase the com-
putational time of a single calculation, a sensitivity analysis was done to determine the minimum amount of reactors required to accurately predict CO emissions.

To test how the amount of reactors affects calculated CO emissions, a simple plug flow reactor receiving the exhaust from the combustion of propane and air at an equivalence ratio at 0.4 was simulated. The equivalence ratio was set to 0.4 to track the slower reaction rates associated with low temperature combustor. The amount of PSR’s within a given PFR was varied over a constant length. The results shown in Figure 5.9 reveal that if more than twenty-five PSR’s are used in a given PFR calculation, there will be less...
than 1% error in the resulting convergence calculation of the CO emission index ($EICO$).

Each PSR and PFR are able to calculate combustion based on files which contain thermodynamic and transport properties of given reactions. Each reservoir is embedded with these chemical reactions and species. The file that contains these kinetic properties are called chemical mechanisms, and the choice of mechanism is important to the combustion that is trying to be replicated.

### 5.2.4 Chemical Mechanisms

To perform chemical kinetic based calculations within a given reactor in Cantera, first an appropriate chemical mechanism must be chosen. There are many different types of chemical mechanisms available depending on the fuel that is being used for the analysis. In addition, more detailed chemical mechanisms can exponentially increase the computational time of a given analysis.

For this report, two chemical mechanisms were considered. The first chemical mechanism was created at the University of California at Berkeley by a team of engineers lead by Smith called GRI30 26. GRI30 contains the detailed combustion of propane ($C_3H_8$) and methane ($CH_4$) 26. The second is the detailed combustion of jet fuel (assumed to be $C_{10}H_{22}$), developed and made available by Westbrook 28. The amount of reactions and species in each mechanism can be seen in Table 5.1.

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Species</th>
<th>Reactions</th>
</tr>
</thead>
<tbody>
<tr>
<td>GRI30</td>
<td>53</td>
<td>325</td>
</tr>
<tr>
<td>Jet Fuel</td>
<td>1421</td>
<td>7851</td>
</tr>
</tbody>
</table>

Table 5.1: Comparison of species and reactions from different chemical mechanisms
Although the jet fuel mechanism contains an accurate account of jet fuel dissociation to CO and production of NO\textsubscript{x}, the carbon-hydrogen ratio and the amount of air required to stoichiometrically react with propane is similar to that of jet fuel. For these reasons, the amount of carbon atoms available to dissociate to CO is similar. As a result, propane has the potential to accurately predict CO from the combustion of jet fuel.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Higher Heating Value (kJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propane</td>
<td>50368</td>
</tr>
<tr>
<td>Jet Fuel</td>
<td>48020</td>
</tr>
</tbody>
</table>

Table 5.2: Higher heating value of fuels

Another key aspect of using the detailed propane mechanism over the jet fuel mechanism is that the temperature produced through the combustion of propane will be higher than that of jet fuel. The higher temperature is a result of propane having a higher heating value than jet fuel as seen in Table 5.2. To correct for the amount of energy entering the system, a quick correction factor was developed to change the amount of fuel entering the combustor based on the difference in higher heating value (\textit{HHV}). Through changing the amount of fuel, the amount of internal energy available to the system is altered. The corrected mass flow rate of fuel is obtained from the expression

\[
\dot{m}_{\text{eff,f}} = \frac{HHV_{\text{Jet}}}{HHV_{\text{Propane}}} \dot{m}_f.
\]  

(5.12)

Using Equation (5.12) is important because the GRI30 mechanism will take less time to replicate the combustion of propane gas than the detailed mechanism of jet fuel. This theory was tested using the Cantera software replicating the combustion of jet fuel and propane within a reactor at an equivalence ratio of 1 (\(\phi = 1\)). As seen in Table 5.3, using a single processor, the propane mechanism took approximately 4.24 seconds where as the jet fuel mechanism takes approximately 1861.32 seconds. When developing models which include multiple reactors and recirculation of flow, the use of a jet fuel mechanism
<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Computational Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GRI30</td>
<td>4.24</td>
</tr>
<tr>
<td>Jet Fuel</td>
<td>1861.32</td>
</tr>
</tbody>
</table>

Table 5.3: Calculation time for the combustion of propane and jet fuel ($\phi = 1$) using a single processor.

could result in calculation times lasting days. On the other hand the use of the propane can reduce the computational time to mere minutes.

### 5.2.5 Limitations

Based on the factors that would affect CO formation, the use of a propane fuel mechanism could result in an under-prediction in CO concentrations. This result is due to the high temperatures associated with propane combustion compared to the combustion of jet fuel. The higher temperatures of combustion will promote the oxidation of CO molecules resulting in an under-prediction of CO.

Another limitation of using chemical kinetics to determine CO emissions is that chemical kinetics only documents the evolution of gaseous phase chemical species. Although the use of chemical kinetics will be able to replicate the results of combustion between a gaseous fuel and air, the fuel first enters the combustor as a liquid. As a result, a second model working in conjunction with the Cantera software was developed to account for liquid fuel evaporation and droplet size.

### 5.3 Liquid Droplet Model

The third aspect of the proposed model that will be focused on is the use of liquid fuels. As discussed in previous sections, the use of evaporation physics is imperative to
determining proper CO emission trends. Furthermore, as chemical kinetic calculations only include gaseous species, a separate model is needed to account for liquid fuel physics. For the liquid droplet model, a similar approach was used in past industrial models with the addition of mean droplet size calculations [18].

5.3.1 Mean Droplet Size

Unlike any previous model, before any chemical kinetic calculations are performed, the mean droplet size of liquid fuel entering the combustor must be determined. As discussed in Section 3.3.1, there have been many mean droplet size correlations that have been developed based on the type and geometry of the atomizer used. To determine which correlation performs the best based on the conditions set by each engine, a test was performed.

Engine B

In Engine B a duplex based pressure atomizer was used to break up fuel as it enters the combustion chamber. As a result, the mean droplet size was calculated for each engine condition assuming a US flow number of 2.25. The resulting mean droplet sizes calculated using each correlation for Engine B can be seen in Figure 5.10.

Although the mean droplet sizes are not known for each of these conditions, it can be assumed that a reasonable estimation of the mean droplet size at idle conditions should be between 50 and 200 microns. The assumed range in mean droplet size was developed based on mean droplet sizes that would enable combustion while preventing flameout. With a calculated mean droplet size of 50 microns and below, the fuel evaporates almost instantaneously as it enters the combustor; thus having little affect on CO emissions. If the calculated mean droplet size is 200 microns or over, the liquid fuel may not be able to evaporate enough fuel to sustain combustion; resulting in flameout. A mean droplet
Figure 5.10: Mean droplet sizes calculated for all ICAO conditions using Engine B combustor inlet conditions

size ranging from 50 to 200 microns allows the model to operate for idle conditions while accounting for changes in mean droplet size. Furthermore, a correct correlation should reduce the mean droplet size for high power as the combustion efficiency improves. A lower mean droplet size would mean that the fuel is better atomized and will take less time to evaporate thus improving the efficiency of combustion. From the results, most of the correlations underestimate the mean droplet size of the fuel entering the combustion chamber. From the result seen in Figure 5.10, the correlation that provides the best estimate of mean droplet size for idle conditions while predicting a reduced mean droplet size for increasing thrust conditions is the Radcliffe correlation. Although the Jasuja and Lefebvre correlations conform to the assumed mean droplet size range, the correlations estimate the droplet size closer to the assumed minimum allowable droplet size. Consequently, the mean droplet size of liquid fuel entering the combustion chamber
will assume to have the same mean droplet size as calculated by the Radcliffe correlation.

**Engine C**

As discussed in Section 4.3, Engine B and Engine C were significantly similar including the use of pressure atomizers. To determine the mean droplet size entering the combustor chamber, pressure atomizer correlations were tested based on ICAO conditions for Engine C. Results of using various pressure atomizer correlations to calculate the mean droplet size for Engine C can be seen in Figure 5.11.

![Figure 5.11: Mean droplet sizes calculated for all ICAO conditions using Engine C combustor inlet conditions](image)

Using a similar methodology that was used to determine the ideal mean droplet size correlation for Engine B, the results show that the Radcliffe correlation is ideal for calculating mean droplet sizes for Engine C conditions. As a result, during the calculation process, the inlet conditions of the combustion chamber will assist in calculating the
mean droplet size of the fuel entering the combustion chamber for both Engine B and Engine C. Inlet fuel entering specific reactors will assume to have the same mean droplet size as calculated using the Radcliffe correlation.

**Engine D**

Unlike the previous cases, Engine D uses airblast atomizers. As a result a second analysis was performed to determine which correlation would best estimate the mean droplet size of liquid fuel entering the combustor. The results of using each correlation discussed in Section 3.3.1 can be seen in Table 5.4 assuming an orifice diameter of 2.75 mm.

<table>
<thead>
<tr>
<th>Condition (%)</th>
<th>Lefebvre &amp; Rink</th>
<th>Inamura &amp; Nagai</th>
<th>Elkotb</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>78.7</td>
<td>937.5</td>
<td>49.2</td>
</tr>
<tr>
<td>30</td>
<td>53.0</td>
<td>900.2</td>
<td>40.8</td>
</tr>
<tr>
<td>85</td>
<td>51.7</td>
<td>790.2</td>
<td>46.2</td>
</tr>
<tr>
<td>100</td>
<td>53.5</td>
<td>773.1</td>
<td>48.6</td>
</tr>
</tbody>
</table>

Table 5.4: Results of using airblast correlations to calculate mean droplet size for Engine D combustor

Similar assumptions were used to choose the mean droplet size correlation for the airblast atomizer as the pressure atomizer. From the results, the Lefebvre and Rink correlation captures the large droplet size produced from the low power conditions and the reduced mean droplet sizes at high power conditions. Unfortunately, the Inamura and Nagai correlation predicts a significantly large mean droplet size, where as the Elkotb correlation predicts a similar mean droplet size for all ICAO conditions. Similar to the pressure atomizer correlation, liquid fuel entering the combustor from the airblast atomizer will assume to have the same mean droplet size as calculated by the Lefebvre and Rink correlation.
5.3.2 Droplet Evaporation

Once the mean droplet size of liquid fuel entering the combustion chamber is determined using the correlations discussed in the previous section, the mean droplet size must be altered based on conditions within a given reactor. Depending on the time contained within a given reactor, the droplet will change its overall size. To calculate the rate of evaporation within a given reactor, the methodology discussed in Section 3.3.2 was used.

The $d^2$ law that was discussed assumes a perfectly spherical and uniform steady state evaporation. Along with the equations for rate of evaporation, the $d^2$ law, as seen in Equation (3.31), is able to take the rate of evaporation ($\lambda$) and determine a change in diameter of the droplet based on the time within a given reactor ($t$). Once the change in diameter of the droplet is calculated, the resulting amount of fuel that is assumed to be evaporated is entered into the reactor as un-combusted fuel. This process is captured using the expression

$$\dot{m}_{gas} = \dot{m}_{liquid} \left(1 - \frac{SMD_{out}^3}{SMD_{in}^3}\right).$$

Unlike past models which attempted to use a correlation to adjust the fuel within a given reactor such as the Rizk model, the new model assumes that the volume evaporated is equalled to the amount of fuel entering a reactor. The ratio of fuel evaporating is determined based on the change in volume from the droplet size entering ($SMD_{in}$) to the droplet size exiting the reactor ($SMD_{out}$). As a result, the amount of gaseous fuel ($\dot{m}_{gas}$) entering the reactor is a percentage of the liquid fuel entering the reactor ($\dot{m}_{liquid}$). To prevent any error within the calculation, limitations within the model were set to prevent the amount of gaseous fuel being less than zero or more than the amount of liquid fuel entering the combustion chamber. The methodology behind the model is illustrated in Figure 5.12.
Figure 5.12: Methodology behind evaporation model

In the combustor models, many different inputs can enter a given reactor depending on the assumed flow. Each reactor contains a set mean droplet size which corresponds to the average droplet size exiting a given reactor. In the case of multiple inputs containing different mean droplet sizes another innovation to the model was required.

As each input would have a corresponding mean droplet size for liquid fuel contained within the reactor, a weight average system was developed. The weighted average is based on the amount of fuel being added to the reactor ($\dot{m}_{\text{liquid},i}$) and corresponding mean droplet size ($SMD_i$) from the total amount of inputs. The mean droplet size weighted average is therefore written as

$$SMD_{in} = \frac{SMD_{out,i}\dot{m}_{\text{liquid},i} + SMD_{out,i+1}\dot{m}_{\text{liquid},i+1} + \ldots + SMD_{out,n}\dot{m}_{\text{liquid},n}}{\dot{m}_{\text{liquid},i} + \dot{m}_{\text{liquid},i+1} + \ldots + \dot{m}_{\text{liquid},n}},$$

where $n$ is the total number of inputs. The result of using this model is that the mean droplet size and amount of fuel still in liquid form must be tracked throughout the combustion chamber. To reduce the amount of calculations and possible convergence problems, the model allows the user to choose which reactors use the evaporation model and which assume the fuel has been completely evaporated. In the reactor models developed for this thesis, it was assumed that once the flow reached the recirculation reactors and intermediate zone, the liquid fuel was assumed to be fully evaporated. As little com-
bustion occurs downstream of the primary zone, the chemical kinetic mechanism should keep the assumed evaporated fuel as unburned fuel within the kinetic mechanism.

5.3.3 Methodology Limitations

Although the evaporation model is able to capture evaporation based on generalized physics, the model is limited to calculating a single droplet size for the entire contents of fuel. In all combustion chambers, the size of fuel droplets at any given position is represented by a distribution of varies droplet sizes. As a result, the assumed amount of evaporated fuel could be different depending on the distribution of droplets throughout the combustion chamber.

5.4 Summary of Newly Proposed Model

In summary, the new proposed model focuses on three key characteristics, the complex internal combustor flow field, combustion chemistry and liquid fuel evaporation. Each model was developed based on past methodologies to further the progress of the methods and to capture both the chemistry and physics of CO production within a gas turbine combustion chamber.

The internal combustor flow field is captured using a similar reactor network development methodology as the Laval model, which uses cold flow CFD to make assumptions about the reactor network configuration and flow splits between reactors [13]. A new aspect of the model however is developing a tangential reactor to track material in between fuel nozzles. Used in all reactor network based models, the combustion chemistry is captured through the use of chemical mechanisms within a network of PSR and PFR reactors to track the concentration of CO throughout the combustion chamber. Similar to the Rizk model, a propane mechanism is used to simplify the calculation process and reduce
the computational time [23]. The evaporation model was developed with correlations
developed to determine mean droplet sizes and evaporation principles to determine the
amount of fuel evaporating in each reactor. An innovative method was developed to cal-
culate the amount of fuel evaporating in a given reactor and a tracking system to follow
the mean droplet size as fuel travels through the combustion chamber.

With a new methodology, the next step is to test the methodology against known data.
In future chapters the methodology will be validated against test cases discussed in Chap-
ter [4]. Furthermore, results from the new proposed model will be compared against past
methods to determine the best method for predicting CO emissions.
Chapter 6

Engine A Combustor Analysis

Using the Engine A combustor discussed in Section 4.1, an analysis was performed on CO emissions using both global and local approaches. In this chapter, the global correlation results will be compared to data collected for Jet-A1 fuel. For the local approach, the purpose of using the can combustor is to prove that a reactor based methodology could accurately predict CO emissions using chemical kinetic based calculations. As a result an analysis was performed on the can combustor using a reactor based methodology and data for gaseous methane fuel.

6.1 Global Approach

The first methodology that was analysed to determine CO emissions from Engine A was the global correlations. The correlations used in this analysis include:

- Mellor
- Lefebvre
- Rizk

For each correlation, two different calculations were performed. The first calculation was done assuming perfect atomization within the primary zone. The second calculation was performed using a simple evaporation model to alter the amount of fuel being
burned in the primary zone. From comparing the results of these calculations, the affect of evaporation on CO emissions in each correlation can be revealed. In addition to calculating the CO emissions with and without atomization, the assumed temperatures within the primary zone of the can combustor was determined assuming equilibrium and non-equilibrium conditions. To calculate the equilibrium temperature of the gas within the primary zone of the combustion chamber, a program known as NASA GUI was used. By inserting the inlet conditions, properties of fuel and air and the localized equivalence ratio, NASA GUI calculates the equilibrium temperature within the primary zone of the combustion chamber. The equilibrium temperature represents the maximum temperature possible for the equivalence ratio given. To calculate the non-equilibrium temperature, a reactor was defined by the volume of the primary zone and chemical kinetics was used to estimate the completeness of the combustion process.

6.1.1 Mellor Correlation

Although the Mellor correlation does not have any direct variables that account for the affect of atomization, unlike the Rizk and Lefebvre correlations; however, the temperature within the primary zone could be affected by atomization. As atomization regulates the amount of fuel being burned within the combustion chamber, the equivalence ratio and temperature will change accordingly. The results of using the Mellor correlation to
calculate the CO emissions for liquid Jet-A1 at all ICAO conditions can be seen in Table 6.1.

<table>
<thead>
<tr>
<th>Engine Condition (%)</th>
<th>Measured</th>
<th>Equilibrium</th>
<th>Equilibrium + Atomization</th>
<th>Non-Ideal</th>
<th>Non-Ideal + Atomization</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>100.00</td>
<td>50.21</td>
<td>50.21</td>
<td>48.68</td>
<td>50.21</td>
</tr>
<tr>
<td>30</td>
<td>33.29</td>
<td>30.51</td>
<td>30.51</td>
<td>29.40</td>
<td>30.51</td>
</tr>
<tr>
<td>60</td>
<td>20.11</td>
<td>31.62</td>
<td>31.62</td>
<td>30.65</td>
<td>31.62</td>
</tr>
<tr>
<td>90</td>
<td>8.04</td>
<td>31.90</td>
<td>31.90</td>
<td>31.21</td>
<td>31.90</td>
</tr>
<tr>
<td>100</td>
<td>2.91</td>
<td>31.35</td>
<td>31.35</td>
<td>30.93</td>
<td>31.35</td>
</tr>
</tbody>
</table>

Table 6.1: Comparison between Mellor correlation and emissions data for Jet-A1 at all ICAO conditions

Although the Mellor correlation performed well at predicting emissions at 30% thrust condition, the Mellor correlation does not produce a large enough range in predicted CO emissions for the remaining conditions. In addition, the lack of atomization characteristics prevents the correlation from predicting higher emissions at idle conditions. The small range of values produced by the Mellor correlation can be associated with the method which the correlation was developed. Since the experimental data that was used to develop the correlation was a simple set up, the coefficients may not be tuned to predict CO emissions for the complexities of a can combustor.

### 6.1.2 Lefebvre Correlation

The same inputs used to calculate CO emissions for the Mellor correlation were applied to the Lefebvre correlation. The calculated CO emissions using the Lefebvre correlation
for a can combustor burning Jet-A1 fuel for all ICAO conditions can be seen in Table 6.2.

<table>
<thead>
<tr>
<th>Engine Condition (%)</th>
<th>EICO/EICO at 7% Thrust Condition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Measured</td>
</tr>
<tr>
<td>7</td>
<td>100.00</td>
</tr>
<tr>
<td>30</td>
<td>33.29</td>
</tr>
<tr>
<td>60</td>
<td>20.11</td>
</tr>
<tr>
<td>90</td>
<td>8.04</td>
</tr>
<tr>
<td>100</td>
<td>2.91</td>
</tr>
</tbody>
</table>

Table 6.2: Comparison between Lefebvre correlation and emissions data for Jet-A1 at all ICAO conditions

From the results, the correlation was able to accurately predict the exponential decay of CO emissions with the increase in thrust conditions. In addition, with atomization characteristics, the Lefebvre correlation increases the estimated CO emissions based on the use of atomization. Unfortunately, the correlation significantly over-predicts for all ICAO conditions. This error can once again be associated with the combustors used to develop the correlation. From Section 3.1.2 it was determine that the Lefebvre correlation was developed using emissions data from annular based combustors. The smaller area and different configuration could result in a over-prediction of CO emissions.

### 6.1.3 Rizk Correlation

Since the Rizk correlation was developed using a similar methodology to the Lefebvre correlation it can be assumed that the Rizk correlation may produce similar trends. The
calculated CO emissions using the Rizk correlation for a can combustor burning Jet-A1 fuel at all ICAO conditions can be seen in Table 6.3.

<table>
<thead>
<tr>
<th>Engine Condition (%)</th>
<th>EICO/EICO at 7% Thrust Condition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Measured</td>
</tr>
<tr>
<td>7</td>
<td>100.00</td>
</tr>
<tr>
<td>30</td>
<td>33.29</td>
</tr>
<tr>
<td>60</td>
<td>20.11</td>
</tr>
<tr>
<td>90</td>
<td>8.04</td>
</tr>
<tr>
<td>100</td>
<td>2.91</td>
</tr>
</tbody>
</table>

Table 6.3: Comparison between Rizk correlation and emissions data for Jet-A1 at all ICAO conditions

As predicted, the results of using the Rizk correlation are similar to that of the Lefebvre correlation. The Rizk correlation was accurately able to predict the exponential decaying emissions as a result of increasing thrust levels as well as an increase in CO emissions with the use of atomization. Unfortunately, like the Lefebvre correlation, the Rizk correlation over-predicts CO emissions at low level thrust conditions but works well at predicting CO emissions at high power conditions. These results suggest that the Rizk correlation performed better at predicting the dissociation of CO at high power conditions than the other global correlations. The error produced at low power conditions is a result of the experimental data used to develop the correlation. Since the correlation was developed using annular based combustors, the Rizk correlation, like the Lefebvre correlation could produce inaccurate values based on the assumed coefficients in the equation.
6.2 Local Approach

Unlike the global correlations which require simple inputs associated within the primary zone, the local approaches require reactor networks to apply chemical kinetics. The purpose of applying a localized approach to the Engine A combustor is to prove that using a reactor network along with chemical kinetics can accurately predict CO emissions. For this analysis, a can combustor model was developed to predict CO emissions from the combustion of gaseous methane fuel. As a result, each reactor model uses the GRI30 chemical kinetic mechanism to predicted the detailed combustion of methane gas. As detailed in the proposed model, the mechanism is applied to each reactor to determine the CO concentration throughout the combustor.

The first step in the analysis is to develop a reactor network for the can combustor. The reactor network was developed by first gaining an understanding of the internal flow field. A cold flow CFD of Engine A was developed by Pandey at the Indian Institute of Technology, seen in Figure 6.2, was observed to gain a better understanding of the flow.

![Figure 6.2: Cold flow CFD for the top half of the Engine A combustor][21]

From the cold flow CFD, the first assumption about the internal flow field is that the symmetrical flow pattern produced by the double toroidal flow generates the same conditions in the top half and bottom half of the combustor. As a result, the reactor network will be developed based on the top half of the combustor and applied to the entire primary zone volume. The reactor network analysis started with a simplistic model and develop
into a more complex model based on the predicted emissions. The simplistic reactor network contained three reactors, one representing the primary zone, intermediate zone and dilution zone; the reactor definition can be seen in Figure 6.3.

Figure 6.3: Simple Engine A combustor reactor network based on cold flow CFD [21]

The simple reactor network included a PSR within the primary zone of the combustor and plug flow reactors representing the intermediate and dilution zones. Assumptions on inlet air within each reactor was based on the percentage inlet air determined from

Figure 6.4: Comparison between actual and predicted CO emission levels using the simple Engine A combustor reactor network
the original analysis \[29\]. From the known data, the predicted CO emissions from the combustion of gaseous methane fuel were compared to the measured values.

From the results seen in Figure 6.4 the simple network configuration was able to predict the proper trends of CO emissions as the engine thrust condition increased. However, the model over-predicts CO emissions for idle thrust conditions. It was determined that the reactor configuration was too simple and that the average conditions over the entire primary zone were too simplified. As a result, the reactor network was altered to include reactors near the wall of the combustion chamber as well as the center of the combustion chamber. The complex reactor configuration can be seen in Figure 6.5.

Figure 6.5: Complex Engine A combustor reactor network developed based on cold flow CFD \[21\]

Inlet air entering each reactor model was assumed based on their position and trajectory provided by the cold flow CFD. The complex model was developed based on the reactor configuration developed for the localized Rizk model discussed in Section 3.2.1. The fuel/air mixtures trajectory are defined by percentage flows leaving a from reactor to reactor and is assumed based on the cold flow CFD.

The predicted CO emissions using the complex network configuration can be seen in Figure 6.6. Using a more complex reactor network produces a much more accurate
Figure 6.6: Comparison between actual and predicted CO emission levels using the complex Engine A combustor reactor network representation of CO emissions produced from the combustion of gaseous methane fuel within the can combustor. Through developing a model that is able to give a more accurate representation of the localized equivalence ratios within the can combustor, the predicted CO emissions have become accurate within 15% error for all thrust conditions. In addition, the average time taken to calculate each condition takes 237 seconds, well within a single day. Consequently, by accurately predicting CO emissions within 15% error using a simplified approach has proven that the use of reactors coupled with chemical kinetics can accurately predict CO emissions for all ICAO conditions.

6.3 Summary of Engine A Combustor Analysis

From the analysis done on the global correlations, each method was able to accurate replicate the trends of reduced CO emissions with increase thrust conditions. Each cor-
relation was not able to predict within 15% at lower power conditions. The Mellor correlation under-predicted the amount of CO produced at lower power conditions while the Lefebvre and Rizk correlation both over-predicted CO emissions. The error in the Mellor correlation was determined to be a result of the apparatus used to develop the correlation. Error from the Lefebvre and Rizk model was determined to be a result of the experimental data used to develop the coefficients within each equation. As the data used to develop the coefficients was based on annular combustors, the correlations could not predict CO emissions within 15% error from the combustion of Jet-A1 fuel at ICAO conditions.

Since the Engine A combustor contained validation data using gaseous methane fuel, the can combustor was used to prove that PSR and PFR reactors coupled with chemical kinetics can accurately predict CO emissions for a combustion chamber. After two iterations, a reactor network containing near wall and centralized reactors was able to predict CO emissions to within 15% error for all ICAO conditions. Using the GRI30 chemical kinetic mechanism to follow the evolution of methane gas combustion the localized equivalence ratios allowed the can combustor model to predict CO emissions. As a result, the model was able to prove that PSR and PFR reactors coupled with chemical kinetics can accurately predict CO emissions.
Chapter 7

Engine B Combustor Analysis

After completing the analysis for Engine A, a can combustor, the focus of the project shifted to determining CO emissions for an annular type combustor. Unlike the Engine A combustor, which has a defined uniform primary zone, Engine B contains a single interconnected, concentric combustion chamber with multiple nozzles and zones in which the fuel may not reach. For the global correlations, this represents the overall primary zone geometry used to analyse CO emissions. For the local approaches, the combustor

Figure 7.1: Cold flow CFD of Engine B combustor, produced by the project industrial partner within the plane of the nozzle
will be divided into reactors in both the cross sectional and tangential directions. Dividing the combustor will be performed with the use of cold flow CFD provided by the project industrial partner; The cold flow CFD in the plane of the nozzle can be seen in Figure 7.1. From the cold flow CFD, the Engine B combustor contains a single toroid within the primary zone. As flow recirculates within the primary zone, fuel/air travelling to the intermediate zone expands from the inner diameter of the engine to the outer diameter. The fuel/air mixture is then quenched by the dilution jets and continues downstream of the combustor.

7.1 Global Approach

For the global correlation analysis, the primary zone of the combustor was defined by the highlighted area seen in Figure 7.2. To determine the conditions within the primary zone of the combustion chamber a non-equilibrium based approach was performed using the Cantera software and the GRI30 mechanism. Furthermore each correlation was analysed using atomization calculations as discussed in Section 5.3.1.

![Diagram of Nozzle Plane](image)

Figure 7.2: Assumed primary zone for global correlation analysis

The resulting emissions calculated using the Mellor, Lefebvre and Rizk correlations for
the Engine B combustor can be seen in Figure 7.3. From the measured results, each of the
global correlations under-predicts the CO emissions produced at most ICAO conditions.
The Mellor correlation revealed similar results as the can combustor, showing a small
range of CO emissions calculated for a wide variety of thrust conditions. The Lefebvre
correlation performs the best out of the three global correlations, however still produces
a 50% error at idle conditions. Similar trends were produced by the Lefebvre and Rizk
correlations for Engine B and Engine A combustors, which is accurate to how CO is
produced over different thrust conditions.

![Figure 7.3: CO emissions predicted for Engine B using global correlations for all ICAO conditions](image)

7.2 Local Approach

For the local approach, two different models were analysed. The first model that will
be looked at is the MIT model described in Section 3.2.2. The MIT model was chosen
because it is designed to work for annular combustors and it was not designed to be
Chapter 7. Engine B Combustor Analysis

The second will be the proposed model that was discussed in Chapter 5. Using the cold flow CFD, a similar approach used for the Engine A combustor will be used to develop the reactor network for the Engine B combustor.

7.2.1 MIT Model

As discussed, the MIT model produces a normalized distribution of equivalence ratios within PSR’s throughout the primary zone of a combustor. After leaving the primary zone, the contents of the reactors are transferred to intermediate and dilution zone PFR’s. For the initial analysis, 10 reactors were used within the primary zone of the Engine B combustor. The contents of the primary zone reactors is then transfer to 3 PFR’s representing the intermediate and dilution zones. The reactor configuration based on the combustor geometry and cold flow can be seen in Figure 7.4.

Figure 7.4: Engine B combustor reactor network configuration based on MIT methodology

An analysis was performed by varying the unmixedness parameter between 0.0 and 0.3. The upper limit was chosen to be 0.3 because in developing the normalized distribution of equivalence ratios, an unmixedness parameter above 0.3 will produced negative equiv-
alence ratios due to an increase in standard deviation. The range of equivalence ratios within the primary zone, relative to the mean equivalence ratios at each unmixedness parameter can be seen in Table 7.1. From Table 7.1, the range of equivalence ratios increase as the unmixedness parameter increases. A similar trend is calculated at all thrust conditions.

<table>
<thead>
<tr>
<th>Unmixedness Parameter</th>
<th>Lower Level Deviation ($\phi / \bar{\phi}$)</th>
<th>Upper Level Deviation ($\phi / \bar{\phi}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.865</td>
<td>1.135</td>
</tr>
<tr>
<td>0.10</td>
<td>0.730</td>
<td>1.266</td>
</tr>
<tr>
<td>0.15</td>
<td>0.595</td>
<td>1.405</td>
</tr>
<tr>
<td>0.20</td>
<td>0.460</td>
<td>1.540</td>
</tr>
<tr>
<td>0.25</td>
<td>0.325</td>
<td>1.676</td>
</tr>
<tr>
<td>0.30</td>
<td>0.189</td>
<td>1.806</td>
</tr>
</tbody>
</table>

Table 7.1: Range of primary zone equivalence ratio deviations from the primary zone mean equivalence ratio for Engine B using different unmixedness parameters at 7% thrust conditions

The CO predicted at each unmixedness parameter can be seen in Figure 7.5. From the results, as the unmixed parameter increases, the amount of CO predicted increases as well. The reason for this result is that with a higher unmixed parameter you will have more reactors at very lean and very rich equivalence ratios producing more CO emissions from incomplete combustion. In addition, the results show an accurate trend of CO emissions as thrust increases. Unfortunately, the overall CO is under-predicting compared to the measured values. The time taken to calculate each condition on average took approximately 40 seconds.
Figure 7.5: CO emission index using MIT model for varying unmixedness parameters

Figure 7.6: CO emission index varying the number of reactors for an unmixedness parameter of 0.3 at 7% thrust conditions
A parameter that could affect the resulting CO emissions is the number of reactors within the primary zone. As a result, an analysis was performed to determine if there is any variation in predicted CO emissions depending on the amount of reactors used. For this analysis, an unmixedness parameter of 0.3 was used as it predicts the highest concentration of CO. The results of varying the number of reactors within the primary zone using an unmixedness parameter of 0.3 can be seen in Figure 7.6. The results show that there is little variation in the predicted CO emissions by increasing the number of primary zone reactors.

Through varying the unmixedness parameter and the number of reactors within the primary zone, the overall conclusion with using the MIT model to predict CO emissions for Engine B is similar to the global correlations. The MIT model is able to follow the correct trends of decreasing CO emissions with increasing thrust conditions. Unfortunately, the CO emissions under-predict for all variations of unmixedness parameters and reactor network configurations.

7.2.2 Proposed Model

Another localized approach that was used to determine CO emissions is the proposed model. Unlike the MIT model, the proposed model is defined by the flow not only in the primary zone but also in the intermediate and dilution zones. Using the cold flow CFD supplied by the product industrial partner and the methodology discussed in Section 5.1, the cross sectional reactors were defined as seen in Figure 7.7.

The reactor network uses four reactors within the primary zone to replicate the recirculation zone produced by the single toroid. Furthermore, four reactors were used near the walls of the primary zone to capture CO produced from wall quenching. For the intermediate zone, a single reactor was used to transition the combusted flow from the
Chapter 7. Engine B Combustor Analysis

Figure 7.7: Cross sectional reactor network configuration for Engine B combustor based on cold flow CFD supplied by the project industrial partner.

In addition to having a cross sectional reactor network, an analysis was performed using an assumed fuel trajectory to determine if reactors within the tangential direction are required. The assumed fuel trajectory produced a conical spray with a diameter that was equal to the height of the combustor. After determining the circumferential distance between two adjacent nozzles, the lengths were compared to determine the distance between two adjacent fuel sprays. With a fuel spray diameter of 68 mm and a distance between nozzles of 113 mm, a set of tangential reactors was developed with the same cross sectional reactor network configuration developed in Figure 7.7.

With the reactor network developed, the flow splits were assumed based on the cold flow CFD. After optimizing the flow parameters, the CO emissions predicted for all ICAO
conditions using the above reactor model, chemical kinetics and an evaporation model can be seen in Figure 7.8. The model was able to predict within 20% error for both idle and 30% thrust conditions. Although the model over-predicted for 85% and 100% thrust conditions, the overall trend of decreasing CO emissions with an increase in thrust is accurate. An over-prediction of CO emissions at high power conditions could be the result of low wall temperatures from the optimized flow splits. The average time taken to calculate the CO emissions using the proposed model was approximately 641 seconds. Compared to the MIT model, the proposed model took 16 times longer to calculate due to its increased complexity.

Since the analysis of the Engine B combustor includes liquid fuel, the use of the droplet model that was discussed in Section 5.3 was applied to the reactor network. As a result, an additional test was performed on the proposed model by changing the mean droplet size entering the combustion chamber. Keeping the same flow splits and inlet conditions,
the mean droplet size entering the combustor was increased from 30 microns to 150 microns to see how it affected the overall predicted CO emissions at 7% thrust condition; the results for the mean droplet test can be seen in Figure 7.9. From the graph, the overall CO emissions exponentially increases until the mean droplet size is too large and combustion is no longer possible. The results of this test show that the model is able to capture the affects of mean droplet size and possibly account for flameout as a result of large droplet sizes.

7.3 Summary of Engine B Combustor Analysis

After using global and local approaches to predict CO emissions for Engine B there are many conclusions that can be made. Similar to the results developed for Engine A the Mellor correlation showed a narrow range of CO emissions and issues predicting CO emissions at all ICAO conditions. The Lefebvre correlation performed the best out of all of
the global correlations, however, it under-predicted the amount of CO being produced in
Engine B at all ICAO conditions. Similar results were seen in using the Rizk correlation
which also unpredicted CO emissions for Engine B.

The local approaches showed more promise when predicting CO emissions. Like the
global correlations, the MIT model under-predicted emissions for all Engine B combus-
tor conditions. Overall the proposed model performed the best predicting within 20%
error for both 7% and 30% thrust conditions. In addition, the evaporation model used in
the proposed model was able to predict trends resulting from alteration in mean droplet
size. With a initial analysis performed on a single toroidal annular combustor, the next
step will be to predict CO emissions for a different flow field.
Chapter 8

Engine C Combustor Analysis

The next combustor analysed for this thesis is the combustor from Engine C. The Engine C combustor is similar to the Engine B combustor as it contains the same geometry. The difference between the two combustors is the internal flow field. The Engine B combustor contains a single toroid flow field within the primary zone where as the primary zone of the Engine C combustor contains a double toroid as seen in Figure 4.3. Unfortunately, no cold flow CFD was supplied for the Engine C combustor. As a result, the cross sectional flow field was assumed to be similar to that of the Engine A combustor seen in Section 6.2. Furthermore, no reference information on the measured CO emissions resulting from each ICAO cycle condition was found. The results from each analysis will be compared to the emissions calculated in the analysis of the Engine B combustor. Accurate results for the Engine C combustor analysis of CO emissions will show a decrease in CO compared to that of the Engine B combustor. A reduction in CO emissions occurs within a double toroidal combustor because more fuel/air mixture is able to recirculate back into the primary zone reducing the amount of unburned hydrocarbon and reducing the amount of CO emissions. Both global and localized approaches will be analysed to determine if each approach can account for changes in the internal flow field of the combustion chamber.
8.1 Global Approach

In the global approach, the Mellor, Lefebvre and Rizk correlation were tested assuming atomization and non-equilibrium conditions. The primary zone was assumed to occupy a similar volume as the Engine B combustor. The results of using the global correlations on the double toroidal flow field can be seen in Table 8.1.

<table>
<thead>
<tr>
<th>Thrust Condition (%)</th>
<th>EICO/EICO predicted for Engine B at 7% Thrust Condition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mellor</td>
</tr>
<tr>
<td>Engine B</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>100.00</td>
</tr>
<tr>
<td>30</td>
<td>108.21</td>
</tr>
<tr>
<td>85</td>
<td>96.43</td>
</tr>
<tr>
<td>100</td>
<td>96.76</td>
</tr>
</tbody>
</table>

Table 8.1: Comparison between predict CO emissions for Engine B and Engine C using global correlations

From the results, there is little difference between the CO emissions predicted from Engine B to Engine C. Comparing the results of Engine B and Engine C show that the CO emissions increase for all ICAO conditions. The conclusion from these results is that global based correlations cannot account for changes in combustion chamber flow fields.

8.2 Local Approach

For the local approach, both the MIT model and proposed model were used to predict CO emissions for the double toroidal combustor. The reactor network development from each model was applied to the Engine C combustor using a similar method to the Engine B combustor.
8.2.1 MIT Model

Figure 8.1: Engine C combustor reactor network configuration using the MIT methodology

To predict CO emissions using the MIT model, the development of a reactor network was similar to that used for the Engine B combustor analysis. As stated by Allaire, the MIT model uses a similar unmixedness parameter for combustors with similar geometries. Consequently, the unmixedness parameter used to predict CO emissions for the double toroidal reactor model was set to 0.3. In addition, 10 reactors were used in the primary zone as there was little difference in CO emissions predicted in varying the number of reactors. The overall combustor model can be seen in Figure 8.1.

The results from using the MIT model to predict CO emissions can be seen in Table 8.2. A comparison between the CO predicted for the single toroid in the Engine B combustor and double toroid in the Engine C combustor show that the MIT model predicts that the CO emissions of a double toroidal flow field will be less than that of the single at all ICAO conditions. In addition, the average time taken to complete a single condition was the same for both Engines at approximately 40 sec. Consequently, this proves the MIT model is able to predict alterations in flow fields.
Table 8.2: Comparison between predict CO emissions for Engine B and Engine C using MIT Model

8.2.2 Proposed Model

In predicting CO emissions with the proposed model, a new reactor network was developed to account for the change in flow within the primary zone and throughout the combustor. The development of the reactor network was performed by Hasnain Lanewala to originally predict NO$_x$ emissions. The cross sectional reactor network that was used to capture the double toroidal flow field can be seen in Figure 8.2. The primary zone consisted of 3 PSR reactors, 2 of which representing the recirculation zones. The contents of these reactors were transferred to 8 PFR’s within the intermediate zone, four of which were used to predict near wall conditions. Contents of the intermediate zone reactors were then transferred downstream to 5 PFR’s representing the dilution zone.
Chapter 8. Engine C Combustor Analysis

Table 8.3: Comparison between predict CO emissions for Engine B and Engine C using proposed model

<table>
<thead>
<tr>
<th>Thrust Condition (%)</th>
<th>EICO/EICO predicted for Engine B at 7% Thrust Condition (%)</th>
<th>Engine C</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>100.00</td>
<td>54.54</td>
</tr>
<tr>
<td>30</td>
<td>30.22</td>
<td>19.07</td>
</tr>
<tr>
<td>85</td>
<td>5.32</td>
<td>0.27</td>
</tr>
<tr>
<td>100</td>
<td>7.04</td>
<td>0.39</td>
</tr>
</tbody>
</table>

Since the geometry of the Engine B and Engine C combustor were similar, the amount of nozzles and distance between adjacent nozzles was assumed to be the same. As a result, Hasnain created tangential reactors for the primary zone but combined the intermediate and dilution zone reactors to create a single reactor between both the plane of the nozzle and volume between adjacent nozzles. The results of using the reactor network to predict CO emissions for the double toroidal can be seen in Table 8.3.

From the results, the overall CO emissions predicted for Engine C were lower than the CO emissions predicted for Engine B at all ICAO conditions. Furthermore, the average time taken to calculate the CO emissions using the reactor network was approximately 308 seconds. Consequently, this shows that the proposed model is able to accurately predict varying flow fields within a similar combustor by altering the reactor network configuration.

8.3 Summary of Engine C Combustor Analysis

The objective for the analysis of the Engine C combustor was to determine if the approaches can account for changes in the internal flow field of the combustor. Calculated
CO emissions were compared to predicted emissions for Engine B. With a similar geometry, the results of the single toroidal flow field in the Engine B combustor should predict higher CO than the double toroidal flow field in the Engine C combustor. Unfortunately, the global correlation predictions for Engine C increased compared to the results of Engine B, showing that the global approach cannot account for changes in internal flow fields. The local approaches however performed well in predicting reduced CO emissions for all ICAO conditions. With an analysis performed on a simple annular combustor, the next step is to see how well each approach performs at predicting emissions for a more modern annular combustion chamber.
Chapter 9

Engine D Combustor Analysis

The final combustor analysed in this thesis is the complex geometry of the Engine D combustor. For the analysis of the Engine D combustor, both global and local approaches were applied to the combustor in a similar process as done for the Engine B combustor in Chapter 7. A similar application was used for the analysis of the Engine D combustor due to the comparable flow field. From Figure 9.1, the cold flow CFD reveals a single toroidal flow field with a small intermediate zone; this figure was provided by the project industrial partner within the plane of the nozzle.

Figure 9.1: Cold flow CFD of Engine D combustor produced by the project industrial partner within the plane of the nozzle
industrial partner. Although there is a small intermediate zone, the cold flow reveals that the contents within the intermediate zone recirculates back into the primary zone. Contents at the inter diameter of the intermediate zone are passed to the dilution zone, however, contents at the outer diameter predominately recirculate back into the primary zone. Using this knowledge to define the different zones within the Engine D combustor, both global and local approaches can be applied.

9.1 Global Approach

Once again the Mellor, Lefebvre and Rizk correlations were applied to the Engine D combustor to determine CO emissions. The first step in calculating the CO emissions using the global correlations is to define the primary zone of the combustion chamber. From the cold flow CFD and with an assumed trajectory of the fuel spray the defined volume of the primary zone can be seen in Figure 9.2.

Using the defined primary zone of the combustion chamber, each correlation was first used to predict CO emissions at Engine D combustor ICAO conditions. From the results of using these correlations on the Engine B combustor in Section 7.1 the Mellor corre-

![Figure 9.2: Assumed primary zone for global correlation analysis](image)

...
lation should produce a small range of predicted emissions over the entire cycle while the Lefebvre and Rizk correlations should under-predict at all conditions. The resulting emissions calculated using each correlation for Engine D over all ICAO conditions can be seen in Figure 9.3.

![Figure 9.3: CO emissions predicted for Engine D using global correlations for all ICAO conditions](image)

From these results, the Mellor correlation performed as predicted while the Lefebvre and Rizk correlation over-predicted at 7% thrust conditions. The over-prediction of CO at idle conditions could be a result of the complex combustor geometry. Although there has been a similar trend in results for each correlation, the only conditions that have been analysed were the ICAO conditions. To better develop an understanding of the trends produced from using each correlation, a parametric study was performed using 32 different conditions with varying inlet parameters. The results of using each correlation for all the 32 parametric studies can be seen in Figure 9.4. Results from the parametric studies show consistency in the predicted trends of each correlation.
Figure 9.4: CO emissions predicted for Engine D using global correlations for all parametric conditions

9.2 Local Approach

Once the analysis was completed for the global approaches, the local approaches were compared to emissions data for Engine D. Before any calculations were performed the reactor network was required for both approaches. Both the MIT model and proposed model were used to predict emissions for different thrust conditions.

9.2.1 MIT Model

For the Engine D combustor a similar reactor network to the Engine B and C combustor was used. The primary zone of the combustion chamber was once again divided into 10 PSR’s, which then passed through 4 PFR’s representing the intermediate and dilution zone reactors. The reactor network configuration can be seen in Figure 9.5.

Similar to the global correlations, the MIT model was first compared to ICAO conditions for the Engine D combustor. Since the combustor geometry is different from the Engine
Figure 9.5: Reactor network configuration for the Engine D combustor using the MIT methodology

B combustor, Engine D emissions data was compared to the MIT model results while varying the unmixedness parameter between 0 and 0.3. The results for this analysis can be seen in Figure 9.6.

Figure 9.6: CO emissions predicted for the modern annular combustor using the MIT model for all ICAO conditions
From the results for the ICAO conditions, the MIT model predicted similar results as the analysis for the Engine B combustor. The MIT model under-predicted the CO emissions for all ICAO conditions over all unmixedness parameters. Furthermore, the average time taken to complete a single CO calculation using a single processor was approximately 133 seconds.

9.2.2 Proposed Model

The final analysis of the Engine D combustor was performed using the proposed model. Using the methodology described in Section 5.1, a reactor network was developed for the Engine D combustor. The reactor network consisted of 4 primary zone reactors, a single intermediate zone reactor, 3 dilution zone reactors and 10 near wall reactors distributed among the different zones. The overall reactor network configuration can be seen in Figure 9.7.

![Figure 9.7: Engine D combustor cross sectional reactor network configuration using proposed model methodology](image)

Using the assumed trajectory for the 24 fuel nozzles within the Engine D combustor, the distance between two adjacent nozzles was compared to the assumed diameter of the fuel spray. With a diameter of 43 mm and the distance between adjacent nozzles at 47 mm,
the area between adjacent nozzle trajectories is negligible. As a result, there is no need
for reactors within both the plane of the nozzle and the space between adjacent nozzles.

![Figure 9.8: CO emissions predicted for Engine D using the proposed model for all ICAO conditions](image)

Using only the reactor network developed in the plane of the nozzle, the predicted CO
emissions were compared to the ICAO conditions; the results of using the the reactor
network can be seen in Figure 9.8. The results show that the proposed model predicts
within 20% error for both 7% and 30% thrust conditions. Furthermore, the model under-
predicts high power thrust conditions.

To further test the capabilities of the model, additional tests were performed on alter-
ations to mean droplet size, near wall flow and fuel spray trajectory. The first test
involved altering the mean droplet size while keeping all other flow parameters and inlet
conditions constant. Varying the mean droplet size from 40 microns to 140 microns for
the 7% ICAO thrust condition produced the graph seen in Figure 9.9.
Figure 9.9: CO emissions predicted for Engine D by varying mean droplet size at 7% thrust conditions

Figure 9.10: CO emissions predicted for Engine D for parametric conditions
The final test performed using the proposed model was a parametric study using 32 different combustor configurations with varying inlet conditions. The results of using the reactor network seen in Figure 9.7 to calculate CO emissions for all 32 conditions can be seen in Figure 9.10. Results from the analysis show a under-prediction in CO emissions for all conditions. Since some of these conditions were performed simulating high altitude conditions, the mean droplet size of the liquid fuel entering the combustor could be under-predicted accounting for the reduction in emissions. Furthermore, the humidity for the parametric study was not given. An increase in humidity could reduce the temperature of combustion and increase CO emissions.

9.3 Summary of Engine D Combustor Analysis

The analysis of the Engine D combustor tested each methodologies predictive capability against a modern combustor with a complex geometry. Similar to the results developed for the previous test cases, the Mellor correlation showed a narrow range of CO emissions. In addition, the Lefebvre and Rizk correlations continued to predict exponential declining CO emissions with increasing thrust conditions. The Lefebvre correlation however, over-predicts for low level thrust conditions, while the Rizk correlation over-predicts for idle conditions while under predicting for all other ICAO conditions. Similar results were determined for all parametric conditions.

The local approaches showed similar results to past test cases. The MIT model continued to under-predict emissions for all ICAO conditions for varying unmixedness parameters. The proposed model performed the best once again predicting within 20% error for both 7% and 30% thrust conditions. Similar to the analysis performed on the Engine B combustor, the evaporation model was able to predict trends resulting from alterations in mean droplet. Unfortunately, the proposed model was unable to calculate CO emissions.
within 20% error for all parametric conditions.
Chapter 10

Conclusions

The objective of this thesis was to test and evaluate different methods of predicting CO emissions against a variety of combustor flow fields and geometries. Two different approaches were investigated, global and local. The global approach looked at using a set of equations to quickly solve for the CO production based on inlet conditions and conditions within the primary zone. The local approach looked at methods focusing on the localized conditions within areas of the combustor.

Within the global approach, three different correlations were investigated, the Mellor, Lefebvre and Rizk correlations. The local approach included both the MIT model and a “new proposed methodology” was developed based on past models such as the Laval, Rizk and Industrial based models. The “new proposed methodology” focused on three main characteristics affecting CO emissions; the complex internal combustor flow field, combustion chemistry and liquid fuel evaporation. The internal combustor flow field was captured using assumptions from cold flow computational fluid dynamic calculations. Combustion chemistry was captured using chemical kinetic calculations and ideal reactors. Liquid fuel evaporation was captured using correlations for evaporation and mean droplet size. Each model was tested against combustors from four different engines: En-
gine A, Engine B, Engine C and Engine D.

From each analysis, conclusions were developed based on the results from each model. Unfortunately, the global correlations performed poorly. The Mellor correlations’ lack of droplet size evaporation and the simplistic equation development revealed that the Mellor correlation does not predict over a large enough range of conditions. In each test case, the Mellor correlation under-predicted for low level thrust conditions and over predicted for high level thrust conditions. The Lefebvre and Rizk correlation performed similarly, accurately predicting the exponential decay of CO emissions levels at increasing thrust conditions. However, the Lefebvre and Rizk correlations over-predicted for Engine A and D combustors and under-predicted for Engine B and C combustors thus not properly predicting trends developed from alterations in internal flow fields.

For the local approach, reactor networks were developed and flow parameters were optimized to best predict CO emissions for each case. Unfortunately, the MIT model under-predicted for all test cases, however the MIT model was able to predict trends produced from a change in the internal flow field of the combustor. The proposed model performed the best by predicting CO emissions within 20% error for low level ICAO thrust conditions for Engines B and D combustors. In addition, the model was able to predict a reduction in CO emissions between Engine B and C combustors, revealing that the proposed model is able to account for changes in a combustors internal flow field. Finally, the model was also able to capture trends associated with variation in mean droplet size, predicting flameout conditions associated with an increasing mean droplet size.

From all of the models and correlations that were analysed, the “new proposed methodology” worked the best as it was able to predict trends and accurately predict CO emissions
for most low level thrust conditions. Although the “new proposed methodology” takes longer than the other models, a single calculation using the proposed methodology can be completed well within a single day; saving weeks of computational time compared to that of a CFD code. The improved accuracy using the proposed methodology, coupled with the low computational time make the “new proposed methodology” a viable tool in estimating CO emissions at the preliminary stages of aviation gas turbine combustor chamber design. Before implementing such a tool, more work is needed to not only create a standardized method of generating reactor networks but also reduce some of the assumptions made by the methodology.
Chapter 11

Future Work

There are a few aspects of the proposed model that require additional work to further validate its’ use and assess the limitations of the model. These tests would include validation of mean droplet size correlations, the use of different fuel nozzles, alterations in fuel spray definition, dependence of reactor model configuration, wall cooling affects, the use of detailed or reduced jet fuel based chemical mechanisms and additional combustor geometries and conditions. It will be important to perform these tests using known data from modern aviation engine configurations as modern engines contain complex geometries and flow fields that will be difficult to accurately predict localized conditions using a simplistic methodology. These specific test were chosen based on the profound effect that each can have on predicted CO emissions. Understanding the limitations of the model will assist in the creation of a standardized tool to be used in the preliminary design phase of an aviation gas turbine combustor.

Secondly, from the variations in the flow of the fuel/air mixture, the model is able to accurately predict changes in trends. The next step is to develop a method for calculating the percent flow splits from reactor to reactor based on the cold flow CFD or other calculation methods. The best method for calculating this assumption would be
integrating the flow split calculations based on the interpretation of velocity contours, within the cold flow CFD calculations.

Another recommendation for future work is to attempt to use a similar methodology to solve for NO\textsubscript{x} emissions. Although the proposed model has been developed focusing on CO emissions, attempting to combine the use of CO and NO\textsubscript{x} emissions can potentially make the preliminary design emissions analysis more efficient. With additional tests and validation of methodology assumptions, the proposed model could accurately provide emissions predictions at the preliminary design phase. In addition, validation of CO trends allow the proposed methodology to assist companies in altering details in internal flow field that could promote CO reduction and produce more environmentally friendly engines.

The last recommendation is to expand on what has been developed to include the prediction of heat transfer and operability. From the results of using the proposed model to analyse variations in mean droplet size, the model has already shown promise in predicting operability conditions such as flame-out. The next step would be to expand the functionally of the model to track other operability conditions and heat transfer especially near the wall of the combustor. As near wall conditions can affect CO formations within the combustor, heat transfer at the wall will be paramount to improving the proposed model.
References


