Prediction of Emissions for Lean-Premixed Gas Turbine Combustors

by

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Abstract

A preliminary design methodology for lean-premixed combustors was developed at Carleton University, but lacked an emissions-prediction tool. An evaluation of the methods available for quantifying emissions is undertaken, and a chemical reactor network (CRN) is selected as the ideal method for predicting emissions. A general set of procedures focusing on determining flow splits and volumes, representing the internal flowfield of the combustor, is developed using published empirical and semi-empirical correlations. The correlations are validated using available experimental data, and compared against CFD methods for selected cases. Results show good accuracy compared to simple CFD methods, and are competitive with the more sophisticated CFD methods in predicting experimental values. The developed CRN model is applied to an existing lean-premixed combustor, and the emissions results obtained from the model show good agreement with experimental emissions data. Finally, the resulting reactor network is applied to the preliminary lean-premixed combustor created at Carleton University to confirm the ability of this particular design to reduce emissions. Results show higher-than-expected amounts of NO_x formation, but lower-than-expected amounts of CO formation. Overall, the preliminary CRN model efficiently predicts emissions with reasonable accuracy compared to a CFD-based approach, with the added advantage of being able to directly integrate into the combustor design methodology, allowing for immediate iterations.

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Nomenclature

Abbreviations

CF	Centre Flow
CFD	Computational Fluid Dynamics
CFZ	Centre Flame Zone
CMC	Conditional Moment Closure
CREK	Combustion Reaction Equilibrium and Kinetics
CRN	Chemical Reactor Network
CRZ	Corner Recirculation Zone
CV	Control Volume
DC	Dome-Cooling
DJ	Dilution Jet
DLE	Dry-Low Emissions
DLN	Dry-Low NO _x
DNS	Direct Numerical Simulation
DOE-HAT	Department of Energy Humid Air Turbine
DRZ	Dome Recirculation Zone
DZ	Dilution Zone
EDM	Eddy-Dissipation Model
EDC	Eddy-Dissipation Concept
FZ	Flame Zone
GRI-Mech	Gas Research Institute Mechanism
IF	Inner Flow

IFZ	Inner Flame Zone
IRZ	Inner Recirculation Zone
JP	Jet Propellant
LBO	Lean Blowout
LDKM	Localized Dynamic Kinetic Energy Model
LEM	Linear Eddy Model
LES	Large Eddy Simulation
LRR	Launder, Reece, and Rodi
MFZ	Main Flame Zone
MIX	Mix reactor
OF	Outer Flow
OFZ	Outer Flame Zone
PDF	Probability Density Function
PFR	Plug Flow Reactor
PFZ	Post-Flame Zone
P-LP	Preliminary Lean-Premixed
PMZ	Premixing Zone
ppm	Parts per Million
ppmvd	Parts per Million corrected to Dry Volume
PSR	Perfectly Stirred Reactor
PZ	Primary Zone or Pilot-flame Zone
RANS	Reynolds-Averaged-Navier-Stokes
RES	Reservoir

RQL	Rich-Quench-Lean
RNG	Renormalization Group
RSM	Reynolds Stress Model
SSG	Speziale, Sarker, and Gatski
SW	Swirler
UHC	Unburned Hydrocarbon
WALE	Wall-Adapting Local Eddy-viscosity
WC	Wall-Cooling
WSR	Well-Stirred Reactor

English Symbols

a	Major radius of an ellipse [m]
A	Area [m^2], empirical constant for Eddy-dissipation model, and Air
A_k	Pre-exponential factor [cm^3, mol, s]
A_{SW}	Swirler flow area [m^2]
b	Minor radius of an ellipse [m]
B	Empirical constant for Eddy-dissipation model
$\mathbb{C}$	Centerline
c_p	Constant-pressure specific heat of the mixture [$J/kg \cdot K$]
$c_{p,i}$	Constant-pressure specific heat of the i^{th} species [$J/kg \cdot K$]
C_D	Discharge coefficient
$C_{D,SW}$	Swirler discharge coefficient
C_{D90°	Orifice discharge coefficient

$C_{1\epsilon}$	Turbulence closure coefficient
$C_{2\epsilon}$	Turbulence closure coefficient
C_μ	Turbulence closure coefficient
d_0	Jet orifice diameter [m]
D	Diameter [m]
Da	Damköhler number (Equation 2-33 on page 36)
$D_{T,ij}$	Turbulence diffusion [m^2/s]
$D_{L,ij}$	Molecular diffusion [m^2/s]
E_A	Activation energy [cal/mol]
f	Flow fraction or Mixture fraction
F	Fuel
G_k	Generation of turbulence kinetic energy [J]
G_ϕ	Angular momentum flux (Equation 2-45 on page 58) [J]
G_x	Axial momentum flux (Equation 2-46 on page 58) [N]
h	Expansion ratio (Equation 2-51 on page 61)
h_i	Specific enthalpy of the i^{th} species [J/kg]
$h_{f,i}^o$	Specific enthalpy of formation for the i^{th} species [J/kg]
$\hat{h}$	Heat transfer coefficient [W/m^2K]
H	Step height [m]
i	Chemical species index
k	Reaction rate coefficient [various units], Turbulence kinetic energy [J]
l	Intersection length of the recirculation zone to the swirler hub [m]
L	Length [m]

m	Mass [kg]
$\dot{m}$	Mass flow rate [kg/s]
M	Third-body collision partner
M_{ANG}	Axial flux of angular momentum (Equation 2-45 on page 58) [N]
MW_i	Molecular weight of the i^{th} species [$kg/kmol$]
n	Temperature exponent
n, m	Reaction order
N	Number of species
N_R	Number of reactions
$p(f)$	Probability density function
$\mathcal{P}$	Perimeter [m]
P	Pressure [Pa]
P_{ij}	Stress production [m^2/s^3]
$\dot{Q}$	Rate of heat transfer [W]
r	Radius [m]
r'_{ij}, r''_{ij}	Reaction order of reactants and products of species i in reaction j
R_j	Rate of progress of reaction j (Equation 2-25 on page 28) [$kmol/m^3s$]
R_u	Universal gas constant [$J/(kmol \cdot K)$]
S	Unmixedness parameter (Equation 2-52 on page 64)
$\overline{S}_{ij}$	Strain-rate tensor [$1/s$]
S_n	Swirl number (Equation 2-47 on page 59)
S_D	Dump plane swirl number

t	Time [s]
t_R	Average residence time a particular mixture spends within a specified region (Equation 2-3 on page 12) [s]
T	Temperature [K]
T_{in}	Dilution jet temperature [K]
T_{PZ}	Average primary zone temperature [K]
u	Axial velocity [m/s]
v'_{ij}, v''_{ij}	Stoichiometric coefficients for reactants and products of species i in reaction j
V	Volume [m^3], volumetric flow rate [m^3/s]
w	Tangential velocity [m/s]
W_j	Dilution jet mass flow rate [kg/s]
W_m	Mass flow rate entrained upstream of the dilution jet [kg/s]
x	Distance along the x-axis [m]
x_R	Reattachment length (Equation 2-50 on page 61) [m]
X_i	Mole fraction of the i^{th} species [kmol/kmol]
y	Distance along the y-axis [m]
Y_C	Dilution jet penetration distance [m]
Y_i	Mass fraction of the i^{th} species [kg/kg]
Y_0	Inlet radius [m]
Y_1	Combustor radius [m]
z_R	Corner recirculation reattachment length (Equation 2-50 on page 61) [m]

Greek Symbols

β_0	Jet angle [<i>deg</i>]
δ_{ij}	Kronecker's delta function
δ_0	Corner reattachment length in the absence of swirl [<i>m</i>]
Δx	Incremental distance along the x-axis [<i>m</i>]
ϵ	Turbulence dissipation rate [m^2/s^3]
ϵ_{ij}	Turbulence dissipation transport [m^2/s^3]
θ_v	Swirler vane turning angle [<i>deg</i>]
μ	Laminar viscosity [Ns/m^2]
μ_t	Eddy-viscosity [Ns/m^2]
Π_{ij}	Pressure strain transport [m^2/s^3]
ρ	Gas density [kg/m^3]
σ_k	Turbulence closure coefficient
σ_ϵ	Turbulence closure coefficient
σ_ϕ	Standard deviation of fuel-air equivalence ratio
σ_m	Mean fuel-air equivalence ratio
τ_{chem}	Characteristic chemical time [<i>s</i>]
τ_{flow}	Characteristic mixing time [<i>s</i>]
τ_{ij}	Sub-grid turbulence or Reynolds stress [N/m^2]
τ_{kk}	Isotropic portion of sub-grid turbulence or Reynolds stress [N/m^2]
ϕ	Equivalence ratio defined as the actual fuel-air ratio divided by fuel-air ratio at the stoichiometric condition (Equation 2-2 on page 11)
ϕ_i	Instantaneous properties of a gas

$\dot{\omega}_i$	Net rate of production/consumption of the i^{th} species (Equation 2-24 on page 28) [$kmol/m^3s$]
------------------	--

Subscripts

<i>air</i>	Properties of air
<i>b</i>	Backward reaction
<i>c</i>	Combustor properties
<i>CF</i>	Centre flow
<i>CFZ</i>	Centre flame zone
<i>CRZ</i>	Corner recirculation zone
<i>d</i>	Dome properties
<i>DJ</i>	Dilution jet
<i>DZ</i>	Dilution zone
<i>f</i>	Forward reaction, properties of mixture fraction
<i>fuel</i>	Properties of the fuel
<i>g</i>	Gas properties
<i>h</i>	Swirler hub
<i>i</i>	Chemical species index
<i>i, j, k</i>	Index of the three grid directions, x, y, z
<i>IF</i>	Inner flow
<i>IFZ</i>	Inner flame zone
<i>IRZ</i>	Inner recirculation zone
<i>j</i>	Dilution jet conditions, Chemical reaction index

max	Maximum value
min	Minimum value
OFZ	Outer flame zone
OF	Outer flow
p	Properties of primary stream
PFZ	Post-flame zone
PZ	Primary zone
r	Recirculation properties
ref	Reference value
s	Properties of secondary stream
SW	Swirler
t	Swirler tip
w	Combustor and reactor wall properties
x, y, z	Cartesian spatial co-ordinates
3	Combustor inlet conditions

Superscripts

$*$	Reactor inlet conditions
-----	--------------------------

Other

$[X_i]$	Molar concentration of species i [$kmol/m^3$]
$\sim$	Indicates Favre-averaged value

1 Introduction

Stringent governmental regulations for gas turbine emissions combined with the ever-increasing pressure ratios and temperatures of next-generation gas turbine engines have prompted significant modifications to the combustion chamber [1-3]. The primary goals of early conventional diffusion flame combustor designs were to achieve flame stability as well as high combustion efficiency, which is the ratio of actual energy released to the theoretical energy potential of the fuel [4]. In the current climate, however, reduction of pollutants such as nitrogen oxides (NO_x), carbon monoxide (CO), and unburned hydrocarbons (UHC) has gained importance while still emphasizing the capabilities of conventional designs [3,5]. Of the modern combustor concepts, lean-premixed combustion has been successfully used to reduce emissions in industrial gas turbine engines [6]. The lack of available methodologies to create such a design led to Carleton University's development of a preliminary design methodology for a lean-premixed combustor [5,7]. At this time, a tool that can be directly incorporated into the preliminary design process for assessing the emission potential of such a design is required.

In this thesis, the methods that are available for quantifying emissions are explored, and the development of a tool for assessing emission potential is outlined and applied to the new design. The proceeding sections briefly highlight the motivation behind emissions-reducing technologies and the development of lean-premixed combustors that require a design tool that can be easily implemented to predict emissions.

1.1 Progression of Emissions-Reducing Technologies

An overview of the primary pollutants that are generated in the gas turbine combustion process is shown in Table 1-1. In addition to exerting harmful effects on health, emissions containing NO_x , CO, and UHC are also known to cause ozone depletion, acid rain, and smog [6,8,9]. In general, the mechanisms of oxides of nitrogen formation can be classified into four categories: 1) Thermal NO, 2) Prompt NO, 3) Nitrous oxide NO, and 4) Fuel NO [6]. Carbon monoxide and unburned hydrocarbons are products of incomplete combustion which are commonly combustor-design related [10]. An overview of the formation mechanisms of these pollutants in the combustion process is given in Chapter 2.

Table 1-1: Constituents originating from the combustion process [10].

Constituents	% By Weight	Remarks
Nitrogen (N_2)	74.16	Mostly inert, from atmosphere
Oxygen (O_2)	16.47	From excess air
Carbon Dioxide (CO_2)	5.47	Product of complete combustion
Water (H_2O)	2.34	Product of complete combustion
Argon (A)	1.26	Inert, from atmosphere
Unburned Hydrocarbons (UHC)	Trace	Product of incomplete combustion
Carbon Monoxide (CO)	Trace	Product of incomplete combustion
Oxides of Nitrogen (NO_x)	Trace	Atmospheric and fuel-bound nitrogen
Oxides of Sulphur (SO_x)	Trace	From Sulphur in fuel

Escalating environmental and health concerns have stimulated government intervention in controlling emissions [9]. The United States Environmental Protection Agency imposed regulations which require gas turbine manufacturers to reduce emissions

based on best available technology [6,11]. This has led to the development of water or steam injection to control the NO_x emission levels by acting as a heat sink to reduce the peak flame temperatures in the combustion chamber [9]. Even though this new development was highly successful in reducing NO_x levels, dramatic increases in CO and UHC were noticed [12]. As a result, innovative designs for satisfying conflicting requirements, such as achieving high efficiency, low NO_x , low CO, low UHC emissions and flame stability, were still necessary. This spawned new concepts such as rich-quench-lean (RQL), catalytic, and dry low NO_x (DLN) or dry low emission (DLE) combustors [2,9].

The RQL concept functions on the basis that combustion temperature and, in turn, NO_x production is lower at both fuel-lean and fuel-rich conditions compared to near stoichiometric conditions [6,9]. In the RQL design, the fuel-rich primary zone is followed by rapid quenching by the dilution air, allowing for a lean burn zone. Unfortunately, a brief period of stoichiometric conditions is inevitable during the transition from rich to lean conditions. Therefore, the effectiveness of this concept is said to be limited by the rate at which dilution air can quench the rich mixture [9].

In catalytic combustion systems, catalysts are used to reduce equivalence ratios for combustion below the lean flammability limits of fuel-air mixture, resulting in reduced flame temperatures [9]. Even though this seems to be a promising solution to reduce emissions, it is limited by the catalyst substrate materials' inability to withstand combustion temperatures over prolonged periods [9].

Figure 1-1: Typical air split for (a) conventional and (b) lean-premixed combustors; modified from [5,7].

The DLE combustion systems, which evolved from DLN, employ concepts such as fuel-staging, variable geometry and lean-premixing to reduce emissions to ultra low levels [5]. In lean-premixed designs, the objective is to premix the fuel and air at fuel-lean conditions (less than 0.65) prior to combustion in order to reduce the extent of local regions of high temperatures within the flame [2,6,9]. This is done primarily in the premixer before the mixture enters the combustion chamber via the swirler (Figure 1-1).

The swirler produces a highly turbulent swirling flow which results in the formation of a recirculation zone. This feature stabilizes the flame by providing stable, hot combustion products to ignite the fresh reactants. Unlike conventional combustor designs, the lean-premixed design utilizes the majority of the air for combustion rather than for cooling the liner walls, as shown in Figure 1-1. Consequently, advanced cooling schemes such as augmented backside cooled liners that eliminate air injection through liner walls are used [13]. Coincidentally, this also results in reducing CO emissions, since liner cooling in the primary zone often leads to quenching or freezing CO-converting reactions [6,13]. To achieve low NO_x emissions, it is important to keep the combustion zone within a narrow band of temperatures over a variety of operating conditions (as shown in Figure 1-2) [2,6]. A low equivalence ratio, and therefore low temperature, leads to high CO, UHC and poor stability, while equivalence ratios close to stoichiometric yield stability, but high NO_x formation [2].

To control the equivalence ratio in the primary zone, lean-premixed combustion is commonly equipped with either variable geometry or fuel-staging for direct control of the mixture composition over a wide range of operation [2,6,13]. Variable geometry is a way of modulating the airflow distribution in the combustor. Common methods are variable-area swirlers to control airflow in the primary zone and variable openings into the dilution zone [2,6]. Fuel-staging is used to control local fuel-air ratio by switching fuel flow from one zone to another to keep a constant combustion temperature [2,6]. These techniques are always coupled to complex control and feedback mechanisms to manage the fuel-air mixture in the combustor [6].

Figure 1-2: Temperature range for low emissions [6].

1.2 Existing Design Methodology

The evolution of emission-reducing technologies has significantly changed several aspects of gas turbine combustor designs. Dodds and Bahr [14] indicated that new combustor designs are developed by modifying previously established combustor geometries through a trial-and-error approach using expensive engine development programs. Typically, these programs allow the manufacturer to develop proprietary design rules based on experimental data. To overcome the use of costly experimentation and unattainable design rules, several researchers have published generalized sets of empirical, semi-empirical, and analytical models for combustor designs. However, these published design methodologies by authors such as Sawyer [15], Dodds and Bahr [14], and Mattingly *et al.* [16] outline only preliminary designs for conventional combustors. This led to the initial undertaking by Charest [5], and later by Capurro [7], to use these

resources to formulate a preliminary design methodology for a lean-premixed combustor. A CFD simulation on this design helped to verify the temperature and structural integrity requirements for the combustor [5]. This study also produced preliminary data on emissions output, which was thought to be under-estimated. Since then, a specific tool to accurately evaluate the emissions output of the lean-premixed combustor that could be intrinsic to the preliminary design has not been developed. As demonstrated in Figure 1-3, the integration of emissions prediction would fulfill a crucial internal step in the combustor design pathway.

Figure 1-3: Combustor design flowchart.

1.3 Motivation and Objectives

The primary motivation behind this thesis is to develop a methodology to quantify the emissions output from a lean-premixed combustor that can be seamlessly incorporated into the existing lean-premixed combustor preliminary design methodology developed by Charest [5] and Capurro [7].

The three most common methods for predicting emissions are: 1) design-specific empirical correlation, 2) chemical reactor modeling, and 3) computational fluid dynamics (CFD) as shown in Figure 1-4. Existing design-specific empirical correlations are unique to a specific combustor geometry and cannot be used to predict new designs, in particular lean-premixed combustors. In chemical reactor modeling, important combustion features are represented by idealized chemical reactors to create a chemical reactor network (CRN), which can employ a full set of chemical kinetic reactions to describe any combustion process. The flowfield features in the chemical reactor modeling approach can be determined by three methods: 1) flowfield correlations (based on empirical relations), 2) cold-flow CFD, and 3) hot-flow CFD without detailed chemistry as shown in Figure 1-4. The hot-flow CFD approach differs from the cold-flow CFD approach in that the latter does not account for the effects of temperature and hence density variations in the combustor when establishing the flowfield through momentum and mass conservation. The final method, labelled simply as CFD, utilizes detailed chemical reactions integrated into the flowfield computations, and is considered to be the most elaborate method to model the flow and reaction processes in a combustor. Unfortunately, it is hampered by long computational time required for a converged and quantitatively accurate solution for useful emissions prediction. This is especially true

when dealing with a high number of chemical kinetic reactions needed to predict CO and NO_x emissions.

Figure 1-4: Hierarchy of emission prediction methods for gas turbine combustion.

The current state-of-the-art method to predict emissions is hot-flow CFD combined with CRN, which can be considered as a compromise between highly complex CFD with detailed chemistry and simple design-specific empirical correlations. However, this process still takes a considerable amount of time in setting up, running, and post-processing the hot-flow CFD solution before a reasonable reactor network can be constructed. For the purposes of preliminary design iterations, a method that can provide relatively accurate emissions predictions to allow for rapid modifications to the design is needed. Flowfield correlations combined with CRN is one method that could possibly meet this demand for new combustor designs.

The objective of the present work is to develop a methodology to build a chemical reactor network to represent a lean-premixed combustor for predicting emissions without the use of CFD. A general set of procedures focused on determining flow splits and volumes that represent the internal flowfield of the combustor is developed using published empirical and semi-empirical correlations describing the flowfield. The correlations are validated using available experimental data, and compared against CFD methods for selected cases. The developed chemical reactor network (CRN) is then used to model an existing lean-premixed combustor with experimental data to assess the prediction quality. As part of this evaluation, to determine the degree of complexity required for the CRN to adequately represent a combustion system, comparisons are made between CRN models containing decreasing numbers of reactors. Finally, the resulting reactor network is applied to the preliminary lean-premixed combustor created at Carleton University [5] to confirm the ability of this particular design to reduce emissions compared to its design goals.

2 Literature Review

This chapter reviews the feasibility and degree of complexity of the three different methods for predicting emissions outlined in the previous chapter. Prior to examining each method, a brief review of the mechanisms that lead to the gas turbine combustor emissions is presented. The chapter concludes with a review of combustor flow patterns that are essential for the development of a chemical reactor network.

A few common combustion-pertaining concepts that recur throughout the thesis require initial clarification. These are stoichiometry, equivalence ratio and residence time.

Stoichiometry

Stoichiometric condition is achieved when the oxidizer and, hence, the air is just sufficient to burn all of the fuel completely [17]. Considering this ideal combustion process, the stoichiometric fuel-air ratio, $(F/A)_{stoic}$, is determined by:

$$(F/A)_{stoic} = \frac{m_{fuel}}{m_{air}} \quad (2-1)$$

where m_{fuel} and m_{air} are the mass of the fuel and air, respectively.

Equivalence Ratio

The definition of equivalence ratio is given as the actual fuel-air ratio divided by fuel-air ratio at the stoichiometric condition [17]:

$$\phi = \frac{(F/A)_{actual}}{(F/A)_{stoic}} \quad (2-2)$$

For a particular fuel-air mixture, the mixture is fuel-lean for $\phi < 1$ and fuel-rich for $\phi > 1$. An equivalence ratio equal to unity indicates the stoichiometric condition.

Residence Time

The mean residence time is defined as the average time a particular mixture spends within a specified region of space:

$$t_R = \frac{\rho V}{\dot{m}} \quad (2-3)$$

where ρ is the mixture density, V is the volume, and $\dot{m}$ is the mass flow rate.

2.1 Mechanisms of Gas Turbine Combustor Emissions

To properly model a combustor, a solid understanding of the pertinent chemical reactions and the effects of the combustor geometry on these reactions is needed. More specifically, the chemical kinetic mechanisms that incorporate formation chemistry must have accurate reaction steps and rate data for the modeling process [18].

The main species of concern in gas turbine combustion emissions are CO, NO_x, and UHC. The main cause of these emissions can be related to operating conditions. At a low power the concentrations of CO and UHC are at their highest, and as power is increased, leading to an increase in flame temperature, these concentrations decrease [6]. Unfortunately, NO_x opposes this trend in that its concentration is lowest at low-power settings, but increases with higher power. A review of reaction mechanisms and the pathways to pollutant formation is provided next.

2.1.1 Reaction Mechanisms

Chemical reaction rates control the rate of combustion and determine the formation of pollutants in most combustion processes [17]. The study of chemical kinetics is a division of physical chemistry that looks into elementary reactions and their rates that define the detailed chemical pathways from reactants to products [17]. The resulting collection of elementary reaction steps to describe an overall reaction is called a reaction mechanism [17]. However, due to the large number of reactions and the difficulties in obtaining the reaction rates, very few existing fuel-oxidizer reaction mechanisms are complete. In combustion research, a wide variety of mechanisms are used. These range from the least complex one-step global mechanisms, that describe the overall reaction with no intermediate steps, to complete mechanisms which are composed of all possible elementary reactions [17]. In general, they are all based on experimental measurements that express the rate at which a species is consumed, for example in a bimolecular reaction ($A + B \rightarrow C + D$) by [17]:

$$\frac{d[X_A]}{dt} = -k(T)[X_A]^n[X_B]^m \quad (2-4)$$

where $[X_A]$ is the molar concentration of species A, $k(T)$ is the temperature-dependent reaction rate coefficient, and n, m are the reaction orders. The reaction rate coefficient, which is a strong function of temperature, is determined through collision theory and is represented by an empirical modified-Arrhenius form given by [17]:

$$k(T) = A_k T^n e^{(-E_A/R_u T)} \quad (2-5)$$

where, R_u is the universal gas constant, n is the temperature exponent, A_k is the pre-exponential factor, and E_A is the activation energy. The last three parameters are generally determined experimentally [17]. For detailed information on these derivations, the reader may refer to the textbook by Turns [17].

The global and quasi-global mechanisms developed by Westbrook and Dryer [19] for a variety of hydrocarbons are commonly used in simple gas turbine combustion analyses [5]. Reduced mechanisms which are created by trade-off studies between complexity and accuracy have also been used in more detailed combustion analyses [18]. One such mechanism is the Kollrack mechanism for Jet-A fuel that has been incorporated into numerous studies using chemical reactor modeling of gas turbine combustors [1,16,20]. One of the most complex mechanisms that has been used in chemical reactor modeling is the Gas Research Institute Mechanism version 3.0 (commonly referred to as GRI-Mech 3.0) [21], optimized for methane and natural gas combustion [22-24]. This mechanism consists of 325 elementary reactions involving 53 species. Reduced versions for methane combustion have also been used extensively, such as the Miller-Bowman mechanism [18,24-26]. Most, if not all, of these reduced mechanisms that are used to study combustion systems include reactions that are known to be involved in pollutant formation; these reactions are discussed in the next section.

2.1.2 Oxides of Nitrogen (NO_x)

The oxides of nitrogen consist of nitric oxide (NO) and nitrogen dioxide (NO_2). The formation of NO_2 results from the oxidation of NO, therefore the net NO_x is not affected by the amount of NO_2 formed [9]. The four main mechanisms for NO formation

are: 1) Thermal, 2) Prompt, 3) Nitrous Oxide (N₂O), and 4) Fuel-bound nitrogen. A description of each of these mechanisms and the parameters that influence them is provided next.

Thermal NO

Also known as the Zeldovich mechanism, thermal NO is aptly named due to its high sensitivity to temperature [6,9,27]. The formation of NO primarily results from the oxidation of air-bound nitrogen in high temperature regions, generally above 1800 K, in the combustion process [9]. This agrees with studies by Correa and Smooke [28], which showed that thermal NO is prominent near stoichiometric conditions. The reactions that represent the formation of thermal NO are commonly given by the extended Zeldovich mechanism [6,18]:

Nicol [18] states that for methane-air combustion in the flame zone, 80 percent of the NO formation occurs through Reaction 2-7 while 15 percent occurs through Reaction 2-8. In the post-flame region, the contribution of NO from Reaction 2-8 diminishes to zero due to the depletion of OH-radical concentration [18]. Reaction 2-6 is considered very slow with a high activation energy (hence its significance only above 1800 K), compared to Reaction 2-7; therefore, these reactions are limited by the rate at which the first reaction (2-6) can produce nitrogen atoms [18]. Both reactions (2-6 and 2-7) are relatively slow

compared to combustion reactions, and thus, theoretically, shortening the residence time at high temperatures can decrease the final NO emitted [17].

Prompt NO

Originally termed the Fenimore mechanism, as it was proposed by Fenimore in 1971 [6], prompt NO is the formation of cyano-compounds that are converted to NO [18]. The main reaction responsible for this pathway is shown below:

For lean-premixed combustion, this reaction takes place very early in the flame zone since the CH-radical is short-lived [18]. This explains why prompt NO is commonly referred to as the mechanism that accounts for NO early in the flame region [6,9]. The conversion of hydrogen cyanide (HCN) and N from Reaction 2-9 to NO is quite complex involving more than 20 reactions [26], thus detail will not be provided. The reader is encouraged to refer to the work of Miller and Bowman [26] for a more thorough explanation.

Experimental studies using lean methane-air flames at ambient pressures by Leonard and Correa [29] revealed that the prompt mechanism is dominant below flame temperatures of 1850 K. However, at high pressures, typical of gas turbine combustors, lean-premixed methane combustion testing conducted by Nicol *et al.* [30] showed prompt NO to be negligible and not to play a significant role in the total NO_x emitted.

Nitrous Oxide NO

An important pathway for NO formation for lean combustion conditions ($\phi < 0.8$) is the nitrous oxide (N_2O) route [18]. This pathway was first proposed by Malte and Pratt [31] for which the main reactions involved are:

where M is the third-body collision partner. The main source of N_2O formation is through forward reaction of Reaction 2-10, which is then transformed into NO by recombination due to hydrogen radicals (Reaction 2-11) or oxygen radicals (Reaction 2-12). In the combustor flame zone, Nicol [18] affirms that for lean-premixed conditions, reactions 2-11 and 2-12 produce equal amounts of NO. However, as oxygen radicals are depleted in the flame zone, the post-flame zone is dominated by Reaction 2-11 (95 percent conversion) [18]. Furthermore, the NH created from Reaction 2-11 further reacts to form NO. As a result, for every N_2O molecule, two molecules of NO are formed [18].

Early studies by Correa and Smooke [28] revealed that N_2O is the dominant mechanism in lean-premixed combustion compared to the thermal and prompt NO mechanisms. This agreed with studies conducted by Nicol *et al.* [30], which showed that at the leanest conditions the N_2O mechanism was dominant, while at richer conditions the dominant mechanism was thermal NO. Furthermore, for ultra low NO_x combustors (less than 10 ppm), the NO contribution of the N_2O pathway increases and approaches 100 percent.

Fuel NO

Fuel NO mechanism concerns gas turbines that operate on nitrogen-containing fuels such as distillates which may contain up to 1.8 percent nitrogen [6,9]. The nitrogen-bound fuels generally lead to HCN and, to a lesser extent, ammonia (NH_3) through pyrolysis, which is the chemical decomposition of organic fuels when heated in the absence of oxygen [5,9]. The conversion of HCN to NO generally follows the same pathway as the prompt mechanism described above [9,18,26]. The conversion of NH_3 to NO is equally complex, and details of this pathway can be found in the work by Miller and Bowman [26].

With regards to new low-emission gas turbine power plants, which typically use natural gas, fuel NO is of little concern. This is because fuels such as natural gas contain less than 0.06 percent of fuel-bound nitrogen [6].

2.1.3 Carbon Monoxide (CO)

Poor combustion efficiency in a gas turbine combustor is closely linked with the formation of CO emissions. Formation of CO has been known to be sensitive to combustor inlet temperature, combustion pressure, primary zone equivalence ratio, and mean fuel droplet size for liquid fuels [6].

Primary zone equivalence ratio, and hence flame temperature, requires a delicate balance during the combustion process. Starting at a lean condition, increasing equivalence ratio is known to reduce CO emissions reaching a minimum just below stoichiometric. However, past this point, further increases in equivalence ratio increases

CO emissions [6]. The reactions that are commonly used to explain these processes are given below [17,32,33]:

It is evident that the population of H and OH radicals plays a large role in the oxidation of CO to CO₂ [32,33]. Low equivalence ratios reduce the temperature in the flame and post-flame zones leading to quenching of OH radical formation in Reaction 2-13 and attenuating CO in Reaction 2-15. At a high equivalence ratio, generally above 1800 K, the lack of oxygen available to replenish the OH radicals (Reaction 2-14) also leads to increase in CO (Reaction 2-15) [6,32,33]. Additionally, it has been noted at high temperatures, CO by chemical dissociation of CO₂ (Reaction 2-16) starts to become significant [6]. Generally, the main location for CO formation is in the flame zone where fast fuel-consuming reactions take place. The CO only starts to oxidize with radicals when the competing CH_x radical levels decrease significantly, typically in the post-flame zone [34]. Considering these competing factors, CO production is said to be highly nonlinear with respect to temperature and oxygen fraction [33].

Other factors such as pressure and combustor liner wall-cooling also play an important role in the formation and destruction of CO emissions. It has been reported that increased pressure reduces CO emissions for both low and high equivalence ratios by accelerating the rate of conversion of CO into CO₂ and suppressing chemical

dissociation, respectively [6,17,35]. Although at fixed pressures, changes in temperatures can have the opposite effects as discussed above [17]. Formation of CO resulting from liner wall-cooling is due to the migration of cooling air into the primary zone leading to abrupt quenching of the reactions mentioned above [6]. Thus, the interaction between liner wall-cooling and the primary flow is important in controlling CO emissions.

2.1.4 Unburned Hydrocarbon (UHC)

All species exiting the combustor containing carbon atoms, except for CO, CO₂, and nitrogen containing species, fall under the umbrella of unburned hydrocarbons [24]. In general, factors that influence CO emissions also influence UHC emissions. However, the pathways of UHC formation are considered to be more complex than that of CO emissions [6]. Factors that are known to affect UHC formation are poor atomization for liquid fuels, poor burning rates, and quenching effects from cooling air.

Depending on the droplet sizes achieved from atomization, large mean diameters can lead to poor evaporation rates and incomplete burning in the residence time available for combustion [6]. Conversely, over-mixing of excess air in lean-premixed combustion can lead to extremely lean mixtures that may escape the combustion process and exit unburned [6,36]. Even though there are various sources that lead to the formation of UHCs, little research has been done in this area since the quantification of UHC emissions from these sources is not straightforward [36].

With the current knowledge of formation mechanisms of NO_x, CO, and UHC having been explained, the three methods of emissions prediction summarized in Figure

1-4 are reviewed next, in the order of design-specific correlations, computational fluid dynamics, and chemical reactor modeling.

2.2 Design-Specific Correlations

Empirical correlations for emissions prediction are derived by relating known historical emissions to engine-specific conditions such as combustor inlet pressure (P_3), inlet temperature (T_3), and air and fuel mass flow rates [6,37]. Conversely, the semi-empirical approach is based on the assumption that CO and NO_x exhaust concentrations are governed by mean residence time in the combustion zone, chemical reaction rates, and mixing rates [6,38]. These three factors are commonly derived using combustor size, liner pressure loss, airflow proportions, and the parameters used for empirical correlations as noted above [6]. Example correlations for these two approaches can be found in the published literature [6,37-39].

Empirical and semi-empirical correlations allow one to predict accurate results quickly for conditions compatible with the historical datasets on which they are based. However, the general applicability to combustor designs on which the correlations are not based is poor [37]. The success of the design-specific correlations is said to be very dependent on input parameters, and accurate estimations of these parameters are required for a reliable emission prediction [37,39].

2.3 Computational Fluid Dynamics

Next to experimental testing, computational fluid dynamics is considered to be the gold standard for predicting emissions for gas turbine combustors in the development phases. However, modeling turbulent combustion associated with gas turbine combustors is a complex problem [40,41]. In particular, predicting emissions in lean-premixed combustors is difficult due to the complexity of the chemistry and the interactions with the turbulent fluctuations [42]. An outline of the overall numerical solution procedure for a comprehensive combustion model is shown in Figure 2-1. Appropriate representation of each block in Figure 2-1 greatly influences the outcome of the simulation [43]. Some of these factors are discussed in this section, but the reader is encouraged to consult the works by Wilcox [44], Peters [45], and Veynante and Vervisch [41] for complete descriptions regarding turbulence and turbulent combustion modeling.

Figure 2-1: Numerical solution procedure for a comprehensive combustion model [43].

2.3.1 Turbulence Modeling

In a turbulent flow, the ratio of smallest to largest turbulence scales (also known as eddies) decreases rapidly as the Reynolds number increases [44]. Presence of these eddies exerts a powerful effect during combustion, since the interaction of these eddies with the mean flowfield dramatically enhances mixing and transport [41]. Capturing the small scales becomes very difficult with finite spatial and temporal meshing techniques, even though the Navier-Stokes equations describe both laminar and turbulent flow without additional information [46]. Typically, in order to predict the effects of turbulence, turbulence models are developed to account for these effects without resorting to extremely fine spatial and temporal meshes. There are three main techniques for turbulent flow predictions: 1) Direct Numerical Simulation (DNS), 2) Large Eddy Simulation (LES), and 3) Reynolds-Averaged Navier-Stokes (RANS) models [40].

Direct Numerical Simulation (DNS)

The most accurate of these techniques is DNS, which numerically solves the full Navier-Stokes equations without the requirement of any additional modeling [47]. To do so, the computational temporal and spatial mesh must contain extremely fine increments to fully resolve the entire range of turbulence scales [40]. The computational cost to resolve the entire range of scales is very high, which is especially true for high Reynolds numbers associated with gas turbine combustors [46,47].

Large Eddy Simulation (LES)

The state of the art in combustion modeling in industrial gas turbines is large eddy simulation (LES) [47]. In this approach, the smaller eddies are filtered and are modeled using a sub-grid-scale turbulence model, while the larger energy-carrying eddies are resolved and hence are represented explicitly [40]. The advantage for this approach is two-fold. First, by modeling less of the turbulence spectrum, the error introduced by turbulence modeling is reduced [46]. Secondly, the smaller eddies which receive energy from the large eddies are closer to isotropic behaviour and can be modeled more universally [46,48]. Unlike DNS, the filtering in LES utilizes fewer computational resources since the computational mesh is less refined, but it is still significantly higher than the RANS models discussed next [7].

As a result of filtering, the filtered form of the Navier-Stokes equations contains additional unknown terms, which are grouped into a single sub-grid-scale turbulence term, known as the sub-grid turbulence stress, which requires modeling. Typically, the sub-grid-scale model employs the Boussinesq hypothesis, which states the effects of turbulence on the mean flowfield to be similar to the effects of molecular viscosity [44]. This approach correlates the sub-grid turbulence stress, τ_{ij} , to the resolved strain-rate tensor, $\bar{S}_{ij}$, by a scaling factor called the eddy-viscosity, μ_t , to give the following form:

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\mu_t\bar{S}_{ij} \quad (2-17)$$

where δ_{ij} is the Kronecker's delta function and τ_{kk} is the isotropic part of the sub-grid turbulence stresses [46]. The Smagorinsky-Lilly, dynamic Smagorinsky-Lilly, Wall-Adapting Local Eddy-Viscosity (WALE), and Local Dynamic Kinetic Energy (LDKM)

models define the method by which the eddy-viscosity is modeled [46]. The last of these two methods are the most common models used in combustion modeling [48-51].

Reynolds-Averaged Navier-Stokes (RANS) Models

The most commonly used technique for combustion modeling is RANS-based models. In this approach, modifications of the unsteady Navier-Stokes equations are made by decomposing the dependent variables into time-mean and fluctuating components and time-averaging the entire set of governing equations over a time period that is long compared to the time scales of turbulence activity to produce the RANS equations [46]. For combustion modeling, Reynolds-averaging is replaced by Favre-averaging to account for density fluctuations associated with heat release [40]. As a consequence of the averaging procedure, RANS equations introduce additional unknown terms known as Reynolds stresses that require additional equations to be solved numerically. These additional equations classify the type of turbulence or closure model for RANS equations [44]. These closure models can be classified into two groups: 1) Eddy-viscosity models and 2) Reynolds stress models (RSM).

The most commonly used eddy-viscosity model in combustion modeling is the two-equation k - ϵ model, where k is the turbulence kinetic energy and ϵ is the turbulence dissipation rate [42]. Similar to the LES sub-grid turbulence stresses, the Boussinesq hypothesis is used here to relate the Reynolds stresses, τ_{ij} , to the mean strain-rate tensor as follows:

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\mu_t S_{ij} \quad (2-18)$$

where δ_{ij} is the Kronecker's delta function, τ_{kk} is the isotropic part of the Reynolds stresses, and μ_t is the eddy-viscosity calculated using additional transport equations for k and ϵ . The equations to calculate these terms are given below in a simplified form; more information on these transport equations is given in the work of Wilcox [44]:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \epsilon \quad (2-19)$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_i}(\rho \epsilon u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} \frac{\epsilon}{k} G_k - C_{2\epsilon} \rho \frac{\epsilon^2}{k} \quad (2-20)$$

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon} \quad (2-21)$$

where G_k represents the generation of turbulence kinetic energy, μ is the laminar (molecular) viscosity, and σ_k , σ_ϵ , $C_{1\epsilon}$, $C_{2\epsilon}$, and C_μ are model coefficients which are determined empirically. The drawback to this approach is that μ_t is assumed to be an isotropic scalar quantity (i.e. no directional dependence), which has been shown experimentally to be not true even in relatively simple turbulent flows [47]. This is especially troublesome in highly swirling flows common in gas turbine combustors, which exhibit streamline curvature and highly anisotropic turbulence, leading to inaccurate predictions of the flowfield [52-54]. To resolve this aspect of the model, various modifications have been suggested. The two most common forms are the renormalization group (RNG) k - ϵ [55] and realizable k - ϵ models [56]. In brief, the latter model incorporates a new formulation of the eddy-viscosity and a new transport equation for turbulence eddy dissipation rate, while the former includes a dynamically-computed $C_{2\epsilon}$ term in Equation 2-20 [46].

An alternative to the eddy-viscosity models are the Reynolds stress models (RSM), which abandon the isotropic turbulence assumption and solve transport equations for each of the terms in the Reynolds stress tensor [46]. A simplified form of the Reynolds stress transport equation derived by taking the moments of the Navier-Stokes equations is given below [46]:

$$\frac{\partial}{\partial x_k} (\rho u_k \tau_{ij}) = -D_{T,ij} + D_{L,ij} - P_{ij} + \Pi_{ij} - \epsilon_{ij} \quad (2-22)$$

where $D_{T,ij}$ is the turbulence diffusion, $D_{L,ij}$ is the molecular diffusion, P_{ij} is the Reynolds stress production, Π_{ij} is the pressure-strain, and ϵ_{ij} is the dissipation term. Of these terms, $D_{T,ij}$, Π_{ij} , and ϵ_{ij} require modeling to close the equation. It is commonly said that the success of the RSM models depends on how the pressure-strain and dissipation terms are modeled. The latter term is commonly treated in similar fashion to the k - ϵ models (Equation 2-20 and 2-21) and is considered to be the weakest link in the RSM technique [52]. The pressure-strain term is modeled using either the linear correlation method developed by Launder *et al.* [57] or a quadratic relationship developed by Speziale *et al.* [58] typically referred to as LRR-RSM and SSG-RSM, respectively. It has been said that generally increasing the order of the pressure-strain correlation has a positive effect on the solution accuracy [52]. These RSM models have had good success in modeling gas turbine combustors [53,59]

2.3.2 Turbulent Combustion Modeling

In its most complete form, application of CFD to combustion modeling involves the solution of the energy conservation and species conservation equations in addition to the Navier-Stokes equations (mass and momentum conservation) [41]. From the species conservation equation emerges the net rate of production/consumption of species i , $\dot{\omega}_i$, that must be solved for closure.

Considering N_R reactions involving N species, the general form of chemical reactions can be written as:

where X_i is the species i , N is the number of species, and v'_{ij} and v''_{ij} are the stoichiometric coefficients for reactant and product i in reaction j , respectively. Then the net rate of production/consumption of species i , $\dot{\omega}_i$, can be computed as the sum of the rate of progress over the N_R reactions in which species i participates:

$$\dot{\omega}_i = MW_i \sum_{j=1}^{N_R} (v''_{ij} - v'_{ij}) R_j \quad (2-24)$$

where MW_i is the molecular weight of species i and R_j is the rate of progress for reaction j . Here the R_j term, which is similar to Equation 2-4, is given in a more general form as:

$$R_j = k_{fj} \prod_{i=1}^N [X_i]^{r'_{ij}} - k_{bj} \prod_{i=1}^N [X_i]^{r''_{ij}} \quad (2-25)$$

where $[X_i]$ is the molar concentration of species i , r'_{ij} and r''_{ij} represent the reaction order of reactant and product i in reaction j , and k_{fj} and k_{bj} are the forward and backward reaction rate constants for reaction j as described in Equation 2-5 earlier:

$$k_{fj}, k_{bj} = A_k T^n e^{(-E_A/R_u T)} \quad (2-26)$$

where, R_u is the universal gas constant, n is the temperature exponent, A_k is the pre-exponential factor, and E_A is the activation energy.

The filtering or time-averaging of the net rate of production/consumption from Equations 2-24 to 2-26, in the context of the LES and RANS approaches, yields additional unknown terms, requiring simplifying assumptions. These simplified assumptions define the type of turbulent combustion models [42]. Typical turbulent combustion models are the eddy-dissipation model (EDM), eddy-dissipation concept (EDC), assumed probability density function (PDF), laminar flamelet, and linear eddy model (LEM). A summary of the advantages and disadvantages of each of the models is provided by Brewster *et al.* [42]. In general, these models can be classified according to the type of treatment of the chemical reactions: 1) fast chemistry and 2) finite-rate chemistry. Fast chemistry neglects kinetic limitations and assumes instantaneous reaction, limited only by turbulent mixing [42]. Finite-rate chemistry, on the other hand, with an appropriate chemical mechanism, can simulate the production of kinetically-controlled species such as the emissions from a gas turbine combustor [46]. This treatment typically applies to EDC, assumed PDF, and LEM models for premixed combustion. Most of the methods described above fall outside the scope of this thesis, therefore, a brief description of a select few methods will be provided next.

Finite-Rate Model

The simplest of the turbulent combustion models, namely the finite-rate model, assumes reacting species are premixed or the turbulent mixing time-scale is very fast compared to the reaction time-scale, essentially ignoring turbulent mixing [43]. The rate of progress variable (R_j), in this case, is evaluated using Equations 2-25 and 2-26 using a specified chemical reaction mechanism for application of interest. This model is useful for laminar flames, but is generally considered inaccurate for turbulent flames since turbulence-chemistry interactions are not accounted for [46].

Eddy-Dissipation Model

In contrast to the finite-rate model, eddy-dissipation model (EDM) assumes the reactions occur on a much faster time-scale than the mixing time-scale, leading the model to ignore chemical kinetic rates [43]. This concept was developed by Magnussen and Hjertager [60] based on the eddy-breakup model suggested by Spalding [61], which relates the rate of progress to the dissipation rate of the turbulence eddies containing products and reactants [43]. The rate of progress of reaction j is given by the limiting value (smaller) of the two expressions [62]:

$$R_j = A \frac{\epsilon}{k} \min \left(\frac{[X_i]}{v'_{ij}} \right) \quad (2-27)$$

$$R_j = AB \frac{\epsilon}{k} \left(\frac{\sum_P [X_i] MW_i}{\sum_P v'_{ij} MW_i} \right) \quad (2-28)$$

where $[X_i]$ in Equation 2-27 represents the minimum molar concentration of species i among reacting species only, $[X_i]$ in Equation 2-28 is the molar concentration of all

product species P in the reaction j , and A and B are empirical constants. It is clear from the above equations that the dissipation rate is assumed to be the ratio of the turbulence dissipation to the turbulence kinetic energy, ϵ/k . The empirical constants, A and B , are “tuned” for the reacting flow application of interest and are not generalized [43,45].

To simultaneously account for mixing and finite-rate chemistry, a modified version of this approach, commonly used in combustion models, uses the finite-rate model along with the eddy-dissipation model [22,24,43]. This approach selects the limiting value of rate of progress of reaction j among Equations 2-25, 2-27, and 2-28.

The EDM and finite-rate/EDM are, however, said to produce good results for one- to two-step reaction mechanisms only. This is because, in a multi-step reaction mechanism, the Arrhenius reaction rate coefficients are different for each reaction, whereas in the EDM approach, every reaction has the same eddy-dissipation rate [46]. Consequently, the finite-rate/EDM approach is commonly only used in simple combustion models to predict the heat release.

Assumed Probability Density Function (PDF) Method

In the assumed PDF method, the typical approach is to assume fast chemistry, in which the instantaneous properties of the gas are in equilibrium and can be calculated from a conserved scalar variable known as the mixture fraction, f [42]. This relationship can be generalized as:

$$\phi_i = \phi_i(f) \quad (2-29)$$

where ϕ_i represents the instantaneous species mass fraction, density, or temperature of the gas. The mixture fraction defines the degree of “mixedness” of primary (m_p) and secondary mass constituents (m_s), which are fuel and oxidizer streams in non-premixed combustion applications [43]:

$$f = \frac{m_p}{m_p + m_s} \quad (2-30)$$

Under the assumption of equal turbulence diffusivities for all gas phase species, the species conservation equation can be reduced to a single transport equation for the mixture fraction, f [46]. The assumption of equal turbulence diffusivities is said to be reasonable in turbulent flows, in which the turbulence diffusion overwhelms the molecular diffusion [46]. To account for turbulence, the resulting transport equation for f is solved for its Favre-averaged mean value, $\tilde{f}$, and its variance, $\widetilde{f'^2}$, which represents the fluctuating mixture fractions about its mean value. In the same way, to calculate averaged values of the variables that depend on f (Equation 2-29), an assumed-shape PDF, $p(f)$, describing the temporal fluctuations of f in the turbulent flow, is used [46]. This relationship is given by:

$$\tilde{\phi}_i = \int_0^1 p(f) \phi_i(f) df \quad (2-31)$$

The shape of the PDF is selected based on its similarity to experimentally-observed fluctuations. Detailed derivations of this procedure are found in the work of Eaton *et al.* [43].

The above approach is restricted to only fast-chemistry non-premixed combustion. To account for premixed combustion that applies finite-rate chemistry, an improved version of this approach was developed by Zuo *et al.* [63] by adding another conserved scalar called the reaction progress variable:

$$\theta = \frac{Y_{f,max} - Y_f}{Y_{f,max} - Y_{f,min}} \quad (2-32)$$

where Y_f is the mass fraction of fuel species, and $Y_{f,min}$ and $Y_{f,max}$ are the minimum and maximum values of the mass fraction of fuel species. The addition of this conserved scalar requires the use of a joint-PDF, $p(f, \theta)$, to calculate the averaged-instantaneous variables, $\tilde{\phi}_t$. Here, the mixture fraction and reaction progress variables are assumed to be mutually independent, thus making the joint-PDF separable for integrating each variable independently [42]. The detailed derivation of this improved approach is complex; one may refer to the work of Zuo *et al.* [63] for a more thorough explanation. Validation of this model against experimental data showed reasonable prediction of emissions for both premixed and diffusion turbulent combustion [63]. However, it has been noted that the use of reaction mechanisms involving more than two or three steps can become significantly more time-consuming computationally [42].

Even though the bulk of available research on CFD-based combustor modeling focuses on the interaction between the turbulence and chemistry, two other major factors affecting CFD modeling are geometric complexity and heat transfer effects. Significant resources must be put into creating a spatial grid that appropriately represents the swirlers, cooling holes, film-cooling slots and other complex features of the combustor

[42]. Furthermore, heat transfer due to convection and radiation must also be properly modeled to achieve good agreement between the simulation and experimental results. A comprehensive review of CFD simulations that use turbulence and combustion modeling for gas turbine combustors is provided by Mongia [53,64], and separately by Brewster *et al.* [42].

In conclusion, turbulence alone requires considerable computational effort to resolve the complex flow in the gas turbine combustor. The addition of combustion in a turbulent flow increases the computational requirements even more. Accurate prediction of emissions requires turbulent combustion models based on finite-rate chemistry. For this to be successful, the model should allow for a detailed chemical mechanism to be used to resolve all the pathways for pollutant formation. However, the more detailed the chemical mechanism becomes, the higher is the computing cost [3,23]. Overall, a substantial amount of computational work is needed to obtain a satisfactory solution for emissions in modern gas turbine combustors using CFD techniques. For example, the use of a RANS-based approach with turbulent combustion modeling to simulate the flow and reaction processes of a simple combustor would require computing times in the order of days on today's computational platforms.

2.4 Chemical Reactor Modeling

The alternative to the aforementioned methods for combustor modeling is the use of elementary chemical reactors such as perfectly stirred reactors (PSR) and plug flow reactors (PFR) that employ detailed reaction mechanisms to represent various features of the combustor flowfield. To create a network containing these reactors, an understanding

of the combustor internal flowfield is required to determine the size of the reactors (i.e. volume) and their integration with the combustor flowpath (i.e. air and fuel partitioning, cooling flows, residence times, etc.). Three methods of constructing a combustor model using a chemical reactor network exist: 1) flowfield features are estimated using empirical and semi-empirical correlations, 2) flowfield features are estimated using cold-flow CFD simulations, and 3) flowfield features are estimated using simple hot-flow CFD simulations. The third methodology is the most commonly used, and the second method is rarely used. The hot-flow CFD method starts first with a proper turbulence model and a turbulent combustion model using a simple two- to three-step reaction mechanism for the desired fuel and oxidizer to establish the flowfield, accounting for the effects of the prevailing heat release. The resulting solution is used to extract volumes and flow splits for specific flowfield regions (e.g. recirculation zones) based on the flow temperature, velocity, and chemical species concentrations. This information is then used to represent the specific flowfield regions by idealized reactors such as non-reactive mixers (MIX), PSRs, and PFRs. The hot-flow CFD method, considered to be a relatively efficient way to analyze new combustors, still takes a considerable amount of time in setting up, running, and post-processing a CFD simulation before a reasonable reactor network can be made. The alternative is to use available empirical and semi-empirical correlations that describe the flowfield features to construct a chemical reactor network. The next section focuses on this alternative and provides a brief introduction to the reactor theory followed by a review of the chemical reactor networks used to represent gas turbine combustors. It concludes with a review of the available correlations that describe the combustor flowfield.

2.4.1 Idealized Chemical Reactors

The reacting flow is governed by the mass, momentum, energy and species mass conservation equations. As discussed earlier, a solution for the full set of governing equations is difficult and time-consuming. Idealized chemical reactors make a number of assumptions that significantly reduce the complexity of the reacting flow by decoupling the fluid dynamics and chemical processes [22,24,37]. In essence, idealized reactors provide the building blocks for modeling complex flows, such as gas turbine combustors, to examine the chemical behaviour that leads to pollutant formation [17]. A brief overview of the main types of idealized reactors and their relevance to the modeling of combustors is given next.

Perfectly Stirred Reactor

A schematic of a perfectly stirred reactor (PSR) is shown in Figure 2-2a. A PSR is also known as a well-stirred reactor (WSR) as described by Longwell and Weiss [17]. The contents of a PSR are perfectly mixed and are assumed to be spatially uniform due to high diffusion rates and/or forced turbulent mixing [17,65]. As a consequence, the rate of conversion of reactants to products is limited by chemical reaction rates rather than mixing. This situation is commonly described by the use of the Damköhler number (Da), which characterizes the chemical kinetics constraint in the mixture. The Damköhler number is the ratio of the characteristic mixing time (τ_{flow}) to the characteristic chemical reaction time (τ_{chem}):

$$Da = \frac{\tau_{flow}}{\tau_{chem}} \quad (2-33)$$

For PSR conditions, the Damköhler number approaches zero to indicate the rate of conversion to be completely dependent on chemical kinetics of the mixture [37]. This assumption allows the mathematical model to neglect mixing effects, leading to a large reduction in computational effort. As a consequence, the mathematical model is capable of utilizing detailed chemical reaction mechanisms [65].

The detailed derivation of the mathematical model for the PSR can be found in the works of Kee *et al.* [66] and Meeks *et al.* [65]. Briefly, the mass conservation for the individual species, is given by:

$$\frac{dY_i}{dt} = \frac{\dot{\omega}_i MW_i}{\rho} + \frac{\dot{m}}{\rho V} (Y_i^* - Y_i) \quad (2-34)$$

where i indicates the i^{th} species, $\dot{\omega}_i$ is the net rate of production/consumption, MW_i is the molecular weight, V is the mixture volume, $\dot{m}$ is the mass flow rate of the mixture, ρ is the density of the mixture calculated from the ideal gas equation of state, Y_i is the mass fraction of the i^{th} species, and the superscript $*$ indicates inlet conditions. Equation 2-34 equates the rate at which the mass of species i accumulates within the control volume to the sum of the rate at which species i is generated and the net rate of the mass flow of species i into the control volume [17].

The energy equation for the individual species is given by:

$$c_p \frac{dT}{dt} = \frac{\dot{m}}{\rho V} \sum_{i=1}^N Y_i^* (h_i^* - h_i) - \sum_{i=1}^N \frac{h_i \dot{\omega}_i MW_i}{\rho} + \frac{\dot{Q}}{\rho V} \quad (2-35)$$

where $\dot{Q}$ is the rate of heat transfer into the control volume, T is the reactor temperature, N is the number of species, and, assuming ideal gas behaviour, the specific enthalpy of the i^{th} species h_i is given by:

$$h_i = h_{f,i}^o + \int_{T_{ref}}^T c_{p,i} dT \quad (2-36)$$

where $h_{f,i}^o$ is the enthalpy of formation at the reference temperature T_{ref} , and $c_{p,i}$ is the specific heat of the i^{th} species calculated using polynomial parameterization [67]. For steady-state conditions, the above equations are a set of coupled nonlinear algebraic equations that can be solved, for example, using a version of the damped Newton's method [17,65,66].

Figure 2-2: Schematic of (a) a PSR and (b) a PFR.

Plug Flow Reactor

The plug flow reactor (PFR) is an ideal reactor commonly used for tube/channel flow in chemical engineering (Figure 2-2b). The general characteristic of the PFR is that it assumes there is no mixing in the axial (flow) direction, but perfect mixing in the radial (perpendicular to the flow) direction [68]. It is considered to be a steady, one-dimensional inviscid flow with ideal gas behaviour [37]. A detailed derivation of the PFR theory can be found in the work of Kee *et al.* [66]. The mass, momentum, species, and energy conservation equations describing the flow are given by:

$$\frac{d(\rho u_x)}{dx} = 0 \quad (2-37)$$

$$\frac{dP}{dx} + \rho u_x \frac{du_x}{dx} = 0 \quad (2-38)$$

$$\frac{dY_i}{dx} - \frac{\dot{\omega}_i MW_i}{\rho u_x} = 0 \quad (2-39)$$

$$\rho u_x c_p \frac{dT}{dx} = \frac{\hat{h} \mathcal{P}}{A} (T_w - T) - \sum_{i=1}^N h_i \dot{\omega}_i MW_i \quad (2-40)$$

where c_p is the specific heat of the mixture, ρ is the density of the mixture, u_x is the axial velocity, A is the channel cross-sectional area, P is the pressure, $\hat{h}$ is the convective heat-transfer coefficient of the channel wall, $\mathcal{P}$ is the channel perimeter, T_w is the channel wall temperature, N is the number of species, and MW_i is the molecular weights of the individual species. The system of equations represents a set of ordinary differential equations that can be solved numerically [66].

Relevance to Combustor Modeling

Idealized reactors such as a PSR and a PFR have been used extensively in complex reactor networks for gas turbine combustor modeling, as reviewed in the next section. The high turbulence intensity associated with gas turbine combustors is the main characteristic that allows for the incorporation of PSRs into combustor modeling [8,24]. Turbulence intensity, defined as the local velocity fluctuations divided by the local time-mean velocity, is typically reported to be in the range of 150 to 200 percent for gas turbines, since mean velocities in the recirculation boundaries can approach near zero values [69,70]. Consequently, the use of PSRs is usually confined to the primary flame zone which encompasses the intensively-mixed recirculation zone that stabilizes the flame [1,2,8]. The strong turbulence in this region tends to have short characteristic mixing times relative to characteristic chemical times, translating to low Damköhler numbers. This is supported by the work of Allaire [37], who mentions that as turbulence intensity increases, the Damköhler number decreases. This is the ideal condition for the implementation of a PSR since the Damköhler number in a PSR is essentially zero. In addition to representing the flame zone in the combustor, a PSR is also commonly used to model a non-reacting mixer (MIX) to mix combustion products with dilution air [1]. This is accomplished by treating the PSR model with the chemical reactions disabled.

Unlike the PSR, the PFR is used in lower turbulence intensity regions of the post-combustion zones of the gas turbine combustor [24,25,31]. This region represents the secondary burn-up or flame relaxation zone where the reactions continue towards completion with very little mixing [1,2].

2.4.2 Chemical Reactor Networks

The use of chemical reactors to model a gas turbine combustor was initially introduced by Bragg in 1953 [71]. The Bragg combustor used a WSR (also known as a PSR) followed by a PFR to distinguish the primary and secondary zones of the gas turbine combustor, respectively (Figure 2-3) [16]. Although this configuration has been widely used in gas turbine combustor development [25], studies by Sturgess and Shouse [1] have concluded that a single reactor representation of the primary zone is an unacceptable over-simplification. In order to accurately model real combustion systems, many reactors (a chemical reactor network) are required to describe the complex flowfields and boundary conditions [17,22].

Figure 2-3: Bragg combustor; modified from [16].

To create a chemical reactor network (CRN) that accurately represents a gas turbine combustor, the major aerodynamic features, such as recirculation and cooling flow mixing, should be identified. This modeling technique is commonly referred to as zonal combustion modeling originally proposed by Swithenbank in 1970 [22]. Sturgess and Shouse [1] state that to include realistic chemistry in this modeling technique, it is necessary to accurately know the reactor types (PSR, PFR, or MIX), volumes, mass

exchange rates between them and the connectivity linking the reactors that idealize the aerodynamic features. In the context of implementing a chemical reactor network, three possible methods exist to determine the combustor internal flowfield features and their interactions with each other: 1) empirical/semi-empirical correlations [20,23,37,72], 2) cold-flow CFD simulations [3], and 3) hot-flow CFD simulations [1,22,24]. The advantages and disadvantages are listed in Table 2-1. In general, one method's advantages are the other method's disadvantages. For example, the correlations-based CRN can easily accommodate changes to the combustor design parameters, whereas CFD-based CRN is fixed for one specific combustor simulation and is therefore less adaptable.

Table 2-1: Comparisons of flowfield estimation methods.

Methods	Advantages	Disadvantages
Correlations-Based	<ul style="list-style-type: none"> - Quick - More adaptable - Easy to implement 	<ul style="list-style-type: none"> - Accuracy depends on correlation - Difficult to obtain flowfield correlation
CFD-Based	<ul style="list-style-type: none"> - Accurate - Flowfield is well-defined 	<ul style="list-style-type: none"> - Time-consuming - Less adaptable - Difficult to implement

Flowfield based on CFD Methods

CFD is the most commonly used method to obtain the flowfield features to build a CRN by idealized chemical reactors. This approach takes advantage of CFD's ability to reliably calculate the aerodynamic features (or zones of interest) inside a combustor and complements its deficiency in predicting emissions with reactor models [73]. As

discussed in the previous section, incorporating kinetics-limited chemistry to predict emission is difficult and time-consuming with CFD methods. However, reactor models can easily handle the large number of detailed chemical reactions to provide chemical kinetic effects on emissions with properly defined zones.

The CFD methods use either cold-flow simulations [3] or more time-consuming hot-flow simulations involving two- or three-step reaction mechanisms to predict the proper heat release [1,22,24]. The justification for using cold-flow simulation is the high Reynolds number characteristics of gas turbine combustors, which is said to allow cold-flow simulations to depict hot-flow details fairly well [3]. This, however, is in conflict with other studies, which show flowfield differences in reacting and non-reacting cases [70,74]. To remedy this problem, most CFD-based CRNs use hot-flow CFD solutions that utilize two-step global reaction mechanisms to resolve the thermal expansion effects on the flowfield features [1,22,24]. The resulting solution is used to extract volumes and flow splits (distribution of the flow throughout the combustor) based on the flow temperature, velocity, and chemical species concentrations [1,22,24]. Details on specific methods are discussed in the review of the available hot-flow CFD methods.

Based on the assumption that the fundamental flowfield within the combustor, once calculated by CFD, does not change substantially as blowout is approached and as operating conditions such as combustor inlet temperature, pressure and overall fuel-air ratio are varied, Sturgess and Shouse [1] developed a hot-flow CFD-based CRN model. The model shown in Figure 2-4 was developed to study the lean blowout (LBO) conditions of a simplified annular conventional gas turbine combustor. The CFD

simulation used the standard $k-\epsilon$ turbulence model and eddy-dissipation model (EDM) for predicting heat release. To define the major features, various indirect methods were used to determine the volume, mass flow rate, mean residence time, mean equivalence ratio, and the degree of mixing from the CFD solution [1]. In addition to using three-dimensional fluid flow topology, dissipation gradient analysis and streak-line tracking methods were used to represent an equivalent network of connected reactors [1,75]. A similar approach was extended by Sturgess [75] to calculate emissions using an abbreviated reaction mechanism for Jet-A/JP-5/JP-8 fuel [16]. However, the model for this study was designed for a perforated-plate flame holder instead of a gas turbine combustor.

Figure 2-4: CRN model based on hot-flow CFD solution [1].

A more sophisticated CRN model based on a hot-flow CFD solution for a dry-low emission (DLE) industrial gas turbine was developed by Novosselov [22] to predict

exhaust emissions. The 2D-axisymmetric CFD simulation utilized the University of Washington's eight-step global mechanism for methane to build the 31-element CRN model made of MIX, PSR, and PFR reactors (Figure 2-5). Of the eight-step global mechanisms, three reactions are used for methane oxidation and the remaining five nitrogen chemistry mechanisms are used for post-processing the CFD solution for NO_x formation (the list of eight-step reactions can be found in the work of Novosselov [22]). The CFD simulation used the RSM turbulence model and finite-rate/eddy-dissipation model for turbulence-chemistry interaction. Based on the CFD solution, the combustor volume was divided into five distinct regions characterized by physical properties of the flow and flame behaviour: 1) main flame zone (MFZ), 2) pilot flame zone (PZ), 3) centre recirculation zone (CRZ), 4) dome recirculation zone (DRZ), and 5) post-flame zone (PFZ). The determination of the flow parameters in each region was based on CFD results, namely velocity, pressure, temperature, and chemical species concentrations; details can be found in the dissertation by Novosselov [22]. In the flame zone, the model used several PSRs in series to spread out the flame by allowing the flame to progress and produce intermediate and incomplete products of combustion, which were eventually consumed as the final state of the flame was reached. The author modeled the recirculation zone using a PFR due to low turbulence intensity found in the CFD solution. To accurately depict the premixer commonly used in DLE combustors, cross-mixing between the streams of different fuel-air ratios was used to smooth out the fuel-air ratio, accounting for the effects of turbulent mixing. The post-flame zone was modeled by PFRs followed by a MIX reactor to simulate dilution at the combustor exit.

and the finite-rate/eddy-dissipation model for turbulence-chemistry interaction similar to that of Novosselov described above. The corresponding CRN from the CFD solution, shown in Figure 2-7, was made of 24 reactors and divided into the five zones described by Novosselov [22]. One of the main differences was the use of PSR to simulate the recirculation flow instead of the PFR used for Novosselov's model. Russo *et al.* [24] state that this decision was made because of the high turbulent intensity predicted in the 2D-CFD solution; however, the author acknowledges further investigation is needed for its validity. The other difference was the exclusion of fuel-air mixing effects that were effectively used in the study by Novosselov [22].

Figure 2-6: Flowfield division of a micro GT combustor [24].

Figure 2-7: CRN for micro gas turbine combustor [24].

The CRN simulation was conducted with an in-house code using both GRI-Mech 3.0 [21] and a reduced mechanism for methane proposed by Miller and Bowman [26]. The predicted emissions by the CRN model were then compared to experimental measurements at varying thermal load conditions from 60 percent to 100 percent. The results summarized in Figure 2-8, where emissions are reported in parts per million corrected to dry volume (ppmvd), showed good agreement between predicted and experimental values for NO_x formation. However, CO emission was under-predicted at lower thermal load conditions. This may have been due to major flowfield and flame shape changes that could not be adapted to the CRN model with fixed volume and flow splits determined by a single CFD solution.

Figure 2-8: Results of CRN model for the micro gas turbine combustor [24].

Flowfield based on Empirical Correlation Methods

For the CFD-based CRN models discussed previously, there is a large time investment in the CFD solution and post-processing before a workable reactor network can be built [1]. The motivation behind this method is the notion that only one CFD solution is required for one particular combustor to evaluate the emissions through CRN models [1,22]. However, the study by Russo *et al.* [24] maintained that different thermal loading conditions require different CRN models based on the proper loading CFD results since the reactor volumes and flowfield features are significantly modified. Furthermore, physical changes made to a combustor in development cannot be accommodated easily by the CFD-based CRN since a new CFD solution and CRN model will be required for each version of the combustor [1]. Thus, adaptability and quick on-the-fly results are not possible. An alternative would be the empirical and semi-empirical models that employ correlations to quantify reactor volumes and flow splits to represent the combustor flowfield.

The first such model that applied zonal modeling was the work by Swithenbank *et al.* [72] to represent an experimental combustor using seven reactors (Figure 2-9). The model used combustor design approximations and entrainment theory based on the geometry to determine the sizes of the reactor volumes and flow splits. Details of their methods are outlined in the next section. The incorporation of a PFR for the recycle reactor was determined from water model studies of the combustor, which showed little turbulence along the recycle flow path. The secondary and dilution zones incorporate a WSR (also known as a PSR) followed by a PFR with the assumption that the jet turbulence dissipates rapidly due to impingement of radially opposed jets leading to little

additional mixing after the WSR [8]. Unfortunately, the model was only used to predict performance variables of the combustor and the pollutant emission capabilities were not explored.

Figure 2-9: CRN for an experimental combustor by Swithenbank [72].

To predict emissions for an experimental ALF-502 (Honeywell Aerospace, NJ, USA) gas turbine combustor, a zonal reactor model was developed by Rubins and Pratt [20]. Dimensional and configuration data were combined with water tunnel data to identify the combustor flow patterns that were to be represented by chemical reactors (Figure 2-10). The resulting simple CRN, shown in Figure 2-11, was developed ignoring recycle flow effects and mass exchanges between main flow and dilution flows from the walls. The simplifications made in the CRN model were justified by the need for trends in emissions rather than precise results. The CRN model was tested using the CREK code with Kollrack's 30-reaction mechanism for Jet-A fuel [16]. The predicted trend of CO concentration was similar to experimental data. However, the accuracy of the prediction

was dependent on the combustors' ability to approach the instantaneous mixing that is modeled by the stirred reactors.

Figure 2-10: Idealized zones of the combustor derived from water tunnel tests [20].

Figure 2-11: CRN model for experimental ALF-502 combustor [20].

Roby *et al.* [23] developed an analytical tool to create a reactor model to predict pollutant formation and efficiency characteristics of high fuel-air-ratio combustors. The design tool makes use of engine-operating conditions, air distribution, and geometry inputs to create a set of generalized design rules to identify the reactors and flow splits

required to create a CRN. Unfortunately, none of the design rules or methodology used to create CRNs for combustors were published. Their work, however, showed results of the design tool's ability to create a CRN for a generic lean-premixed combustor called Combustor "A". In the CRN shown in Figure 2-12, two PSRs are used to model the effect of unmixedness in the primary reaction zone, while two PFRs are included to capture the wall-cooling effects of the combustor. The CRN predictions were obtained using the CHEMKIN II code (FORTRAN-based subroutines developed by Sandia National Laboratories which are discussed in Chapter 3) and GRI-Mech 3.0 [21] mechanism for methane. The results compared to experimental measurements showed the correct values of NO_x and CO emissions over a wide range of equivalence ratios.

Figure 2-12: CRN model for Combustor A [23].

A more recent CRN was developed by Allaire [37] for predicting emissions for the purpose of assessing design modifications of conventional gas turbine combustors as a policy-making tool. The generalized CRN model shown in Figure 2-13 is composed of a parallel array of PSRs followed by a series of PFRs to represent the primary,

intermediate, and dilution zones. The reactor volumes and flow splits were obtained from scaled schematics of particular combustors and correlations, respectively. The parallel arrangement of 16 PSRs was used to account for unmixedness in the primary zone. This was calculated from calibrating the model with available certification data for each engine being analyzed. The whole arrangement was simulated using CHEMKIN 4.0 with GRI-Mech 3.0 [21] reaction mechanism for propane combustion. The results showed good correlations with certification emissions data and design-specific semi-empirical correlations, but the model is only useful in predicting trends. The author suggests that more correct physical representation of the nature of gas turbine combustors (i.e. flowfield features, such as flame and recirculation zones) should be used to improve predictive capabilities.

Figure 2-13: A generalized CRN model modified from [37].

2.4.3 Combustor Flowfield Features

To develop a proper chemical reactor network for a modern gas turbine combustor, an adequate representation of the internal flow features is needed [20]. In reviewing existing CRNs provided above, particular attention must be paid to the following features in a lean-premixed combustor: the coupling of flame and recirculation in the primary zone, secondary burn-up in the dilution zone, homogeneity of the premixer, and wall-cooling effects. This section reviews the available information in the literature to describe these features along with a general overview of combustor volumes.

Overall Volumes

At the preliminary design stage of gas turbine combustors, the geometry and air flow proportions through the swirler, air injection, and wall-cooling are known [5,7], as summarized in Appendix A. Typically, estimations of the primary, secondary, and dilution zone volumes of a conventional combustor are made according to the air injection locations [5]. These injection points determine the start and end of a particular zone. Using this approximation in a lean-premixed combustor, the primary and dilution zones are divided by the dilution air injection location. As a result, the volumes of the primary and dilution zone are known from preliminary design variables (Appendix A).

Primary Zone

The inner recirculation zone in a modern combustor is primarily driven by highly swirling flow and augmented by combustion air jets to produce the desired flow reversal needed to stabilize the flame [6]. The strength of the swirl is defined by the swirl number,

which is the ratio of angular momentum flux to axial momentum flux [77]; more information is provided in later sections. Typically, swirl numbers greater than 0.5 result in strong adverse pressure gradients in the axial direction, yielding reduction of velocity along the axial flow direction, ultimately resulting in flow reversal. An idealized flow pattern in the primary zone is shown in Figure 2-14. Two separate zones can be identified in the region: high-energy swirling flow along the outer envelope (A in Figure 2-14) and core flow consisting of high radial velocities and reverse flow in the centre (B in Figure 2-14) [78]. The dotted line (C in Figure 2-14) around the core indicates a zero axial velocity where transition from downstream flow to reverse flow takes place [70,74,78]. Between the outer envelope and the zero axial velocity line, the local turbulence intensity and shear rates are said to be high while the reverse flow near the centre is associated with lower turbulence intensity [22,70,74,78,79]. Furthermore, the flame is typically situated along the highly turbulent region and anchored from the centerbody of the swirler [70,74]. Another feature shown in Figure 2-14 is the corner recirculation zone (D), which is a consequence of the sudden expansion of the flow leaving the swirler [48,80]. The size and impact of this corner recirculation is difficult to determine, but higher swirling flow intensities lead to shorter reattachment length of the outer flow to the wall [48,80-83].

With this overall view of the primary zone, three regions can be modeled separately: 1) Corner recirculation zone (CRZ) representing region D in Figure 2-14, 2) Flame zone (FZ) representing regions A and C, and 3) Inner recirculation zone (IRZ) representing region B. The flame between the two recirculation zones is typically

represented by PSRs due to the high turbulence intensity present in this region [22,23]. This region interacts with the corner and inner recirculation flows. There are varying opinions on the arrangements of the PSRs to represent the flame regions, as seen in the preceding review section. It is common to represent high burning regions as a single PSR; however, some researchers have represented this region as two to three PSRs in series to spread out the flame [22,24]. The inner recirculation zone can be modeled by a single PFR to represent the low turbulence intensity characteristics exhibited in this region [22,72]. Alternatively, Sturgess and Shouse [1] suggest that the turbulence intensity present in the region is more than sufficient to be modeled as a PSR. This technique was utilized in the model by Russo *et al.* [24]. Typically, the inner recirculation region interacts with the main flame. The corner recirculation zone is modeled similarly to the IRZ and it interacts with the flame.

Figure 2-14: Primary zone flow.

Limited sources are available to describe the volumes and the interaction between the primary zone regions. Roberts *et al.* [84] describe a method to determine the zero

axial velocity boundary (C in Figure 2-14) by using semi-empirical correlations based on the work by Kind and Youssef [78]:

$$\frac{M_{ANG} r_c}{\rho_g V^2} = \frac{2\pi r_c}{3A_{sw}^2 C_{D,sw}} \tan \theta_v (r_t^3 - r_h^3) \quad (2-41)$$

The non-dimensional term on the left-hand side is described by the axial flux of angular momentum leaving the swirler defined below (M_{ANG} or G_ϕ), radius of the combustor (r_c), the gas density (ρ_g), and the axial volumetric flow rate (V). The right-hand side is composed of swirler flow area (A_{sw}), swirler vane turning angle (θ_v), swirler hub and tip radii (r_h and r_t), and swirler discharge coefficient given by:

$$C_{D,sw} = C_{D90^\circ} \cos \theta_v \quad (2-42)$$

According to Mattingly *et al.* [16], the discharge coefficient C_{D90° is taken to be 0.64. The value of the non-dimensional term is then used along with the correlation in Figure 2-15 to determine the boundary radius, r_r , where r_w is equal to the combustor radius, r_c . It should be noted that the above correlation was derived based on a non-reacting flow. This was justified by experiments by Kind and Youssef [78] that showed the outlines of recirculation flow to remain virtually unaffected by combusting flow, with only the velocities being enhanced. This agrees with a recent experimental study by Wicksall *et al.* [85] that showed no significant change in the size of the recirculation zone in a confined swirling flow when chemical reactions were introduced. Wicksall *et al.* [85] suggest this may be due to the radial expansion being constrained by the combustor walls.

Figure 2-15: Recirculation radius function; modified from [84].

From the experimental results of Beer and Chigier [77], the axial length of the recirculation region can be estimated by:

$$L = 1.62 S_n D_t \quad (2-43)$$

where D_t is the swirler tip diameter and S_n is the swirl number defined as the ratio of angular momentum flux (G_ϕ) to axial momentum flux (G_x) [77,86]:

$$S_n = \frac{G_\phi}{G_x r_t} \quad (2-44)$$

$$G_\phi = \int_0^R (wr) \rho u 2\pi r dr \quad (2-45)$$

$$G_x = \int_0^R u \rho u 2\pi r dr + \int_0^R P 2\pi r dr \quad (2-46)$$

where u is the axial velocity, w is the tangential velocity, P is the static pressure, and R is the radius of the swirler exit. While the swirl number is calculated from measured values of velocity and static pressure profiles, it can also be estimated geometrically [86]. For axial swirlers, swirl number is estimated by:

$$S_n = \frac{2}{3} \left[\frac{1 - (r_h/r_t)^3}{1 - (r_h/r_t)^2} \right] \tan \theta_v \quad (2-47)$$

To predict the flame zone defined in Figure 2-14 (regions A and C) Mattingly *et al.* [16] suggest the volume can be assumed to be one-eighth of the recirculation volume. The fact that a change in the axial length of the recirculation region would affect the size of the flame zone can be readily appreciated. Studies by Beer and Chigier [77] have shown that the recirculation height and length do not change independently of one another. Therefore, the estimation by Mattingly *et al.* [16], though perhaps oversimplified, may still be valid for determining the flame size.

Another possible method to define the volumes proposed by Swithenbank *et al.* [72] is to proportionally size the regions according to the amount of mass flow entrained in the region. Sources to determine the mass flow interaction between the different regions in the primary zone are also limited. One method proposed by Mattingly *et al.* [16] mentions the rate of entrainment of swirler air ($\dot{m}_{SW}$) into the recirculation zone at high swirl numbers ($S_n < 2.5$) can be approximated by:

$$\frac{\dot{m}_r}{\dot{m}_{SW}} = 0.1(S_n)^3 \quad (2-48)$$

where $\dot{m}_r$ is the mass flow rate recycled, as shown in Figure 2-16. This correlation was based on the experimental work performed by Mathur and Maccallum [87] who extensively studied swirling air jets from vane swirlers.

A separate study by Swithenbank *et al.* [72] used the simple free jet entrainment model developed by Ricou and Spalding [88] to calculate the amount of upstream flow entrained ($\dot{m}_m$) into the dilution jet ($\dot{m}_{DJ}$), as shown in Figure 2-16:

$$\frac{\dot{m}_m}{\dot{m}_{DJ}} = 0.32 \left(\frac{Y_c}{d_0} \right) \left(\frac{\rho}{\rho_j C_D} \right)^{1/2} \quad (2-49)$$

where $\dot{m}_{DJ}$ is the jet mass flow rate, Y_c is the distance penetrated by the jet, d_0 is the jet orifice diameter, C_D is the orifice discharge coefficient, and ρ, ρ_j are the hot- and jet-gas densities. Although this model was developed for non-reacting flows, reviews by Han and Mungal [89] indicated that the coefficient value of 0.32 can be replaced by 0.16 for reacting flows.

Figure 2-16: Primary zone airflow distributions.

For a combustor design, as demonstrated in Figure 2-14, a corner recirculation zone is created in part by a sudden expansion at the exit of the premixer. Conversely, in a design with a gradual expansion as shown in Figure 2-16, the induced axial pressure gradient is strong enough to force the outer flow to diminish the corner recirculation zone [5,15,80]. One possible way to estimate the volume enclosed by the corner recirculation zone is to determine the location of axial reattachment of the outer flow to the wall (Figure 2-17). This method is complicated since several factors influence the reattachment length, for example swirl number, heat release, and expansion ratio (ratio of combustor radius, r_c to inlet flow radius, r_t) [48,70,81,90]. One source by Vanierschot and Van den Bulck [81] surveyed multiple sources that studied the influence of swirl on reattachment length (z_R) and derived an analytical expression as a function of swirl number at the dump plane (S_D), expansion ratio (h), and reattachment length in the absence of swirl (δ_0):

$$z_R = \frac{r_t \delta_0}{1 + \delta_0^2 S_D^2} \left(\sqrt{(h^2 - 1) \delta_0^2 S_D^2 + h^2 - 1} \right) \quad (2-50)$$

$$h = \frac{r_c}{r_t - r_h} \quad (2-51)$$

The no-swirl reattachment length can be approximated using correlations provided by Eaton and Johnston [91] based on backward-facing-step calculations (Figure 2-18) where x_R is equal to z_R and $Y0$ and $Y1$ are equal to r_c and r_t , respectively.

Figure 2-17: Volume of corner recirculation zone.

Figure 2-18: Reattachment length as a function of expansion ratio [91].

Dilution Zone

In the secondary burn-up region of the combustor, the flow is commonly modeled using PFRs [1,20,22-24,37,72]. This is a valid assumption, considering the flow is uniform in the cross-section perpendicular to the gas flow following the intense mixing in the primary zone [20,25]. As discussed in previous sections for a PFR, under these conditions the reactions proceed at a finite rate with negligible axial mixing [25]. Typically, the dilution flow is represented by two distinct flows as seen in Figure 2-19: outer flow interacting with wall-cooling and core flow from the post-flame region [22-24]. The mass flow rate of the outer flow can be calculated using Equation 2-49, which calculates the amount of upstream flow entrained in the dilution jet. The remaining upstream flow not entrained in the jet is defined to be the core flow. The length of the dilution region (L_{DZ}) is defined by the distance from the dilution jet to the exit of the combustor. Near the combustor exit, the outer and core streams from the PFRs combine to mix together in a MIX reactor prior to exiting the combustor.

Figure 2-19: Flow interaction in the dilution zone.

Premixer

In modern gas turbine combustors, a premixer (Figure 2-20) is commonly used in lean-premixed designs to facilitate fuel evaporation (for liquid fuel) and mix fuel and air vigorously prior to combustion [7]. Ideally, the fuel-air mixture should be fully mixed at the exit of the premixer; however, in practice this is not the case and the degree of mixedness is the primary performance variable of the device [5,92]. The common terminology used for this parameter is unmixedness (S) and is described by Mikus and Heywood [93] as:

$$S = \frac{\sigma_\phi}{\phi_m} \quad (2-52)$$

where σ_ϕ is the standard deviation of the fuel-air equivalence ratio about the mean fuel-air equivalence ratio, ϕ_m . A standard deviation value of zero corresponds to perfect premixing in which the combustor burns at the mean equivalence ratio [92]. Sturgess *et al.* [94] suggest ϕ_m should be less than 0.7 and S should be less than 0.25 for typical lean-premixed combustion. Numerous studies have shown the consequence of unmixedness is a significant increase in NO_x emissions [95-97]. As a result, one possible way for improving CRN emission predictions is to incorporate the effect of unmixedness.

Figure 2-20: Premixer concept [5].

Sturgess and Shouse [1] state that the effect of unmixedness can be accounted for by replacing each individual reactor in a CRN with a parallel array of like-reactors. The total inlet flow is then distributed using a Gaussian approach along the array to describe the degree of mixing. Based on the works by Razdan *et al.* [95], a Gaussian equivalence ratio distribution best represents the local fuel concentration. Furthermore, the authors suggest 10 to 13 parallel reactors to be adequate to describe unmixedness, which agrees with the model of Allaire [37] discussed in the previous section. Similarly, Nicol *et al.* [25] used a Gaussian distribution of the fuel-air equivalence ratio given by:

$$g(\phi) = \frac{1}{\sigma_\phi \sqrt{2\pi}} \exp \left(-\frac{(\phi - \phi_m)^2}{2\sigma_\phi^2} \right) \quad (2-53)$$

to describe the unmixedness of the primary zone mass flow rate. Five discrete mass flow rates at the fuel-air equivalence ratio shown in Figure 2-21 were incorporated into a parallel arrangement of PSRs to simulate unmixedness in a CRN model (Figure 2-22). Results showed the assimilation of the unmixedness model successfully represented the behaviour of the experimentally-determined data [25]. Furthermore, it was demonstrated

that the leanest regions resulted in the highest production of CO emissions and the richest regions resulted in the highest NO_x emission.

Figure 2-21: Discrete normal Gaussian distribution of fuel-air equivalence ratio [25].

Figure 2-22: CRN model to account for unmixedness [25].

Alternatively, Novosselov [22] used a linear variation of fuel-air distribution with a non-uniform air mass flux profile at the premixer exit divided into three parallel streams (Figure 2-23). The linear variation was used to enhance the equivalence ratio variation

caused by non-uniform distribution of air mass flux [22]. To represent the effects of turbulent mixing between the three streams, Novosselov [22] incorporated cross-mixing to achieve uniform equivalence ratio downstream of the premixer exit. The results showed increases in NO_x emissions and flame temperatures for the linear fuel-air distribution compared to the uniform fuel-air distribution. This was attributed to local high fuel-air equivalence ratios.

Figure 2-23: Premixer exit streams to account for fuel-air distribution [22].

Wall-Cooling Effects

Another contributor of emissions discussed in earlier sections is the wall-cooling effect. In general, separate regions are not required to model the effects of cooling air entering through liner walls. Many models [20,37,72] have incorporated all wall-cooling flows into the core flow reactors, which may incorrectly diminish the CO and UHC emission production [94]. It may be more representative to use an outer flow region of PFRs to incorporate the cooling flows into the combustor as discussed previously [23,72].

3 Methodology

Considering the flowfield patterns of the combustor and the mechanism of emission formation, this chapter outlines a methodology to create a chemical reactor network (CRN) for a lean-premixed combustor based on the empirical and semi-empirical correlation method. The chapter begins with the selection of a suitable library of subroutines that solve the governing equations of the PSR and the PFR, and allows for a straightforward implementation of a network consisting of these reactors. This is followed by the idealized reactor representation of the combustor flowfield features.

3.1 Numerical Implementation

Libraries of subroutines such as CHEMKIN III, a group of FORTRAN subroutines [65,68,98] created by Sandia National Laboratories, are the most commonly used in solving the governing equations of the PSR and PFR to model a CRN [23,24,37]. The primary advantage of the CHEMKIN subroutine library is that it allows for easy incorporation of subroutines in a FORTRAN environment [23,24]. However, a more recent version of this software, namely CHEMKIN 4.1, maintained and distributed by ReactionDesign Inc. (San Diego, CA, USA), is only available commercially. The need for an open source code that can be incorporated into a design methodology led to a C++ based code for chemically reacting flow called Cantera. Originally developed for the chemical process industry by Professor David Goodwin at the California Institute of Technology, it has now gained popularity in combustion research [23]. A critical review of the available subroutines for chemical reactor modeling by Roby *et al.* [23] showed

Cantera to be one of the most promising software packages; however, they selected CHEMKIN due to Cantera's lack of a PFR subroutine. A new version of Cantera (version 1.7) has since updated the software package to incorporate a PFR model, and is thus suitable for use in the current research.

The basic structure of Cantera is shown in Figure 3-1. The software supports large reaction mechanisms and multiple user interfaces such as MATLAB (The MathWorks Inc, Natick, MA, USA), Python (Python Software Foundation, DE, USA), FORTRAN 90, and C++. However, only C++ is able to directly interface with the Cantera "kernel" without going through a library of functions. Consequently, Visual Studio C++ 2003 (Microsoft Corp. Redmond, WA) was used to implement Cantera for the present reactor network code. Details on Cantera's structure and its functionality can be found in the user manuals by Goodwin [67,99]. An introduction to reactor modeling using Cantera as well as a comparison with industry standard CHEMKIN is provided in Appendix B.

Figure 3-1: Cantera structure [67].

The PSR and PFR reactors in Cantera are represented by Reactor and FlowReactor objects, respectively. For MIX reactor, the Reactor object can be used with the chemistry disabled. The inputs required to describe each reactor are given in Table 3-1. In addition to the reactors used, an object known as a Reservoir (RES) is used to represent a container which stores a particular mixture at specified conditions. For example, for an incoming premixed air and fuel from the premixer, a Reservoir can be set to have the proper molar composition, temperature, and pressure to represent the mixture. The described reservoirs and reactors are connected using mass flow controllers and valves to provide constant mass flow and to maintain specified upstream pressure by adjusting its mass flow rate. Details of the connectivity of each of the objects are provided in Appendix B.

Table 3-1: Required inputs for reactor type.

Inputs	Reactor Types		
	PSR	PFR	MIX
Mass Flow Rate (kg/s)	X	X	X
Temperature (K)	X	X	X
Pressure (Pa)	X	X	X
Length (m)		X	
Volume (m³)	X	X	X

The proceeding sections describe the reactor modules that utilize the PSR, PFR, MIX and RES objects of Cantera to describe the reactor network representing a lean-premixed gas turbine combustor.

3.2 Chemical Reactor Network

The flowfield features of a lean-premixed combustor as identified in the previous chapter are shown in Figure 3-2. In the primary zone (PZ), the main features that were identified are the flame zone (FZ), corner recirculation zone (CRZ), the inner recirculation zone (IRZ), and the post-flame zone (PFZ). The flame zone is further divided into three zones: outer (OFZ), centre (CFZ), and inner (IFZ) flame zones. The dilution zone (DZ) is considered as one large region. In addition to these features, a premixing zone (PMZ) was also incorporated to test the effects of the mixedness of fuel and air from the premixer. The proposed chemical reactor model representing these flowfield features is shown in Figure 3-3. The rationale for the selection of the ideal reactors and the determination of volumes and flow splits for representing these features is described in the proceeding sections.

Figure 3-2: Idealized combustor flowfield.

Figure 3-3: Proposed chemical reactor model for a lean-premixed combustor.

3.2.1 Primary Zone

Flame Zones

The literature review revealed that the location of the intense flame region is commonly situated at the edge of the recirculation zone where combustion products combine with fresh reactants for continuous burning. This region is considered to have a high degree of turbulence that promotes rapid mixing. A recent study by Strakey *et al.* [100] showed this highly turbulent shear layer region to be associated with small Damköhler numbers ($Da \ll 1$) which is appropriately modeled by a PSR. In typical lean-premixed combustors, two recirculation zones are defined. These are the corner (CRZ) and inner (IRZ) recirculation zones as shown in Figure 3-4. Therefore, two intense flame regions that are represented by PSRs are modeled; these are labelled as outer flame zone (OFZ) and inner flame zone (IFZ) in the flame zone reactor model in Figure 3-5. These

two flame zones are defined to converge into one central flame zone (CFZ) represented by a PSR before entering the post-flame zone (PFZ) PSR. This configuration is consistent with the models developed by both Novosselov [22] and Russo *et al.* [24] using a CFD-based solution.

Figure 3-4: Primary zone flowfield.

The fuel and air flow entering the flame zone reactor model are determined by the premixing zone (PMZ) model. The output of the OFZ reactor is split three ways: 1) flow into the CRZ for recycling (*a* in Figure 3-4), 2) flow converging into the CFZ (*b*), and 3) flow into the dilution zone (DZ) along the wall (*c*). The output of the CFZ reactor enters the PFZ. As for the PFZ reactor, a fraction of the flow enters the IRZ for recycling (*d*), and the remaining portion flows into the dilution zone (*e*). Details of the volumes and flow split calculations are given in the next section.

Figure 3-5: Flame zone reactor model.

Recirculation Zones

Unlike the flame zone, which is consistently modeled by a PSR, the recirculation zone has been modeled by a PFR in some reactor models [22,72] and by a PSR in others [1,24]. The use of a PFR can be attributed to the relatively low turbulence intensity in this region compared to the edge of the recirculation zone (shear layer), leading to the assumption that only a small amount of axial mixing is present. However, the study by Strakey *et al.* [100] discussed above indicated that the Damköhler number in the corner and inner recirculation zones are less than unity, which can be appropriately modeled by a PSR. This agrees with the model by Sturgess and Shouse [1] who represented the recirculation regions by a PSR. Consequently, the current model incorporates a PSR to model both inner and corner recirculation zones as shown in Figure 3-6.

The flow entering the recirculation zones is related to the flame zone reactor discussed above. Depending on the combustor design, dome-cooling air flow is mixed in the CRZ reactor.

Figure 3-6: (a) Inner and (b) Corner recirculation reactor models.

3.2.2 Dilution Zone and Wall-Cooling

With the diminishing turbulence downstream of the primary zone, the dilution zone is most effectively represented by PFRs [1,22-24]. The main function of this zone is to complete the combustion of the mixture leaving the primary zone by oxidizing the remaining CO to CO₂. As discussed previously, the dilution zone should ideally be divided into two separate flows, outer and core flows, similar to the CRNs produced by Russo *et al.* [24] and Novosselov [22] (Figure 3-2). However, due to a lack of correlations that define the volumes separately for outer and core flows, the dilution zone is considered to be one large region. In this region, the flows entering from the OFZ and PFZ combine with the dilution air in the MIX reactor (Figure 3-7). The product of the MIX reactor is then fed into the PFR to allow reactions to take place along the length of the reactor, before exiting into the turbine (Figure 3-7).

Figure 3-7: Dilution zone reactor model.

3.2.3 Premixer

The premixing zone reactor model was based on the work by Nicol *et al.* [25]. Three reservoirs are created to represent discrete Gaussian distribution of the fuel-air equivalence ratio as shown in Figure 3-8 and Figure 3-9. The centre reservoir (RES_{CF}) supplies the CFZ reactor with the mean equivalence ratio given by the preliminary design. The outer reservoirs (RES_{OF} and RES_{IF}) supply slightly lean (ϕ_{OF}) and slightly rich (ϕ_{IF}) equivalence ratios to the OFZ and IFZ, respectively. The Gaussian distribution is normalized to set 50 percent of incoming mass flow rate at mean equivalence condition while 25 percent each at ϕ_{OF} and ϕ_{IF} as suggested by Nicol *et al.* [25].

Figure 3-8: Discrete equivalence ratio distribution.

Figure 3-9: Premixing zone reactor model.

3.3 Reactor Volumes and Flow Splits

With the reactor network defined, the reactor volumes and flow splits are determined in this section. The main features of the combustor and the volumes they encompass are schematically shown in Figure 3-10.

Figure 3-10: Reactor volumes.

3.3.1 Volumes

Inner Recirculation Zone (IRZ)

The volume of the inner recirculation zone shown in Figure 3-10 can be represented by an ellipsoid partially intersecting the swirler hub at the location where the flame is said to be anchored. The corresponding height and lengths of the ellipsoid are calculated using the correlations obtained from Roberts *et al.* [84] and Beer and Chigier [77] respectively, as discussed in the previous chapter. The validity of these correlations

will be discussed in detail in the next chapter. The expressions discussed in Chapter 2 are repeated here for completeness. For the height of the inner recirculation ellipsoid, the expression given by Roberts *et al.* [84] is:

$$\frac{M_{ANG} r_c}{\rho_g V^2} = \frac{2\pi r_c}{3A_{sw}^2 C_{D,sw}} \tan \theta_v (r_t^3 - r_h^3) \quad (3-1)$$

where M_{ANG} is the axial flux of angular momentum leaving the swirler, r_c is the radius of the combustor, ρ_g is the gas density, V is the axial volumetric flow rate, A_{sw} is the swirler flow area, θ_v is the swirler vane turning angle, r_h and r_t are the swirler hub and tip radii, and $C_{D,sw}$ is the swirler discharge coefficient given by:

$$C_{D,sw} = C_{D90^\circ} \cos \theta_v \quad (3-2)$$

where C_{D90° is the discharge coefficient taken to be 0.64 [16]. The correlation given in Figure 2-15 was digitized and the curve was fitted using Curve Fitting Toolbox (MATLAB) to give the following expression for inner recirculation height as a function of Equation 3-1:

$$r_{IRZ} = r_c \left[-0.478 \left(\frac{M_{ANG} r_c}{\rho_g V^2} \right)^{-0.761} + 0.945 \right] \quad (3-3)$$

The length of the inner recirculation zone was estimated using the correlation provided by Beer and Chigier [77]:

$$L_{IRZ} = 1.62 S_n (2r_t) \quad (3-4)$$

where S_n is the swirl number, which is given by the preliminary design (Appendix A).

With the calculated values for height and length of the inner recirculation zone, the volume of the ellipsoid can be determined. First, the intersection of the ellipse with the swirler must be found (as shown in Figure 3-11). The equation of an ellipse is given by:

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \quad (3-5)$$

Where b is the inner recirculation height (r_{IRZ}) and a is:

$$a = \frac{l + L_{IRZ}}{2} \quad (3-6)$$

Solving Equations 3-5 and 3-6 for the intersection point l with $x = l$ and $y = r_h$ gives:

$$l = L_{IRZ} \left(\frac{r_{IRZ}^2 - r_h^2 + 2(r_{IRZ}^4 - r_{IRZ}^2 r_h^2)^{1/2}}{3r_{IRZ}^2 + r_h^2} \right) \quad (3-7)$$

Figure 3-11: Intersection of ellipse to the swirler hub.

The portion of the volume that represents the inner recirculation zone is then calculated using the formula for a volume of revolution around the x-axis [101]:

$$V = \int_{-r}^r \pi [f(x)]^2 dx \quad (3-8)$$

$$V_{IRZ} = 2\pi b^2 \int_0^a \left(1 - \frac{x^2}{a^2}\right) dx - \pi b^2 \int_{-a}^{-l} \left(1 - \frac{x^2}{a^2}\right) dx \quad (3-9)$$

Corner Recirculation Zone (CRZ)

The corner recirculation zone shown in Figure 3-10 encompasses the area enclosed from the edge of the swirler tip (r_t) to the reattachment of the swirling flow to the outer wall. The correlation given by Vanierschot and Van den Bulck [81] as described in the previous chapter is used to calculate the axial reattachment length, L_{CRZ} :

$$L_{CRZ} = \frac{r_t \delta_0}{1 + \delta_0^2 S_D^2} \left(\sqrt{(h^2 - 1) \delta_0^2 S_D^2 + h^2} - 1 \right) \quad (3-10)$$

where S_D is the swirl number at the dump plane, h is the expansion ratio, and δ_0 is the reattachment length in the absence of swirl. The non-swirling reattachment length δ_0 is calculated using the following expression as a function of expansion ratio (h) from the correlation of Figure 2-18:

$$\delta_0 = 2.496h + 3.383 \quad (3-11)$$

where the expansion ratio is:

$$h = \frac{r_c}{r_t - r_h} \quad (3-12)$$

where r_h is the swirler hub radius and r_c is the combustor radius. Using the corner reattachment length, the volume of the corner recirculation zone can be calculated by

integrating the region bounded by curves $f_1(x)$ and $f_2(x)$, as shown in Figure 3-12. The curves can be represented simply by the line equation:

$$f_1(x) = \frac{r_c - r_t}{L_{CRZ}} x + r_t \quad (3-13)$$

$$f_2(x) = r_c \quad (3-14)$$

Using the formula for a volume of revolution (Equation 3-8):

$$V_{CRZ} = \int_0^{L_{CRZ}} \pi [r_c]^2 dx - \int_0^{L_{CRZ}} \pi \left[\frac{r_c - r_t}{L_{CRZ}} x + r_t \right]^2 dx \quad (3-15)$$

If the combustor design has a tapered corner, the above procedure is repeated to calculate the region bounded by curves $f_2(x)$ and $f_3(x)$ and is subtracted from the volume calculated previously.

Figure 3-12: Corner recirculation area

Flame Zones

As suggested by Mattingly *et al.* [16], the intensively mixed zone representing the flame region can be approximated by assuming the volume is one-eighth of the recirculation zone. Therefore, the volumes of the outer and inner flame zones (OFZ and IFZ) are:

$$V_{OFZ} = \frac{1}{8} V_{CRZ} \quad (3-16)$$

$$V_{IFZ} = \frac{1}{8} V_{IRZ} \quad (3-17)$$

The validity of this estimation was discussed in Chapter 2. More detail on the sensitivity of this estimation is provided in the proceeding chapters. The outer and inner flame zones combine to mix in the centre flame zone (CFZ), therefore the CFZ volume is taken to be the sum of the OFZ and IFZ volumes:

$$V_{CFZ} = V_{OFZ} + V_{IFZ} \quad (3-18)$$

Finally, the post-flame zone is assumed to occupy the remaining volume of the primary zone:

$$V_{PFZ} = V_{PZ} - V_{OFZ} - V_{CFZ} - V_{IFZ} - V_{CRZ} - V_{IRZ} \quad (3-19)$$

where V_{PZ} is the volume of the primary zone which is given by the preliminary combustor design (Appendix A).

Dilution Zone

The volume and length of the dilution zone, V_{DZ} and L_{DZ} , are dictated by the preliminary combustor design (Appendix A).

3.3.2 Flow Splits

The major flow splits, such as the amount of flow entering through the premixer, dome, dilution, and wall-cooling, are predetermined from the preliminary combustor design (Table 3-2). From these parameters, the important flow splits that need to be determined are the proportion of premixer flow entering the flame zones, the amount of combusted products entering the recirculation zones, and the flow into the dilution zone.

Table 3-2: Preliminary combustor design flow split variables.

Flow Split	Fraction of Total Air Flow ($\dot{m}_a$)
Swirler	f_{SW}
Dome-Cooling	f_{DC}
Wall-Cooling	f_{WC}
Dilution Jet	f_{DJ}

Premixer

As described in the previous section, mixing of fuel and air is accomplished in the premixer. For the premixing zone reactor model, an unmixedness parameter (S) of 0.25 is selected based on the suggestion by Sturgess *et al.* [94] for lean-premixed combustors. Combining this with the given mean equivalence ratio from the preliminary combustor design, the standard deviation of the equivalence ratio about the mean is calculated:

$$\sigma_{\phi} = S \cdot \phi_m \quad (3-20)$$

To set the mass flow rates according to the normal distribution (Equation 2-53) as was done in the work of Nicol *et al.* [25], the mean equivalence ratio is set equal to 50 percent of total mass flow rate to exit the RES_{CF} reservoir (f_{CF}) (refer to Figure 3-8 and Figure 3-9). The fraction exiting the RES_{OF} (f_{OF}) and RES_{IF} (f_{IF}) reservoirs are set to 25 percent of the total mass flow rate. To calculate the equivalence ratios for the corresponding reservoirs (ϕ_{OF} and ϕ_{IF}), the following relation based on Equation 2-53 is used:

$$\frac{g(\phi)}{g(\phi_m)} = \frac{f_{OF,IF}}{f_{CF}} \quad (3-21)$$

$$\phi_{OF,IF} = \phi_m \pm \sigma_{\phi} \sqrt{\ln \left(\frac{f_{OF,IF}}{f_{CF}} \right)^{-2}} \quad (3-22)$$

The lower equivalence ratio is ϕ_{OF} and the higher value is ϕ_{IF} .

Primary Zone

Fraction of flow entering the OFZ, CFZ, and IFZ shown in Figure 3-13 is equal to the flow exiting the RES_{OF}, RES_{CF}, and RES_{IF} reservoirs described above, respectively:

$$f_{OFZ} = f_{OF} = 0.25 \quad (3-23)$$

$$f_{CFZ} = f_{CF} = 0.5 \quad (3-24)$$

$$f_{IFZ} = f_{IF} = 0.25 \quad (3-25)$$

At split point 1 (S1) in Figure 3-13, the fraction of flow exiting the OFZ is split three ways. Due to the lack of correlations describing the flow interaction at this point, fractions are based on experimental results by Coghe *et al.* [102] and on the works of Russo *et al.* [24] and Novosselov [22]:

$$f_{OFZ,DZ} = 0.5 \quad (3-26)$$

$$f_{OFZ,CFZ} = 0.4 \quad (3-27)$$

$$f_{OFZ,CRZ} = 0.1 \quad (3-28)$$

where $f_{OFZ,DZ}$ is the fraction of OFZ flow entering the DZ, $f_{OFZ,CFZ}$ is the fraction of OFZ flow entering the CFZ, and $f_{OFZ,CRZ}$ is the fraction of OFZ flow entering the CRZ. Detailed discussions on the selection of these fractions and sensitivity of the predicted emissions to their values are discussed in the proceeding chapters.

Figure 3-13: Primary zone flow splits.

At split point 2 (S2), the correlation given by Mattingly *et al.* [16] is used to describe the amount of flow entrained in the inner recirculation zone (IRZ) as a fraction of total swirler flow:

$$\frac{\dot{m}_r}{\dot{m}_{sw}} = 0.1(S_n)^3 \quad (3-29)$$

$$f_{PFZ,IRZ} = \frac{\dot{m}_{sw}}{\dot{m}_{PFZ}} 0.1(S_n)^3 \quad (3-30)$$

where $\dot{m}_r$ is the mass flow rate recycled, $\dot{m}_{sw}$ is the mass flow rate through the swirler, $\dot{m}_{PFZ}$ is the mass flow rate through the PFZ reactor, and S_n is the swirl number. The remaining flow from the PFZ reactor enters the MIX reactor in the dilution zone.

Dilution Zone

All of the flows entering the dilution zone are as described above and are repeated below for completeness.

$$f_{OFZ,DZ} = 0.5 \quad (3-31)$$

$$f_{PFZ,DZ} = 1.0 - f_{PFZ,IRZ} \quad (3-32)$$

The dilution jet flow mixes with the flow from the post-flame and outer flame zones in the MIX reactor shown in Figure 3-7.

4 Validation

Before arriving at the final step of predicting emissions with the proposed CRN, the accuracy with which the aforementioned correlations can successfully predict the flowfield features (volumes and flow splits) must be determined. More specifically, the ability of these correlations to predict these flow patterns in comparison to CFD methods of varying complexity, which are typically used in developing a CRN, is to be established. In combustors, the recirculation zones exert the greatest influence on flame shape, flame stability, and heat release rate, and consequently on emissions [103]. This chapter provides a detailed look at the prediction of the corner and inner recirculation zones by using representative cases of typical gas turbine combustor flows. Following this is an examination of the validity of calculations related to the flame and post-flame zones, and of the flow splits in the primary zone. The accuracies of the overall primary and dilution zone sizes are not discussed, since they are solely determined by the preliminary design of the combustor.

4.1 Primary Zone

4.1.1 Recirculation Zones

To identify how the correlations method of determining the recirculation zone sizes compares with CFD methods, two cases representing typical gas turbine combustor flows are used. The general requirements for these cases were:

1. Sudden expansion combustor creating a corner recirculation

2. Sufficiently strong swirling flow, inducing inner recirculation
3. Availability of experimental data and CFD solutions

The basic representation of the combustor for all cases discussed hereafter is shown in Figure 4-1.

Figure 4-1: Generic confined swirling flow combustor.

Table 4-1: Combustor geometry parameters for Case 1 and Case 2.

Parameter	Case 1: Nejad <i>et al.</i> [104]	Case 2: Dellenback <i>et al.</i> [105]
Combustor Length, L_C , (cm)	185	104
Combustor Radius, r_C , (cm)	7.62	4.93
Swirler Tip Radius, r_t , (cm)	5.08	2.54
Swirler Hub Radius, r_h , (cm)	0.95	n/a
Swirler Angle, θ_v (deg)	36	n/a
Swirl Number, S_n	0.5	0.6

The first case is based on the work by Nejad *et al.* [104], where the flowfield of a cold-flow dump combustor was measured using two-component laser velocimetry. The inlet flow at Reynolds number of 125,000 (based on the inlet diameter) passed through

axial swirlers which imparted sufficient swirl to induce an inner recirculation zone. The pertinent parameters for this combustor (Case 1) are listed in Table 4-1. For this case, along with the correlations, the turbulence models used in the CFD methods to predict the recirculation zones are the standard $k-\epsilon$ model, RSM-based LRR and SSG models, as introduced in Chapter 2. The predicted parameters and their respective sources are listed in Table 4-2. It should be noted that all dimensions in this table are normalized with respect to the step height of the combustor ($H = r_c - r_t$) to be consistent with reported values. Compared to experimental results, the $k-\epsilon$ model performs the worst by under-predicting both the inner recirculation height and length by roughly 38 and 81 percent, respectively, while the more complex RSM-SSG model predicted these dimensions to within 10 percent. The correlations-based method performs better than the $k-\epsilon$ and RSM-LRR models by under-predicting the height and length by approximately 20 and 26 percent. The substantial under-prediction of the $k-\epsilon$ model compared to the experimental data is due to the model's inability to adapt to sudden changes in strain caused by swirl [106]. This conclusion was noted in a similar combustor study comparing the standard $k-\epsilon$ model, RNG $k-\epsilon$ and RSM-LRR models [54]. In the same study, it was noted that RNG $k-\epsilon$ model, which is designed to perform better in situations with high strain rates, only showed minor improvements over the standard $k-\epsilon$ model. On the other hand, the RSM-LRR and RSM-SSG models, which resolve the anisotropic nature of turbulent flow, are able to handle the swirling flow in this case.

The length of the corner recirculation zone is predicted to within 10 percent by all methods with the RSM-LRR providing the best result. Overall, only the more

computationally-intensive RSM-SSG model is able to outperform the correlations-based prediction for this case.

Table 4-2: Experimental and predicted dimensions for Case 1.

Method	Source	L_{CRZ}/H	r_{IRZ}/H	L_{IRZ}/H
Experimental	Nejad <i>et al.</i> [104]	3.20	0.40	4.40
CFD – Standard $k-\epsilon$	Lai [107]	3.53	0.25	0.84
CFD – RSM-LRR	Lai [107]	3.15	0.55	5.96
CFD – RSM-SSG	Lu and Semiao [108]	n/a	0.37	4.50
Correlations	Equations 3-10, 3-3, 3-4	3.39	0.32	3.24

Based on the work of Dellenback *et al.* [105], Case 2 provides swirling flow into a sudden expansion tube. The Reynolds number for this flow was 30,000, based on the inlet diameter. All other parameters for this case are given in Table 4-1 (Case 2) above. Unlike the first case, the swirl is not produced by axial swirlers, but rather produced from tangential jet injection. As such, the correlations for the recirculation height (Equation 3-3), which is based on axial swirlers, cannot be used. For this case, the turbulence models compared in predicting the recirculation zones are the standard $k-\epsilon$ model, RSM-LRR model, and LES using the Smagorinsky-Lilly model to represent the sub-grid-scale turbulence. The predicted parameters and their respective sources are listed in Table 4-3. All dimensions in this table are normalized with respect to the inlet diameter ($D_t = 2r_t$) to be consistent with reported values. For Case 2, again the standard $k-\epsilon$ model performs the worst by under-predicting the height and length by 43 and 58 percent, respectively. The correlations-based method is equally poor in predicting the recirculation length

compared to experimental results. The most complex of the CFD models, LES, best predicts the recirculation height and length to within 20 and 10 percent (under-predicted), respectively. These results are in agreement with a study by Wang *et al.* [103], who compared experimental combustor results to LES simulations and found predictions to be within the same range. The prediction of the corner recirculation length is best predicted by correlations and LES methods while the standard $k-\epsilon$ model performs the worst.

Table 4-3: Experimental and predicted dimensions for Case 2.

Method	Source	L_{CRZ}/D_t	r_{IRZ}/D_t	L_{IRZ}/D_t
Experimental	Dellenback <i>et al.</i> [105]	1.20	0.30	3.0
CFD – Standard $k-\epsilon$	Chang <i>et al.</i> [109]	0.45	0.17	1.25
CFD – RSM-LRR	De Langhe <i>et al.</i> [110]	1.00	0.19	2.5
CFD – LES	Schluter [111]	1.25	0.25	2.75
Correlations	Equations 3-10, 3-3, 3-4	1.22	n/a	1.00

In considering these cases, the use of the correlations-based method is justifiable in predicting the sizes of the recirculation zones. Though there are discrepancies compared to experimental results, the relative accuracy in predicting volumes is quite reasonable when compared to advanced versions of CFD-based methods. Moreover, the correlations-based method predicts these volumes by using only a fraction of the computing time used in CFD-based methods. Based on these two cases, the correlations-based method under-predicts the corner and inner recirculation zone volumes to within 10 and 50 percent accuracies, respectively, compared to experimental data. However, the

standard $k-\epsilon$ model appears to further under-predict the recirculation zone volumes. This can lead to an incorrect prediction of the emissions output.

4.1.2 Flame Zone

The flame is located in the shear layers of the recirculation zones. As a result, its volumes are closely related to that of the recirculation zones. The correlation by Mattingly *et al.* [16] uses this notion to predict the flame zone to be one-eighth or 12.5 percent of the recirculation zone volume. This estimation agrees well with that of the CRNs created by Russo *et al.* [24] and Novosselov [22], who predicted the flame zone sizes to be 16 and 15 percent of the recirculation zone volumes, respectively, using hot-flow CFD methods. The accuracy with which the flame zone volume is estimated is directly dependent on the prediction of recirculation zone volumes, which have been validated in the experimental cases outlined previously. Further validation of the flame zone volume itself would be beneficial using actual experimental data on reacting flows. The next chapter elaborates on the sensitivity of the emissions prediction to variations in flame zone and recirculation zone volumes of a lean-premixed combustor.

4.1.3 Post-Flame Zone

After identifying the recirculation and flame zone volumes within the primary zone, the residual volume is considered to be the post-flame zone. The accuracy of this estimation is thus dependent on the prediction of other zones occupying the primary zone.

4.1.4 Primary Zone Flow Splits

In addition to defining volumes, mass flow rate entering and exiting each reactor is an important parameter that must be predicted in order to create a CRN. The partitioning of flow amongst the various chemical reactors ultimately determines, in conjunction with the reactors' volumes, the time that species reside in each reactor. In other words, the partitioning influences the residence time for reactions to occur, which then determines the amount of emissions formed.

Equations 3-26 to 3-28 are used to describe the flow splits from the outer flame zone. From the flow exiting this zone, roughly 10 percent, or 2.5 percent of total mass flow, is recycled into the corner recirculation zone. Due to the lack of correlations available to predict this fraction, this value was obtained from similar reactor network studies [22,24] and comparisons to an experimental study by Coghe *et al.* [102]. The experimental study showed the fraction of flow recycled in the corner to be between 2 and 5 percent of the total flow entering through the swirlers. The remaining flow was distributed between the outer and centre flows, based on the work of Russo *et al.* [24] and Novosselov [22]. The subsequent chapter expands on the sensitivity of the emissions prediction to variations in the flow distributions of a lean-premixed combustor.

The mass flow recycled into the inner recirculation zone from the post-flame zone is calculated by Equation 3-30, which is based on experimental results of Mathur and Maccallum [87]. To verify this correlation, calculated fractions of total mass flow recycled in an experimental study by Schmittel *et al.* [112] showed approximately 8 and 20 percent for swirl numbers of 0.9 and 1.4, respectively. Accordingly, using this correlation, these fractions were predicted to be 7 and 27 percent for swirl numbers of 0.9

and 1.4, respectively. The discrepancies between the experimental and predicted values are explained in predicting the emissions of the lean-premixed combustor in the next chapter.

4.2 Dilution Zone

The volume of the dilution zone is solely determined from the preliminary design, while the mass flow rates entering this zone are determined from the primary zone flowfield features. This zone serves to combine all the flows exiting the primary zone to complete the oxidation of the remaining CO to CO₂. Ideally, as mentioned in the preceding chapters, it is preferable to have two separate zones, an outer flow near the wall and a core flow in the centre of the combustor, to properly handle CO destruction. However, this separation of zones is not possible due to the lack of applicable correlations.

4.3 Emissions Prediction

Having evaluated the volume and flow split correlations, the chemical reactor network is applied to two combustors for emissions prediction: 1) a lean-premixed combustor with experimental emissions data and 2) the preliminary lean-premixed combustor developed at Carleton University. The first case is used to provide feedback on the capabilities of the CRN, while the second case is the motivation behind the development of the present CRN.

4.3.1 DOE-HAT Combustor

The first case is based on the work by Bhargava *et al.* [113] and Cannon *et al.* [51] on a lean-premixed combustor from a U.S. Department of Energy (DOE)-sponsored Humid Air Turbine (HAT) project. The basic dimensions of the DOE-HAT combustor are shown in Figure 4-2 and the specifications required for the analysis are given in Table 4-4. This case was chosen due to the simplicity of the combustor, which has no dome- or dilution-cooling that can lead to excessive pollutant formation. In addition to the experimental measurements, Cannon *et al.* [51] provide CFD-predicted emissions data using LES and RANS-based RNG $k-\epsilon$ models. With this information, the ability of the correlations-based CRN to predict emissions can then be compared to the three aforementioned existing methods.

The experimental measurements were made using a three-hole water-cooled suction probe situated 38.1 cm downstream of the inlet plane (Figure 4-2). One port was located at the combustor centerline and two ports (180° apart) were located 4.3 cm away from the centerline [51]. For the LES prediction, the sub-grid-scale turbulence was modeled using Localized Dynamic Kinetic energy Model (LDKM) and a two-step assumed-PDF method was used to model the unresolved turbulence-chemistry interactions. The latter method uses a two-step chemical mechanism (shown below) in which fuel oxidizes to CO and then the CO oxidizes to equilibrium products at finite rates.

A decoupled NO_x transport equation was separately solved at each time-step using the thermal NO mechanism discussed previously in Chapter 2. This treatment for thermal NO is based on the assumption that fuel combustion is complete before NO formation becomes significant, thereby uncoupling the two processes [17]. This treatment is common for most CFD simulations to reduce the computing cost [17,42]. For the steady-state RANS calculations, Cannon *et al.* [51] used RNG $k-\epsilon$ model to account for the effects of turbulence and the same turbulence-chemistry interaction model as the LES case. For both cases, a $1/16^{\text{th}}$ sector of the premixer was simulated to provide the necessary exit profiles of velocity, pressure, temperature, turbulence quantities and equivalence ratio for boundary condition mapping.

The DOE-HAT combustor serves as a baseline to validate the proposed CRN and the correlations described in preceding sections. Furthermore, the proposed full CRN (8 reactors) was reduced in number to 5 and 2 reactors to examine the degree of complexity required to successfully predict emissions for this simple lean-premixed combustor. Of note, one parameter commonly obtained from preliminary combustor design is the length of the primary zone, which is not available on this combustor. Based on combustor design methodologies of Sawyer [15], the primary zone length is taken to be three-quarters of the combustor diameter.

Figure 4-2: Specifications of the DOE-HAT combustor.

Table 4-4: Flow parameters for DOE-HAT combustor.

Parameter	Value
Combustor Inlet Temperature (K)	734
Combustor Inlet Pressure (MPa)	1.378
Fuel Type	CH ₄ (methane)
Mean Equivalence Ratio, ϕ_m	0.58, 0.5, 0.42
Swirler Air (kg/s)	0.96
Swirl Number, S_n	0.6
Swirl Angle, θ_v (deg)	45

4.3.2 P-LP Combustor

Although a preliminary lean-premixed (P-LP) combustor was developed by Charest [5] at Carleton University, and deemed successful in meeting temperature and structural requirements, the preliminary design had not included a specific tool to

The CFD simulation used by Charest is compared to the present correlations-based CRN to predict the emissions output. Charest predicted the emissions output using a two-step Westbrook and Dryer global mechanism for fuel oxidization of decane, as shown below. However, fluid properties of Jet-A were used to calculate the thermodynamic properties, since fluid properties of decane were not available in the CFD code used [5].

NO_x was post-processed using a two-step thermal NO mechanism (Equation 2-6 and Equation 2-7 in Chapter 2). Heat transfer and radiation models were incorporated using total energy and differential approximation methods, respectively [5].

Table 4-5: Parameters for the P-LP combustor.

Parameter	Value
Combustor Inlet Temperature (K)	575
Combustor Inlet Pressure (MPa)	0.8
Fuel Type	C ₁₂ H ₂₃ (Jet-A)
Mean Equivalence Ratio, ϕ_m	0.55
Swirler Air (kg/s)	2.48
Dilution Air (kg/s)	2.91
Swirl Number, S_n	1.2
Swirl Angle, θ_v (deg)	60

The correlations-based CRN model is applied to these two test cases. The first case, which uses methane-air for combustion, utilizes the industry standard GRI-Mech 3.0 [21] chemical reaction mechanism for the reactor network calculations. Due to the large number of chemical reactions, the reader can consult the work of Smith *et al.* [21] for a detailed list of the chemical reactions for GRI-Mech 3.0. For the second case, which uses Jet-A ($C_{12}H_{23}$) as the fuel, Kollrack's 30-reaction mechanism for $C_{12}H_{23}$ -air combustion is used from the works of Mattingly *et al.* [16]. The list of the chemical reactions for the Jet-A reaction mechanism is provided in Appendix D. For both cases, the reactor network assumes adiabatic combustion (i.e. no heat loss). This is a simplified assumption made due to the constraints of the reactor network code.

5 Results and Discussion

This chapter presents the emissions predictions of the two combustor cases outlined in the preceding chapter: 1) the DOE-HAT combustor and 2) the P-LP combustor. The emissions presented are all corrected to 15 percent excess oxygen on a dry basis to compare with the experimental emissions reported by Cannon *et al.* [51]. The correction formulas are given in Appendix E.

5.1 DOE-HAT Combustor

The reactor network used for the DOE-HAT combustor is shown in Figure 5-1. The main difference from the more elaborate network shown in Chapter 3 is that the dome- and dilution-cooling air is removed to adapt to the DOE-HAT combustor. The network consists of six PSRs to represent the primary zone, one MIX and one PFR to represent the dilution zone, and a premixing zone to model the effects of fuel-air unmixedness.

Figure 5-1: DOE-HAT combustor chemical reactor network with 8 reactors.

5.1.1 Emission Predictions Compared to Experimental Results

The reactor network's ability to predict the DOE-HAT combustor's experimental emissions data for carbon monoxide (CO) is shown in Figure 5-2 for three equivalence ratios which are typical of industrial lean-premixed gas turbine combustors [6]. The results show that with the uniform-equivalence-ratio inflow, CO emission is predicted to within 21 and 8 percent for equivalence ratios of 0.58 and 0.50, respectively. The addition of the premixing model, assuming fuel-air is not perfectly mixed (non-uniform-equivalence-ratio inflow) prior to entering the combustor, shows no difference in CO output compared to the uniformly-mixed model, which was not expected. Studies by Nicol *et al.* [25] showed that the non-uniform-equivalence-ratio inflow should lead to increases in CO output compared to the uniform-equivalence-ratio inflow. Furthermore, at the leanest condition (0.42), the predictions significantly deviate from the experimental results. As discussed next, both of these discrepancies are believed to be attributed to the improper modeling of the dilution zone, which, due to the lack of correlations describing the flow in this zone, is modeled by a single PFR.

As discussed in previous chapters, the flow in the dilution zone is typically split into two flow regions: an outer flow near the wall and a core flow along the centre of the combustor. This is done primarily to represent the lower equivalence ratio along the combustor wall, which leads to reduced conversion of CO to CO₂, resulting in increased CO output in the outer flow [25]. To verify this concept, the dilution zone was modeled by two separate PFRs representing the outer (OF) and core flows (CF) before combining in the MIX reactor, as shown in Figure 5-3. The volume for the outer flow was assumed to be 10 percent of the total dilution zone volume, according to visual inspection of the

equivalence ratio distribution of the hot-flow LES solution of the same combustor by Cannon *et al.* [51]. The flow originating from the outer-flame zone (OFZ) is directed to the outer dilution region. Similarly, the flow originating from the post-flame zone (PFZ) is directed to the core dilution region as shown in Figure 5-3. The resulting CRN consisting of 9 reactors using the modified dilution zone is shown in Figure 5-4. The result of this modification on CO output is shown in Figure 5-5. The separation of the dilution zone correctly predicts the trend of increased CO output for the leanest case and displays sensitivity to the equivalence ratio non-uniformity at the inlet. To accurately predict CO output, proper division of the dilution zone is thus necessary based on physical properties of the flowfield as demonstrated in this test case. Based on sensitivity studies examining the variation of the outer flow portion, as detailed in Appendix C, an increase in its size within the dilution zone leads to decreased CO output and vice versa. This is expected since the increase in the outer flow volume increases the residence time allowing CO to further oxidize to CO₂. These changes are more sensitive to the leanest equivalence ratio than to the higher equivalence ratios; however, further correlations based on experimental results are required to verify the effects in the leanest case. Considering this, the remaining discussion will keep the modified representation of the dilution zone for the proposed CRN (Figure 5-4).

Figure 5-2: CO emission for the DOE-HAT combustor using the 8-reactor CRN.

Figure 5-3: Dilution zone represented by (a) single flow and (b) two separate flows.

Figure 5-4: DOE-HAT combustor chemical reactor network with 9 reactors.

Figure 5-5: CO emissions for the DOE-HAT combustor using the 9-reactor CRN.

The comparison of predicted NO_x output to the experimental data for three equivalence ratios using the 9-reactor CRN is shown in Figure 5-6. The uniform-equivalence-ratio inflow under-predicts the experimental data by roughly 38, 45, and 41 percent for equivalence ratios of 0.58, 0.50, and 0.42, respectively. For the condition of the non-uniform-equivalence-ratio inflow, which is more representative of a real combustor inlet, the NO_x predictions are over-predicted by 38, 40, and 23 percent for equivalence ratios of 0.58, 0.50, and 0.42, respectively. The substantial increase in NO_x output as a result of the non-uniform-equivalence-ratio inflow compared to the uniform case indicates a strong temperature dependence of NO_x production, which agrees with similar studies [22,25,72]. The region of richer fuel-air mixtures created by the non-uniform-equivalence-ratio inflow leads to local increases in temperature, which consequently increases the NO_x production significantly. At the same time, the leaner region created by the non-uniform-equivalence-ratio inflow increases the formation of CO, which leads to a better agreement of the results to the experimental data (Figure 5-5). This is precisely what is reported in the study by Nicol *et al.* [25], in which the leanest regions of the combustion from inlet unmixedness led to an increase in CO emitted, while the richest regions led to an increase in NO_x emitted.

Figure 5-6: NO_x emissions for the DOE-HAT combustor using the 9-reactor CRN.

Although the predicted emissions are comparable to the experimental results, the over-prediction of CO, and more specifically NO_x output with the non-uniform-equivalence-ratio inflow condition, requires more attention. Three factors are identified as possible causes for the discrepancies in emissions predictions: 1) the unmixedness parameter assumption for the non-uniform-equivalence-ratio inflow, 2) the absence of heat loss near the combustor walls, and 3) the sensitivity to predicted volumes and flow splits which typically are not in perfect agreement with their experimental counterparts.

Unmixedness Parameter

The importance of the non-uniform-equivalence-ratio inflow condition is clearly evident in comparisons of the CRN results to the experimental data set presented thus far. As described in previous chapters, the parameter used to vary the equivalence ratio

inflow is the unmixedness parameter, S . The effect of increasing this parameter from zero, which indicates perfect mixing (uniform equivalence ratio), leads to the outer flow of the CRN model receiving increasingly leaner mixture and the inner flow receiving increasingly richer mixture. The actual unmixedness parameter of combustors is typically found experimentally; however, for the DOE-HAT combustor, this was not provided. As a result, a value of 0.25 based on the recommendation of Sturgess *et al.* [94] for typical lean-premixed combustors was used in the present CRN. The effect of varying the unmixedness parameter on emissions prediction for a mean equivalence ratio of 0.50 is shown in Figure 5-7 and Figure 5-8 for CO and NO_x, respectively. In these figures, the experimentally-determined emission is shown by a dashed line for reference. Increases in the unmixedness parameter lead to increases in CO and NO_x output; however, this is more pronounced for the latter value. As displayed in Figure 5-8, the substantial increase in NO_x supports the non-linear temperature dependence of NO_x production. For comparison, the inlet conditions for a mean equivalence ratio of 0.50 used for the hot-flow LES simulation by Cannon *et al.* [51] showed the equivalence ratio to reach approximately 0.35 and 0.60 at the outer and inner regions of the premixer exit, respectively. For the present model, at the same mean equivalence ratio, the unmixedness parameter of 0.25 yields outer and inner equivalence ratios of 0.35 and 0.64, respectively. Assuming the equivalence ratio distribution used by Cannon *et al.* [51] is correct, the discrepancy in the inner equivalence ratio leads to decreases of 4 and 35 percent for CO and NO_x emissions, respectively, compared to the originally predicted values. This results in a more accurate prediction of the experimental data.

Figure 5-7: Effect of unmixedness on CO formation for $\phi_m = 0.50$.

Figure 5-8: Effect of unmixedness on NO_x formation for $\phi_m = 0.50$.

Heat Transfer

Another possible reason for the higher NO_x formation in predicted emissions may be the adiabatic walls assumption used in the CRN model. As noted in a study by Shehata [114], this assumption has an effect on the near-wall NO_x and CO formation, since typically heat transfer near the walls results in a reduction of temperature, leading to decreased NO_x and increased CO close to the walls. To approximate the effect of heat loss near the walls, the temperature in the outer flow of the CRN is decreased by reducing the outer flow equivalence ratio. The results, shown in Figure 5-9, reveal NO_x output is not highly sensitive to large reductions in outer flow temperature as compared to CO output. This seems to indicate that the reduction in temperature in the outer flow has a significant effect on decreasing the oxidation rate of CO to CO_2 to produce more CO, while exerting only minor effects on NO_x , which is typically produced in the high temperature core region of the flow [25]. Although, for this particular combustor, the heat loss is reported to be small due to the ceramic-lined combustor wall [51], it is clear that the effect of including heat loss near the walls can have a significant effect on CO output, and less so for NO_x output. A method to quantify the effects of heat loss should be incorporated into the CRN model in future studies.

Figure 5-9: Effect of reducing the outer flow temperature on NO_x and CO emissions.

Sensitivity of Predicted Emissions to Volumes and Flow Splits

The sensitivity of predicted emissions to variations in calculated volumes and flow splits, shown in Figure 5-10, is another potential source of discrepancy between predicted and experimental emissions data. A detailed analysis of the effects of varying the volumes and flow splits about their predicted values is given in Appendix C. A summary of these studies is provided in Table 5-1 and Table 5-2, showing the percent change of NO_x and CO, respectively, when the predicted volume or flow split is decreased to half its value or increased by 1.5 times its value. It should be noted in Table 5-2 that only flow splits S1 and S2 in Figure 5-10 are listed, since no significant changes in CO emissions were noted in varying the volumes or flow split S3. Evidently, the largest relative change in emissions is caused by variations in the S1 and S2 flow splits,

which describe the exit flow of the outer flame zone (OFZ). Unfortunately, this is also the location where no correlations were used to predict the flow split due to the lack of pertinent published studies, and these particular flow splits were estimated using comparisons to similar reactor networks [22,24]. The noted sensitivity of this location is primarily due to the change in mean residence time as a result of changes in the amount of mass flow entering the core region. As indicated in Table 5-1, an increase in mass flow rate into the core region (S2) leads to a decrease in NO_x by roughly 17 percent. This can be explained by looking at the equation below for the mean residence time:

$$t_R = \frac{\rho V}{\dot{m}} \quad (5-1)$$

where ρ is the density, V is the reactor volume, and $\dot{m}$ is the mass flow rate through the reactor. This equation shows that an increase in mass flow rate results in a decrease in the mean residence time. As discussed in detail in Chapter 2, the reduction of residence time in the primary zone results in decreased NO_x formation. For the present CRN, the fraction of mass flow from the outer flame zone entering the core region (S2) is 0.4, while the fraction entering the dilution zone (S1) is 0.5. It is uncertain as to whether this estimation accurately describes the flow in this region, and further analysis is needed based on experimental studies.

In summary, varying individual volumes and flow splits does not cause significant changes to the predicted emissions, with the sole exception being the variation of flow splits at the outer flame zone. Therefore, with respect to the prediction of the volumes and flow splits, the overall uncertainty of emissions prediction using this CRN model hinges on the prediction of the outer flame zone flow splits. Significant variations in this

parameter (+/- 50 percent) result in 17 percent change in NO_x output and 10 percent change in CO output. Although, these large variations in flow splits are not expected, as further correlations based on experimental studies become available, the actual impact of these flow splits on emissions output can be elucidated.

Figure 5-10: Volumes and flow splits in the primary zone.

Table 5-1: Percent change in NO_x in varying the volumes and flow splits predicted.
Negative value indicates decrease in NO_x .

Location	1/2 of Predicted Value	1.5X Predicted Value
Volume: OFZ, CFZ, and IFZ	-6%	+3%
Volume: CRZ	< -1%	+3%
Volume: IRZ	-6%	+3%
Flow Split: S1	-17%	+17%
Flow Split: S2	+17%	-17%
Flow Split: S3	< -1%	< +1%

Table 5-2: Percent change in CO in varying the volumes and flow splits predicted.
Negative value indicates decrease in CO.

Location	1/2 of Predicted Value	1.5X Predicted Value
Flow Split: S1	-10%	+10%
Flow Split: S2	+10%	-10%

5.1.2 Emissions Prediction Compared to CFD Models

In addition to the experimental results, the predicted emissions from the hot-flow LES and RNG $k-\epsilon$ model simulations by Cannon *et al.* [51] are compared to present CRN-predicted values in Figure 5-11 and Figure 5-12. These CFD models, as outlined in Chapter 4, used the assumed-PDF approach for turbulence-chemistry interaction, which employed a two-step chemical reaction mechanism for heat release and CO formation. The NO_x formation was calculated by post-processing the CFD solution using only the three-step thermal NO mechanism. Considering this, to compare the CRN model predictions with the LES and RNG $k-\epsilon$ models' predictions, reactions involving NO_x formation other than thermal NO are removed from the GRI-Mech 3.0 mechanism. However, the same procedure could not be applied to remove all other CO-forming reactions excluding the one used in the CFD model. This is due to the complexity of the CO-forming reactions described in the full GRI-Mech 3.0 mechanism. In the figures, the CRN using the reduced mechanism is labelled "CRN-Reduced Mechanism", while the one using the full GRI-Mech 3.0 mechanism is labelled "CRN-Full Mechanism". In the case of using the full reaction mechanism, the CRN model performs better for all equivalence ratios in predicting the CO emissions compared to LES and RNG $k-\epsilon$ models. For NO_x prediction, the LES model outperforms the CRN and RNG $k-\epsilon$ models

when compared to experimental data. The relatively accurate prediction of the LES model is interesting since only the thermal NO mechanisms were used in both LES and RNG $k-\epsilon$ models. This provides misleading evidence suggesting that other NO mechanisms are not as important. In observing the results of the CRN model with the reduced mechanism, there is a significant contribution of the other NO-forming reactions. The results show a 30, 50, and 75 percent decrease in NO_x emission for equivalence ratios of 0.58, 0.50, and 0.42, respectively, when compared to the CRN using the full mechanism. This indicates that, at the higher equivalence ratio, thermal NO is dominant and at the lower case it is the N_2O pathway, since prompt mechanism is said to be virtually non-existent at elevated pressures common to gas turbine combustors [18,30]. This outcome indicates that the LES model significantly over-predicts the NO_x formation for higher equivalence ratios, while the RNG $k-\epsilon$ model over-predicts for an equivalence ratio of 0.50. A review of similar flow conditions involving lean-premixed combustion studies using LES simulations showed temperature fluctuations in the primary zone to be significantly over-predicted compared to experimental results [49,50]. Furthermore, velocity fluctuations in the shear layers of the corner and inner recirculation zones are over-predicted. Therefore, excessive peaks in temperature may result in unrealistic NO_x formation due to the non-linear temperature behaviour of thermal NO formation. On the other hand, for RNG $k-\epsilon$ simulations, the model has been reported to under-predict the turbulence near the shear layers [107]. This explains the reduced prediction of NO_x using the same chemistry as the LES model.

Figure 5-11: CRN-based prediction of CO emissions compared with CFD-based predictions and experimental data.

Figure 5-12: CRN-based prediction of NO_x emissions compared with CFD-based predictions and experimental data.

5.1.3 Reactor Network Complexity

To ascertain the lowest degree of complexity of the reactor network required to predict emissions accurately, the baseline chemical reactor network (9 reactors) was systematically reduced in the number of reactors. The CRNs consisting of 9, 8, 5, and 2 reactors are shown in Figure 5-13. For the 8-reactor case, the volumes of the two PFRs in the dilution zone are combined. For the 5-reactor case, the volumes of the outer, centre, and inner flame zones are combined into one central PSR. The 2-reactor case combines all of the PSRs in the primary zone. In order to compare the predicted emissions with the 5- and 2-reactor cases, which cannot include the non-uniform-equivalence-ratio inflow, the 9- and 8-reactor cases are considered with uniform-equivalence-ratio inflow.

(a)

(b)

(c)

(d)

Figure 5-13: Reduction of reactor network: (a) 9 reactors, (b) 8 reactors, (c) 5 reactors, and (d) 2 reactors.

The effect of variation of reactor network size is shown for CO and NO_x formation in Figure 5-14 and Figure 5-15, respectively. For CO emissions, aside from the leanest equivalence ratio, there is very little difference in the predicted values for varying reactor network size. However, at the leanest condition, only the 9-reactor model is able properly predict the CO emitted. The reason behind this, as discussed previously, is the separation of the outer and core flows in the dilution zone in the 9-reactor model. This separation leads to the cooler outer flow to convert CO to CO₂ at a slower rate than the hotter core flow. As a result, Nicol *et al.* [25] state that accurate prediction of CO emissions requires more complex arrangement of chemical reactors along the wall and dilution zones to represent CO-forming conditions, such as lean combustion and quenching of hot combustion products with cooling air.

For NO_x formation, there is very little difference between the different reactor network sizes. Contrary to expectations, the 2-reactor model is almost 20 percent better at predicting NO_x at an equivalence ratio of 0.5 compared to the 9-reactor model. This result indicates that the 2-reactor model is perhaps better at predicting NO_x for this particular combustor. In fact, for lean-premixed combustors, Nicol *et al.* [25] state that since the highest rates of NO_x formation occur in one major location, namely the inner flame zone (or at the edge of the inner recirculation zone), a complex arrangement of reactors is not necessary. However, this does not fully explain why a 2-reactor model performs better than the 9-reactor model for the uniform-equivalence-ratio inflow. In examining this result, it is seen that the residence time, which is the average time each species remains in a reactor, ultimately affects the NO_x formation. For the 5-reactor model, the residence time is higher compared to the 9- and 8-reactor models since the flame zones have

combined to make a larger zone, allowing more time for the mixture to react, which then leads to a rise in the average temperature (Figure 5-16). This trend is also seen with the 2-reactor model, where all the zones in the primary zone combine to make one large zone leading to an increase in the average temperature (Figure 5-16). The outcome agrees with published results, which state longer residence times lead to increased NO_x formation at high temperatures [18]. This result indicates that the residence times in the 9- and 8-reactor cases are under-predicted. This is consistent with the under-prediction of the corner and inner recirculation zone volumes discussed in Chapter 4, which results in decreased residence time. Therefore, for the uniformly-mixed equivalence ratio inflow condition, the 2-reactor model should perform equivalently to the 9-reactor model with accurately predicted residence times. However, reduced reactor models such as the 2-reactor model cannot account for the unmixedness of fuel-air of typical lean-premixed combustors in predicting NO_x formation. The inclusion of the non-uniform-equivalence-ratio inflow in the 9-reactor model significantly increases the NO_x formation predicted, which is more representative of the experimentally-measured data as discussed in previous sections.

Figure 5-14: Effect of reducing the number of reactors on CO emission.

Figure 5-15: Effect of reducing the number of reactors on NO_x emission.

Figure 5-16: Average temperatures in the primary zone.

5.2 P-LP Combustor

The work presented thus far has demonstrated that a properly constructed CRN can be more reliable in predicting emissions than more computationally-intensive CFD-based methods. Consequently, the present CRN model is used to verify the preliminary findings of Charest [5] regarding emissions on the P-LP Combustor that was obtained on the basis of a CFD method. The emissions goal of this design was to meet NO_x and CO limits of 30 and 10 ppm, respectively [5].

The reactor network used for the P-LP combustor is shown in Figure 5-17. The main difference between this CRN and the one used for the DOE-HAT combustor is the addition of the dilution jet in the dilution zone. This addition requires a MIX reactor to mix the different flows entering the outer flow with the dilution jet prior to entering the

outer flow (OF) PFR. Because there are no adequate correlations to separate the dilution zone flow, the dilution jet properties from Charest's [5] CFD solution were employed to define two separate volumes and flow splits. The flow split dividing the dilution zone is determined using a simple entrainment model commonly used for free jets as described in Chapter 2, and is given below:

$$\frac{\dot{m}_m}{\dot{m}_{DJ}} = 0.16 \left(\frac{Y_C}{d_0} \right) \left(\frac{\rho}{\rho_j C_D} \right)^{1/2} \quad (5-2)$$

where $\dot{m}_m$ is the mass flow rate entrained into the dilution jet, $\dot{m}_{DJ}$ is the mass flow rate of the dilution jet, Y_C is the penetration distance of the dilution jet, d_0 is the jet orifice diameter equal to 0.01 m, C_D is the orifice discharge coefficient equal to 0.64 [16], and ρ and ρ_j are the hot- and jet-gas densities. The dilution jet penetration distance, as shown in Figure 5-18, was estimated from Charest's [5] CFD solution to be 0.12 m. This distance was also used as the dividing line for the outer and core flow region volumes. The hot- and jet-gas densities are calculated within the CRN model's subroutines. Due to the large amount of dilution jet entering the dilution zone compared to the main flow (2.916 kg/s vs. 2.484 kg/s), the predicted entrainment will exceed the mass flow available from the outer flame zone (OFZ), thus the remaining mass flow is entrained from the post-flame zone (PFZ). This is indicated by a dashed arrow connecting the flow exiting the PFZ to the MIX reactor in Figure 5-17. Due to the strong interaction between the dilution jet and main flow, the CRN model is used to examine the sensitivity of the emissions to the selected jet penetration distance. Significant variations in this parameter (+/- 50 percent) yield less than 15 percent change in NO_x output and less than 33 percent in CO output.

However, the predicted jet penetration distance should not vary as widely as tested in this sensitivity study and, as such, the resulting changes in emissions are deemed minimal.

Figure 5-17: Reactor network for the P-LP combustor.

Figure 5-18: Dilution jet entry and entrainment model parameters.

The results of the P-LP combustor simulation are shown in Figure 5-19 and Figure 5-20 for CO and NO_x emissions, respectively. The values are compared to the preliminary hot-flow CFD simulation reported by Charest [5] for the P-LP combustor using a standard $k-\epsilon$ model for turbulence modeling and a finite-rate/eddy-dissipation model for turbulence-chemistry interaction, as mentioned previously. Additionally, the hot-flow CFD simulation by Charest used a uniform-equivalence-ratio inflow, which is not representative of a real combustor. To allow comparison between CFD- and CRN-predicted emissions, the CRN model predicts both the uniform- and the non-uniform-equivalence-ratio inflow. These are indicated as “Uniform Inflow” and “Non-uniform Inflow” in Figure 5-19 and Figure 5-20. The CO emission predicted by the CRN for both uniform and non-uniform cases is within the range of the value predicted by the CFD-based approach, and meets the design goal of 10 ppm. However, for NO_x prediction, the CRN model prediction using both the uniform and non-uniform cases are significantly different from the uniform inflow CFD prediction, exceeding the design goal of 30 ppm. Going from non-uniform inflow condition to uniform inflow condition for the CRN model yields a 36 percent drop in NO_x. The remaining discrepancy between the CRN and CFD models for the uniform inflow cases may be attributed to two main reasons: 1) the difference in the use of thermal NO mechanism and 2) the volume prediction of the inner recirculation zone.

Figure 5-19: CO emissions for the P-LP combustor predicted by CFD and CRN models.

Figure 5-20: NO_x emissions for the P-LP combustor predicted by CFD and CRN models.

Thermal NO Mechanism

To systematically resolve the predicted NO_x discrepancy between the uniform inflow CFD case and the uniform inflow CRN case, first the CRN model's reaction mechanism, which includes the three-step mechanism as shown below, is modified to only include the two-step thermal NO mechanism (Reaction 5-5 is removed).

The result of the CRN using the two-step thermal NO mechanism shows a 15 percent decrease in NO_x when compared to the uniform inflow CRN case using three-step thermal NO mechanism as seen in Figure 5-21. This result is consistent with the results of Nicol [18], who showed that 15 percent of the NO from the total NO produced by the thermal mechanism is due to Reaction 5-5. Based on this finding, the CFD-based method used by Charest [5] lacks a crucial step in the thermal NO formation pathway in predicting total NO_x .

Next, the relative accuracy of the CFD model's ability to predict the inner recirculation size is examined since, as noted in Chapter 4, the standard $k-\epsilon$ model cannot predict the recirculation zone properly. Using Case 1 from Chapter 4 as a basis, the standard $k-\epsilon$ model under-predicted the recirculation height and length by 38 and 81 percent, respectively, compared to experimentally-measured values. Comparatively, the empirical correlations under-predicted the same values by 20 and 26 percent, respectively. Comparing the extent of under-prediction of inner recirculation size by the

standard $k-\epsilon$ model to that of correlations could partially explain the discrepancy in the NO_x emissions between the CRN and CFD models, since the majority of the NO_x is formed in this region. To confirm this postulate, this difference was applied to the uniform inflow CRN case using the two-step thermal NO mechanism by reducing the size of the inner recirculation height and length by 18 and 55 percent, respectively. The result, illustrated in Figure 5-21 labelled “CRN - Modified IRZ Volume”, shows a 22 percent decrease in NO_x compared to the uniform inflow CRN case using the two-step thermal NO mechanism. This agrees with the earlier discussions of the reduction of volume resulting in a decrease in NO_x .

Figure 5-21: Response of NO_x formation due to model changes.

In spite of these adjustments bringing the CRN- and CFD-based predictions closer to each other with respect to the flowfield upon which the emission predictions are based, the prediction of the CRN still does not agree with the CFD-based prediction. One other factor that may account for the lower NO_x predicted by the CFD model may be the inclusion of a heat transfer and radiation model to account for the wall-cooling. As mentioned in preceding sections, this can lead to a reduction in the temperatures near the wall, and thereby reduce the NO_x emission output. However, in examining the production of NO_x near the outer flow regions of the combustor in the CRN model, very little is formed here compared to the core flow region. Thus there remains a gap between the CFD-based and the CRN-based predictions even when accounting for heat transfer near the walls.

Certainly there are differences in the underlying assumptions between the two approaches, as demonstrated through this exercise. However, the flexibility of the CRN model allows it to analyze various assumptions on-the-fly and, in turn, reduce these perceived differences.

In summary, the evaluation of the PL-P combustor using the CRN model shows the combustor to produce large amounts of NO_x compared to its target value of 30 ppm. This outcome was not expected, since the combustor was originally designed to achieve low NO_x output. On the contrary, the predicted CO emissions fall well under the target value of 10 ppm, which better supports the overall objective of the combustor design. At this point, the CRN-based predictions are preliminary, having been proven against a single test case. However, based on this initial evidence from the DOE-HAT test case, the

CRN model provides a reliable estimate of emissions of a lean-premixed combustor. Additionally, this model is advantageous because of its ability to efficiently calculate emissions output compared to computationally-intensive CFD-based methods, and can be used as a basis for further iterations to the combustor design methodology.

6 Conclusions and Recommendations

6.1 Conclusions

A preliminary design methodology for lean-premixed combustors was developed by Charest [5] and Capurro [7] at Carleton University. However, before any experimental testing could be conducted, an emissions-prediction tool, which had not been included in their original procedure, was deemed essential. In the work presented in this thesis, an evaluation of the methods available for quantifying emissions is undertaken and chemical reactor modeling using correlations is identified as the ideal method for predicting emissions efficiently. An outline of a methodology to implement a chemical reactor network (CRN) based on preliminary design parameters is provided, and includes a premixing model to account for imperfect mixing in the premixer, which is typical of a lean-premixed combustor.

The selected correlations to predict the volumes and flow splits for the CRN model are validated using simplified test cases representing gas turbine combustors. In this context, the correlations-based predictions are compared to CFD-based predictions and experimental values. Results show good accuracy compared to simple CFD methods, and are competitive with the more sophisticated CFD methods in predicting experimental values. For emissions prediction, the developed CRN model is used to evaluate two lean-premixed combustors: the DOE-HAT combustor and the P-LP combustor.

The emissions predicted for the DOE-HAT combustor using the CRN model show good agreement with experimental results when the premixing model is utilized. Comparing the experimental results to the CRN, LES and RNG $k-\epsilon$ models reveals the

relative inaccuracy of the latter two methods in predicting emissions. There are two factors in the proposed CRN model that can potentially affect the emissions prediction. The first is proper representation of the dilution zone as two separate regions; however, this is only relevant at lean equivalence ratios approaching the lean-flammability limit. Secondly, variation of the flow splits at the outer flame zone can affect emissions prediction. Both of these factors warrant closer examination as correlations based on experimental studies become available.

Finally, the CRN model is applied to the preliminary lean-premixed combustor (P-LP) developed at Carleton University. Results show higher-than-expected amounts of NO_x formation, but lower-than-expected amounts of CO formation, for a lean-premixed combustor design.

The preliminary validations using the DOE-HAT combustor confirm the reliability of the present CRN-based model and the ability of this tool to more time-efficiently predict emissions than a CFD-based approach without compromising accuracy. Moreover, the CRN-based model can directly integrate into the combustor design methodology to allow for immediate iterations.

6.2 Recommendations

The recommendations for future work include:

- Proper representation of the dilution zone by separating the flow into outer and core flows
- Analysis of the flow interaction with the determined zones of interest to provide better correlations for flow splits

- More descriptive correlations of the flame zone volume
- Inclusion of heat transfer from the reactors to the environment, allowing for superior assessment of the combustor wall-cooling and, in turn, better prediction of NO_x and CO emission.

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Appendix A. Preliminary Design Output Variables

Table A-1: Preliminary design output variables [5].

Parameter	Description
S_n	Swirl number for combustor swirler
T_{PZ}	Estimated flame temperature
V_{ref}	Reference velocity
f_{an}	Fraction of mass flow through annulus
f_{DJ}	Fraction of mass flow through dilution holes
f_{DZ}	Fraction of mass flow in dilution zone
f_{SW}	Fraction of mass flow through premixer
f_{PZ}	Fraction of mass flow in primary zone
ϕ_{DZ}	Dilution zone equivalence ratio
ϕ_{PZ}	Primary zone equivalence ratio
A_{an}	Annulus flow area
C_D	Dilution hole discharge coefficient
D_{DJ}	Dilution hole diameter
D_c	Combustor liner diameter
D_t	Swirler tip diameter
D_h	Swirler hub diameter
D_{ref}	Combustor casing diameter
L_{DZ}	Dilution zone length
L_{PZ}	Primary zone length
V_{DZ}	Dilution zone volume
V_{PZ}	Primary zone volume

Appendix B. Cantera & Reactor Networks

Cantera is a library of subroutines for reacting flow problems which include numerical solutions to the governing equations of the PSR and PFR. The source code of Cantera and its corresponding user manual and instructions for installation can be obtained from <http://sourceforge.net/projects/cantera>. To begin working with Cantera, intermediate knowledge of C++ is needed if one wishes to work in the C++ environment, such as Microsoft Visual Studio C++. However, modules for using Cantera with more straightforward software such as MATLAB or Python can also be downloaded and used. Details on the basic structure and error-handling of Cantera is described in the Cantera C++ User Guide [67].

The main objects that are used to describe a reactor network are Reactor and FlowReactor which represent a perfectly stirred reactor (PSR) and a plug flow reactor (PFR), respectively. Additionally, Reservoir object is used to represent inlet flow conditions such as air and fuel mixtures. The connections between the reactor objects in a network are made by assigning Valves and MassFlowController objects to regulate pressure and mass flow rates. The following sections will briefly describe each of these objects and how they are implemented in a reactor network.

B.1 Reactors

Reactor - PSR

The connectivity of the Reactor object is shown in Figure B-1. The Reactor must be connected to a flow controller at the inlet and outlet before connecting to another reactor or Reservoir. Operating parameters required to use the Reactor object include the designation of a chemical reaction mechanism and a reactor volume. All other parameters, such as pressure and temperature, are obtained from the incoming flow.

Figure B-1: Connectivity of Reactor object.

FlowReactor - PFR

The connectivity of the FlowReactor object is shown in Figure B-2. Similar to the Reactor, FlowReactor must be connected to a flow controller at the inlet and outlet before connecting to another reactor or Reservoir. Operating parameters required to use FlowReactor include the designation of a reaction mechanism, reactor area, and length. Again, like the Reactor object, all other parameters are specified from the incoming flow.

Figure B-2: Connectivity of FlowReactor object.

Reservoir

The connectivity of the Reservoir object is shown in Figure B-3. The Reservoir is similar to a Reactor, except that the state of the contents, once set, does not change [99]. The contents of the Reservoir are defined by assigning the reaction mechanism to be used and the state of the mixture (i.e. temperature, pressure, and molar composition). The Reservoir is designed to be connected to Reactors/FlowReactors to provide a specified inlet condition [99]. The Reservoir is also used to output final exhaust flow from Reactor/FlowReactor.

Figure B-3: Connectivity of Reservoir object.

B.2 Flow Controllers

MassFlowController

The connectivity of the MassFlowController object is shown in Figure B-4. The controller can be connected to either Reactor or Reservoir objects with a specified mass flow rate to provide constant mass flow between the reactors [67]. Typically, mass flow controllers are used between Reservoirs and Reactor/FlowReactors and in the case of back flow (moving upstream) between Reactor/FlowReactors and Reactor/FlowReactors.

Figure B-4: Connectivity of MassFlowController object.

Valve

The connectivity of the Valve object is shown in Figure B-5. The controller is connected between Reactors/FlowReactors to maintain a specified upstream pressure by adjusting its mass flow rate [99]. The object is designed to regulate the exhaust flow rate from a Reactor/FlowReactor and is installed on an outlet of a Reactor/FlowReactor to be controlled [99].

Figure B-5: Connectivity of Valve object.

B.3 Implementation

To begin a basic calculation for a reactor, as with any C++ code, header files and variables needed to utilize the subroutines must be declared. For Cantera, the main header files or subroutines that are required to calculate the chemical kinetics, the thermodynamics properties, and the governing equations of the PSR and PFR, are: Cantera.h, IdalGasMix.h, and zerodim.h. These are shown in the sample code below. This is followed by specifying the reaction mechanism to be used and initializing the mixture by specifying the temperature, pressure, and the molar composition. The sample code shown below employs a stoichiometric fuel-air ratio of methane and air using the GRI 3.0-Mech reaction mechanism. Once this is done, to simulate a particular reactor, the proper reservoirs and flow controllers are specified, as discussed next.

```

#include <cantera/Cantera.h>
#include <cantera/zerodim.h>
#include <cantera/IdealGasMix.h>

using namespace std;

// Declare variables such as temperature (T3), pressure (P3), volume
of PSRs and PFRs (V), lengths of PFRs (L), mass flow rate of the
mixture:
double T3, P3, V, L, mdotmix;

int main()
{
    // Define reaction mechanism to be used for the mixture and
    name it 'GasMix'
    IdealGasMix GasMix("gri30.cti", "gri30");

    // Set the state of the mixture
    GasMix.setState_TPX(T3, P3, "CH4:1.0, O2:2.0, N2:7.52");

    ...
    // Add code for reservoirs and reactors
}

```

Perfectly Stirred Reactor (PSR) Implementation

For a simple PSR simulation as shown in Figure B-6, the corresponding sample code is given below. For organization, the sample code first defines the reservoirs required to model the PSR: an “Inlet” reservoir for storing the mixture contents and an “Exhaust” reservoir for discharging the contents of the PSR. Following this step, the PSR is defined as “Zone” and initialized by specifying the reaction mechanism to be used and its volume. Next, the appropriate controllers are defined: a MassFlowController (MFCIn) to specify the mass flow rate of the mixture entering “Zone1” and a Valve (VOut) to regulate the pressure in between “Zone1” and the “Exhaust” reservoir. Finally, the PSR is added to a reactor network before the governing equations of the PSR are solved to steady-state conditions. Once the algorithm solves the reactor network to steady state, the properties of the contents can be outputted as desired.

Figure B-6: Simple PSR simulation.

```

// Setup a reservoir containing the fuel-air mixture and call it
'Inlet'
Reservoir Inlet;
Inlet.insert(GasMix);

// Setup a reservoir for the products of the reactor to exit to and
call it 'Exhaust'
Reservoir Exhaust;
Exhaust.insert(air);

// Setup a PSR and call it 'Zone1'
Reactor Zone1;
// Specify the reaction mechanism to be used for the calculations
Zone1.insert(GasMix);
// Specify the volume of the reactor, V
Zone1.setInitialVolume(V);

// Install a mass flow controller between the Inlet reservoir and the
Zone1 PSR and call it 'MFCIn'
MassFlowController MFCIn;
// Connect the reservoir and PSR using the controller
MFCIn.install(Inlet, Zone1);
// Set the mass flow rate entering the reactor
MFCIn.setMassFlowRate(mdotmix);

// Install a valve to control the pressure between the Zone1 PSR and
the Exhaust reservoir and call it 'VOut'
Valve VOut;
// Connect the PSR and reservoir using the controller
VOut.install(Zone1, Exhaust);
VOut.setParameters(1, &Kv);

// Create a reactor network called NET, and add the reactor to it
ReactorNet NET;
NET.addReactor(&Zone1);

// Solve reactor from time, t, to steady state
t = 0.0;
while (t<SteadyState) {
    NET.step(SteadyState);
    T = NET.time();
}
// Specify parameters of the reactor contents for output

```

Plug Flow Reactor (PFR)

The implementation of the PFR, as shown in Figure B-7, follows the same procedure as the PSR. To be concise, the highlighted portions (indicated by dashed lines) of the PSR sample code are replaced by the sample code below for PFR implementation.

Figure B-7: Simple PFR simulation.

```

// Setup a PFR and call it 'Zone1'
FlowReactor Zone1;
// Specify the reaction mechanism to be used for the calculations
Zone1.insert(GasMix);
// Specify the volume of the reactor, V
Zone1.setInitialVolume(V);
// Specify the mass flow rate
Zone1.setMassFlowRate(mdotmix);

// Solve PFR along the distance L starting from zero
D = 0.0;
while (D<L) {
    NET.step(L);
    D = NET.distance()/(V/A);
    // Specify parameters of the reactor contents for output
}
  
```

MIX Reactor

The MIX reactor is commonly used to mix multiple flow streams before entering a PFR. The MIX reactor is implemented similarly to the PSR, with the chemical reactions disabled. To do this, the following code is added after setting up the reactor:

```

// Disable chemical reactions in the Zone1 reactor
Zone1.disableChemistry();
  
```

B.4 Comparison of Cantera and CHEMKIN

To verify Cantera-based calculations to the industry standard CHEMKIN software (Version 4.1, ReactionDesign Inc., San Diego, CA, USA), a tutorial of a generic gas turbine combustor from CHEMKIN documentation [115] was used. The generic combustor reactor network using CHEMKIN tool-set is shown in Figure B-8. The primary zone cluster represented by P SRs consists of: 1) mixing zone that combines primary air and premixed fuel, 2) flame zone that combines mixing zone products, secondary air, and recirculation products, and 3) recirculation zone. The dilution zone consists of a post-flame zone represented by a PFR.

Figure B-8: Generic gas turbine CRN.

The equivalent reactor network using Cantera is shown in Figure B-9 using the guidelines discussed above.

Figure B-9: Cantera flow diagram of generic gas turbine CRN.

The network was solved using GRI-Mech 3.0 for methane-air combustion using the listed variables in Table B-1 given from the CHEMKIN documentation [115]. The flow splits between the reactors are given in Table B-2.

The results of the comparison are shown in Figure B-10 and Figure B-11 for the primary zone cluster and PFR, respectively. For both the primary zone and PFR, the Cantera calculations are in good agreement with the calculations of CHEMKIN.

Table B-1: Variables for the generic gas turbine.

Parameter	Value
Fuel Type	CH ₄ (Methane)
Primary Air Temperature (K)	650
Premix Temperature (K)	800
Secondary Air Temperature (K)	670
Pressure (MPa)	1.0
Premix Equivalence Ratio, ϕ_{premix}	0.6
Primary Air (kg/s)	0.05
Premix (kg/s)	0.5
Secondary Air (kg/s)	0.1
Mixing Zone Volume (m ³)	5.8×10^{-5}
Flame Zone Volume (m ³)	5.9×10^{-4}
Recirculation Zone Volume (m ³)	1.2×10^{-4}
Post Flame Zone Area (m ²)	7.8×10^{-3}
Post Flame Zone Length (m)	5.0×10^{-2}

Table B-2: Reactor flow fractions of the generic gas turbine.

Reactor Flow Direction	Flow Fraction
Mixing Zone to Flame Zone	1.0
Recirculation Zone to Mixing Zone	0.15
Recirculation Zone to Flame Zone	0.85
Flame Zone to Recirculation Zone	0.2
Flame Zone to Post Flame Zone	0.8

Figure B-10: Comparison of primary zone cluster calculations.

Figure B-11: Comparison of PFR calculations.

Appendix C. Sensitivity Studies

This section uses the baseline combustor, namely the DOE-HAT combustor, to analyze the effects of changing the correlations-based volumes and flow splits on the prediction of NO_x and CO emissions. The 9-reactor network with the premixing zone model to account for non-uniform-equivalence-ratio inflow of 0.58 was used for all the calculations. All the figures shown in this section indicate the experimental emissions measurement as a dashed line for reference.

C.1 Corner Recirculation Zone Volume

The corner recirculation zone (CRZ) volume is calculated using the correlation given by Vanierschot and Van den Bulck [81]. The sensitivity of predicted emissions to variations in CRZ volume results in marginal changes in NO_x (~3 percent) and no significant changes in CO output, as shown in Figure C-1. In a non-uniform mixing condition, this region contains leanest mixtures in the combustor, thus exhibiting minor NO_x sensitivity. On the other hand, lean mixtures typically result in more CO emissions, but in this case, the reactions occur close to the inlet of the combustor, leaving enough time for the majority of the CO produced to oxidize to CO_2 at the combustor exit.

Figure C-1: Sensitivity of corner recirculation zone (CRZ) volume variation in predicting (a) CO and (b) NO_x emissions.

C.2 Inner Recirculation Zone Volume

The inner recirculation zone (IRZ) volume is calculated using the correlations by Roberts *et al.* [84] and Beer and Chigier [77]. The sensitivity of predicted emissions to variations in IRZ volume results in a 6 percent decrease in NO_x when the volume was decreased by 50 percent, and 3 percent increase in NO_x when the volume was increased by 50 percent, as shown in Figure C-2b. Unlike the CRZ, the IRZ is associated with the richer mixture leading to higher temperatures which promote more NO_x formation. Therefore, increasing the volume of the IRZ results in increased residence time, allowing for more NO_x to form. In contrast, due to the higher temperatures associated in this region, the rate of oxidation of CO to CO₂ is increased, resulting in negligible changes in CO output as a result of varying the IRZ volume, as shown in Figure C-2a.

Figure C-2: Sensitivity of inner recirculation zone (IRZ) volume variation in predicting (a) CO and (b) NO_x emissions.

C.3 Flame Zone Volume

The flame zone volumes are assumed to be one-eighth the fraction of the recirculation zone volumes according to Mattingly *et al.* [16]. The results of varying the flame zone volume about the predicted value are shown in Figure C-3 for CO and NO_x output. No significant change in CO output is seen in varying the flame zone volume. A 50 percent decrease in the predicted volume shows NO_x to decrease by roughly 6 percent. The reduction in NO_x is a consequence of decreased residence time caused by the reduction of the volume. Similarly, the increase in NO_x seen for increased flame zone volume is a consequence of increased residence time.

Figure C-3: Sensitivity of flame zone (FZ) volume variation in predicting (a) CO and (b) NO_x emissions.

C.4 Split Dilution Zone Volume

In order to properly represent the dilution zone, two separate regions are delineated. For the DOE-HAT combustor, the volume of the outer flow in the dilution zone is determined from CFD-based results of Cannon *et al.* [51]. The sensitivity of predicted emissions to variations in the predicted outer flow volume is shown in Figure C-4 for both CO and NO_x output for equivalence ratios of 0.58 and 0.42. The results show no changes in both CO and NO_x for the higher equivalence ratio; however, at the leanest case, CO output changes significantly with variations in the outer flow volume. This is expected since the increase in the outer flow volume increases the residence time allowing CO to further oxidize to CO₂. This reveals the importance of an accurate representation of the outer flow volume to predict CO emissions for this case.

Figure C-4: Sensitivity of outer flow (OF) volume variation in predicting (a) CO and (b) NO_x emissions for equivalence ratios 0.58 and 0.42.

C.5 Primary Zone Volume

Typically, the primary zone volume is provided by the combustor design methodology; however, for the DOE-HAT combustor, this parameter was not available. As a result, the primary zone length (and, in turn, the volume) was predicted based on the correlation given by Sawyer [15]. The sensitivity of predicted emissions to variations in the predicted primary zone volume is shown in Figure C-5 for both CO and NO_x output. No significant changes in emissions are seen in varying this value.

Figure C-5: Sensitivity of primary zone (PZ) volume variation in predicting (a) CO and (b) NO_x emissions.

C.6 Outer Flame Zone Flow Split

Output at the outer flame zone (OFZ) splits into three streams: 1) corner recirculation zone (CRZ), 2) dilution zone (DZ), and 3) centre flame zone (CFZ). Of these flow splits, the fraction entering the CFZ is based on the work of Coghe *et al.* [102] and it is determined to be 10 percent. The remaining flow is split 50-40 with respect to DZ and CFZ. The sensitivity of predicted emissions to variations in these flow splits is shown in Figure C-6 for both CO and NO_x output. The largest discrepancy lies in the variation of the DZ and CFZ flow splits, which describe the exit flow of the outer flame zone (OFZ). Unfortunately, this is also the location where no correlations were used to predict the flow split due to the lack of pertinent published studies. The sensitivity of this location is primarily due to the change in mean residence time as a result of the change in the amount of mass flow entering the core region. A 50 percent increase in mass flow into the core region (CFZ) leads to an increase in residence time, and consequently results in a decrease in NO_x by roughly 17 percent. A 50 percent increase in the amount

of mass flow into the core region results in decreased CO by roughly 10 percent. This can be explained by the fact that lower amounts of CO formed early in the combustion process are oxidized in the outer dilution zone, while the majority of the CO enters the hotter core region, accelerating the oxidation process.

Figure C-6: Sensitivity of OFZ flow split variation in predicting (a) CO and (b) NO_x emissions. The circle indicates flow split selected.

C.7 Post-Flame Zone Flow Split

The fraction of flow entering the inner recirculation zone (IRZ) from the post-flame zone (PFZ) exit is calculated using the correlation by Mattingly *et al.* [16]. The sensitivity of predicted emission to variations in this predicted value is shown in Figure C-7 for both CO and NO_x output. No appreciable changes in emissions are noticed for these variations.

Figure C-7: Sensitivity of PFZ flow split variation in predicting (a) CO and (b) NO_x emissions.

Appendix D. Jet-A Reaction Mechanism

Table D-1: Jet-A reaction mechanism [16].

Step	Reaction	A_k	n	E_A
1	$C_{12}H_{23} + O_2 \rightarrow 5C_2H_4 + C_2H_4 + O_2$	3.01995×10^7	1.5	15697.3
2	$C_{12}H_{23} + OH \rightarrow 6C_2H_4 + O$	1.99526×10^{10}	1.0	8941.5
3	$C_2H_4 + H \rightleftharpoons C_2H_3 + H_2$	3.01995×10^{13}	0.0	18876.5
4	$H + H + M \rightleftharpoons H_2 + M$	1.99526×10^{15}	-1.0	0
5	$O + O + M \rightleftharpoons O_2 + M$	1.00000×10^{14}	-1.0	0
6	$H + OH + M \rightleftharpoons H_2O + M$	7.07945×10^{16}	-1.0	0
7	$H + O_2 \rightleftharpoons OH + O$	2.23872×10^{14}	0.0	16690.8
8	$O + H_2 \rightleftharpoons OH + H$	1.73780×10^{13}	0.0	9398.5
9	$CO + OH \rightleftharpoons CO_2 + H$	1.77828×10^{12}	7.0	-13909
10	$H + H_2O \rightleftharpoons OH + H_2$	8.31763×10^{13}	0.0	19969.3
11	$CH_3 + O_2 \rightleftharpoons CH_2O + OH$	1.00000×10^{12}	0.0	7948
12	$HO_2 + M \rightleftharpoons H + O_2 + M$	2.08929×10^{15}	0.0	45701
13	$HO_2 + H \rightleftharpoons 2OH$	7.76247×10^{12}	0.0	1887.6
14	$CH_2O + OH \rightleftharpoons H_2O + HCO$	7.94328×10^{13}	0.0	4212.4
15	$O + H_2O \rightleftharpoons 2OH$	5.75439×10^{13}	0.0	17883
16	$N_2 + O \rightleftharpoons NO + N$	1.00000×10^{12}	0.0	49675
17	$N + O_2 \rightleftharpoons NO + O$	1.00000×10^8	1.0	3974
18	$N + OH \rightleftharpoons NO + H$	1.00000×10^{12}	0.0	0
19	$HCO + O_2 \rightleftharpoons HO_2 + CO$	3.01995×10^{13}	0.0	13909
20	$HCO + OH \rightleftharpoons H_2O + CO$	1.99526×10^{13}	0.0	0
21	$C_2H_4 + OH \rightleftharpoons C_2H_3 + H_2O$	6.02559×10^{12}	0.0	3477.3
22	$CH_2O + HO_2 \rightleftharpoons HCO + 2OH$	1.00000×10^{12}	0.0	8941.5
23	$C_2H_2 + HO_2 \rightleftharpoons HCO + CH_2O$	1.99526×10^{12}	0.0	10928.5
24	$C_2H_3 + O_2 \rightleftharpoons C_2H_2 + HO_2$	1.69824×10^{12}	0.0	9935
25	$NO + HO_2 \rightleftharpoons NO_2 + OH$	1.00000×10^6	1.0	0
26	$C_2H_4 + O \rightleftharpoons CH_3 + HCO$	8.51138×10^{12}	0.0	2980.5
27	$C_2H_4 + HO_2 \rightleftharpoons CH_3 + HCO + OH$	7.94328×10^{12}	0.0	9935
28	$H_2 + CH_3 \rightleftharpoons CH_4 + H$	1.00000×10^{10}	-1.5	14187.2
29	$C_2H_2 + OH \rightleftharpoons CH_3 + CO$	1.58489×10^{11}	0.0	4967.5
30	$CH_3 + O \rightleftharpoons CH_2O + H$	1.28824×10^{14}	0.0	1987

The reaction rate coefficient corresponding to the above reactions is given by:

$$k(T) = A_k T^n e^{(-E_A/R_u T)} \quad (\text{D-1})$$

where R_u is the universal gas constant with units $\text{cal}/(\text{mol} \cdot \text{K})$, E_A is the activation energy with units cal/mol , n is the temperature exponent, A_k is the pre-exponential factor with units involving $\text{cm}^3, \text{mol}, \text{s}$, and T is the temperature with units K .

Appendix E. Emissions Correction Formulas

To compare experimental data from different combustors, emissions are commonly corrected to 15 percent excess oxygen on a dry basis [6]. To calculate the dry basis mass fraction of species i ($Y_{i,dry}$) according to Turns [17]:

$$Y_{i,dry} = \frac{Y_{i,wet}}{1 - Y_{H_2O}} \quad (E-1)$$

where $Y_{i,wet}$ is the mass fraction of species i with H_2O present in the products and Y_{H_2O} is the mass fraction of H_2O . This is followed by a correction formula to reference the dry mass fraction of species i to 15 percent excess O_2 :

$$Y_{i,15\% \text{ excess } O_2 \text{ dry}} = \frac{(20.9 - 15)}{(20.9 - Y_{O_2,dry})} \cdot Y_{i,dry} \quad (E-2)$$

where O_2 content ($Y_{O_2,dry}$) is expressed in percentage by volume [6].