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Mathematical Modeling of Combustion Processes

by

Abdul Wahab

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degree of Master of Science

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It is with my deepest gratitude and warmest affection that I dedicate this thesis to my Parents and Supervisors who have been constant source of knowledge and inspiration for me in this whole period.



CERTIFICATE OF APPROVAL

Mathematical Modeling of Combustion Processes

by

Abdul Wahab

(MME173003)

THESIS EXAMINING COMMITTEE

S. No.	Examiner	Name	Organization
(a)	External Examiner	Dr. Talha Irfan Khan	IST, Islamabad
(b)	Internal Examiner	Dr. M. Mahabat Khan	CUST, Islamabad
(c)	Supervisor	Dr. Khawar Naveed Abbasi	CUST, Islamabad

Dr. Khawar Naveed Abbasi

Thesis Supervisor

November, 2021

Dr. M. Mahabat Khan
Head
Dept. of Mechanical Engineering
November, 2021

Dr. Imtiaz Ahmad Taj
Dean
Faculty of Engineering
November, 2021

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Abstract

Combustion is extremely important to our existence on this planet. A glance around the surroundings shows the importance of combustion in daily life. Industry economic development relies heavily on combustion. Combustion occurs in engines like gas turbines, spark ignition, ramjet, etc. Gas turbine combustion objectives are to provide the required temperature rise to operate the turbine. Three codes are developed with a modern user interface by the name HPFLAME, TPEQUIL and UVFLAME in Microsoft visual basic. The development of combustion codes has optimized the engine cycle by eliminating the need for hand calculations. The correct prediction of engine combustor performance is crucial for an efficient engine cycle. In this work, an approach has been developed for obtaining the combustor theoretical performance and to compare numerical and analytical results. HPFLAME code computes equilibrium mole fractions, adiabatic flame temperature at constant pressure, mixture enthalpy, mixture specific heat, specific heat ratio, mixture molecular weight and moles of fuel per mole of products. UVFLAME code computes equilibrium mole fractions, adiabatic flame temperature at constant volume, product pressure, mixture enthalpy, mixture specific heat, specific heat ratio, mixture molecular weight and moles of fuel per mole of products. TPEQUIL code computes equilibrium mole fractions, mixture enthalpy, mixture specific heat, specific heat ratio, mixture molecular weight and moles of fuel per mole of products. The code is validated with NASA chemical equilibrium analysis software results, Honegger (Kansas state university) results, Peters (Germany) results, Ufot and Douglas results.

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Abbreviations

Ar	Argon
C	Carbon
CO	Carbon Monoxide
H	Hydrogen
N	Nitrogen
NO	Nitric Oxide
O	Oxygen

Symbols

A_{ij}	$\partial f_i / \partial x_j$
dQ/dt	Rate of Heat Transfer
f_i	Nonlinear function of mole fractions
F	fuel/air equivalence ratio
h	Enthalpy per unit mass
h_i	Enthalpy per mole of species i except where otherwise defined
h_r	Reactant enthalpy per unit mass
K_i	Partial Pressure equilibrium constant
m	Mass or number of H atoms in fuel molecule
n	Number of Carbon atoms in fuel molecule
p	Pressure
r, r', r''	Proportions of N_2, O_2, Ar in air
R	Specific Gas Constant of Mixture
R_O	Universal Gas Constant
t	Time
T	Temperature
T_{ij}	$\partial x_i / \partial x_j$
T_w	Gas side wall surface temperature
u	Internal energy per unit mass
V	Volume
x_i	Mole fraction
ζ	Gas constant correction factor
<i>overdot</i>	indicates d/dt

Chapter 1

Introduction

Combustion involves highly exothermic chemical reactions that produces heat. Combustion systems utilize the energy of chemical species generated during this burning process for power generation, transportation and to provide power and heat for numerous applications. Combustion and chemistry are related in numerous ways. The outcome of a burning fuel in terms of its energy, regarding the generation of power, work and harmful emissions, depends on the molecular nature of the respective hydrocarbon fuel. It is required to design an efficient and low emission combustion systems. A closer inspection of the chemical reactions and molecular properties of hydrocarbon fuel is desirable. Information about reaction species, equilibrium nature and potentially hazardous combustion by-products is crucial for safety considerations. Moreover, hydrocarbon fuel can be utilized for energy storage. Combustion processes can also be used to synthesize hydrocarbon fuel with appealing properties.

Chemical knowledge is desirable to understand the behavior of combustion processes. Desirable knowledge includes computation of thermodynamic properties after the combustion reaction and relevant description about the chemical processes that occur during the reactive transformations from the air and fuel to the product species under the initial conditions. Combustion processes can be tailored, described and improved by taking chemical knowledge into account. Combining combustion theory, empirical relations, observations, model development

and numerical analysis of uncertainties enables quantitative or qualitative predictions for many combustion systems of practical significance.

This thesis highlights some of the numerical investigations for combustion reactions with a main focus on numerically predicting thermodynamic properties of hydrocarbon fuels. It attempts to provide knowledge of burning of hydrocarbon fuel with air and a guide to numerical schemes.

In recent years multiple researches on combustion flame temperature have been carried out to study the application of numerical calculations and revealed that the use of computer simulation in vehicle engine design can have accountable significance. Study of numerical techniques includes study of combustion chemical reaction, chemical equilibrium equations, Navier Stokes equations and solving these equations using matrices. This chapter explains briefly about Background of the Study, Research Scope and Thesis overview. The research aims and objectives are also presented in this chapter.

1.1 Background of the Study

Combustion is one of the most focused areas of research in the current era. Spark Ignition engine and turbine engine combustion is the area of concern for manufacturers to increase the effectiveness of a locomotive. Combustion occurs in every car, motor bikes, ships, railway trains, airplanes and rockets. The fuel efficient gas turbine engine is the key element for power in aeroplanes and power generation industry. Similarly internal combustion engine is used for power and heat generation in an automobile industry.

Internal combustion engine works on the principle of constant volume combustion. The internal combustion engine consists of a cylinder where fuel and air mixture is ignited. The engine cycle is discretized into four phases. These phases are termed as intake of fuel-air mixture, compression due to piston force, expansion due to combustion and exhaust of fuel-air mixture. The internal combustion engine comprises of piston, connecting rod, cylinder housing, intake valve, exhaust valve

and a cam mechanism. A mixture of air and hydrocarbon fuel is feeded inside combustion cylinder to generate heat and power. The valve attached at the top of the combustion cylinder allows the air and fuel mixture to enter the cylinder. The opening of this valve is important which would allow the required quantity of air to fuel mixture. The air to fuel mixture is also denoted by equivalence ratio. The equivalence ratio is different at different engine rotation speed. The nearly exact amount of equivalence ratio and its effect on flame temperature can be studied by numerical analysis. The greater the flame temperature, the greater will be power produced.

Volumetric efficiency of the internal combustion engine is defined as the ratio of volume of fuel-air intake charge to the volume of combustion geometry. The efficiency of internal combustion engine depends on the equivalence ratio and type of fuel.

Gas turbine engine works on the principle of constant pressure combustion. An aero-derivative or stationary gas turbine follows a brayton cycle. Its an open cycle that has compressor for increasing the pressure of air, combustion chamber for increasing the temperature of the air and fuel mixture and a turbine for producing required power. The combustion chamber is positioned between the compressor and turbine assembly.

Gas turbines are air breathing engine which require hydrocarbon fuel for combustion. Air flows into the intake section where straight vanes are located to streamline the freshly incoming air. The air then passes through the axial or radial compressor which increases the pressure as well as temperature of air. Atomized Fuel is sprayed inside combustion liner to generate heat energy which would result in rise of temperature of fuel-air mixture. These heated and pressurized gases enters the axial turbine to produce power. The compressor and turbine are connected with a shaft. Part of turbine power is required to drive compressor. Rest of the turbine power is either utilized to provide shaft power or to provide thrust force. The shaft power generated by turbine is used to drive electric generator, pump, external compressor or propellers. The efficiency of the Brayton

cycle is dependent upon compressor pressure ratio, turbine inlet temperature and efficiencies of the gas turbine engine components.

Gas turbines can be designed to use several different fuels such as kerosene fuel, jet fuel, natural gas or hydrogen gas. The efficiency of gas turbine engine is dependent upon fuel to air ratio and type of fuel. The value of burning flame temperature inside combustion chamber can be studied by numerical analysis. Different numerical schemes are presented by different authors. The accurate prediction of thermodynamic properties of species inside combustion chamber depends upon the numerical scheme.

1.2 Research Scope and Objectives

Borman and Olikara [1] has written two subroutines with a test main program. The subroutines can only compute mole fractions, molecular weight, enthalpy, gas constant and internal energy. The subroutine can also compute partial differential of mole fractions and other thermodynamic properties. The subroutine only accepts inputs and outputs in MS-DOS user interface. The main aim of this work is to developed a user friendly softwares.

The scope of this research aims to:

1. Study of existing code subjected to various input.
2. Study of governing linear and partial derivative equations.
3. Solution of linear and partial derivative equations using numerical techniques.
4. Comparing numerical results of old and new code.
5. Optimization of engine combustion flame properties.

Based on the above research scope following research objectives have been established:

1. Analytical modeling of selected chemical reaction.
2. Derivation of linear and partial differential equations for chemical reaction. Linear equations for calculating mole fractions. Partial differential equations for calculating $(\partial x_i / \partial T, \partial x_i / \partial P, \partial x_i / \partial F)$ rate of change of species mole fractions with

equivalence ratio (F), pressure (P) and temperature (T). Also performed derivation for rate of change of enthalpy, combination gas constant and outcome compound internal energy with reference to equivalence ratio (F), pressure (p) and temperature (T).

3. Calculation of the combustion chemical reaction for any hydrocarbon fuel; the required steadiness mole fractions and the partial derivatives of the mole fractions with reference to equivalence ratio, pressure and temperature. These calculations for variable composition of air was not performed in borman algorithm.
4. Calculation of outcome combination enthalpy, combination gas constant, combination internal energy and the partial derivatives of blend with reference to equivalence ratio, pressure and temperature.
5. Calculation of the flame properties of Constant Pressure Combustion.
6. Calculation of the flame properties of Constant Volume Combustion.
7. Compare the results of various hydrocarbon fuels.
8. Validation of new code with old Borman FORTRAN code.
9. Validation of new code with NASA Chemical Equilibrium Analysis code and other international reputed sources.
10. Case studies.

1.3 Research Methodology

The type of research that will be used in this study is quantitative research. Quantitative researchers aim to gather an in-depth understanding of combustion analysis and the mathematical modeling that govern combustion. The research contained analytical analysis, numerical modeling and numerical analysis. The numerical analysis on combustion was performed to obtain flame temperature calculations. For this objective, a code was written which calculates flame properties. Therefore, with the help of these essentials calculations were performed to design the combustion chamber under given conditions. Also validations for various numerical analysis has been presented which are used for calculating flame properties. The numerical and analytical analysis were performed. The numerical

analysis includes analytical modeling and solution. The numerical analysis was conducted to resolve the set of differential equations. To determine the results of flame calculations the partial derivative equations were solved. However code was written to solve the equations rapidly. The flame properties for constant volume combustion and constant pressure combustion were determined through calculations. Microsoft Visual Basic software is used for designing the user interface as well as for programming. In this research object oriented programming theme is selected. The user interface is designed so that calculations are started using one click Calculate button. Three different codes named HPFlame, TPEquil and UVFlame are written in Microsoft Visual Basic.

The data collected by codes are validated against NASA Chemical Equilibrium Analysis code and other international reputed data. Different case studies are conducted on recuperation/regeneration (air preheated) and spark ignition engine exhaust gas recirculation. Background information of complete combustion, water-gas equilibrium, full equilibrium and NASA chemical equilibrium analysis is given. Numerical methods for solving nonlinear equations with Gaussian Elimination and Newton Raphson technique is given. Possible limitations of the codes are temperature in the range from 100 K to 5000 K. The code cannot predict flame properties outside this range. The outcomes of burning are presumed to be ideal gases. This guess is not effective at enormously extreme pressures. The code cannot grip the creation of free carbon.

1.4 Thesis Overview

This thesis comprises of five chapters. Chapter 1, presented the background of a computer software package for computing properties of equilibrium combustion products as well as flame properties. It also includes aims and objectives of the research. Also, the methodology of research was sentenced in this chapter. Comprehensive literature review is presented in Chapter 2, in which studies of last decade was presented, which includes History and Combustion Exhaust Emission for Gas turbine and Spark Ignition Engine. Chapter 3, discusses the

detail description of the stoichiometry, water gas equilibrium, full equilibrium, energy model devising, Steadiness thermodynamics, Lessening in Sum of Equations, the preliminary valuation of mole fractions and taking derivatives of the mole fractions. The chapter 3 deals with the study of enthalpy and Internal Energy, Calculation of Partial Derivatives of Gas Constant of mixture, Enthalpy and Internal Energy, Curve Fitting of Equilibrium Constants, Newton Method for Single Variable, Gaussian Elimination with Backward Substitution.

Chapter 4 deals with code development. Flowcharts for HPFlame, TPEquil and UVFlame Software are specified at the end of the chapter 4.

Chapter 5 deals with Complete Combustion(no dissociation) Adiabatic Flame Temperature at Constant Pressure, Complete Combustion(no dissociation) Adiabatic Flame Temperature at Constant Volume, Visual Basic Code Validation with Borman Code & NASA Code, Code Validation with other References. Case Studies are presented in chapter 5.

The results are discussed and concluded. References [2] are given at the end of the thesis.

Chapter 2

Literature Review

2.1 Thermodynamic Properties

Various vehicles like Motor Car, Diesel Car, Commercial Aeroplane, Fighter Aircraft, Unmanned Aerial Vehicle, Unmanned Combat Aerial Vehicle and Tomahawks requires combustion to propel. Out of the many parameters changing during combustion, temperature is the main parameter. Combustion occurring in a cylinder follows two paths. First path is the burning of any fuel at constant pressure. Second path is the burning of any fuel at constant volume. Both processes increases the temperature of the products mixture. During combustion fuels like hydrocarbon fuel reacts with the air or oxidizer to form product compounds which are also known as species.

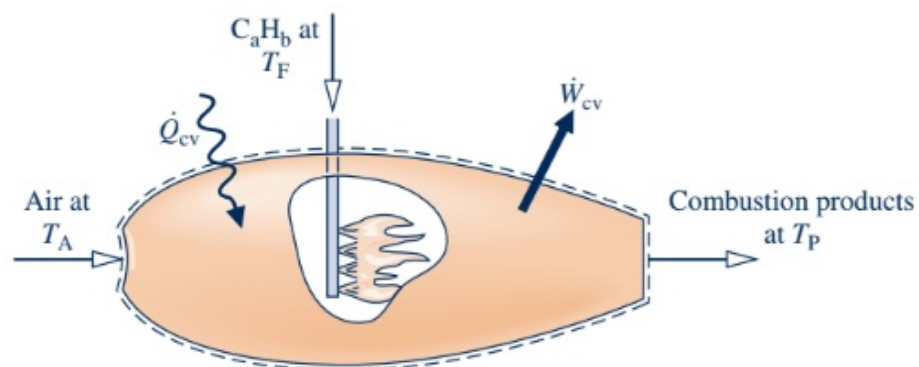


FIGURE 2.1: Reactor at steady state (Reproduced as it is from [3])

The combustion process occurring in turbojet, turbofan, turboshaft and ramjet engine is known as constant pressure combustion. The combustion process occurring in spark ignition engine and diesel engine is known as constant volume combustion. Considering combustion occurring at constant pressure as shown in figure 2.1 [3]. Air is entering the combustion chamber at temperature T_A . Fuel is entering at the fuel injectors at temperature T_F . During the burning process, there are two ways of energy transfer between the combustion chamber and the surroundings. One way is through heat transfer or rate of change of heat transfer Q_{CV} and the other way through work done or rate of change of work W_{CV} . Due to chemical reaction the temperature of the product mixture would rise and some amount would be liberated to the environment. In case of an insulation between combustion chamber and the surroundings, zero energy is transferred to the surroundings. This results in maximum temperature of the product species. The maximum temperature of the product species is known as adiabatic combustion temperature or adiabatic flame temperature.

The adiabatic flame temperature computed for turbo engine combustion chamber and ramjet engine combustion chamber is known as adiabatic flame temperature at constant pressure. The adiabatic flame temperature calculated for spark ignition engine combustion chamber and diesel engine combustion chamber is known as adiabatic flame temperature at constant volume.

Mixture molecular weight is equal to the sum of individual species mole fractions multiplied by the species molecular weight.

Specific heat at constant pressure is defined as rate of change of enthalpy with respect to temperature.

Specific heat at constant volume is defined as rate of change of internal energy with respect to temperature.

Specific heat ratio is defined as ratio of specific heat at constant pressure to the specific heat at constant volume.

Enthalpy is also considered as a thermodynamic quantity equivalent to the total heat content of a system. It is equal to the internal energy of the system plus the

product of pressure and volume. Mixture enthalpy is defined as the total enthalpy of the product mixture divided by the mixture average molecular weight.

The combustion inside a cylinder is modelled by the first law of thermodynamics. The mathematical model is applied to single complete cylinder. The cylinder domain can be subdivided into subsystems. In that case first law of thermodynamics is applied to subsystems. Mathematical models of Spark Ignition engine combustion was studied by [4] Blumberg & Kummer. Mathematical models of Diesel engine combustion was studied by [5] Borman , Myers & Uyehara. Stratified charge engine combustion model (“stratified charge” refers to the working fluids and fuel vapors entering the cylinder) was studied by Evers , Myers & Uyehara [6]. The product species in present work are considered to be at equilibrium state. This was also studied by Newhall [7] for the computation of combustion reaction chemical kinetics parameters. Considering today's world there is a need to compute product species molecular weight, internal energy, enthalpy and mole fractions at equilibrium state. Equilibrium internal energy computation was also studied by Pye and Tizard [8]. Several scientist by the name Powell [9], Newhall [10], Steffensen [11] and Gordon [12] studied the numerical techniques to evaluate thermodynamic properties and species mole fractions using computer.

Olikara and Borman developed a computer subroutine as a case of the full equilibrium model being useful to the C,H,N,O fuel. The code solves for species N_2 , H , CO_2 , O , H_2O , N , O_2 , OH , NO , CO , H_2 with the help of seven equilibrium reactions and four atom balance expressions, one each for Carbon, Oxygen, Hydrogen and Nitrogen. The Borman subroutine was written to solve Internal Combustion locomotive Simulations and is freely inserted as a subprogram to solve Gas Turbine Engine and Ramjet Engine Simulations.

In 1996 Gordon [12], working at NASA Glenn Research Center, write a computer program by the name Chemical Equilibrium Analysis also known as CEA. The code is updated every year so that new features are incorporated into it. This code can calculate product species mole fractions and other thermodynamic properties of the mixture. This code has the ability to solve for four hundred species.

The Code CEA can compute for oblique shock in a rocket nozzle. The code CEA is considered to be most power code in calculating thermodynamic properties of the combustion outcome. The NASA Chemical Equilibrium Analysis Code does not work on the principle of equilibrium constants. The NASA Chemical Equilibrium Analysis Code employs algorithm to minimize either the Helmholtz or Gibbs energies, subject to atom balance constraints.

The current code is capable of solving twelve species as compared to four hundred species in NASA program. It computes with the vapor state outcomes of burning of hydrocarbon fuels (covering N,O,H,C atoms) and air. This code is capable of calculating the partial derivatives of internal energy and molecular weight which are supportive when mathematically calculating the differential model in time by means of the technique of [13] Borman. The Borman code provides a fast way of computation analogous to the procedure of the regression analysis model assumed in Reference [14] Krieger & Borman.

2.2 Computer Codes for Calculating Flame properties

Computer programs were written in Microsoft Visual Basic with good user interface and robust algorithm. Three different programs were written that computes adiabatic flame temperature and other mixture properties. The programs along with their description and limitations are given below.

2.2.1 HPFlame Program

“HP” stands for “Constant Enthalpy” and “Constant Pressure”. Constant Enthalpy means enthalpy of reactants are equal to enthalpy of products. Constant pressure means combustion is taking place at constant pressure. This constant pressure combustion process is also known as isobaric process. A process in which

a gas does work on its environment at constant pressure is called an isobaric process. Generally in isobaric process, the walls of the combustion chamber remains fixed. The input parameters of HPFlame code are type of fuel, equivalence ratio, guess temperature, pressure and enthalpy of reactants. The HPFlame code works on System International units. The code can be adjusted to defined composition of air. The user interface of the HPFlame code is shown in appendix A.

Upon clicking of calculate button, main program is executed. The main program first call for TABLES () subroutine to load molecular weight, enthalpy and specific heat for twelve species. The subroutine also loads $\log K_P$ for seven equilibrium reaction in the arrays for faster computation speed. The main program then calls for PER () subroutine which call for EQMD () subroutine to compute mole fractions and the partial derivatives of mole fractions with respect to pressure, temperature and equivalence ratio. The PER () subroutine computes molecular weight, gas constant, enthalpy and internal energy. The PER () subroutine also computes partial derivatives of molecular weight, gas constant, enthalpy and internal energy with respect to pressure, temperature and equivalence ratio. The main program then updates change in temperature and the iteration continues till change in temperature is less than or equal to 0.01.

The HPFlame Code works on the principle of Borman and Olikara algorithm. The borman algorithm states that to solve for thirteen unknowns (12 species + number of moles of fuel per mole of products) , five atom balance equation plus sum of all the mole fractions add up to unity plus seven chemical equilibrium equations are required. In order to accelerate the convergence, borman algorithm assumes that the only product species are H_2 , CO , O_2 , H_2O , CO_2 , N_2 and Ar . This algorithm is embedded in present work with modern user interface.

The HPFlame temperature has built in thermodynamic tables in the range of 100 K \sim 5000 K. The code cannot calculate external to this temperature array. The code cannot grip the creation of free carbon. The outcomes of burning are expected to be ideal gases. The statement is not effective at exceedingly extreme pressures.

2.2.2 TPEquil Program

“TP” stands for “Temperature” and “Pressure”. “EQUIL” means chemical equilibrium. TPEquil code computes product species mole fraction and thermodynamic properties of mixture at predefined temperature and pressure. The combustion process can be constant pressure or constant volume. For constant pressure combustion, temperature and pressure are specified for turbojet, turbofan, turboshaft and ramjet engine combustion chamber calculations. For constant volume combustion, temperature and pressure are specified for spark ignition and diesel engine combustion chamber calculations. The input parameters of TPEquil code are type of fuel, equivalence ratio, temperature and pressure. The TPEquil code works on System International units. The code can be adjusted to defined composition of air. The user interface of the TPEquil code is shown in appendix A. Upon clicking of calculate button, main program is executed. The main program first call for TABLES () subroutine to load molecular weight, enthalpy and specific heat for twelve species. The subroutine also loads $\log K_P$ for seven equilibrium reaction in the arrays for faster computation speed. The main program then calls for PER () subroutine which call for EQMD () subroutine to compute mole fractions and the partial derivatives of mole fractions with respect to pressure, temperature and equivalence ratio. The PER () subroutine computes molecular weight, gas constant, enthalpy and internal energy. The PER () subroutine also computes partial derivatives of molecular weight, gas constant, enthalpy and internal energy with respect to pressure, temperature and equivalence ratio. The main program then updates thermodynamic properties of the mixture such as mixture molecular weight, mixture enthalpy, mixture specific heat, specific heat ratio and moles of fuel per mole of products. The main program also updates product species mole fractions.

The TPEquil Code works on the principle of Borman and Olikara algorithm. The borman algorithm states that to solve for thirteen unknowns (12 species + number of moles of fuel per mole of products) , five atom balance equation plus sum of all the mole fractions add up to unity plus seven chemical equilibrium equations are required. In order to accelerate the convergence, borman algorithm assumes that

the only product species are H_2 , CO , O_2 , H_2O , CO_2 , N_2 and Ar . This algorithm is embedded in present work with modern user interface.

The TPEquil temperature has built in thermodynamic tables in the range of 100 K \sim 5000 K. The code cannot calculate external to this temperature array. The code cannot grip the creation of free carbon. The outcomes of burning are expected to be ideal gases. The statement is not effective at exceedingly extreme pressures.

2.2.3 UVFlame Program

“UV” stands for “Constant Internal Energy” and “Constant Volume”. Constant Internal Energy means Internal energy of reactants are equal to internal energy of products. Constant volume means combustion is taking place at constant volume. This constant volume combustion process is also known as isochoric process. A thermodynamic process during which the volume of the closed system undergoing such a process remains constant. This process is also known as isovolumetric process or an isometric process. Generally in isochoric process, the walls of the combustion chamber moved in order to keep volume fixed. The input parameters of UVFlame code are type of fuel, equivalence ratio, guess product temperature, reactant temperature, reactant pressure, enthalpy of reactants, moles of reactant and molecular weight of reactants. The UVFlame code works on System International units. The code can be adjusted to defined composition of air. The user interface of the UVFlame code is shown in appendix A. Upon clicking of calculate button, main program is executed. The main program first call for TABLES () subroutine to load molecular weight, enthalpy and specific heat for twelve species. The subroutine also loads $\log K_P$ for seven equilibrium reaction in the arrays for faster computation speed. The main program then calls for PER () subroutine which call for EQMD () subroutine to compute mole fractions and the partial derivatives of mole fractions with respect to pressure, temperature and equivalence ratio. The PER () subroutine computes molecular weight, gas constant, enthalpy and internal energy. The PER () subroutine also computes partial derivatives of molecular weight, gas constant, enthalpy and internal energy with respect to pressure, temperature and equivalence ratio. The main program then updates

change in temperature and the iteration continues till change in temperature is less than or equal to 0.01. The UVFlame Code works on the principle of Borman and Olikara algorithm. The borman algorithm states that to solve for thirteen unknowns (12 species + number of moles of fuel per mole of products) , five atom balance equation plus sum of all the mole fractions add up to unity plus seven chemical equilibrium equations are required. In order to accelerate the convergence, borman algorithm assumes that the only product species are H_2 , CO , O_2 , H_2O , CO_2 , N_2 and Ar . This algorithm is embedded in present work with modern user interface.

The UVFlame temperature has built in thermodynamic tables in the range of 100 K \sim 5000 K. The code cannot calculate external to this temperature array. The code cannot grip the creation of free carbon. The outcomes of burning are expected to be ideal gases. The statement is not effective at exceedingly extreme pressures.

2.3 Gas Turbine Emissions

Due to the health consideration and safety requirement of the environment gas turbine and internal combustion engine emissions are the major public concerns. For the previous ten years lot of research is conducted in terms of technology and the regulations for controlling emissions. The need for both civil as well as military aviation has raised the requirement of fuel consumption and air transport has become the fastest developing energy use sectors. During the past decade fixed gas turbines technology has emerged and has made its roots in power sector and oil & gas industry. Due to the above mentioned reasons there is an immense need of combustion engineer to solve problems relevant to pollutant emissions.

2.3.1 Exhausts of Gas Turbine Engine

The species CO , water vapor (H_2O), carbon dioxide (CO_2), particulate matter (mainly carbon), unburned hydrocarbons (UHC), NO_x and atmospheric oxygen

and nitrogen in large quantities are the exhaust of an aircraft gas turbine engine. Both CO_2 and H_2O are not considered as contaminants because they are the usual outcome of comprehensive burning of a hydrocarbon fuel. By burning less fuel both CO_2 and H_2O contribute less to the global warming. Both direct operating costs and pollution are reduced by improvement in engine thermal efficiency.

A list of major pollutants are shown in Table 2.1. Carbon monoxide (CO) decreases the magnitude of the blood to consume oxygen and can source asphyxiation and even expiry in high concentrations [15]. Unburned hydrocarbons (UHC) combine with NOx to form photochemical smog and they are toxic. Particulate matter (generally called soot or smoke) causes soiling of the atmosphere and creates problems of exhaust visibility. Particulate matter is non toxic at the stages released but modern readings by Seaton [16] specify a robust link between breathing illnesses, asthma and air contamination by gathering of minor bits/particles in the (mcg) microgram scale. Barium which is heavy metal of some smoke suppressants add additional pollutant to the drain gases. The complex at high emission ranks NO from NOx($NO + NO_2$) causes destruction to plant lifespan and add complexity to acid rain [15]. It also donate to the generation of photochemical pollution at sea-level.

Pollutants	Outcome
Carbon-Monoxide (CO)	Poisonous
Unburned-Hydrocarbons (UHC)	Poisonous
Particulate Matter (C)	Noticeable
Oxides of Nitrogen (NOx)	Poisonous, predecessor of chemical smog, reduction of ozone in stratosphere
Oxides of Sulphur (SOx)	Poisonous, corrosive

TABLE 2.1: Principal Pollutants Emitted by Gas Turbines [15]

Aircraft engines contributes less to the overall NOx emissions as compared to other sources. In United States (USA), NOx productions from aero-engines justify for only around two out of a hundred of the overall releases countrywide from all bases [17]. On a worldwide origin, NOx releases from aero-engines create not as

much of 3% of all manufactured machine NO_x releases. Moreover formation of ozone in the Troposphere (the zone that ranges from water level to roughly 12 km top of the earth's level) is caused by these emissions. This is the zone in which ground stationary power turbines and subsonic turbo engine works. The relevant ozone reaction mechanisms are



2.3.2 Pollutant Formation Mechanisms

The presence of above mentioned contaminants in gas turbine drain can be linked straight to the concentration histories, time, temperature of the burning procedure. The contaminant creation varies from one burning can to another and for any assumed combustor, with variations in environment/operating situations [15]. The causes of contaminant creation is such that the aggregation of Carbon-Monoxide (CO) and Unburned-hydrocarbons (UHC) are lowest at high power and highest at low power conditions. Inversely NO_x and smoke reach extreme values at the peak power condition and are justly irrelevant at diminished power settings.

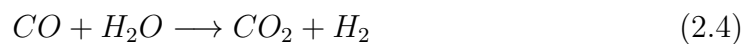
2.3.2.1 Generation of Carbon Monoxide (CO)

Huge quantities of Carbon Monoxide (CO) is generated due to the absence of adequate oxygen to form Carbon Dioxide (CO₂) when a combustion reaction is fed with large quantity of fuel. For the combustion when fuel to air ratio is stoichiometric or discreetly fuel lean, substantial quantities of Carbon monoxide (CO) will also be existing due to the dissociation of Carbon dioxide (CO₂). Due to the admittance of bleed air at the secondary holes of the combustor liner to reduce temperature of the burning outcomes it is possible to lessen the production of Carbon monoxide (CO) to a diminished level. Once formed, carbon monoxide

(CO) is moderately unaffected by oxidation and in many real-world applications carbon monoxide (CO) oxidation is rate determining with reference to the accomplishment of comprehensive burning. The key chemical reaction eliminating Carbon Monoxide (CO) at high temperature is



This is a firm reaction over a comprehensive temperature series. The reaction at lesser temperatures



is vital as a means of eliminating Carbon Monoxide (CO).

The key aspects persuading burning efficiency and hence CO releases are combustor and engine inflow temperatures, burning pressure and primary region equivalence ratio. The key aspects persuading combustion efficiency and hence CO releases are mean drop size of the injector spray with liquid fuels.

2.3.2.2 Unburned Hydrocarbons

The term “Unburned Hydrocarbon” relates to the products that come out of the combustor in terms of drops or vapor and combustion product species of lower molecular weight as a result of thermal degradation. Unburned hydrocarbons are a results of insufficient burning rates, poor atomization, the chilling properties of film-cooling air or any grouping of these. The reaction chemical kinetics of Unburned Hydrocarbon development are more intricate than carbon monoxide creation. Through experimentation it is revealed that the factors influencing carbon monoxide and unburned hydrocarbon emissions are common.

2.3.2.3 Smoke

Smoke is generated in the flame in the fuel rich region due to the creation of finely separated soot particles [15]. Smoke is generated at the exhaust. In old

combustors it is always near to the fuel spray nozzle. There is a region in conventional combustor where burned combustion outcomes transfer upstream towards the fuel injectors. The gases recirculates in the combustor. In this region fuel vapors pockets are entrapped in oxygen lacking gases at high temperature. Soot is produced in large quantities in fuel rich zones. Some of the soot developed in the primary zone is expended in the later stages of combustor. A combustor consists of two zones according to the smoke standpoint. The primary zone in which soot is produced and intermediate zone where soot is consumed at some rate. There is also a zone known as dilution zone on high temperature combustor. The method of noting soot at the drain is the subtraction between two large numbers. Through measurement it is revealed that the exhaust gases contains typically of carbon (Ninety six percent) and a combination of oxygen, hydrogen and other elements. Soot is not formed at balance conditions. It is produced at far richer conditions than the one condition at primary regions of gas turbines. It is not possible to expect its rate of creation and last concentration from chemical kinetic data or thermodynamic information. The speed of soot creation is predicted by atomization processes and fuel to air ratio.

2.3.2.4 Oxides of Nitrogen

Oxidation to NO_2 occurs from nitric oxide NO in combustion successively. For this objective, it is required to combine NO and NO_2 collectively and define outcomes in relations of NO_x , other than NO. It can be formed by four dissimilar mechanisms: nitrous oxide mechanism, thermal NO, fuel NO and prompt NO.

2.3.2.4.1 Thermal Nitric Oxide The oxidation of atmospheric nitrogen in the post flame gases and in high temperature areas of the flame produces thermal nitric oxide. It starts at a noteworthy rate only at temperatures above around 1850 K and the process is endothermic. Extended Zeldovich mechanism is utilized for the planned reaction arrangements for thermal Nitric Oxide (NO). The reactions are as follows:



2.3.2.4.2 Nitrous Oxide Formation Mechanism Agreeing to Nicol et al. [18], the reaction is started by this mechanism



and the nitrous oxide (N_2O) created is then oxidized to Nitric Oxide (NO) primarily by the reaction



but also by the reactions



2.3.2.4.3 Prompt Nitric Oxide Considering positive circumstances, NO is created initially in the flame area - a point that is in conflict with the clue of a kinetically orderly process. Considering Nicol [18], the starting reaction is



The equilibrium of the quick Nitric Oxide (NO) mechanism comprises of the oxidation of the Nitrogen (N) atoms and Hydrogen Cyanide (HCN) molecules. Beneath lean premixed conditions, the Hydrogen Cyanide (HCN) oxidizes to Nitric Oxide

(NO) mostly by a order of reactions including $\text{HCN} \Rightarrow \text{CN} \Rightarrow \text{NCO} \Rightarrow \text{NO}$. The Nitrogen (N) atom responds largely by the Zeldovich reaction of second order.

2.3.2.4.4 Fuel Nitric Oxide Formation Low concentrate fuels hold little than 0.06% of organically fused nitrogen (typically recognized as fuel bound nitrogen; FBN), but the weighty concentrates may comprise as plentiful as 1.8%. Throughout burning, some of this nitrogen rejoins to made the so-termed fuel NO. The portion of nitrogen experiencing this variation rises only gently with rising flame temperature. Considering gaseous fuels, natural gases cover slight or no fuel bound nitrogen but particular is originated in some processes and low British thermal unit gases. Liable on the grade of nitrogen transformation, fuel NO can characterize a substantial amount of the total Nitric oxide (NO) [19].

Nicol [18] critically inspected the comparative offerings of the countless mechanisms argued above to the overall NO_x releases formed by a lean-premixed combustor consuming fuel methane, considering fuel Nitric oxide (NO) is zero. The outcomes of the learning shows that at comparatively high temperatures of around 1900 K and equivalence ratios of around 0.8, the influences are around 60% thermal, 10% N_2O and 30% prompt. With falls in temperature and equivalence ratio, the offerings completed by N_2O and prompt NO rise considerably until, at a temperature of 1500 K and an equivalence ratio of around 0.6, the comparative influences to the total NO_x releases become 5% thermal, 30% N_2O and 65% prompt. At the lowermost equivalence ratios ($\varphi = 0.50.6$), the main basis of NO_x is that made by the N_2O sequence. These outcomes evidently have countless significance to the project of ultra-low NO_x lean premixed combustors.

2.3.3 Pollutants Lessening by Control of Flame Temperature

The utmost significant up till now is the temperature of the combustion reaction of all the aspects persuading contaminant releases from gas turbine combustors. As indicated in Figure 2.2 this can vary from 1000 K at low power process to 2500 K

at high power process with conservative combustors. The figure 2.2 below shows that excessive Carbon Monoxide (CO) is produced at temperatures below around 1670 K (Kelvin). Too much volumes of NO_x are created at temperatures elevated than about 1900 K (Kelvin). Merely in the equally thin range of temperatures between 1670 K and 1900 K are the proportions of NO_x and Carbon Monoxide (CO) below 15 and 25 ppmv individually. Over the total power range of the engine the elementary goal of all the numerous methods towards little emissions combustors is to sustain the combustion region or regions within a equally thin array of temperatures.

2.3.3.1 Variable Geometry

In order to lower temperature at primary zone bleed air is supplied to the inlet of combustor at conditions of maximum power. This is also done to deliver acceptable film cooling air.

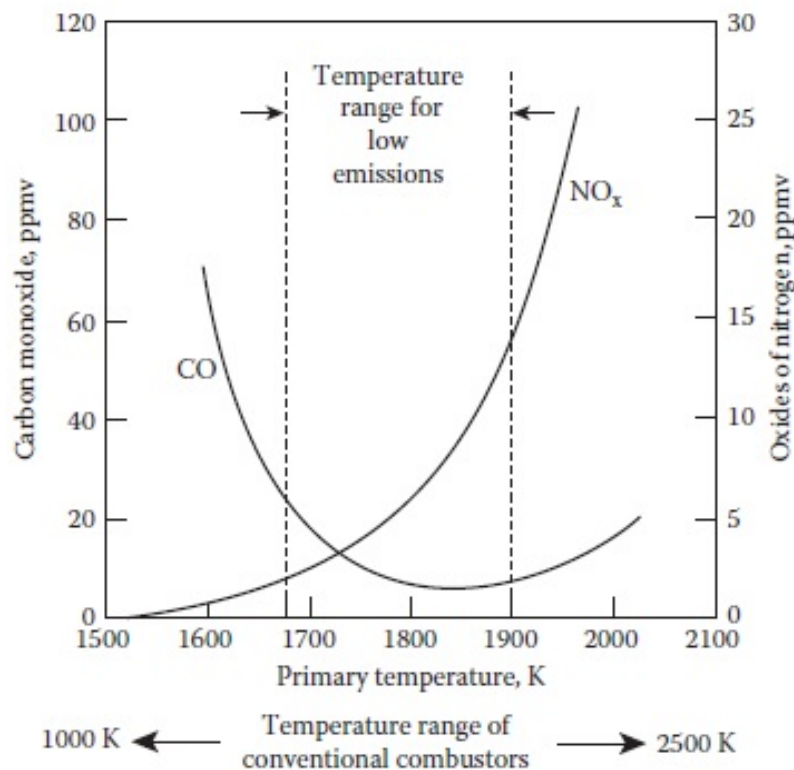


FIGURE 2.2: Influence of primary-zone temperature on CO and NO_x emissions [15]

When engine power is reduced, in order to maintain major region temperature within the diminishing emissions range bleed air is supplied to the dilution zone as shown in Figure 2.2 above. To control the airflow inside combustor variable area swirlers or adjustable air openings into the dilution zone are used. Some systems are also installed with the combination of these. The intricate control and response mechanisms that incline to rise price and reduce dependability and weight is the main disadvantages to all systems of adjustable geometry. Variable geometry combustors are installed in combination with premix pre-vaporize fuel-injection systems. It is probable to circumvent the high NO_x forming areas, local high temperature, formed by the existence of fuel droplets in the burning cylinder. For many years adjustable mechanism has been used in large industrial Gas Turbine locomotives. There have been rare successes of this system in low scale to average size gas turbines due to dimensions and rate restrictions and also because of alarms concerning working dependability [20].

2.3.3.2 Staged Combustion

With variations in combustor power settings, the burning temperature is handled to within equally thin boundaries by exchanging air from one region to another with variable-geometry systems.

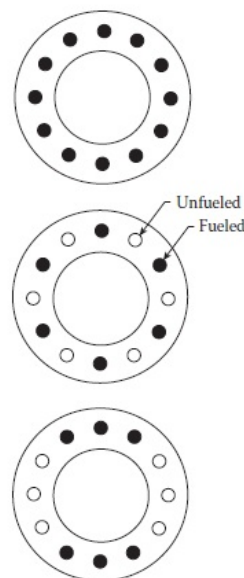


FIGURE 2.3: Illustration of the use of selective fuel injection [15]

The airflow supply within step burning units stays constant. To sustain a fairly constant burning temperature the fuel flow is swapped from one zone to another. One uncertain technique of fuel staging is by “selective fuel injection”, as explained by Bahr [21].

The fuel is delivered merely to designated groupings of fuel injectors at relight, engine idle settings and lightoff as shown in Figure 2.3 with this technique. Power settings above idle is the only full accompaniment of fuel injectors installed. The aim of this intonation schem is to increase the temperature of the restricted burning regions at low power process and the equivalence ratio. This approach not only reduces Unburned Hydrocarbon (UHC) and Carbon Monoxide (CO) releases but also has the extra benefit of spreading the lean blowout boundary to lesser equivalence ratios.

2.3.4 Dry Low Oxides of Nitrogen Combustor Design

In the strategy of Dry Low-Oxides of Nitrogen (DLN) combustors for stationary gas turbines, there are two main performance standards to be met. One noticeable necessity is that of controlling the distinction of releases planes across the load array of the locomotive and gathering the emissions objectives at base load on equally gas and liquid fuels as noted by Davis [22]. Likewise important condition for fidelity system survivability to attain steady burning at all working settings, acceptable levels of combustion noise and worthy system response to fast load variations. Also there is a requirement for swapping easily from gas to liquid fuel, and vice versa. Combustors of this type are known as “dry low emissions” (DLE) combustors or “dry low-NO_x” (DLN) combustors.

2.4 Spark Ignition Engine Pollutants

The primary sources of troposphere pollutions are petrol engines (Spark Ignition) and diesel engines. After combustion in spark ignition engines the gases exiting engine are termed as : nitric oxide (NO) (oxides of nitrogen), nitrogen dioxide

(NO_2) in small quantity jointly recognized as NO_x , carbon monoxide (CO) and carbon based mixtures which are non-reacted or moderately reacted fuel hydrocarbons (HC). The comparative quantities of these "engine-out emission" [23] that enter exhaust are subject to combustor design and functioning surroundings. They are of order NO_x (500–1000 ppm or 20 g/kg fuel); CO (about 1% or 150 g/kg fuel) and hydrocarbons HC (2000 ppm or 15 g/kg fuel). Catalytic converters in the exhaust system reduces engine out emissions by over 90%. Piston exhaust gases, fuel disappearance and discharge to the air through openings in the fuel system, particularly after combustor closed down were historically additional causes of not burning hydrocarbons. However, in recent combustors these nonexhaust bases are handled by transferring the blow-by gases from the crankcase to the combustor entering system and by expelling the petroleum reservoir through a vapor absorbing carbon cannister which is removed with some of the engine entering air during standard combustor operation.

In diesel combustor drain, concentrations of NO_x are similar to those from Spark Ignition engines. Diesel hydrocarbon releases are important, though drain concentrations are much lesser than standard Spark Ignition engine range. The drain hydrocarbons may also condense to create white smoke during combustor initiating and running. Precise hydrocarbon mixtures in the drain gases are the basis of diesel odor. Diesel combustor are a noteworthy basis of particulate releases; between about 0.2% and 0.5% of the fuel mass is released as minor (10 to 500 nm diameter) particles, which contain mainly of soot with added hydrocarbon elements. Diesel combustors are not a primarily cause of carbon monoxide emissions.

The procedures by which contaminants create within the combustion zone of a conventional spark ignition locomotive are shown in Figure 2.4 and 2.5. The schematic demonstrate the combustion zone during four dissimilar stages of the engine working cycle: compression state, combustion state, expansion state and exhaust state. Nitric oxide (NO) creates in the elevated temperature scorched gases after the flame through chemical sequences linking nitrogen and oxygen atoms and molecules: where nitrogen-oxygen system does not achieve chemical steadiness. The greater the scorched gas temperature, the greater is the amount

of growth of Nitric oxide (NO). As the scorched gases cool through the expansion cycle the reactions connecting Nitric oxide (NO) are restricted, and produce Nitric oxide (NO) concentrations fine in additional of stages agreeing to steadiness at drain conditions. Carbon monoxide is similarly created during the burning course.

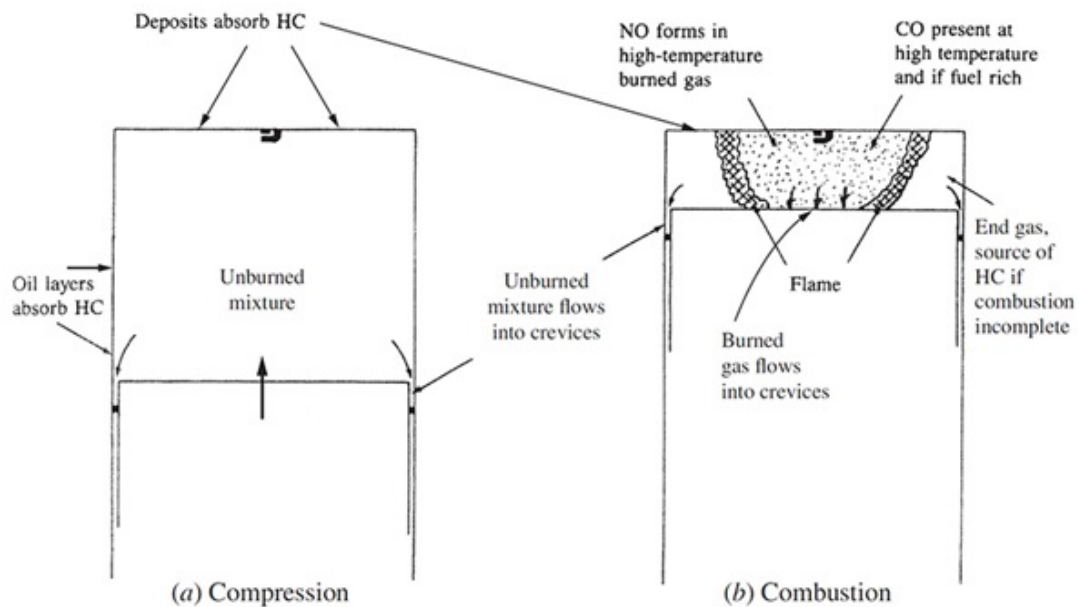


FIGURE 2.4: Summary of HC CO and NO pollutant formation mechanisms in a spark-ignition engine during compression and combustion [23]

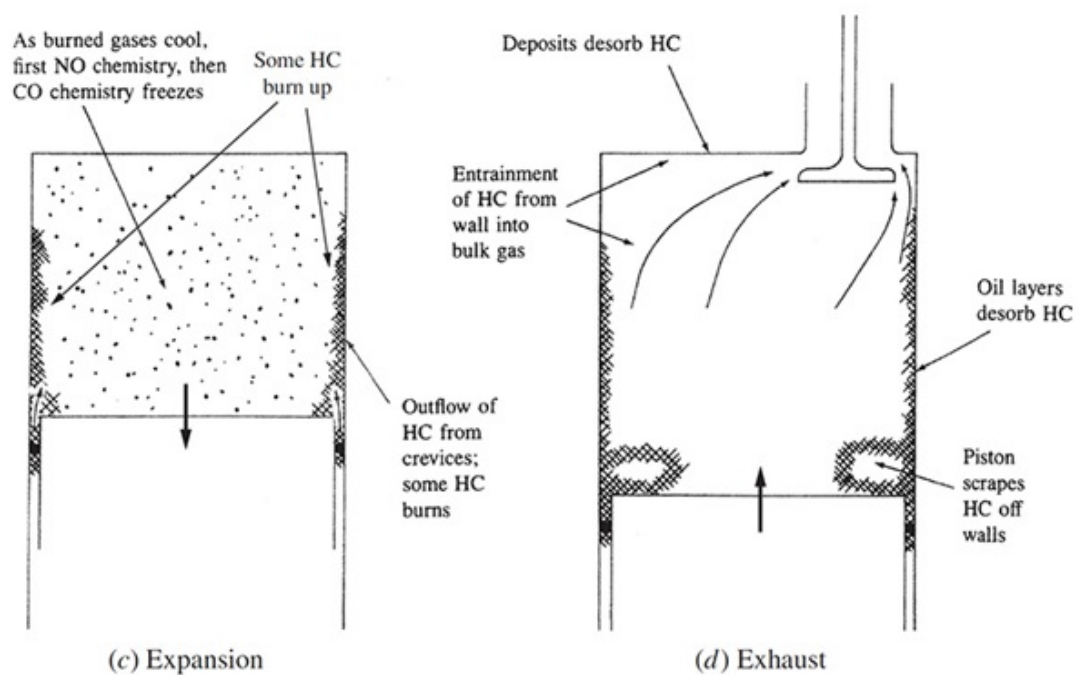


FIGURE 2.5: Summary of HC CO and NO pollutant formation mechanisms in a spark ignition engine during expansion and exhaust [23]

With rich fuel to air mixtures, there is inadequate oxygen to scorch completely all the carbon in the petrol to Carbon dioxide (CO_2). With fuel lean mixtures, due to the dissociation in the high temperature products creates substantial carbon monoxide levels. In the advanced stages of expansion cycle, the Carbon monoxide (CO) oxidation procedure also halts as the scorched mixture temperature drops. The supreme significant ratio in defining spark ignition locomotive drain releases is the relative air to fuel ratio. Figure 2.6 displays the variation of Nitric oxide (NO), Carbon monoxide (CO) and Hydrocarbon (HC) drain releases with the parameter (Air/Fuel Ratio). The spark ignition combustor has generally been functioned close to stoichiometric condition or marginally fuel rich to guarantee even and dependable process.

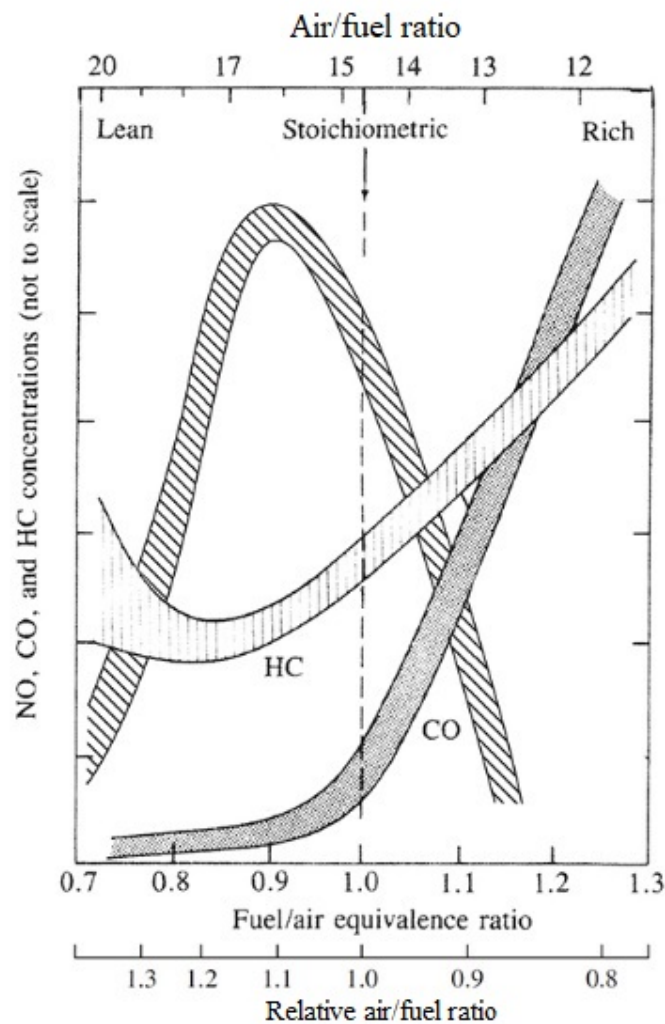


FIGURE 2.6: Variation of HC, CO, and NO concentration in the exhaust of a conventional spark-ignition engine with relative air-fuel ratio and fuel/air equivalence ratio [23]

Figure 2.6 displays that fuel lean mixtures give lesser Carbon monoxide (CO) and Hydrocarbon (HC) drain releases until the combustion grade becomes deprived (and finally backfire happens), when Hydrocarbon (HC) drain releases rise abruptly and combustor working becomes unpredictable. However Nitric oxide (NO) emissions crown about 10% lean of stoichiometric. The profiles of these curves point out the difficulties of drain release control. In a cold combustor, when fuel vaporization is sluggish, the fuel flow may be amplified to offer a simply flammable marginally rich combination in the chamber. Thus increasing Carbon monoxide (CO) and Hydrocarbon (HC) drain releases. At part load settings, lean combinations could be used which would create lesser Hydrocarbon (HC) and Carbon monoxide (CO) drain releases (at least until the burning quality declines), but Nitric oxide (NO) emissions would be high. Usage of recycled exhaust to thinned the combustor entering combination depresses the Nitric oxide (NO) levels, but also depreciates burning grade. Numerous engine control systems uses Exhaust gas recirculation system (EGR) for stoichiometric mixtures. Note that the maximum power stages are gained from the combustor with marginally fuel rich stoichiometric combinations and no recovered drain to thinned the arriving mixture. Also numerous drain release control methods are essential to decrease engine out releases of all three contaminants over all combustor working cycles.

2.4.1 Technical Alternatives for Controlling Spark Ignition Engine NO_x

Three way catalytic converter is installed in all modern spark ignition combustor vehicles as a part of the exhaust system. There are three methods catalytic converter controls three pollutants: carbon monoxide (CO), which reacts with oxygen in the converter to form carbon dioxide (CO_2); unburned hydrocarbons (UHC), which react with oxygen to form carbon dioxide (CO_2) and water vapor (H_2O); and NO_x, which is lessened over the catalyst to nitrogen and water or carbon dioxide (CO_2). The three-way catalyst was designed in the 1970s. It is not expensive and is fuel economic. It causes less problems to performance,

maintenance and drivability. A modern spark ignition engine traveler automobile correctly designed and functioning in standard settings has a very little quantity of NO_x existent in the exhaust of the engine. The NO_x problem is still a major concerned as huge traffic enhance health danger and pollution problematic.

Diesel engine vehicles mechanism of controlling NO_x is more complicated. To control NO_x most modern diesel engine automobiles include exhaust gas recirculation (EGR) in design. In Exhaust Gas Recirculation (EGR) system a percentage of the exhaust gas is fed back into the combustion chamber where it reacts with the fresh intake air to reduce NO_x. This decreases the oxygen content and rises the water vapor content of the combustion mixture. Feeding Exhaust Gas has the result of dropping peak combustion temperature. Because additional NO_x is generated as peak combustion temperature increases, Exhaust Gas Recirculation (EGR) efficiently diminishes the amount of NO_x created by the engine. A proper design of the engine is required because feeding excessive amount of exhaust gas would rise $PM_{2.5}$ and lessen fuel efficiency.

During Combustion Exhaust Gas Recirculation solves the problem of NO_x formation inside the engine combustor. In order to control NO_x two methods which are also known as “aftertreatment” are used at the exhaust of diesel car. A trap known as lean NO_x trap (LNT) temporarily store NO_x using catalyst. The engine controller rises the fuel inside combustor in order to adjust air to fuel ratio at intervals going from seconds to minutes conditional on functioning settings. At a fuel rich condition the exhaust contains less oxygen and more unburned hydrocarbons which results in a chemical reaction of NO_x stored at the catalyst with the hydrocarbons to form nitrogen and water or carbon dioxide. Another method is Selective catalytic reduction (SCR) where NO_x uses ammonia as a reductant over a catalyst. The urea which contains ammonia is supplied which is stored in solution in a tank of a vehicle. The heavy duty vehicles manufactured today is installed with Selective catalytic reduction (SCR) systems while light duty vehicles are installed with Selective catalytic reduction (SCR) or lean NO_x trap (LNT) system. This is due to the size of the engine, operating characteristics and the raw materials cost.

Exhaust Gas Recirculation (EGR), lean NOx trap (LNT) and Selective catalytic reduction (SCR) are considered to be active system as opposed to the three-way catalytic converter. The vehicle engine controls EGR,LNT and SCR using engine control unit. The engine control unit required maintenance and there is a cost both direct (service charges for refilling a urea tank) and indirect (reduced fuel economy due to fuel rich condition or exhaust gas recirculation). The digital electronic control system stops the “aftertreatment” systems during the vehicle movement due to cost constraints.

Chapter 3

Theoretical Analysis

3.1 Introduction

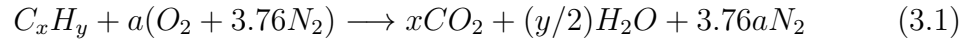
For Gas turbine engines adiabatic flame temperature in the combustor is the temperature of the hot gases at constant pressure after the oxidation process in the combustor. For Spark Ignition engines adiabatic flame temperature in the combustor is the temperature of the hot gases at constant volume after the combustion process. It is so named because there is no energy exchange with the outside surroundings during the adiabatic process. Adiabatic flame temperature calculation for both constant pressure as well as constant volume combustion is important in the design of combustion chamber. Combustor if not designed accordingly will result in the poor efficiency or deterioration of the materials of the combustor which eventually results in premature failure of the combustion chamber.

3.2 Stoichiometry

The stoichiometric amount of air or oxidizer [24] is rightly that quantity required to entirely burn a quantity of fuel. Increasing the supply of the fuel above stoichiometric quantity, the mixture is said to be rich mixture or fuel rich. Decreasing

the supply of the fuel below stoichiometric quantity, the reactant combination is thought to be lean mixture or fuel lean. The stoichiometric air to fuel ratio (by mass) is calculated by solving atom equilibriums, supposing that the fuel counters with air to produce ideal outcomes.

The stoichiometric relation for a hydrocarbon compound (C_xH_y) is expressed as



Where

$$a = x + y/4 \quad (3.2)$$

It is assumed that the basic structure of air is twenty one percent Oxygen (O_2) and seventy nine percent Nitrogen (N_2) (by volume) i.e, for each mole of Oxygen (O_2) in air there are 3.76 moles of Nitrogen (N_2).

The stoichiometric air to fuel fraction is expressed as

$$(A/F)_{stoic} = \left(\frac{m_{air}}{m_{fuel}} \right)_{stoic} = \frac{4.76a}{1} \frac{MW_{air}}{MW_{fuel}} \quad (3.3)$$

Where MW_{air} and MW_{fuel} are the molecular weights of the air and fuel respectively. The equivalence ratio “ F ” is normally related to designate in amount whether a fuel air blend is rich, lean or stoichiometric.

The equivalence fraction is narrated as

$$F = \frac{(A/F)_{stoic}}{A/F} = \frac{(F/A)}{(F/A)_{stoic}} \quad (3.4)$$

For fuel rich combinations $F > 1$ and for fuel lean combination $F < 1$. For a stoichiometric combination “ F ” equals to one.

In numerous combustion applications, the equivalence ratio is the solo most significant aspect in deciding a systems presentation.

3.3 Water-Gas Equilibrium

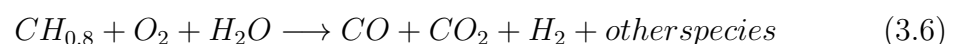
3.3.1 Introduction

In Water-gas shift reaction (WGSR), carbon monoxide and water vapor combines to produce carbon dioxide and hydrogen (Wikipedia) [25]:



The value of water gas shift reaction in industry was realized due to requirement of hydrogen as shown in equation 3.5. In the past, hydrogen was originate by combining steam under extreme pressure with iron to yield iron, hydrogen and iron oxide. With the growth of engineering developments there was a requirement of hydrogen to be used in the Haber Bosch ammonia mixture. A least expensive and effective scheme of hydrogen creation was required. For the solution of this problem, the water gas shift reaction (WGSR) was united with the gasification of coal to yield a clean hydrogen gas. Chemically, coal is an intricate material that can be transformed into a range of outcomes. The gasification of coal is one technique that can create power, liquid fuels, chemicals and hydrogen. Precisely, hydrogen is formed by first combining coal with oxygen and steam under high pressures and temperatures to produce mixture gas, a combination containing mostly of carbon monoxide and hydrogen [26].

Coal gasification reaction (unbalanced):



Once the impurities are detached from the synthesis gas, the carbon monoxide in the gas mixture is combined with steam through the water gas shift reaction

to form extra hydrogen and carbon dioxide. Hydrogen is detached by a parting scheme and the extremely intense carbon dioxide stream can successively be caught and put in storage.

3.3.2 Applications

The water gas shift reaction (WGSR) is a vital engineering model that is employed in the making of hydrocarbons, methanol and hydrogen. It is similarly, frequently employed in combination with steam reforming of methane and added hydrocarbons.

Steam reforming or steam methane reforming is a technique for creating syngas (carbon monoxide and hydrogen) by combining hydrocarbons with water. Generally natural gas is the feedstock (renewable and biological material that can be used directly as a fuel). The core drive of this knowledge is hydrogen making. This water-gas equilibrium is also vital to steam reforming of Carbon monoxide (CO) in the petroleum company.

Another application of water gas shift reaction is the computation of combustion outcome species mole fractions. For stoichiometric condition as given in equation 3.1, the mole fractions can be calculated by atom balances of Carbon, Hydrogen, Nitrogen and Oxygen. But for rich conditions ($F > 1$), additional chemical equilibrium reaction is required. The problem is solved by introducing equilibrium constant values of water gas shift reaction. In the FischerTropsch method, the water gas shift reaction (WGSR) is one of the utmost significant model employed to stabilize the H_2/CO fraction. The FischerTropsch method is a group of chemical models that converts a combination of carbon monoxide and hydrogen into fluid hydrocarbons. The method was initially established by Franz Fischer and Hans Tropsch [27]. It offers a basis of hydrogen at the cost of carbon monoxide, which is vital for the making of concentrated hydrogen for usage in ammonia mixture (Wikipedia) [25].

3.3.3 Calculation of Species Mole fractions by Water-Gas Equilibrium Reaction

To solve for combustion reaction for both rich and lean conditions Water-Gas Equilibrium reaction is introduced in addition to hydrocarbon combustion reaction. This method gives a simple relation that permit the computation of the perfect outcomes of burning (no separation creating negligible species) for equally rich and lean settings. For lean burning, only atom balances equations are required. For rich combustion, single equilibrium reaction is employed additionally 3.5,

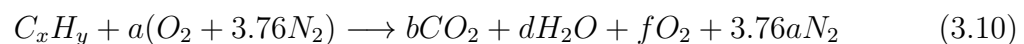
The water gas shift model accounts for the concurrent existence of the imperfect outcomes of burning CO and H_2 . The course of separation is the breakdown of burning outcomes at elevated temperature. Separation is the heat immersion process whereas in burning heat is generated. In Internal Combustion locomotive primarily separation of CO_2 and slight break down of H_2O occurs.



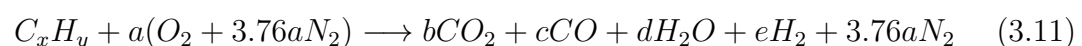
Assuming no dissociation in combustion products, the combustion of any hydrocarbon fuel with basic air is expressed as



For lean or stoichiometric settings ($F \leq 1$) turn out to be



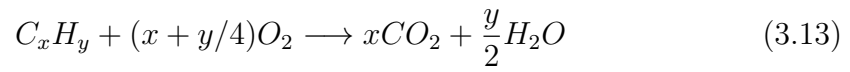
Or for rich conditions ($F > 1$) becomes



Since the coefficient “ a ” in above equation, characterizes the relation of the number of moles of O_2 in the reactants to the number of moles of fuel, one can narrate “ a ” to the equivalence ratio by means of relation $a = x + y/4$ 3.39 i.e.,

$$a = \frac{x + y/4}{F} \quad (3.12)$$

Assuming fuel type and equivalence ratio “ F ” is specified, “ a ” is a known quantity. The relation “ a ” is a result of the stable chemical model for the full burning of a general hydrocarbon fuel C_xH_y derived from equation 3.1:



For stoichiometric or lean burning, the coefficients “ c ” and “ e ” are zero because there is adequate Oxygen (O_2) to have all the fuel Carbon (C) and Hydrogen (H) combine to create Carbon Dioxide (CO_2) and Water (H_2O), correspondingly. The constants b,d and f can be found by Carbon, Hydrogen and Oxygen atom balances, correspondingly; therefore from 3.10

$$b = x \quad (3.14)$$

$$c = 0 \quad (3.15)$$

$$d = y/2 \quad (3.16)$$

$$e = 0 \quad (3.17)$$

$$f = \frac{1 - F}{F}(x + y/4) \quad (3.18)$$

The overall moles of outcomes (per mole of fuel combusted) is evaluated by adding the variables b,c,d,e and f collectively with the $3.76a$ moles of Nitrogen gas (N_2):

$$N_{TOT} = x + y/2 + \frac{x + y/4}{F}(1 - F + 3.76) \quad (3.19)$$

The mole fractions are then calculated by dividing each of the variables mentioned above by overall outcomes moles (N_{TOT}):

Lean or stoichiometric ($F \leq 1$)

$$x_{CO_2} = x/N_{TOT} \quad (3.20)$$

$$x_{CO} = 0 \quad (3.21)$$

$$x_{H_2O} = (y/2)/N_{TOT} \quad (3.22)$$

$$x_{H_2} = 0 \quad (3.23)$$

$$x_{O_2} = \left(\frac{1-F}{F}\right)(x + y/4)/N_{TOT} \quad (3.24)$$

$$x_{N_2} = 3.76(x + y/4)(FN_{TOT}) \quad (3.25)$$

For fuel flow above equivalence ratio ($F > 1$), no oxygen is developed, so the variable “ f ” is zero. To solve for four variables (b, c, d and e), employing the three element level equation (Carbon (C), Hydrogen (H) and Oxygen (O)) and the water-gas shift equilibrium equation [24],

$$K_p = \frac{(P_{CO_2}/P^O)(P_{H_2}/P^O)}{(P_{CO}/P^O)(P_{H_2O}/P^O)} = \frac{b \times e}{c \times d} \quad (3.26)$$

The equilibrium constant of this model express a noteworthy temperature dependency and the equilibrium constant falls with a rise in temperature. More hydrogen development is experienced at lesser temperatures.

The use of above equation 3.26 causes the system of equations for b, c, d and e to be quadratic or nonlinear. Solving the element balances in relation to the unidentified variable “ b ” results in

$$c = x - b \quad (3.27)$$

$$d = 2a - b - x \quad (3.28)$$

$$e = -2a + b + x + y/2 \quad (3.29)$$

Substituting equations above in equation “ K_p ” 3.26 harvests a quadratic model in “ b ” variable, the answer lies

$$b = \frac{2a(K_p - 1) + x + y/2}{2(K_p - 1)} - \frac{1}{2(K_p - 1)} [(2a(K_p - 1) + x + y/2)^2 - 4K_p(K_p - 1)(2ax - x^2)]^{1/2} \quad (3.30)$$

The negative root is computed to vintage accurate (positive) numbers of “ b ”.

$$N_{TOT} = b + c + d + e + 3.76a = x + y/2 + 3.76a \quad (3.31)$$

The mole fractions are stated in relations to “ b ”.

Rich ($F > 1$)

$$x_{CO_2} = b/N_{TOT} \quad (3.32)$$

$$x_{CO} = c/N_{TOT} = (x - b)/N_{TOT} \quad (3.33)$$

$$x_{H_2O} = d/N_{TOT} = (2a - b - x)/N_{TOT} \quad (3.34)$$

$$x_{H_2} = e/N_{TOT} = (-2a + b + x + y/2)/N_{TOT} \quad (3.35)$$

$$x_{O_2} = 0 \quad (3.36)$$

$$x_{N_2} = 3.76a/N_{TOT} \quad (3.37)$$

Subsequently “ K_p ” is temperature dependent and a suitable temperature is nominated. Nevertheless, at distinctive combustion temperatures in the range 2000K-2400K, the compound mole fractions are not sturdily reliant on the selection of temperature. Nominated numbers of “ K_p ” are given in Table 3.1.

T(K)	K_p	T(K)	K_p
298	1.05×10^5	2000	0.2200
500	138.3	2500	0.1635
1000	1.443	3000	0.1378
1500	0.3887	3500	0.1241

TABLE 3.1: Selected values of equilibrium constant K_p for water-gas shift reaction [24]

F	x_{CO}	x_{CO}	% Diff	x_{H_2}	x_{H_2}	% Diff
F	Full Eq	WaterGas	% Diff	Full Eq	WaterGas	% Diff
1.1	0.0317	0.0287	-9.5	0.0095	0.0091	-4.2
1.2	0.0537	0.0533	-0.5	0.0202	0.0203	+0.5
1.3	0.0735	0.0741	+0.8	0.0339	0.0333	-1.8
1.4	0.0903	0.0920	+1.9	0.0494	0.0478	-3.4

TABLE 3.2: CO and H_2 mole fractions for rich combustion C_3H_8 $P = 1atm$
 $K_p = 0.193$ ($T = 2200K$) [24]

Table 3.2 shows comparison between the approximate method above and the full equilibrium calculations for Carbon monoxide (CO) and Hydrogen (H_2) mole fractions for propane air burning outcomes. The equilibrium constant for the water gas shift model is assessed at $2200K$ (Kelvin) for complete equivalence ratios. It is observed that for equivalence ratio $F \geq 1.2$, the approximate methods and the full equilibrium (water-gas equilibrium) produce concentrations that vary by solitary a little percent. As equivalence ratio “ F ” approaches one, the modest model (water-gas equilibrium) becomes progressively imprecise because detachment is ignored.

3.4 Full Equilibrium

Since Water-Gas Equilibrium method is not accurate for equivalence ratio close to unity and for fuel rich mixtures, a full equilibrium method was devised.

An example of Full Equilibrium model calculation for constant pressure (one atm) burning of propane with air is given in figure 3.1 and figure 3.2 where it has been supposed that the only combustion outcomes are N , N_2 , NO , O , O_2 , OH , H , H_2 , H_2O , CO and CO_2 . The variation of adiabatic flame temperature and the main outcome compounds as a relation of equivalence ratio is revealed in figure 3.1. Major products of lean combustion are Nitrogen (N_2), Oxygen (O_2), Carbon Dioxide (CO_2) and Water (H_2O). Major products of rich combustion are Nitrogen (N_2), Hydrogen (H_2), Carbon monoxide (CO), Carbon Dioxide (CO_2)

and Water (H_2O). The maximum adiabatic flame temperature $2278.4K$ happens at a marginally rich equivalence ratio ($F \approx 1.05$) instead of at stoichiometric. The water mole fraction is also maximum at equivalence ratio ($F \approx 1.15$).

Due to the heat capacity and the heat of combustion of the outcomes ($N_{prod} \cdot \overline{C_{p,prod}}$) declining beyond equivalence ratio ($F = 1$), the extreme temperature is at a marginally rich equivalence ratio. The heat capacity declines further quickly with equivalence ratio (F) than heat of combustion (ΔH_c) for equivalence ratios between $F = 1$ and $F(T_{max})$. Heat of combustion (ΔH_c) declines further quickly as compared to the heat capacity between equivalence ratio $F(T_{max})$ and beyond. The reduction in heat capacity is subject to the lessening in number of outcome moles shaped per mole of fuel combusted with the lessening in the mean specific heat being lesser important. The instantaneous existence of Oxygen (O_2), Carbon Monoxide (CO), and Hydrogen (H_2) at stoichiometric conditions ($F = 1$) as a result of dissociation is shown in figure 3.1.

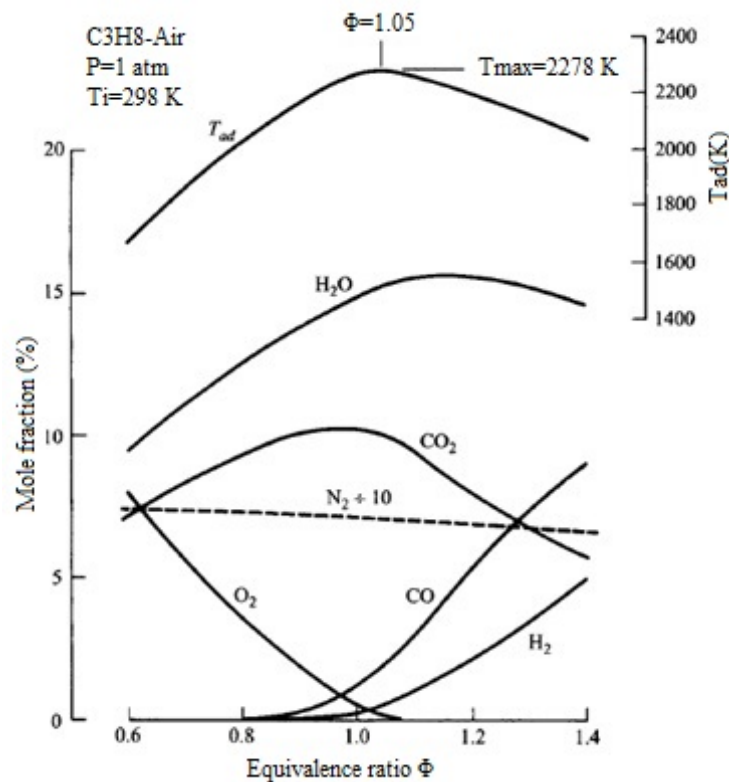


FIGURE 3.1: Equilibrium adiabatic flame temperatures and major product species for propane-air combustion at 1 atm [24]

Under circumstances of “complete combustion” that is no dissociation, species

Oxygen (O_2), Carbon Monoxide (CO) and Hydrogen (H_2) would be zero. The negligible species Carbon Monoxide (CO), Oxygen (O_2), Hydrogen (H_2), Hydroxyl (OH), Nitric Oxide (NO), Carbon Monoxide (CO), Oxygen (O), Hydrogen (H_2) and Hydrogen atom (H) are given in figure 3.2. As shown in figure 3.2 the Oxygen atom (O), hydrogen atom (H) and the diatomic species hydroxyl (OH) and Nitric Oxide (NO) are altogether underneath the 400 ppm level. The Carbon Monoxide (CO) is a negligible specie in lean outcomes. On the other hand the (Oxygen) O_2 is a trivial outcome of rich burning. The Carbon monoxide (CO) and Oxygen (O_2) concentrations are on the top of the graph because they are the main species in rich and lean outcomes correspondingly.

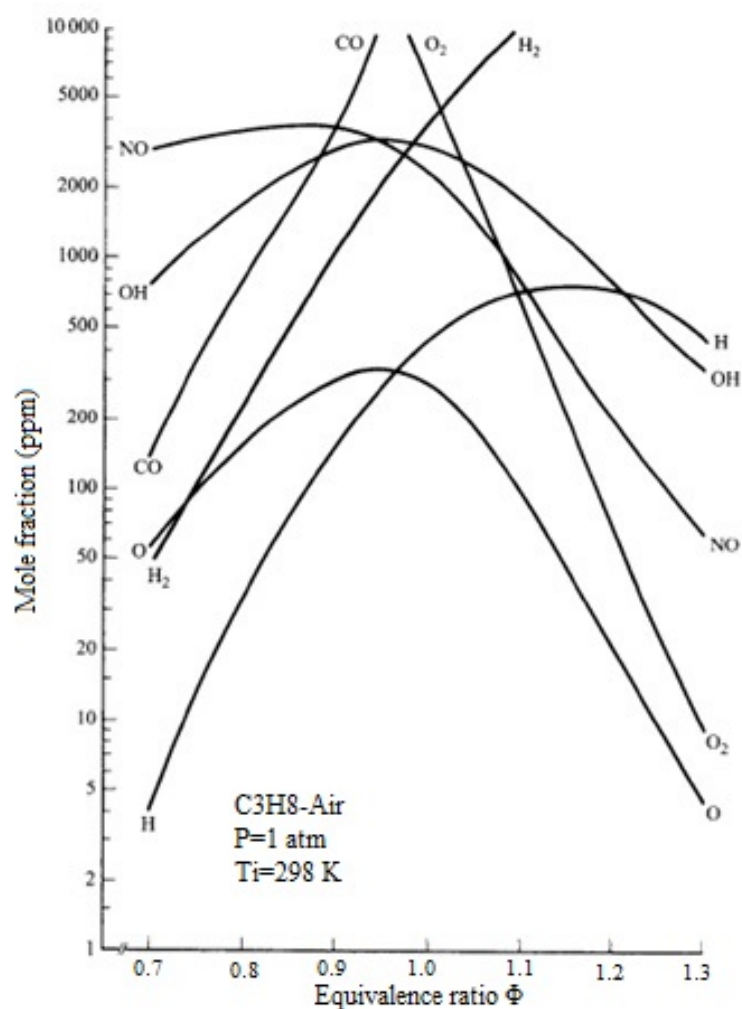


FIGURE 3.2: Minor species distributions for propane-air combustion at 1 atm [24]

As noted the concentration of the hydroxyl radical (OH) is extra than an order of

extent larger than the Oxygen (O) atom and mutually are at the top of the graph at marginally lean of stoichiometric conditions. Also Nitrogen atom (N) levels are numerous orders of magnitude fewer than those of the Oxygen atom (O). The absence of detachment of the Nitrogen (N_2) molecule is a outcome of the robust three-way covalent bond. The Oxygen atom (O) and hydroxyl radical (OH) is utmost in the lean area have associations for the kinetics of Nitric Oxide (NO) creation. Equilibrium Nitric Oxide (NO) levels are smooth and crowning in the lean area while dropping quickly in the rich area. As shown in figure 3.2 Nitric Oxide (NO) concentrations are well beneath the steady state concentrations in most combustion systems. This is due to the fact of relatively slow formation reactions.

3.5 Energy Equation Formulation

The system is divided into cells to treat the cylinder gas system thermodynamically for uniformity of the configuration and temperature of each cell of the system. This concludes that the molar average temperature of the cell can be employed to calculate the internal energy of the cell. For example various theoretical representations employed for the spark ignition locomotive system split the system into subsystems assuming the similar pressure for each subsystem. It is assumed to allocate one temperature for the complete product mass. The primary law for each structure of outcomes is

$$\frac{dmu}{dt} = -p\frac{dV}{dt} + \frac{dQ}{dt} + \Sigma h_i \dot{m}_i \quad (3.38)$$

Where $\frac{dmu}{dt}$ = rate of change of total internal energy mu of system mass m

m =Mass in the system

u =Specific internal energy of the system

h_i =Total specific (stagnation) enthalpy of the mass inflowing or outflowing the system through flow surface i

p =Total pressure in the system

\dot{V} = Rate of volume change of the system

\dot{Q} = Rate of heat transfer through surface

$p \frac{dV}{dt}$ = Rate of mechanical work completed by the system on its limit

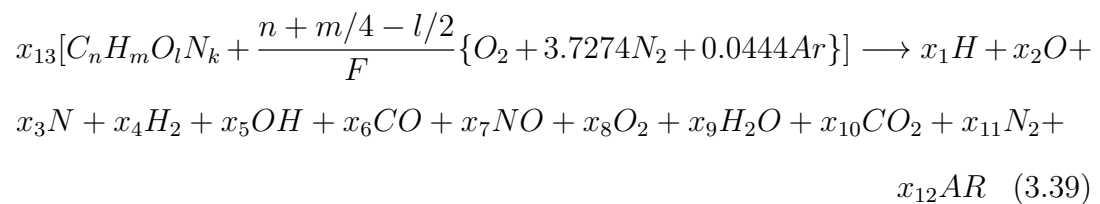
$\frac{dQ}{dt}$ = Rate of heat transfer into the system through system boundary

$h_i \dot{m}_i$ = energy transfer in or out of the system at flow area location i by mass flow rate (\dot{m}_i).

For outflow the enthalpy h_i is the system total enthalpy. For inflow the stagnant absolute enthalpy of the flow stream at the edge is to be utilized. Equation 3.38 postulates that the time change of internal energy in the system is equal to the sum of the time rates at which energy leaves the system due to work $-p \frac{dV}{dt}$, due to heat transfer $\frac{dQ}{dt}$ and due to mass transfer $\Sigma h_i \dot{m}_i$.

3.6 Equilibrium Thermodynamics

Assuming the fuel $C_n H_m O_l N_k$ and air at equivalence ratio “ F ” react and the outcomes focusing temperature “ T ” and pressure “ p ” achieve equilibrium. The numbers “ n ” and “ m ” must be nonzero; “ l ” and “ k ” may or may not be zero.



Where x_1 through x_{12} are mole fractions of the outcome species.

The number x_{13} signifies the moles of fuel that will provide one mole of outcomes.

The left side of the model equation 3.39 is shown as

$$x_{13}[nC + mH + rO_2 + r'N_2 + r''Ar] \quad (3.40)$$

Where

$$r = l/2 + r_O \quad (3.41)$$

$$r' = k/2 + 3.7374r_O \quad (3.42)$$

$$r'' = 0.0444r_O \quad (3.43)$$

$$r_O = (n + m/4 - l/2)/F \quad (3.44)$$

Atom stabilities for the numerous elements give

$$C \text{ balance} : x_6 + x_{10} = nx_{13} \quad (3.45)$$

$$H \text{ balance} : x_1 + 2x_4 + x_5 + 2x_9 = mx_{13} \quad (3.46)$$

$$O \text{ balance} : x_2 + x_5 + x_6 + x_7 + 2x_8 + x_9 + 2x_{10} = 2rx_{13} \quad (3.47)$$

$$N \text{ balance} : x_3 + x_7 + 2x_{11} = 2r'x_{13} \quad (3.48)$$

$$Ar \text{ balance} : x_{12} = r''x_{13} \quad (3.49)$$

The restriction that the mole fraction of all the outcomes add up to one necessitates that

$$\sum_{i=1}^{12} x_i = 1 \quad (3.50)$$

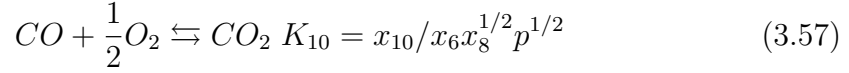
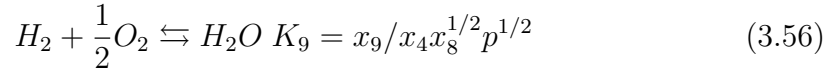
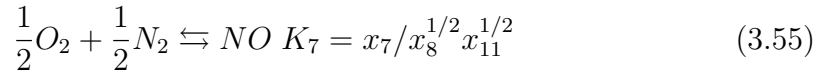
To solve for the thirteen unknowns, seven more equations are required which are supplied by the standards of equilibrium between the outcomes conveyed by the resulting seven non redundant hypothetical reactions.

$$\frac{1}{2}H_2 \rightleftharpoons H \quad K_1 = x_1p^{1/2}/x_4^{1/2} \quad (3.51)$$

$$\frac{1}{2}O_2 \rightleftharpoons O \quad K_2 = x_2p^{1/2}/x_8^{1/2} \quad (3.52)$$

$$\frac{1}{2}N_2 \rightleftharpoons N \quad K_3 = x_3p^{1/2}/x_{11}^{1/2} \quad (3.53)$$

$$\frac{1}{2}H_2 + \frac{1}{2}O_2 \rightleftharpoons OH \quad K_5 = x_5/x_4^{1/2}x_8^{1/2} \quad (3.54)$$



Where symbol “ p ” is the pressure in atmospheres (atm). The equilibrium constants are evaluated from Joint Army Navy Air Force (JANAF Tables) [28] through curve fittings method. Curve fitting details are given in headings below. The equilibrium constants relations can be reordered to relate mole fractions of all the outcomes of burning in terms of x_4, x_6, x_8 and x_{11} . Here x_4, x_6, x_8 and x_{11} are the mole fractions of Hydrogen H_2 , carbon monoxide CO , Oxygen O_2 and Nitrogen N_2 respectively.

$$x_1 = C_1 x_4^{1/2} \quad \text{where } C_1 = K_1/p^{1/2} \quad (3.58)$$

$$x_2 = C_2 x_8^{1/2} \quad \text{where } C_2 = K_2/p^{1/2} \quad (3.59)$$

$$x_3 = C_3 x_{11}^{1/2} \quad \text{where } C_3 = K_3/p^{1/2} \quad (3.60)$$

$$x_5 = C_5 x_4^{1/2} x_8^{1/2} \quad \text{where } C_5 = K_5 \quad (3.61)$$

$$x_7 = C_7 x_8^{1/2} x_{11}^{1/2} \quad \text{where } C_7 = K_7 \quad (3.62)$$

$$x_9 = C_9 x_4 x_8^{1/2} \quad \text{where } C_9 = K_9 p^{1/2} \quad (3.63)$$

$$x_{10} = C_{10} x_6 x_8^{1/2} \quad \text{where } C_{10} = K_{10} p^{1/2} \quad (3.64)$$

3.7 Number of Equations Reduction

Equation 3.45 springs $x_{13} = \frac{1}{n}(x_6 + x_{10})$

Equation 3.49 gives $x_{12} = r'' x_{13} = \frac{r''}{n}(x_6 + x_{10})$ These are now used to eliminate x_{12} and x_{13} in Equations 3.46, 3.47, 3.48 and 3.50

$$x_1 + 2x_4 + x_5 + 2x_9 - \frac{m}{n}(x_6 + x_{10}) = 0 \quad (3.65)$$

$$x_2 + x_5 + x_6 + x_7 + 2x_{10} - \frac{2r}{n}(x_6 + x_{10}) = 0 \quad (3.66)$$

$$x_3 + x_7 + 2x_{11} - \frac{2r'}{n}(x_6 + x_{10}) = 0 \quad (3.67)$$

$$\sum_{i=1}^{11} x_i + \frac{r''}{n}(x_6 + x_{10}) - 1 = 0 \quad (3.68)$$

Denote the ratios

$$\frac{m}{n} = d_1 \quad (3.69)$$

$$\frac{2r}{n} = d_2 \quad (3.70)$$

$$\frac{2r'}{n} = d_3 \quad (3.71)$$

$$\frac{r''}{n} = d_4 \quad (3.72)$$

Now Equations 3.58,3.59,3.60,3.61,3.62,3.63 and 3.64 are utilized in Equations 3.65,3.66,3.67 and 3.68 to remove all variable quantity excluding x_4, x_6, x_8 and x_{11} . The subsequent four nonlinear equations with four unknowns is stated representatively by

$$f_j(x_4, x_6, x_8, x_{11}) = 0 \quad j = 1, 2, 3, 4 \quad (3.73)$$

$$f_1 = (x_1 + 2x_4 + x_5 + 2x_9) - d_1(x_6 + x_{10}) \quad (3.74)$$

$$f_2 = (x_2 + x_5 + x_6 + x_7 + 2x_8 + x_9 + 2x_{10}) - d_2(x_6 + x_{10}) \quad (3.75)$$

$$f_3 = (x_3 + x_7 + 2x_{11}) - d_3(x_6 + x_{10}) \quad (3.76)$$

$$f_4 = d_4(x_6 + x_{10}) + \sum_{i=1}^{11} -1 \quad (3.77)$$

Putting in the values for $x_1, x_2, x_3, x_5, x_7, x_9, x_{10}$ from Equation 3.58 to 3.64

$$f_1 = (C_1x_4^{1/2} + 2x_4 + c_5x - 4^{1/2}x_8^{1/2} + 2C_9x_4x_8^{1/2}) - d_1(x_6 + c_{10}x_6x_8^{1/2}) \quad (3.78)$$

$$f_2 = (C_2x_8^{1/2} + C_5x_4^{1/2}x_8^{1/2} + x_6 + C_7x_8^{1/2}x_{11}^{1/2} + 2x_8 + C_9x_4x_8^{1/2} + 2C_{10}x_6x_8^{1/2}) - d_2(x_6 + C_{10}x_6x_8^{1/2}) \quad (3.79)$$

$$f_3 = (C_3x_{11}^{1/2} + C_7x_8^{1/2}x_{11}^{1/2} + 2x_{11}) - d_3(x_6 + C_{10}x_6x_8^{1/2}) \quad (3.80)$$

$$f_4 = d_4(x_6 + C_{10}x_6x_8^{1/2}) + \sum_{i=1}^{11} x_i - 1 \quad (3.81)$$

Assuming a vector

$$[x_4^{(1)}, x_6^{(1)}, x_8^{(1)}, x_{11}^{(1)}] \quad (3.82)$$

Which is sensibly near to the correct solution vector

$$[x_4^*, x_6^*, x_8^*, x_{11}^*] \quad (3.83)$$

The functions on the left side of the equations can then be extended around the know vector as a Taylors Series. Let

$$\Delta x_i = x_i^* - x_i^{(1)} \quad i = 4, 6, 8, 11 \quad (3.84)$$

Ignoring the partial derivatives of second order and higher, a set of linear equations is obtained where Δx_i are the approximate corrections. Thus

$$f_j + \frac{\partial f_j}{\partial x_4} \Delta x_4 + \frac{\partial f_j}{\partial x_6} \Delta x_6 + \frac{\partial f_j}{\partial x_8} \Delta x_8 + \frac{\partial f_j}{\partial x_{11}} \Delta x_{11} \cong 0 \quad j = 1, 2, 3, 4 \quad (3.85)$$

Where functions f_j and their partial derivatives are calculated at the known vector. This set of linear equations can be solved for Δx_4 , Δx_6 , Δx_8 and Δx_{11} using a Gaussian Matrix elimination method. The better values are then

$$x_i^{(2)} = x_i^{(1)} + \Delta x_i \quad i = 1, 2, 3, 4 \quad (3.86)$$

The x_i is calculated iteratively to get the improved values and hence calculate the partial derivatives and functions. The corrections Δx_i are also computed iteratively and applied. The iterations are continued till the relative changes are less than a stated value. Specifics of the computation of the elements of equation 3.78 to 3.81 are shown in heading (3.9).

3.8 Initial Estimation of Mole Fractions

In order to solve for twelve mole fractions in four unknowns, it is required to guess a values for four unknowns x_4, x_6, x_8 and x_{11} . For that reason it is assumed

that the products are hydrogen, carbon monoxide, oxygen, water, carbon dioxide, nitrogen and argon. All three variables x_4, x_6, x_{11} are expressed in terms of x_8 . Newton raphson method is used to solve for x_8 . To start the solution initial value of x_8 is taken to be one. The reason to guess x_4, x_6, x_8 and x_{11} is to have the convergence of the solution as fast as possible. The following method of estimation is found to be excellent for fast convergence.

Assume that the products are only $H_2, CO, O_2, H_2O, CO_2, N_2$ and Ar . Equation 3.39 becomes

$$x_{13}(nC + mH + rO_2 + r'N_2 + r''AR) \longrightarrow x_4H_2 + x_7CO + x_8O_2 + x_9H_2O + x_{10}CO_2 + x_{11}N_2 + x_{12}Ar \quad (3.87)$$

From carbon C balance and equation 3.64

$$x_6 = \frac{nx_{13}}{1 + C_{10}x_8^{1/2}} \quad (3.88)$$

From the hydrogen H balance and equation 3.63

$$x_4 = \frac{0.5mx_{13}}{1 + C_9x_8^{1/2}} \quad (3.89)$$

From the nitrogen N , argon Ar and oxygen O balances

$$x_{11} = r'x_{13} \quad (3.90)$$

$$x_{12} = r''x_{13} \quad (3.91)$$

$$x_6 + 2x_8 + x_9 + 2x_{10} = 2rx_{13} \quad (3.92)$$

Substituting for x_6, x_9 and x_{10} , reordering terms and dividing through by x_{13}

$$\frac{2C_{10}nx_8^{1/2} + n}{1 + C_{10}x_8^{1/2}} + \frac{0.5C_9mx_8^{1/2}}{1 + C_9x_8^{1/2}} + \frac{2x_8}{x_{13}} - 2r = 0 \quad (3.93)$$

The variable x_{13} is predicted with virtuous precision from the state that the mole fractions add up to one.

$$x_4 + x_6 + \sum_{i=8}^{12} x_i = 1 \quad (3.94)$$

For $F \leq 1$ a virtuous guess of x_{13} is obtained from

$$x_{13} = 1/(m/4 + r + r' + r'') \quad (3.95)$$

For $F > 1$ an approximation of x_{13} can be acquired from

$$x_{13} = 1/(n + m/2 + r' + r'') \quad (3.96)$$

Substitution of the assessed value of x_{13} into equation 3.93 provides an equation in the single unknown x_8 . The derivative of equation 3.93 is given as:

$$\text{Derivative } f'(x) = \frac{(0.25)(2)(n)(C_{10})}{x_8^{1/2}(1 + C_{10}x_8^{1/2})^2} + \frac{(0.5)(0.5)(m)(C_9)}{x_8^{1/2}(1 + C_9x_8^{1/2})^2} + \frac{2}{x_{13}} \quad (3.97)$$

After solving equation 3.93 by Newtons Raphson scheme, the other undisclosed variables are acquired straight by replacement into equations 3.88,3.89 and 3.90.

Initial estimate of $x_8 = 1.0$.

The stopping criteria for solving above equation by Newtons method is $\delta/x_8 \leq 0.01$ ($\delta = f(x)/f'(x)$).

These preliminary guesses can then be used to initiate the solution of equation 3.73 by use of equation 3.85 and 3.86.

3.8.1 Theory of Concave and Convex function

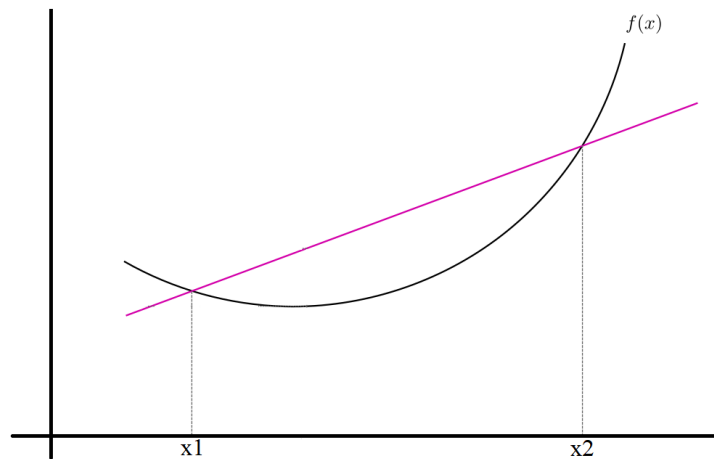


FIGURE 3.3: Convex Function [25]

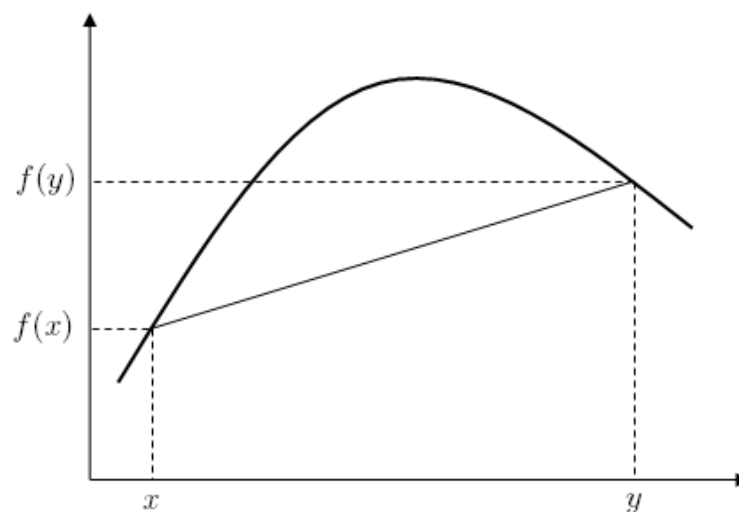


FIGURE 3.4: Concave Function [25]

A real-valued function is called convex if the line segment between any two points on the graph of the function lies above the graph between the two points. Equivalently, a function is convex if its epigraph (the set of points on or above the graph of the function) is a convex set. A twice-differentiable function of a single variable is convex if and only if its second derivative is nonnegative on its entire domain [25]. Well-known examples of convex functions of a single variable include the quadratic function x^2 and the exponential function e^x . In simple terms, a convex function refers to a function that is in the shape of a cup \cup .

Convex functions play an important role in many areas of mathematics. They are especially important in the study of optimization problems where they are distinguished by a number of convenient properties. For instance, a strictly convex function on an open set has no more than one minimum. Even in infinite-dimensional spaces, under suitable additional hypotheses, convex functions continue to satisfy such properties and as a result, they are the most well-understood functionals in the calculus of variations. Convex function is also applied to the probability theory [25].

A real-valued function is called concave if the line segment between any two points on the graph of the function lies below the graph between the two points. A twice-differentiable function of a single variable is concave if and only if its second derivative is negative on its entire domain [25]. A concave function refers to a function that is in the shape of \cap . Concave function are applied to rays bending in the computation of radiowave attenuation in the atmosphere. Similarly they are applied to expected utility theory for choice under uncertainty, cardinal utility functions of risk averse decision makers and in microeconomic theory [25].

3.9 Mole Fraction Computation Equation

The partial derivatives $\frac{\partial x_i}{\partial x_j}$ in addition to T_{ij} is defined as

$$T_{ij} = \frac{\partial x_i}{\partial x_j} \quad i = 1, 2, 3, 5, 7, 9, 10 \quad j = 4, 6, 8, 11 \quad (3.98)$$

$$T_{jj} = \frac{\partial x_j}{\partial x_j} = 1 \quad (3.99)$$

From Equation 3.58 to 3.64 we get

$$T_{14} = 0.5C_1/x_4^{1/2} \quad (3.100)$$

$$T_{28} = 0.5C_2/x_8^{1/2} \quad (3.101)$$

$$T_{311} = 0.5C_3/x_{11}^{1/2} \quad (3.102)$$

$$T_{54} = 0.5C_5x_8^{1/2}/x_4^{1/2} \quad (3.103)$$

$$T_{58} = 0.5C_5x_4^{1/2}/x_8^{1/2} \quad (3.104)$$

$$T_{78} = 0.5C_7x_{11}^{1/2}/x_8^{1/2} \quad (3.105)$$

$$T_{711} = 0.5C_7x_8^{1/2}/x_{11}^{1/2} \quad (3.106)$$

$$T_{94} = C_9x_8^{1/2} \quad (3.107)$$

$$T_{98} = 0.5C_9x_4/x_8^{1/2} \quad (3.108)$$

$$T_{106} = C_{10}x_8^{1/2} \quad (3.109)$$

$$T_{108} = 0.5C_{10}x_6/x_8^{1/2} \quad (3.110)$$

The equation 3.85 in terms of A_{ij} expressed as a matrix equation $[A][\Delta x] = [B]$ is as follows

$$A_{11} = \frac{\partial f_1}{\partial x_4} = T_1 + 2 + T_{54} + 2T_{94} \quad (3.111)$$

$$A_{12} = \frac{\partial f_1}{\partial x_6} = -d_1(1 + T_{106}) \quad (3.112)$$

$$A_{13} = \frac{\partial f_1}{\partial x_8} = T_{58} + 2T_{98} - d_1T_{108} \quad (3.113)$$

$$A_{14} = \frac{\partial f_1}{\partial x_{11}} = 0 \quad (3.114)$$

$$A_{21} = \frac{\partial f_2}{\partial x_4} = T_{54} + T_{94} \quad (3.115)$$

$$A_{22} = \frac{\partial f_2}{\partial x_6} = 1 + 2T_{106} - d_2(1 + T_{106}) \quad (3.116)$$

$$A_{23} = \frac{\partial f_2}{\partial x_8} = T_{28} + T_{58} + T_{78} + 2 + T_{98} + 2T_{108} - d_2T_{108} \quad (3.117)$$

$$A_{24} = \frac{\partial f_2}{\partial x_{11}} = T_{711} \quad (3.118)$$

$$A_{31} = \frac{\partial f_3}{\partial x_4} = 0 \quad (3.119)$$

$$A_{32} = \frac{\partial f_3}{\partial x_6} = -d_3(1 + T_{106}) \quad (3.120)$$

$$A_{33} = \frac{\partial f_3}{\partial x_8} = T_{78} - d_1T_{108} \quad (3.121)$$

$$A_{34} = \frac{\partial f_3}{\partial x_{11}} = T_{311} + T_{711} + 2 \quad (3.122)$$

$$A_{41} = \frac{\partial f_4}{\partial x_4} = T_{14} + 1 + T_{54} + 2 \quad (3.123)$$

$$A_{42} = \frac{\partial f_4}{\partial x_6} = 1 + T_{106} + d_4(1 + T_{106}) \quad (3.124)$$

$$A_{43} = \frac{\partial f_4}{\partial x_8} = T_{28} + T_{58} + T_{78} + 1 + T_{98} + T_{108} + d_4 T_{108} \quad (3.125)$$

$$A_{44} = \frac{\partial f_4}{\partial x_{11}} = T_{311} + T_{711} + 1 \quad (3.126)$$

$$B_1 = -f_1 = -(x_1 + 2x_4 + x_5 + 2x_9) + d_1(x_6 + x_{10}) \quad (3.127)$$

$$B_2 = -f_2 = -(x_2 + x_5 + x_6 + x_7 + 2x_8 + x_9 + 2x_{10}) + d_2(x_6 + x_{10}) \quad (3.128)$$

$$B_3 = -f_3 = -(x_3 + x_7 + 2x_{11}) + d_3(x_6 + x_{10}) \quad (3.129)$$

$$B_4 = -f_4 = 1 - d_4(x_6 + x_{10}) - \sum_{i=1}^{11} x_i \quad (3.130)$$

$$f_1 = (x_1 + 2x_4 + x_5 + 2x_9) - d_1(x_6 + x_{10}) \quad (3.131)$$

$$f_2 = (x_2 + x_5 + x_6 + x_7 + 2x_8 + x_9 + 2x_{10}) - d_2(x_6 + x_{10}) \quad (3.132)$$

$$f_3 = (x_3 + x_7 + 2x_{11}) - d_3(x_6 + x_{10}) \quad (3.133)$$

$$f_4 = d_4(x_6 + x_{10}) + \sum_{i=1}^{11} x_i - 1 \quad (3.134)$$

In matrix form it is written as:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} \begin{bmatrix} \Delta x_4 \\ \Delta x_6 \\ \Delta x_8 \\ \Delta x_{11} \end{bmatrix} = \begin{bmatrix} -f_1 \\ -f_2 \\ -f_3 \\ -f_4 \end{bmatrix}$$

This matrix is solved for $\Delta x_4, \Delta x_6, \Delta x_8, \Delta x_{11}$ using a Gaussian Matrix elimination scheme. The enhanced estimates are

$$x_i^{(2)} = x_i^{(1)} + \Delta x_i \quad i = 1, 2, 3, 4 \quad (3.135)$$

The enhanced vector are employed to assess the partial derivatives and functions. Additional rectifications are computed and put in an application. The loop process is sustained until the comparative deviations in all the variables are less than an indicated number. The Stop Criterion is $|\Delta x_j/x_j| \leq 0.001$ and condition is $|x_j| \geq 10^{-7}$ for $j=1,2,3,4$.

This results in the calculated values of x_4, x_6, x_8, x_{11} . The remaining mole fractions are calculated by the following equations:

$$x_1 = C_1 x_4^{1/2} \quad \text{where} \quad C_1 = K_1/p^{1/2} \quad (3.136)$$

$$x_2 = C_2 x_8^{1/2} \quad \text{where} \quad C_2 = K_2/p^{1/2} \quad (3.137)$$

$$x_3 = C_3 x_{11}^{1/2} \quad \text{where} \quad C_3 = K_3/p^{1/2} \quad (3.138)$$

$$x_5 = C_5 x_4^{1/2} x_8^{1/2} \quad \text{where} \quad C_5 = K_5 \quad (3.139)$$

$$x_7 = C_7 x_8^{1/2} x_{11}^{1/2} \quad \text{where} \quad C_7 = K_7 \quad (3.140)$$

$$x_9 = C_9 x_4 x_8^{1/2} \quad \text{where} \quad C_9 = K_9 p^{1/2} \quad (3.141)$$

$$x_{10} = C_{10} x_6 x_8^{1/2} \quad \text{where} \quad C_{10} = K_{10} p^{1/2} \quad (3.142)$$

3.10 Partial Derivatives of the Mole Fractions

Beginning with equation 3.73, the functions as well as the mole fractions are reliant on pressure, equivalence ratio and temperature. Taking the temperature total derivatives of each equation, four linear synchronized equations in four undisclosed variables are developed.

$$\frac{\partial f_j}{\partial T} + \frac{\partial f_j}{\partial x_4} \frac{\partial x_4}{\partial T} + \frac{\partial f_j}{\partial x_6} \frac{\partial x_6}{\partial T} + \frac{\partial f_j}{\partial x_8} \frac{\partial x_8}{\partial T} + \frac{\partial f_j}{\partial x_{11}} \frac{\partial x_{11}}{\partial T} = 0 \quad j = 1, 2, 3, 4 \quad (3.143)$$

It is observed that the coefficient matrix of the above relations is the Jacobian that appeared in equation 3.85. It is also concluded that the matrices for cracking the partial derivatives with reference to equivalence ratio and pressure is alike but the Temperature (T) is substituted by Pressure (p) or equivalence ratio (F). Models for the calculations of the elements of the coefficient matrix and the constant vector are arranged in Heading (3.11). Equation sets (Equations 3.143 and alike ones for (p) and (F)) are solved in a conventional forward method using the Gaussian Matrix elimination scheme. The lasting partial derivatives of x_1, x_2 etc. are simply attained by employing Equations 3.58 to 3.64 and 3.49 and straight replacement of numbers as shown in Heading (3.11 and 3.12).

The numerical analysis of the steady state mole fractions and partial derivatives of the mole fractions with reference to Temperature (T), Pressure (p), equivalence ratio (F) is supported by a Microsoft Visual Basic.Net coded subroutine EQMD().

3.11 Partial Derivative Computation Equations

Define

$$Y_i = \frac{x_i}{c_i} \quad \text{where } i = 1, 2, 3, 5, 7, 9, 10 \quad (3.144)$$

From equation 3.58 to 3.64 Y_i are perceived to be relations of x_4, x_6, x_8 and x_{11} only

Replacing for x_i from equation above in equation 3.65 to 3.68 and taking derivative with respect to Temperature (T), the partial differential equation is expressed as

$$\frac{\partial f_1}{\partial T} = \frac{\partial C_1}{\partial T} Y_1 + \frac{\partial C_5}{\partial T} Y_5 + 2 \frac{\partial C_9}{\partial T} Y_9 - d_1 \frac{\partial C_{10}}{\partial T} Y_{10} \quad (3.145)$$

$$\frac{\partial f_2}{\partial T} = \frac{\partial C_2}{\partial T} Y_2 + \frac{\partial C_5}{\partial T} Y_5 + \frac{\partial C_7}{\partial T} Y_7 + \frac{\partial C_9}{\partial T} Y_9 + 2 \frac{\partial C_{10}}{\partial T} Y_{10} - d_2 \frac{\partial C_{10}}{\partial T} Y_{10} \quad (3.146)$$

$$\frac{\partial f_3}{\partial T} = \frac{\partial C_3}{\partial T} Y_3 + \frac{\partial C_7}{\partial T} Y_7 - d_3 \frac{\partial C_{10}}{\partial T} Y_{10} \quad (3.147)$$

$$\frac{\partial f_4}{\partial T} = \frac{\partial C_1}{\partial T} Y_1 + \frac{\partial C_2}{\partial T} Y_2 + \frac{\partial C_3}{\partial T} Y_3 + \frac{\partial C_5}{\partial T} Y_5 + \frac{\partial C_7}{\partial T} Y_7 + \frac{\partial C_9}{\partial T} Y_9 + \frac{\partial C_{10}}{\partial T} Y_{10} + d_4 \frac{\partial C_{10}}{\partial T} Y_{10} \quad (3.148)$$

Pressure (p) Partial derivatives are alike but $\partial/\partial T$ is substituted by $\partial/\partial p$. Record that C_5 and C_7 are not relations of pressure (p) and henceforth expressions including $\partial C_5/\partial p$ and $\partial C_7/\partial p$ are zero.

$$\frac{\partial f_1}{\partial p} = \frac{\partial C_1}{\partial p} Y_1 + 2 \frac{\partial C_9}{\partial p} Y_9 - d_1 \frac{\partial C_{10}}{\partial p} Y_{10} \quad (3.149)$$

$$\frac{\partial f_2}{\partial p} = \frac{\partial C_2}{\partial p} Y_2 + \frac{\partial C_9}{\partial p} Y_9 + 2 \frac{\partial C_{10}}{\partial p} Y_{10} - d_2 \frac{\partial C_{10}}{\partial p} Y_{10} \quad (3.150)$$

$$\frac{\partial f_3}{\partial p} = \frac{\partial C_3}{\partial p} Y_3 - d_3 \frac{\partial C_{10}}{\partial p} Y_{10} \quad (3.151)$$

$$\frac{\partial f_4}{\partial p} = \frac{\partial C_1}{\partial p} Y_1 + \frac{\partial C_2}{\partial p} Y_2 + \frac{\partial C_3}{\partial p} Y_2 + \frac{\partial C_9}{\partial p} Y_9 + \frac{\partial C_{10}}{\partial p} Y_{10} + d_4 \frac{\partial C_{10}}{\partial p} Y_{10} \quad (3.152)$$

The parameters d_2, d_3 and d_4 are functions of F but none of the C_i are. Hence

$$\frac{\partial f_1}{\partial F} = -(x_6 + C_{10} Y_{10}) \frac{\partial d_1}{\partial F} = 0 \quad (3.153)$$

$$\frac{\partial f_2}{\partial F} = -(x_6 + C_{10} Y_{10}) \frac{\partial d_2}{\partial F} \quad (3.154)$$

$$\frac{\partial f_3}{\partial F} = -(x_6 + C_{10} Y_{10}) \frac{\partial d_3}{\partial F} \quad (3.155)$$

$$\frac{\partial f_4}{\partial F} = (x_6 + C_{10} Y_{10}) \frac{\partial d_4}{\partial F} \quad (3.156)$$

From the expression for C_i and d_i

$$\frac{\partial C_1}{\partial T} = \frac{dK_1}{dT} / p^{1/2} \quad (3.157)$$

$$\frac{\partial C_2}{\partial T} = \frac{dK_2}{dT} / p^{1/2} \quad (3.158)$$

$$\frac{\partial C_3}{\partial T} = \frac{dK_3}{dT} / p^{1/2} \quad (3.159)$$

$$\frac{\partial C_7}{\partial T} = \frac{dK_7}{dT} \quad (3.160)$$

$$\frac{\partial C_9}{\partial T} = \frac{dK_9}{dT} p^{1/2} \quad (3.161)$$

$$\frac{\partial C_{10}}{\partial T} = \frac{dK_{10}}{dT} p^{1/2} \quad (3.162)$$

$$\frac{\partial C_1}{\partial p} = -\frac{1}{2} \frac{K_1}{p^{3/2}} = -\frac{1}{2} \frac{C_1}{p} \quad (3.163)$$

$$\frac{\partial C_2}{\partial p} = -\frac{1}{2} \frac{C_2}{p} \quad (3.164)$$

$$\frac{\partial C_3}{\partial p} = -\frac{1}{2} \frac{C_3}{p} \quad (3.165)$$

$$\frac{\partial C_9}{\partial p} = \frac{1}{2} \frac{K_9}{p^{1/2}} = \frac{1}{2} \frac{C_9}{p} \quad (3.166)$$

$$\frac{\partial C_{10}}{\partial p} = \frac{1}{2} \frac{C_{10}}{p} \quad (3.167)$$

Define

$$d_5 = -(n + m/4 - l/2)/F^2 \quad (3.168)$$

$$\frac{\partial d_2}{\partial F} = \frac{2}{n} \frac{dr}{dF} = \frac{2}{n} d_5 \quad (3.169)$$

$$\frac{\partial d_3}{\partial F} = \frac{2}{n} \frac{dr'}{dF} = \frac{2}{n} 3.7274 d_5 \quad (3.170)$$

$$\frac{\partial d_4}{\partial F} = \frac{1}{n} \frac{dr''}{dF} = \frac{1}{n} 0.0444 d_5 \quad (3.171)$$

The model used for fitting equilibrium constants K_p is

$$\log_{10} K_p = A \ln(T_A) + B/T_A + C + DT_A + ET_A^2 \quad (3.172)$$

Where $T_A = 0.005T/9$ and T is in $^{\circ}R$

From which we derive

$$\frac{dK_P}{dT} = \frac{0.005}{9} \ln(10) K_p [A/T_A - B/T_A^2 + D + 2ET_A] \quad (3.173)$$

3.12 Computation of Remaining Mole Fractions Partial Derivatives

Taking derivatives of Equation 3.58 to 3.64

$$\frac{\partial x_1}{\partial T} = C_1 \left(\frac{1}{2}\right) x_4^{-1/2} \frac{\partial x_4}{\partial T} + \frac{\partial C_1}{\partial T} x_4^{1/2} \quad (3.174)$$

$$\frac{\partial x_2}{\partial T} = C_2 \left(\frac{1}{2}\right) x_8^{-1/2} \frac{\partial x_8}{\partial T} + \frac{\partial C_2}{\partial T} x_8^{1/2} \quad (3.175)$$

$$\frac{\partial x_3}{\partial T} = C_3 \left(\frac{1}{2}\right) x_{11}^{-1/2} \frac{\partial x_{11}}{\partial T} + \frac{\partial C_3}{\partial T} x_{11}^{1/2} \quad (3.176)$$

$$\frac{\partial x_5}{\partial T} = C_5 \left[\frac{1}{2}\right] \left[x_4^{-1/2} x_8^{1/2} \frac{\partial x_4}{\partial T} + x_4^{1/2} x_8^{-1/2} \frac{\partial x_8}{\partial T} \right] + \frac{\partial C_5}{\partial T} x_4^{1/2} x_8^{1/2} \quad (3.177)$$

$$\frac{\partial x_7}{\partial T} = C_7 \left[\frac{1}{2}\right] \left[x_8^{-1/2} x_{11}^{1/2} \frac{\partial x_8}{\partial T} + x_8^{1/2} x_{11}^{-1/2} \frac{\partial x_{11}}{\partial T} \right] + \frac{\partial C_7}{\partial T} x_8^{1/2} x_{11}^{1/2} \quad (3.178)$$

$$\frac{\partial x_9}{\partial T} = C_9 \left[x_8^{1/2} \frac{\partial x_4}{\partial T} + \frac{1}{2} x_4 x_8^{-1/2} \frac{\partial x_8}{\partial T} \right] + \frac{\partial C_9}{\partial T} x_4 x_8^{1/2} \quad (3.179)$$

$$\frac{\partial x_{10}}{\partial T} = C_{10} \left[x_8^{1/2} \frac{\partial x_6}{\partial T} + \frac{1}{2} x_6 x_8^{-1/2} \frac{\partial x_8}{\partial T} \right] + \frac{\partial C_{10}}{\partial T} x_6 x_8^{1/2} \quad (3.180)$$

$$\frac{\partial x_{12}}{\partial T} = d_4 \left[\frac{\partial x_6}{\partial T} + \frac{\partial x_{10}}{\partial T} \right] \quad (3.181)$$

In order to calculate partial derivative with respect to pressure (p), substitute $\partial/\partial p$ instead of $\partial/\partial T$ in above equations

$$\frac{\partial x_1}{\partial p} = C_1 \left(\frac{1}{2}\right) x_4^{-1/2} \frac{\partial x_4}{\partial p} + \frac{\partial C_1}{\partial p} x_4^{1/2} \quad (3.182)$$

$$\frac{\partial x_2}{\partial p} = C_2 \left(\frac{1}{2}\right) x_8^{-1/2} \frac{\partial x_8}{\partial p} + \frac{\partial C_2}{\partial p} x_8^{1/2} \quad (3.183)$$

$$\frac{\partial x_3}{\partial p} = C_3 \left(\frac{1}{2}\right) x_{11}^{-1/2} \frac{\partial x_{11}}{\partial p} + \frac{\partial C_3}{\partial p} x_{11}^{1/2} \quad (3.184)$$

$$\frac{\partial x_5}{\partial p} = C_5 \left[\frac{1}{2}\right] \left[x_4^{-1/2} x_8^{1/2} \frac{\partial x_4}{\partial p} + x_4^{1/2} x_8^{-1/2} \frac{\partial x_8}{\partial p} \right] + \frac{\partial C_5}{\partial p} x_4^{1/2} x_8^{1/2} \quad (3.185)$$

$$\frac{\partial x_7}{\partial p} = C_7 \left[\frac{1}{2}\right] \left[x_8^{-1/2} x_{11}^{1/2} \frac{\partial x_8}{\partial p} + x_8^{1/2} x_{11}^{-1/2} \frac{\partial x_{11}}{\partial p} \right] + \frac{\partial C_7}{\partial p} x_8^{1/2} x_{11}^{1/2} \quad (3.186)$$

$$\frac{\partial x_9}{\partial p} = C_9 \left[x_8^{1/2} \frac{\partial x_4}{\partial p} + \frac{1}{2} x_4 x_8^{-1/2} \frac{\partial x_8}{\partial p} \right] + \frac{\partial C_9}{\partial p} x_4 x_8^{1/2} \quad (3.187)$$

$$\frac{\partial x_{10}}{\partial p} = C_{10} \left[x_8^{1/2} \frac{\partial x_6}{\partial p} + \frac{1}{2} x_6 x_8^{-1/2} \frac{\partial x_8}{\partial p} \right] + \frac{\partial C_{10}}{\partial p} x_6 x_8^{1/2} \quad (3.188)$$

$$\frac{\partial x_{12}}{\partial p} = d_4 \left[\frac{\partial x_6}{\partial p} + \frac{\partial x_{10}}{\partial p} \right] \quad (3.189)$$

In order to calculate equivalence ratio (F) partial derivatives, assign zero instead of $\partial C_i / \partial T$. Substitute $\partial / \partial F$ instead of $\partial / \partial p$.

$$\frac{\partial x_1}{\partial F} = C_1 \left(\frac{1}{2} \right) x_4^{-1/2} \frac{\partial x_4}{\partial F} \quad (3.190)$$

$$\frac{\partial x_2}{\partial F} = C_2 \left(\frac{1}{2} \right) x_8^{-1/2} \frac{\partial x_8}{\partial F} \quad (3.191)$$

$$\frac{\partial x_3}{\partial F} = C_3 \left(\frac{1}{2} \right) x_{11}^{-1/2} \frac{\partial x_{11}}{\partial F} \quad (3.192)$$

$$\frac{\partial x_5}{\partial F} = C_5 \left[\frac{1}{2} \right] \left[x_4^{-1/2} x_8^{1/2} \frac{\partial x_4}{\partial F} + x_4^{1/2} x_8^{-1/2} \frac{\partial x_8}{\partial F} \right] \quad (3.193)$$

$$\frac{\partial x_7}{\partial F} = C_7 \left[\frac{1}{2} \right] \left[x_8^{-1/2} x_{11}^{1/2} \frac{\partial x_8}{\partial F} + x_8^{1/2} x_{11}^{-1/2} \frac{\partial x_{11}}{\partial F} \right] \quad (3.194)$$

$$\frac{\partial x_9}{\partial F} = C_9 \left[x_8^{1/2} \frac{\partial x_4}{\partial F} + \frac{1}{2} x_4 x_8^{-1/2} \frac{\partial x_8}{\partial F} \right] \quad (3.195)$$

$$\frac{\partial x_{10}}{\partial F} = C_{10} \left[x_8^{1/2} \frac{\partial x_6}{\partial F} + \frac{1}{2} x_6 x_8^{-1/2} \frac{\partial x_8}{\partial F} \right] \quad (3.196)$$

Exception

$$\frac{\partial x_{12}}{\partial F} = d_4 \left[\frac{\partial x_6}{\partial F} + \frac{\partial x_{10}}{\partial F} \right] + \frac{\partial d_4}{\partial F} [x_6 + x_{10}] \quad (3.197)$$

3.13 Computation of Internal Energy and Enthalpy

The computation of absolute enthalpy at temperature (T) is expressed as

Absolute Enthalpy at Temperature T = Enthalpy of formation at standard reference state (T_{ref}, P^0) + Sensible enthalpy change in going from T_{ref} to T

The heat of formation and specific heat values are given in JANAF Thermochemical Tables (reference [28]). The heat of formation and specific heat values are

evaluated from a look up subroutine TABLES (). The mole fractions and partial derivatives of mole fractions calculated from subroutine EQMD() is used to calculate enthalpy of the mixture (h), gas constant (R) of the mixture and molecular weight (M) of the outcomes.

$$M = \sum_{i=1}^{12} x_i M_i \quad (3.198)$$

$$R = R_O / M \quad (3.199)$$

$$h = \sum_{i=1}^{12} h_i / M \quad (3.200)$$

$$u = h - RT \quad (3.201)$$

The partial derivatives are also simply totaled. As a case

$$\frac{\partial M}{\partial T} = \sum_{i=1}^{12} M_i \frac{\partial x_i}{\partial T} \quad (3.202)$$

The relations for the partials of enthalpy (h), internal energy (u) and gas constant (R) with reference to Temperature (T), Pressure (p) and equivalence ratio (F) are specified in heading (3.14). The numerical computation of internal energy (u), enthalpy (h), Gas constant (R) and their partials are evaluated by Visual Basic coded subroutine PER().

3.14 Calculation of Partial Derivatives of Gas Constant (R), Enthalpy (h) and Internal Energy (u)

Considering Equations 3.198 to 3.201

$$\frac{\partial M}{\partial T} = \sum \frac{\partial x_i}{\partial T} M_i \quad (3.203)$$

$$\frac{\partial R}{\partial T} = -\frac{R_O}{M^2} \frac{\partial M}{\partial T} = -\frac{R}{M} \frac{\partial M}{\partial T} \quad (3.204)$$

$$\frac{\partial h}{\partial T} = \frac{1}{M} \left[\sum (x_i \frac{dh_i}{dT} + \frac{\partial x_i}{\partial T} h_i) - \frac{\partial M}{\partial T} h \right] \quad (3.205)$$

$$\frac{\partial u}{\partial T} = \frac{\partial h}{\partial T} - R - \frac{\partial R}{\partial T} T \quad (3.206)$$

Note that $\frac{dh_i}{dT} = C_{pi}$ the specific heats of the outcomes at constant pressure.

In order to calculate pressure (p) partial derivatives and equivalence ratio (F) partial derivatives substitute $\partial/\partial T$ with $\partial/\partial p$ and $\partial/\partial F$ respectively.

$$\frac{\partial M}{\partial p} = \sum \frac{\partial x_i}{\partial p} M_i \quad (3.207)$$

$$\frac{\partial R}{\partial p} = -\frac{R_O}{M^2} \frac{\partial M}{\partial p} = -\frac{R}{M} \frac{\partial M}{\partial p} \quad (3.208)$$

Exceptions are

$$\frac{\partial h}{\partial p} = \frac{1}{M} \left[\sum \frac{\partial x_i}{\partial p} h_i - \frac{\partial M}{\partial p} h \right] \quad (3.209)$$

$$\frac{\partial u}{\partial p} = \frac{\partial h}{\partial p} - \frac{\partial R}{\partial p} T \quad (3.210)$$

Similarly for $\partial/\partial F$

$$\frac{\partial M}{\partial F} = \sum \frac{\partial x_i}{\partial F} M_i \quad (3.211)$$

$$\frac{\partial R}{\partial F} = -\frac{R_O}{M^2} \frac{\partial M}{\partial F} = -\frac{R}{M} \frac{\partial M}{\partial F} \quad (3.212)$$

The exceptions are

$$\frac{\partial h}{\partial F} = \frac{1}{M} \left[\sum \frac{\partial x_i}{\partial F} h_i - \frac{\partial M}{\partial F} h \right] \quad (3.213)$$

$$\frac{\partial u}{\partial F} = \frac{\partial h}{\partial F} - \frac{\partial R}{\partial F} T \quad (3.214)$$

3.15 Computation of Equilibrium Constants

The data for computation of equilibrium constants is taken from Joint Army Navy Air Force (JANAF) [28], where $\log_{10} K_p$ (formation) for all outcomes is expressed as function of the absolute temperature (K). Equilibrium constants for the chemical model considered in the steady state thermodynamics is calculated by the expression

$\log K_p$ is given as:

$$\log K_p(\text{reaction}) = \Sigma \log K_p(\text{formation})\text{products} \\ - \Sigma \log K_p(\text{formation})\text{reactants} \quad (3.215)$$

Theoretical readings ([29]) propose a functional relationship of the type

$$\log K_p = A \ln(T) + \frac{B}{T} + C + DT + ET^2 \quad (3.216)$$

From above expression “ T ” is the absolute temperature and A,B,C,D,E are empirical constants. The above relation is used to calculate the $\log K_p$ which is employed for curve fitting the charted results by way of a least squares fitting code segment.

In order to obtain extreme correctness in a thin array of temperature or lesser correctness in a broader array, a range of 600 to 4000 K ($1080^\circ R$ to $7200^\circ R$) is selected in this report. This range is most appropriate to the understanding of combustion wonders in locomotives.

The $\log_{10} K_p$ expected by the mathematical models are related with the innovative data and the deviations are fewer than 0.0009. (The unique result is arranged only to the third decimal place and hence there is an integral doubt of 0.0005. The nonconformities are not assumed important) A transformed temperature T_A is expressed as $0.005T/9$ where T is in $^\circ R$. A transformed temperature T_A is used in the calculation of $\log_{10} K_p$.

$$\log_{10} K_p = a \ln T_A + \frac{B}{T_A} + C + DT_A + ET_A^2 \quad (3.217)$$

The empirical constants A, B, C, D and E for seven steady state reactions are publicized in table 3.3.

	A	B	C	D	E
$\frac{1}{2}H_2 \rightleftharpoons H$	0.432168	0.267269×10^1	0.267269×10^1	-0.745744×10^{-1}	0.24248×10^{-2}
$\frac{1}{2}O_2 \rightleftharpoons O$	0.310805	-0.12954×10^2	0.321779×10^1	-0.738336×10^{-1}	0.344645×10^{-2}
$\frac{1}{2}N_2 \rightleftharpoons N$	0.389716	-0.245828×10^2	0.314505×10^1	-0.963730×10^{-1}	0.585643×10^{-2}
$\frac{1}{2}H_2 + \frac{1}{2}O_2 \rightleftharpoons OH$	-0.141784	-0.213308×10^1	0.853461	0.355015×10^{-1}	-0.3102×10^{-2}
$\frac{1}{2}O_2 + \frac{1}{2}N_2 \rightleftharpoons NO$	0.150879×10^1	-0.470959×10^1	0.646096	0.272805×10^{-2}	-0.1544×10^{-2}
$H_2 + \frac{1}{2}O_2 \rightleftharpoons H_2O$	-0.752364	0.124210×10^2	-0.260286×10^1	0.259556	-0.1626×10^{-1}
$CO + \frac{1}{2}O_2 \rightleftharpoons CO_2$	-0.415302×10^{-2}	0.148627×10^2	-0.475746×10^1	0.124699	-0.9002×10^{-2}

TABLE 3.3: Constants for the reaction [1]

Chapter 4

Calculation of Flame Properties

The programs works in Microsoft windows environment and input can be given through user interface. The user interface theme is that of Windows 8 & Windows 10. The code files are in executable format, that is no requirement of compilation. The codes input data, process data and output data in SI units. Moreover composition of air can be given as an input to the code. Thermodynamic Tables are integrated within the code thus increasing the execution speed of code.

4.1 General Code Structure

4.1.1 HPFlame Software Code Structure

4.1.1.1 Code Structure

Microsoft Visual Basic.Net software is used as a programming language. First User Interface is designed in Visual Basic Form Designer. Code is written in Visual Basic Form Code Section. One class known as “Public Class HPFlame” is created globally. Subroutine “AboutToolStripMenuItem1_Click” is executed when Help → About is clicked. Subroutine “ExitToolStripMenuItem_Click” ends the program when File → Exit is clicked. Subroutine “Calculatebutton_Click”

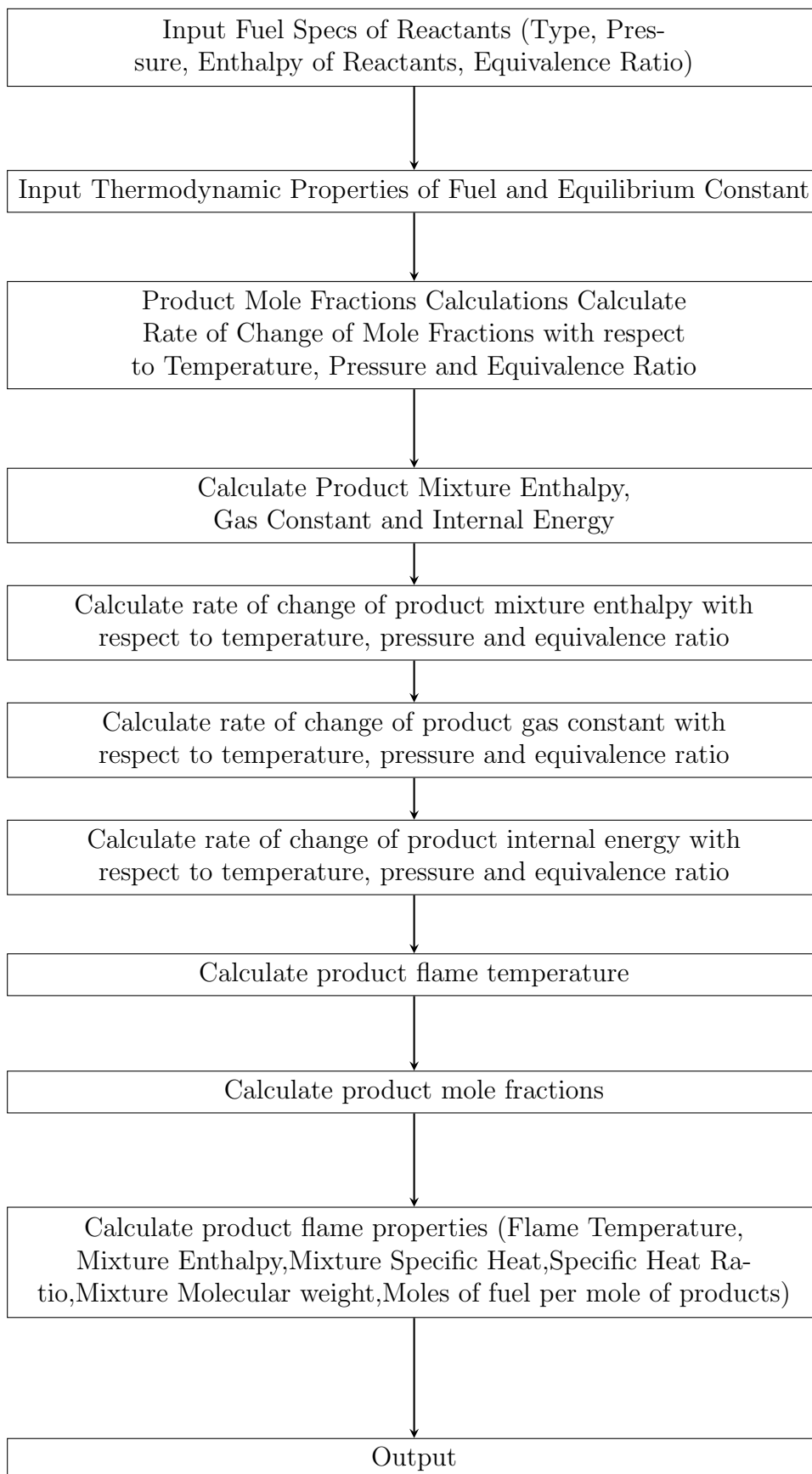


FIGURE 4.1: HPFlame Code Data Flow Diagram

is executed when “Calculate” Button is pressed. The subroutine “Calculatebutton_Click” is the main program. It first load the input variables like fuel type, reactant pressure, guess temperature, equivalence ratio and enthalpy of reactants. The code will call subroutine TABLES() to load arrays for enthalpy, specific heat, molecular weight and equilibrium constants. The code will then convert enthalpy from KJ to Joules. Subroutine PER() is called which would call Subroutine EQMD () to calculate amount fractions and the partial derivatives of these amount fractions with equivalence ratio, temperature and pressure. Subroutine PER() calculates enthalpy, internal energy, gas constant and partial derivatives of these with reference to equivalence ratio, temperature and pressure. Variable “DELTA” is calculated which would update temperature. The loop terminates when DELTA is less than or equal to 0.01 or number of iterations reached 25. The program then outputs variables (Mole Fractions & Flame Properties) in a text boxes. Flame properties like Adiabatic Flame Temperature at constant pressure, mixture enthalpy, mixture specific heat, Specific Heat Ratio, Mixture molecular weight and moles of fuel per moles of outcomes. Subroutine “Sub SERMSG()” deals with the display of error message. HPFlame Visual Basic code defines one global class “HPFlame” and thus follows object oriented programming concept. HPFlame code does not define custom classes or class inheritance. Since only one global class (no hiding of details or black box) is defined there is no need for data abstraction and encapsulation.

4.1.2 TPEquil Software Code Structure

4.1.2.1 Code Structure

Microsoft Visual Basic.Net software is used as a programming language. First User Interface is designed in Visual Basic Form Designer. Code is written in Visual Basic Form Code Section.

One class known as “Public Class TPEquil” is created globally. Subroutine “AboutToolStripMenuItem1_Click” is executed when Help→About is clicked. Subroutine “ExitToolStripMenuItem_Click” ends the program when File→Exit is

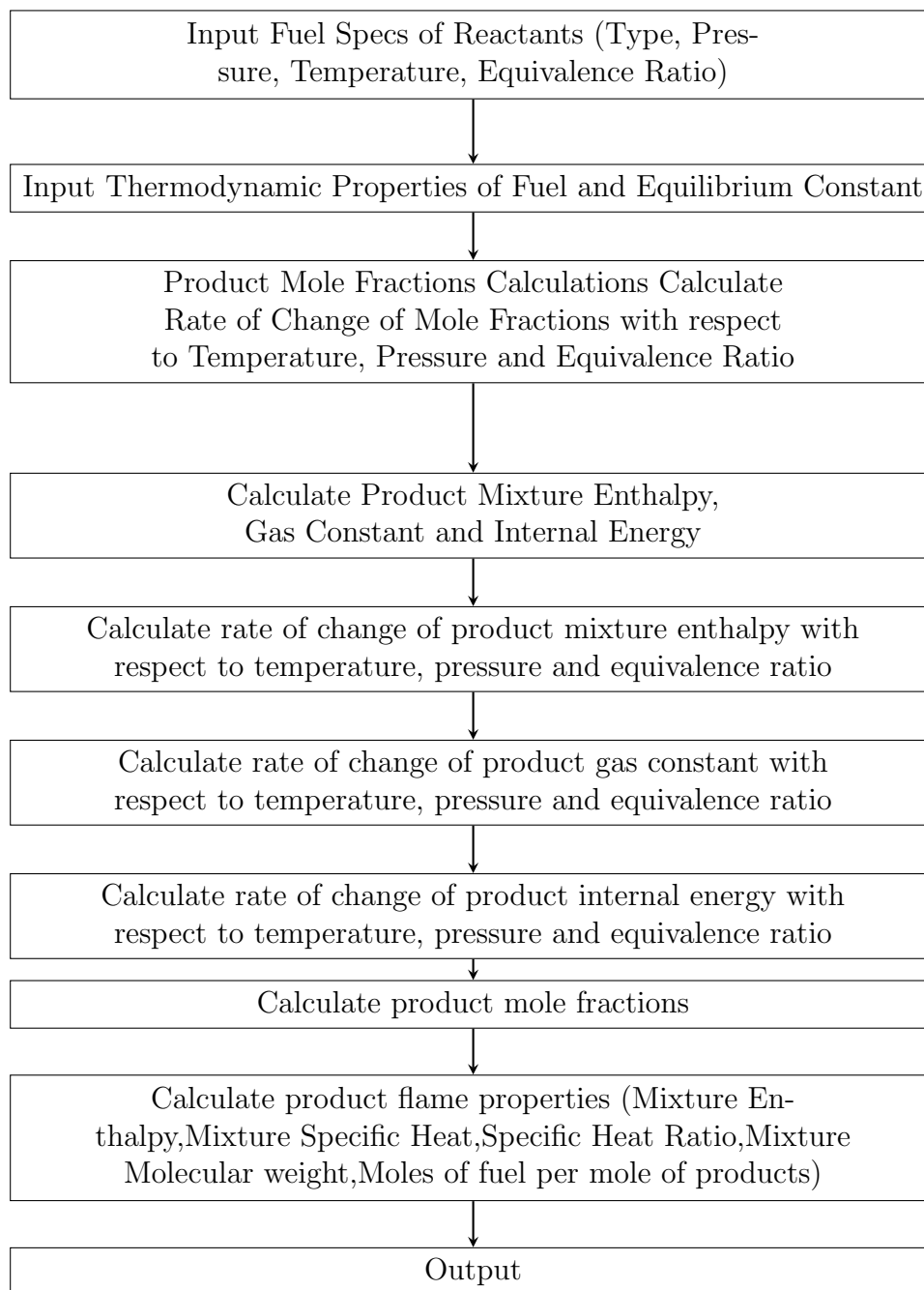


FIGURE 4.2: TPEquil Code Data Flow Diagram

clicked. Subroutine “Calculatebutton_Click” is executed when “Calculate” Button is pressed. The subroutine “Calculatebutton_Click” is the main program. It first load the input variables like fuel type, reactant pressure, product temperature and equivalence ratio. It will call subroutine TABLES() to load arrays for enthalpy, specific heat, molecular weight and equilibrium constants. Subroutine PER() is called which would call Subroutine EQMD () to calculate amount fractions and the partial derivatives of these amount fractions with equivalence ratio,

temperature and pressure. Subroutine PER() calculates enthalpy, internal energy, gas constant and partial derivatives of these with reference to equivalence ratio, pressure and temperature. The program then outputs variables (Mole Fractions & Flame Properties) in a text boxes. Flame properties like mixture enthalpy, mixture specific heat, Specific Heat Ratio, Mixture molecular weight and moles of fuel per moles of outcomes. Subroutine “Sub SERMSG()” deals with the display of error message. TPEquil Visual Basic code defines one global class “TPEquil” and thus follows object oriented programming concept. TPEquil code does not define custom classes or class inheritance. Since only one global class (no hiding of details or black box) is defined there is no need for data abstraction and encapsulation.

4.1.3 UVFlame Software Code Structure

4.1.3.1 Code Structure

Microsoft Visual Basic.Net software is used as a programming language. First User Interface is designed in Visual Basic Form Designer. Code is written in Visual Basic Form Code Section. One class known as “Public Class UVFlame” is created globally. Subroutine “AboutToolStripMenuItem1_Click” is executed when Help→About is clicked. Subroutine “ExitToolStripMenuItem_Click” ends the program when File→Exit is clicked. Subroutine “Calculatebutton_Click” is executed when “Calculate” Button is pressed. The subroutine “Calculatebutton_Click” is the main program. It first load the input variables like fuel type, reactant pressure, reactant temperature, guess product temperature, equivalence ratio, enthalpy of reactants, mole of reactants and molecular weight of source mixture.

The code will calculate pressure based on equation $P = PREAC * T / TREAC$. The code then call subroutine TABLES() to load arrays for enthalpy, specific heat, molecular weight and equilibrium constants. Code will then convert enthalpy from KJ to Joules. Internal Energy is calculated by formula $UREAC = HREAC - XNREAC * 8314.51 * TREAC$.

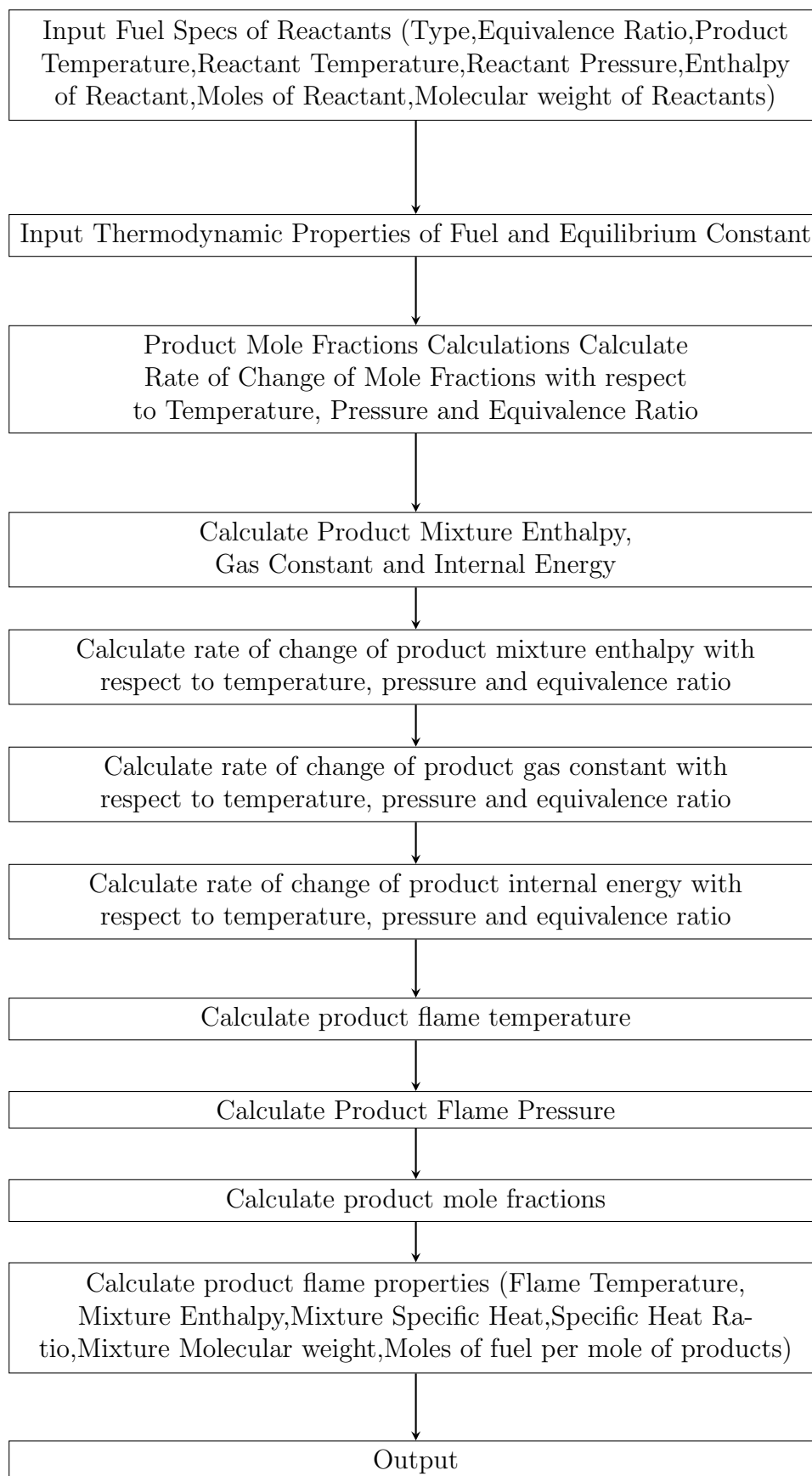


FIGURE 4.3: UVFlame Code Data Flow Diagram

Subroutine PER() is called which would call Subroutine EQMD () to calculate amount fractions and the partial derivatives of these amount fractions with equivalence ratio, temperature and pressure.

Subroutine PER() calculates enthalpy, internal energy, gas constant and partial derivatives of these with reference to equivalence ratio, pressure and temperature. Variable “DELTA” is calculated which would update temperature. Variable Pressure is updated by the formula $P = PREAC * XMREAC * T / (AVM * TREAC)$. The loop terminates when DELTA \leq 0.01 or number of iterations reached 25. The program then outputs variables (Mole Fractions & Flame Properties) in a text boxes.

Flame properties like Adiabatic Flame Temperature at constant volume, product pressure, mixture enthalpy, mixture specific heat, Specific Heat Ratio, Mixture molecular weight and moles of fuel per moles of outcomes.

Subroutine “Sub SERMSG()” deals with the display of error message. UVFlame Visual Basic code defines one global class “UVFlame” and thus follows object oriented programming concept.

UVFlame code does not define custom classes or class inheritance. Since only one global class (no hiding of details or black box) is defined there is no need for data abstraction and encapsulation.

4.2 Flame Properties under Constant Pressure and Enthalpy

A computer program, HPFlame (present work), has been developed to estimate adiabatic flame temperature and other flame properties based on the methodology discussed in Chapter 3. This program calculates the flame properties based upon “Constant Pressure Combustion”.

The program calculates twelve species mole fractions, adiabatic flame temperature at constant pressure, mixture enthalpy, mixture specific heat, specific heat ratio, mixture molecular weight and moles of fuel per mole of outcomes.

The inputs of the program is fuel Type, reactant pressure, guess temperature, equivalence ratio and enthalpy of reactants.

The HPFlame (present work) code algorithm is based on BORMAN [1] algorithm. The difference between HPFlame (present work) code and BORMAN [1]code is that HPFlame (present work) code is in SI units with defined composition of air.

4.3 Flame Properties under Constant Volume and Internal Energy

A computer program, UVFlame (present work), has been developed to estimate adiabatic flame temperature and other flame properties based on the methodology discussed in Chapter 3. This program calculates the flame properties based upon "Constant Volume Combustion". The program calculates twelve species mole fractions, adiabatic flame temperature at constant volume, product pressure, mixture enthalpy, mixture specific heat, specific heat ratio, mixture molecular weight and moles of fuel per mole of outcomes.

The inputs of the program is fuel Type, equivalence ratio, product temperature, reactant temperature, reactant pressure, enthalpy of reactant, moles of reactant, molecular weight of reactants.

The UVFlame (present work) code algorithm is based on BORMAN [1] algorithm. The difference between UVFlame (present work) code and BORMAN [1] code is that UVFlame (present work) code is in SI units with defined composition of air.

4.4 List of All Functions/Subroutine

The subroutine TABLES () is called first within the main program. The main purpose of the TABLES () subroutine is to load thermodynamic data. The composition of air can be adjusted in the subroutine for one mole of oxygen. The

constant used in the subroutine are CALTOJ which converts calories to joules and PSATM which is taken to be one atmosphere. Gas Constant RJOUL is computed from above data. The subroutine then loads enthalpy and specific heat data in an array for *H* Hydrogen, *O* Oxygen, *N* Nitrogen, *H₂* Hydrogen, *OH* Table, *CO* Table, *NO* Table, *O₂* Table, *H₂O* Table, *CO₂* Table, *N₂* Table and *A* Argon Table for different temperature. The temperature values are in the range of 100 K ~ 5000 K. The subroutine then loads LOG Kp values in array for reactions $1/2H_2 \rightleftharpoons H$, $1/2O_2 \rightleftharpoons O$, $1/2N_2 \rightleftharpoons N$, $1/2H_2 + 1/2O_2 \rightleftharpoons OH$, $1/2H_2 + 1/2N_2 \rightleftharpoons NO$, $H_2 + 1/2O_2 \rightleftharpoons H_2O$ and $CO + 1/2O_2 \rightleftharpoons CO_2$. It is assumed that the gases follows ideal behavior. TABLES () subroutine also converts enthalpy and specific heat values from calories to joules.

The subroutine EQMD () is called from subroutine PER () which is called from main program. The purpose of the EQMD () subroutine is to compute product species mole fractions. The inputs of subroutine EQMD () are type of fuel, equivalence ratio, guess product temperature and pressure. The EQMD () subroutine computes twelve species mole fractions and partial derivatives of the species mole fractions with reference to equivalence ratio, pressure and temperature. Primary contents of fuel are hydrogen and carbon. The fuel may or may not contain oxygen and nitrogen atoms. The outcome species are *Ar*, *H*, *H₂*, *O*, *OH*, *N*, *CO*, *N₂*, *CO₂*, *H₂O*, *NO* and *O₂* in vapor state.

The equilibrium constants employed in the code subroutines are stated as relations of temperature in the array (100K to 5000K). The subroutines cannot be utilized external to this boundary limits. The subprogram cannot grip the development of free carbon. It is proved [1] that for equivalence ratio

$$F > \frac{AN + 0.25AM - 0.5AL}{0.5AN - 0.5AL} \quad (4.1)$$

where AN,AM,AL are the figures of C,H and O atoms in fuel molecules, free

carbon is formed. In case of octane fuel C_8H_{16} maximum equivalence ratio (F) is 3.

The outcomes of burning are expected to be ideal gases.

This guess is not effective at extreme pressures ([30]).

Equations used for the computation of species mole fractions are:

$$f_1 = (x_1 + 2x_4 + x_5 + 2x_9) - d_1(x_6 + x_{10}) \quad (4.2)$$

$$f_2 = (x_2 + x_5 + x_6 + x_7 + 2x_8 + x_9 + 2x_{10}) - d_2(x_6 + x_{10}) \quad (4.3)$$

$$f_3 = (x_3 + x_7 + 2x_{11}) - d_3(x_6 + x_{10}) \quad (4.4)$$

$$f_4 = d_4(x_6 + x_{10}) + \sum_{i=1}^{11} x_i - 1 \quad (4.5)$$

Putting in the values for $x_1, x_2, x_3, x_5, x_7, x_9, x_{10}$ from Equation 3.58 to 3.64

$$f_1 = (C_1 x_4^{1/2} + 2x_4 + C_5 x_4^{1/2} x_8^{1/2} + 2C_9 x_4 x_8^{1/2}) - d_1(x_6 + C_{10} x_6 x_8^{1/2}) \quad (4.6)$$

$$f_2 = (C_2 x_8^{1/2} + C_5 x_4^{1/2} x_8^{1/2} + x_6 + C_7 x_8^{1/2} x_{11}^{1/2} + 2x_8 + C_9 x_4 x_8^{1/2} + 2C_{10} x_6 x_8^{1/2}) - d_2(x_6 + C_{10} x_6 x_8^{1/2}) \quad (4.7)$$

$$f_4 = d_4(x_6 + C_{10} x_6 x_8^{1/2}) + \sum_{i=1}^{11} x_i - 1 \quad (4.8)$$

$$\frac{\partial f_j}{\partial T} + \frac{\partial f_j}{\partial x_4} \frac{\partial x_4}{\partial T} + \frac{\partial f_j}{\partial x_6} \frac{\partial x_6}{\partial T} + \frac{\partial f_j}{\partial x_8} \frac{\partial x_8}{\partial T} + \frac{\partial f_j}{\partial x_{11}} \frac{\partial x_{11}}{\partial T} = 0 \quad j = 1, 2, 3, 4 \quad (4.9)$$

Equations used for the computation of mole fractions partial derivatives with reference to temperature are:

$$\frac{\partial x_1}{\partial T} = C_1 \left(\frac{1}{2}\right) x_4^{-1/2} \frac{\partial x_4}{\partial T} + \frac{\partial C_1}{\partial T} x_4^{1/2} \quad (4.10)$$

$$\frac{\partial x_2}{\partial T} = C_2 \left(\frac{1}{2}\right) x_8^{-1/2} \frac{\partial x_8}{\partial T} + \frac{\partial C_2}{\partial T} x_8^{1/2} \quad (4.11)$$

$$\frac{\partial x_3}{\partial T} = C_3 \left(\frac{1}{2}\right) x_{11}^{-1/2} \frac{\partial x_{11}}{\partial T} + \frac{\partial C_3}{\partial T} x_{11}^{1/2} \quad (4.12)$$

$$\frac{\partial x_5}{\partial T} = C_5 \left[\frac{1}{2}\right] \left[x_4^{-1/2} x_8^{1/2} \frac{\partial x_4}{\partial T} + x_4^{1/2} x_8^{-1/2} \frac{\partial x_8}{\partial T} \right] + \frac{\partial C_5}{\partial T} x_4^{1/2} x_8^{1/2} \quad (4.13)$$

$$\frac{\partial x_7}{\partial T} = C_7 \left[\frac{1}{2}\right] \left[x_8^{-1/2} x_{11}^{1/2} \frac{\partial x_8}{\partial T} + x_8^{1/2} x_{11}^{-1/2} \frac{\partial x_{11}}{\partial T} \right] + \frac{\partial C_7}{\partial T} x_8^{1/2} x_{11}^{1/2} \quad (4.14)$$

$$\frac{\partial x_9}{\partial T} = C_9 \left[x_8^{1/2} \frac{\partial x_4}{\partial T} + \frac{1}{2} x_4 x_8^{-1/2} \frac{\partial x_8}{\partial T} \right] + \frac{\partial C_9}{\partial T} x_4 x_8^{1/2} \quad (4.15)$$

$$\frac{\partial x_{10}}{\partial T} = C_{10} \left[x_8^{1/2} \frac{\partial x_6}{\partial T} + \frac{1}{2} x_6 x_8^{-1/2} \frac{\partial x_8}{\partial T} \right] + \frac{\partial C_{10}}{\partial T} x_6 x_8^{1/2} \quad (4.16)$$

$$\frac{\partial x_{12}}{\partial T} = d_4 \left[\frac{\partial x_6}{\partial T} + \frac{\partial x_{10}}{\partial T} \right] \quad (4.17)$$

In order to calculate partial derivative with respect to pressure substitute $\partial/\partial p$ instead of $\partial/\partial T$ in above equations

$$\frac{\partial x_1}{\partial p} = C_1 \left(\frac{1}{2}\right) x_4^{-1/2} \frac{\partial x_4}{\partial p} + \frac{\partial C_1}{\partial p} x_4^{1/2} \quad (4.18)$$

$$\frac{\partial x_2}{\partial p} = C_2 \left(\frac{1}{2}\right) x_8^{-1/2} \frac{\partial x_8}{\partial p} + \frac{\partial C_2}{\partial p} x_8^{1/2} \quad (4.19)$$

$$\frac{\partial x_3}{\partial p} = C_3 \left(\frac{1}{2}\right) x_{11}^{-1/2} \frac{\partial x_{11}}{\partial p} + \frac{\partial C_3}{\partial p} x_{11}^{1/2} \quad (4.20)$$

$$\frac{\partial x_5}{\partial p} = C_5 \left[\frac{1}{2}\right] \left[x_4^{-1/2} x_8^{1/2} \frac{\partial x_4}{\partial p} + x_4^{1/2} x_8^{-1/2} \frac{\partial x_8}{\partial p} \right] + \frac{\partial C_5}{\partial p} x_4^{1/2} x_8^{1/2} \quad (4.21)$$

$$\frac{\partial x_7}{\partial p} = C_7 \left[\frac{1}{2}\right] \left[x_8^{-1/2} x_{11}^{1/2} \frac{\partial x_8}{\partial p} + x_8^{1/2} x_{11}^{-1/2} \frac{\partial x_{11}}{\partial p} \right] + \frac{\partial C_7}{\partial p} x_8^{1/2} x_{11}^{1/2} \quad (4.22)$$

$$\frac{\partial x_9}{\partial p} = C_9 \left[x_8^{1/2} \frac{\partial x_4}{\partial p} + \frac{1}{2} x_4 x_8^{-1/2} \frac{\partial x_8}{\partial p} \right] + \frac{\partial C_9}{\partial p} x_4 x_8^{1/2} \quad (4.23)$$

$$\frac{\partial x_{10}}{\partial p} = C_{10} \left[x_8^{1/2} \frac{\partial x_6}{\partial p} + \frac{1}{2} x_6 x_8^{-1/2} \frac{\partial x_8}{\partial p} \right] + \frac{\partial C_{10}}{\partial p} x_6 x_8^{1/2} \quad (4.24)$$

$$\frac{\partial x_{12}}{\partial p} = d_4 \left[\frac{\partial x_6}{\partial p} + \frac{\partial x_{10}}{\partial p} \right] \quad (4.25)$$

In order to calculate equivalence ratio (F) partial derivatives assign zero instead of $\partial C_i/\partial T$. Substitute $\partial/\partial F$ instead of $\partial/\partial p$.

$$\frac{\partial x_1}{\partial F} = C_1 \left(\frac{1}{2}\right) x_4^{-1/2} \frac{\partial x_4}{\partial F} \quad (4.26)$$

$$\frac{\partial x_2}{\partial F} = C_2 \left(\frac{1}{2}\right) x_8^{-1/2} \frac{\partial x_8}{\partial F} \quad (4.27)$$

$$\frac{\partial x_3}{\partial F} = C_3 \left(\frac{1}{2}\right) x_{11}^{-1/2} \frac{\partial x_{11}}{\partial F} \quad (4.28)$$

$$\frac{\partial x_5}{\partial F} = C_5 \left[\frac{1}{2}\right] \left[x_4^{-1/2} x_8^{1/2} \frac{\partial x_4}{\partial F} + x_4^{1/2} x_8^{-1/2} \frac{\partial x_8}{\partial F} \right] \quad (4.29)$$

$$\frac{\partial x_7}{\partial F} = C_7 \left[\frac{1}{2}\right] \left[x_8^{-1/2} x_{11}^{1/2} \frac{\partial x_8}{\partial F} + x_8^{1/2} x_{11}^{-1/2} \frac{\partial x_{11}}{\partial F} \right] \quad (4.30)$$

$$\frac{\partial x_9}{\partial F} = C_9 \left[x_8^{1/2} \frac{\partial x_4}{\partial F} + \frac{1}{2} x_4 x_8^{-1/2} \frac{\partial x_8}{\partial F} \right] \quad (4.31)$$

$$\frac{\partial x_{10}}{\partial F} = C_{10} \left[x_8^{1/2} \frac{\partial x_6}{\partial F} + \frac{1}{2} x_6 x_8^{-1/2} \frac{\partial x_8}{\partial F} \right] \quad (4.32)$$

Exception

$$\frac{\partial x_{12}}{\partial F} = d_4 \left[\frac{\partial x_6}{\partial F} + \frac{\partial x_{10}}{\partial F} \right] + \frac{\partial d_4}{\partial F} [x_6 + x_{10}] \quad (4.33)$$

The coded subroutine PER () is called from the main program. The subroutine PER () calls for the subroutine EQMD () to compute species mole fractions and partial derivatives of the mole fractions. After executing EQMD () subprogram, the PER() subroutine computes average mixture molecular weight, mixture gas constant, enthalpy and internal energy. The subroutine PER () also computes partial derivatives of gas constant, molecular weight, internal energy and enthalpy with reference to equivalence ratio, pressure and temperature. The inputs of the PER () subroutine is mole fractions and there partial derivatives plus type of fuel, equivalence ratio and pressure.

Equations used for the computation of thermodynamic variables (molecular weight, gas constant, internal energy and enthalpy):

$$M = \sum_{i=1}^{12} x_i M_i \quad (4.34)$$

$$R = R_O / M \quad (4.35)$$

$$h = \sum_{i=1}^{12} h_i / M \quad (4.36)$$

$$u = h - RT \quad (4.37)$$

The partial derivatives are also effortlessly work out. As an instance

$$\frac{\partial M}{\partial T} = \sum_{i=1}^{12} M_i \frac{\partial x_i}{\partial T} \quad (4.38)$$

$$\frac{\partial R}{\partial T} = -\frac{R_O}{M^2} \frac{\partial M}{\partial T} = -\frac{R}{M} \frac{\partial M}{\partial T} \quad (4.39)$$

$$\frac{\partial h}{\partial T} = \frac{1}{M} [\Sigma(x_i \frac{dh_i}{dT} + \frac{\partial x_i}{\partial T} h_i) - \frac{\partial M}{\partial T} h] \quad (4.40)$$

$$\frac{\partial u}{\partial T} = \frac{\partial h}{\partial T} - R - \frac{\partial R}{\partial T} T \quad (4.41)$$

Where $dh_i/dT = C_{pi}$ is the specific heats of the outcomes at constant pressure. In order to calculate pressure (p) partial derivatives and equivalence ratio (F) partial derivatives substitute $\partial/\partial T$ with $\partial/\partial p$ and $\partial/\partial F$ respectively.

$$\frac{\partial M}{\partial p} = \Sigma \frac{\partial x_i}{\partial p} M_i \quad (4.42)$$

$$\frac{\partial R}{\partial p} = -\frac{R_O}{M^2} \frac{\partial M}{\partial p} = -\frac{R}{M} \frac{\partial M}{\partial p} \quad (4.43)$$

Exceptions are

$$\frac{\partial h}{\partial p} = \frac{1}{M} [\Sigma \frac{\partial x_i}{\partial p} h_i - \frac{\partial M}{\partial p} h] \quad (4.44)$$

$$\frac{\partial u}{\partial p} = \frac{\partial h}{\partial p} - \frac{\partial R}{\partial p} T \quad (4.45)$$

Similarly for $\partial/\partial F$

$$\frac{\partial M}{\partial F} = \Sigma \frac{\partial x_i}{\partial F} M_i \quad (4.46)$$

$$\frac{\partial R}{\partial F} = -\frac{R_O}{M^2} \frac{\partial M}{\partial F} = -\frac{R}{M} \frac{\partial M}{\partial F} \quad (4.47)$$

The exceptions are

$$\frac{\partial h}{\partial F} = \frac{1}{M} [\Sigma \frac{\partial x_i}{\partial F} h_i - \frac{\partial M}{\partial F} h] \quad (4.48)$$

$$\frac{\partial u}{\partial F} = \frac{\partial h}{\partial F} - \frac{\partial R}{\partial F} T \quad (4.49)$$

4.4.1 Program Description

Three different programs are written that calculates the combustion products equilibrium compositions: The program description is as follows:

HPFlame (constant enthalpy and pressure = isobaric(pressure=constant) adiabatic) :

HPFlame (present work) is an executable program that computes the adiabatic flame temperature, steady state compositions and properties of the outcomes of burning for adiabatic constant pressure burning with stated fuel blend, equivalence ratio, source enthalpy and inlet pressure.

TPEquil (Temperature Pressure Equilibrium) :

TPEquil (present work) is an executable program that computes burning outcomes, steady state composition and properties for stated fuel, equivalence ratio, outcome temperature and pressure.

UVFlame (constant internal-energy and volume = constant-volume adiabatic):

UVFlame (present work) is an executable program that computes the adiabatic flame temperature, steady state compositions and properties of the outcomes of burning for adiabatic constant volume burning with stated fuel blend, equivalence ratio, source enthalpy and inlet temperature and inlet pressure.

4.4.2 Inputs and Outputs of Code

4.4.2.1 HPFlame

The HPFlame (present work) is coded to compute thermodynamic variables for constant pressure combustion. The inputs of the code are type of fuel, equivalence ratio, assumed temperature, pressure and enthalpy of reactants. The input variables are in SI units. The code HPFlame (This work) computes species mole fractions of oxygen atom O , hydrogen atom H , hydrogen molecule H_2 , nitrogen atom N , hydroxide OH , nitric oxide NO , carbon monoxide CO , water H_2O , oxygen molecule O_2 , nitrogen molecule N_2 and carbon dioxide CO_2 . The code also

computes thermodynamic properties of combustion such as constant pressure adiabatic flame temperature, specific heat of the mixture, average molecular weight, enthalpy of mixture, specific heat ratio and moles of fuel per mole of outcomes.

4.4.2.2 TPEquil

The TPEquil (present work) is coded to compute thermodynamic variables at a given temperature and pressure of combustion. The code assumes combustion reaction to be at equilibrium conditions. The inputs of the code are type of fuel, equivalence ratio, temperature and pressure. The input variables are in SI units. The code TPEquil (This work) computes species mole fractions of oxygen atom O , hydrogen atom H , hydrogen molecule H_2 , Nitrogen atom N , Hydroxide OH , Nitric oxide NO , carbon monoxide CO , Water H_2O , Oxygen molecule O_2 , Nitrogen molecule N_2 and carbon dioxide CO_2 . The code also computes thermodynamic properties of combustion such as specific heat of the mixture, average molecular weight, enthalpy of mixture, specific heat ratio and moles of fuel per mole of outcomes.

4.4.2.3 UVFlame

The UVFlame (present work) is coded to compute thermodynamic variables for constant volume combustion. The inputs of the code are type of fuel, equivalence ratio, assumed product temperature, reactant temperature, reactant pressure, enthalpy of reactants, moles of reactants and molecular weight of reactants. The input variables are in SI units. The code UVFlame (This work) computes species mole fractions of oxygen atom O , hydrogen atom H , hydrogen molecule H_2 , Nitrogen atom N , Hydroxide OH , Nitric oxide NO , carbon monoxide CO , Water H_2O , Oxygen molecule O_2 , Nitrogen molecule N_2 and carbon dioxide CO_2 . The code also computes thermodynamic properties of combustion such as constant volume adiabatic flame temperature, specific heat of the mixture, average molecular weight, enthalpy of mixture, specific heat ratio, product pressure and moles of fuel per mole of outcomes.

4.5 Flowcharts of HPFlame Code, TPEquil Code and UVFlame Code

Figure 4.4 shows the flowchart of the HPFlame code. It has one start and one end. The input parameters are AN,AM,AL,AK,F,T,P,HREAC. The flowchart then call TABLES () subroutine to load enthalpy and heat capacity. Iterations are performed until IT variable reached 25 value. Within the loop, the code calls for PER () subroutine. Variable DELT is computed inside the loop. Temperature is updated by subtracting previous calculated temperature by DELT variable. If DELT variable is less than or equal to 0.01, the code outputs variables temperature, enthalpy, specific heat, specific heat ratio, molecular weight, twelve mole fractions and moles of fuel per mole of products. Within the loop, if DELT variable is greater than 0.01 and IT reached 25 then the code outputs “data not converged”.

Figure 4.5 shows the flowchart of the TPEquil code. It has one start and one end. The input parameters are AN,AM,AL,AK,F,T,P. The flowchart then call TABLES () subroutine to load enthalpy and heat capacity. The code calls for PER () subroutine. The code outputs variables enthalpy, specific heat, specific heat ratio, molecular weight, twelve mole fractions and moles of fuel per mole of products.

Figure 4.6 shows the flowchart of the UVFlame code. It has one start and one end. The input parameters are AN,AM,AL,AK,F,T,P,HREAC,TREAC,PREAC,XNREAC,XMREAC. The flowchart then call TABLES () subroutine to load enthalpy and heat capacity. Iterations are performed until IT variable reached 25 value. Within the loop, the code calls for PER () subroutine. Variable DELT is computed inside the loop. Temperature is updated by subtracting previous calculated temperature by DELT variable. If DELT variable is less than or equal to 0.01, the code outputs variables temperature, enthalpy, specific heat, specific heat ratio, molecular weight, twelve mole fractions and moles of fuel per mole of products. The code then ends with the values displayed on the screen.

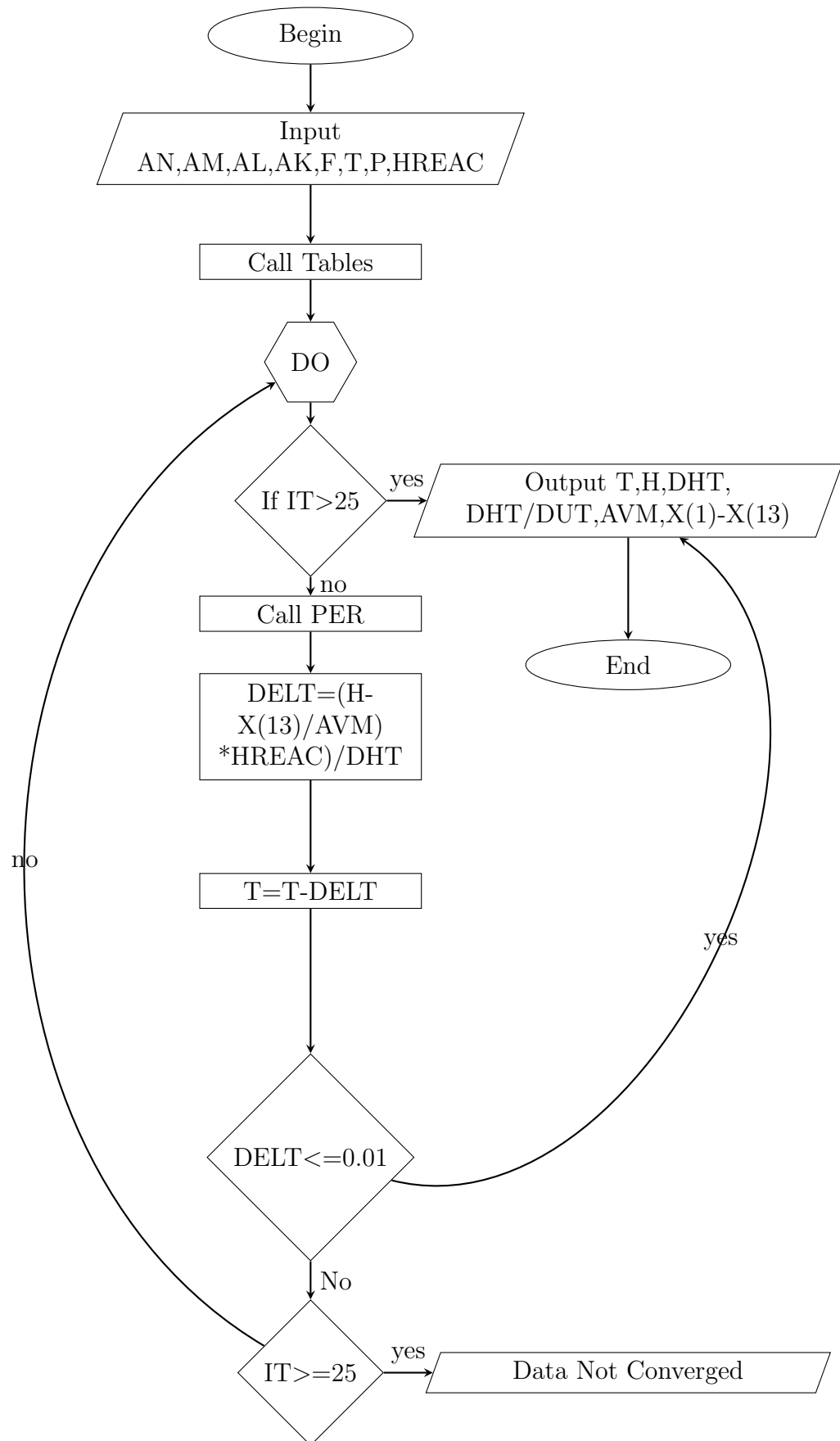


FIGURE 4.4: HPFlame Software Flowchart

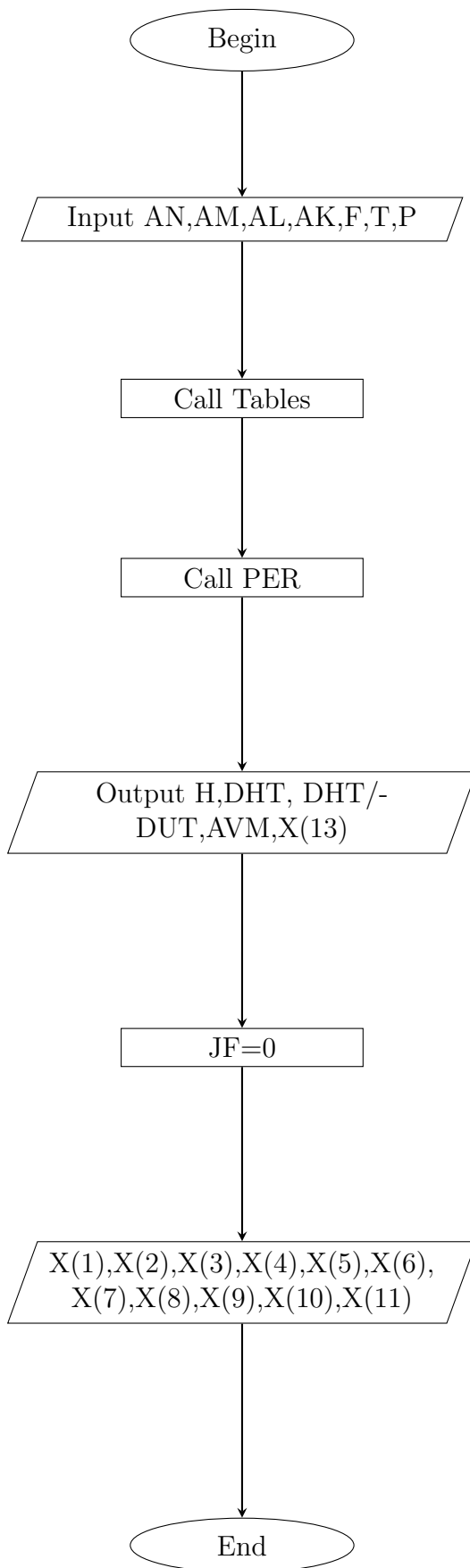


FIGURE 4.5: TPEquil Software Flowchart

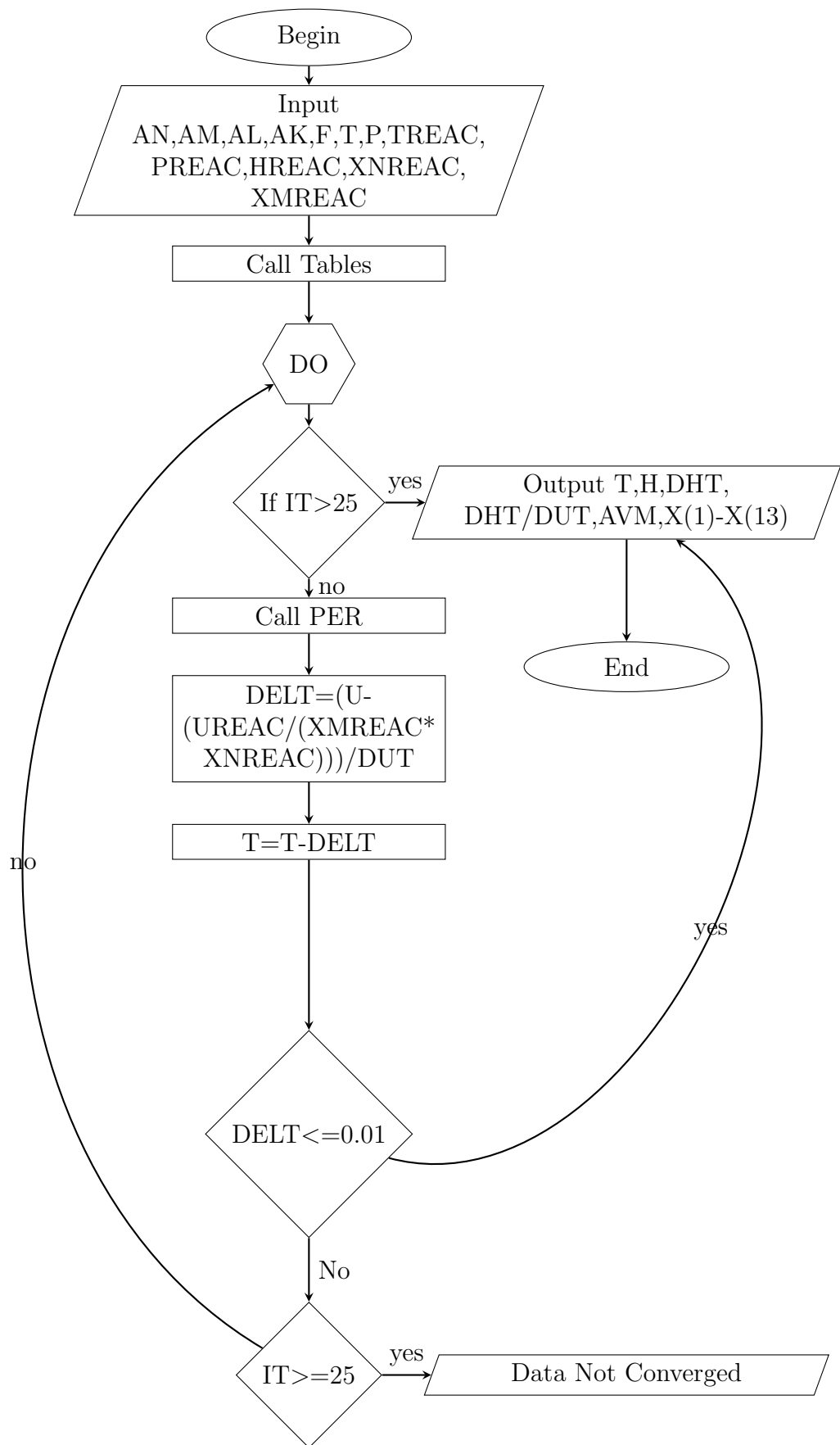


FIGURE 4.6: UVFlame Software Flowchart

Chapter 5

Results and Validation

5.1 Borman Algorithm

Borman Algorithm is based on solving twelve species of any hydrocarbon fuel. The twelve species are H , OH , O , CO , N , H_2O , H_2 , NO , O_2 , N_2 , CO_2 , Ar . Borman model is also known as full equilibrium model. It is experimentally proved [24] that for any hydrocarbon fuel, there are only twelve product species as mentioned in above line. The method to solve for these twelve species is known as full equilibrium model. The Borman code was developed at University of Wisconsin by Olikara and Borman. Borman code unravels for twelve outcomes compound, appealing zero for Argon, seven steadiness chemical models and four atom balance expressions, one each for C,O,H and N. The code was industrialized precisely for spark ignition locomotive and gas turbine locomotive simulations and is inserted as a subprogram in other mathematical numeric codes.

5.2 NASA Chemical Equilibrium Code

One of the leading regularly employed universal steadiness codes is the influential NASA Chemical Equilibrium Analysis (CEA) Code, designated as CEC86. The code is frequently updated so the "86" represents the update year. This code is

skillful in controlling nearly 400 dissimilar species and numerous superior mathematical models are integrated into it.

This code has the capability to perform rocket exhaust cone and shock interactions. These shock calculations are helpful in simulating missile aerodynamics at speed above mach 5.

The academic tactic to the steadiness computation does not involve equilibrium constants. The equilibrium calculations are performed by techniques that are functional to lessen each of two Helmholtz or Gibbs energies related to atom conservation limitations.

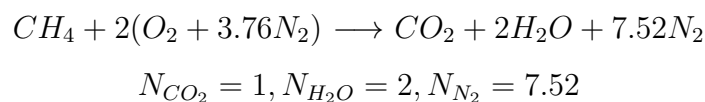
5.3 Case 1 : Constant Pressure Combustion for Methane

5.3.1 Complete Combustion (no dissociation) Adiabatic Flame Temperature at Constant Pressure (Methane)

Assumptions:

- Comprehensive Burning (no detachment), i.e. the outcome combination contains only CO_2, N_2 and H_2O .
- The outcome combination enthalpy is assessed by means of constant specific heats gaged at $(0.5(T_i + T_{ad}))$, where T_{ad} is predicted to be about 2100K)

Combination Arrangement:



Species	Enthalpy of Formation @ 298K	Specific Heat @ 1200K
CH_4	-74831	
CO_2	-393546	56.21
H_2O	-241845	43.87
N_2	0	33.71
O_2	0	

TABLE 5.1: Enthalpy & Specific Heat for Species at 1200K

First Law:

$$\begin{aligned}
 H_{react} &= \sum_{react} N_i \bar{h}_i = H_{prod} = \sum_{prod} N_i \bar{h}_i \\
 H_{react} &= (1)(-74831) + 2(0) + 7.52(O) = -74831 kJ \\
 H_{react} &= (1)(-74831) + 2(0) + 7.52(0) = -74831 kJ \\
 H_{prod} &= \sum N_i [h_{f,i}^{\bar{O}} + \bar{C}_{p,i}(T_{ad} - 298)] \\
 H_{prod} &= (1)[-393546 + 56.21(T_{ad} - 298)] + (2)[-241845 + 43.87(T_{ad} - 298)] + \\
 &\quad (7.52)[0 + 33.71(T_{ad} - 298)]
 \end{aligned}$$

Linking H_{react} to H_{prod} and cracking for T_{ad} produces

$$T_{ad} = 2318K$$

The outcome combination enthalpy is assessed by means of constant specific heats gaged at 1308K ($0.5(T_i + T_{ad})$, where T_{ad} is around 2318K)

Species	Enthalpy of Formation @ 298 K	Specific Heat @ 1308 K
CH_4	-74831	
CO_2	-393546	56.984
H_2O	-241845	45.027
N_2	0	34.113
O_2	0	

TABLE 5.2: Enthalpy & Specific Heat for Species at 1308K

First Law:

$$\begin{aligned}
 H_{react} &= \sum_{react} N_i \bar{h}_i = H_{prod} = \sum_{prod} N_i \bar{h}_i \\
 H_{react} &= (1)(-74831) + 2(0) + 7.52(0) = -74831 kJ \\
 H_{prod} &= \sum N_i [h_{f,i}^{\bar{O}} + \bar{C}_{p,i}(T_{ad} - 298)] \\
 H_{prod} &= (1)[-393546 + 56.984(T_{ad} - 298)] + (2)[-241845 + 45.027(T_{ad} - 298)] \\
 &\quad + (7.52)[0 + 34.113(T_{ad} - 298)]
 \end{aligned}$$

Linking H_{react} to H_{prod} and cracking for T_{ad} produces

$$T_{ad} = 2286.2783K$$

5.3.2 Constant Pressure Combustion present work Validation with Borman Code & NASA Code (Methane)

Consider the conventional problem of calculating the constant pressure adiabatic flame temperature. Considering adiabatic constant pressure burning; first compute the reactant mixture enthalpy. If the fuel heat of formation is not identified it can be assessed using the heating value and H/C ratio.

For extreme pressures the non-ideal effects should be contained within. After computing the reactant enthalpy h_r grip pressure (p) and equivalence ratio (F) constant and compute for temperature (T)

$$h(T, p_O, F_O) - h_r(T_O, p_O, F_O) = 0 \quad (5.1)$$

Using Newtons method

$$T_{n+1} = T_n - \frac{h(T_n, p_O, F_O) - h_r}{(\partial h / \partial T)_n} \quad (5.2)$$

Where T_n is the initial approximation and T_{n+1} is the enhanced approximate.

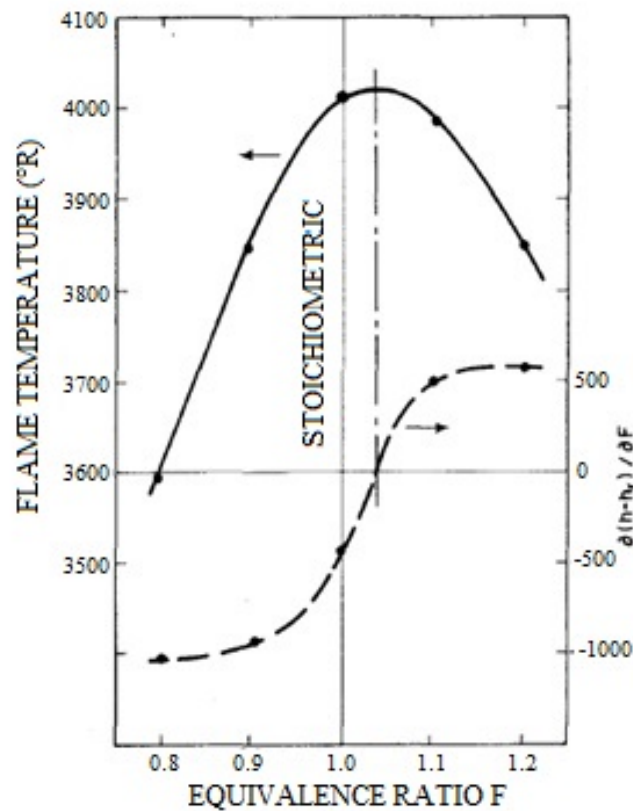


FIGURE 5.1: Adiabatic flame temperature versus equivalence ratio for conditions [1]

The initial guess can be any sensible number but rather greater than the predicted result. As an example take methane at 298K(536.4R), one atmosphere and $F=0.9$. Figure 5.1 displays a plot of the outcome and Table 5.3 displays the liberal estimates of Temperature (T) for the equivalence ratio ($F = 0.9$) case. A graph of $\partial(h - h_r)/\partial F$ at the computed equivalence ratio (F) and temperature (T) numbers of Figure 5.1 gives the dashed spline of Figure 5.1. The zero value on the y axis defines the equivalence ratio (F) at the extreme flame temperature.

Example: Constant Pressure flame temperature

Fuel: CH_4

Equivalence ratio: $F=0.9$

Pressure: $P=101325$ Pa

Temperature (Guess): $T=2000$ K

Reactant enthalpy: $h_r = -74831$ KJ/kmol-fuel

Iter	H	$\partial h / \partial T$	ΔT	T(org)	T(Borman)
1	-463400.71	1634.02	-141.0275	2141.0275	2141.027524
2	-220178.27	1832.536	6.974	2134.05	2134.053484
3	-232926.146	1819.85	0.01775	2134.036	2134.035733
4	-232958.49	1819.82	-1.984×10^{-5}	2134.0357	2134.035753

TABLE 5.3: Calculation of Flame Temperature [1]

Flame Temperature (This Work) at Equivalence Ratio (0.9) = 2134.0357K

Flame Temperature (This Work) at Equivalence Ratio (1) = 2225.565 K

Flame Temperature (NASA) at Equivalence ratio (1) = 2224.93 K

Adiabatic Flame Temperature (Analytical) for complete combustion = 2286.28K

Properties	This Work (a)	Borman Values (b)	% Error (a- b)/a*100
Flame Temperature (K)	2134.0357	2134.04	-2.01×10^{-4}
Mixture Enthalpy (J/kg)	-232958.48678	-233000	-1.78×10^{-2}
Mixture Specific Heat $C_p(J/kg - K)$	1819.8214	1819.82	7.69×10^{-5}
Specific Heat Ratio C_p/C_v	1.2056740	1.2057	-2.16×10^{-3}
Mixture Molecular Weight (kg/kmol)	27.675459	27.6755	-1.48×10^{-4}
Moles of fuel per mole of products	0.0861572	0.08615724	-4.64×10^{-5}

TABLE 5.4: Validation of Flame and Mixture Properties Results

Properties	This Work (a)	NASA CEA (b)	% Error (a-b)/a*100
Flame Temperature (K)	2134.0357	2134.33	-1.38×10^{-2}
Mixture Enthalpy (J/kg)	-232958.48678	-232620	1.45×10^{-1}
Mixture Specific Heat Cp (J/kg-K)	1819.8214	1824.3	-2.46×10^{-1}
Specific Heat Ratio Cp/Cv	1.2056740	1.2119	-5.16×10^{-1}
Mixture Molecular Weight (kg/kmol)	27.675459	27.674	5.27×10^{-3}
Moles of fuel per mole of products	0.0861572	-	-

TABLE 5.5: Comparison of Visual Basic Values and NASA CEA Values

Table below shows the percentage error between this work and borman algorithm.

Mole Fraction	This Work (a)	Borman values (b)	% Error (a-b)/a*100
H	0.000116878	0.00011688	-1.71×10^{-3}
O	0.00023643	0.00023643	0
N	4.6775916×10^{-9}	4.6775916E-09	0
H_2	0.00093566	0.00093566	0
OH	0.00266438	0.00266438	0
CO	0.0023017377	0.00230174	-9.99×10^{-5}
NO	0.003237686	0.00323769	-1.24×10^{-4}
O_2	0.0183908	0.01839082	-1.09×10^{-4}
H_2O	0.1699881799	0.16998818	-5.88×10^{-8}
CO_2	0.08385549	0.08385550	-1.19×10^{-5}
N_2	0.71827272	0.71827272	0

TABLE 5.6: Validation of Species Mole Fraction Results

Mole Fraction	This Work (a)	NASA CEA (b)	% Error (a-b)/a*100
H	0.000116878	0.00012	-2.67
O	0.00023643	0.00024	-1.51
N	4.6775916×10^{-9}	0.00001	0
H_2	0.00093566	0.00093	6.05×10^{-1}
OH	0.00266438	0.00268	-5.86×10^{-1}
CO	0.0023017377	0.00232	-7.93×10^{-1}
NO	0.003237686	0.00305	5.80
O_2	0.0183908	0.01831	4.39×10^{-1}
H_2O	0.1699881799	0.17014	-8.93×10^{-2}
CO_2	0.08385549	0.08391	-6.50×10^{-2}
N_2	0.71827272	0.71829	-2.41×10^{-3}

TABLE 5.7: Comparison of Species Mole Fraction Results

5.3.3 Function Concavity and Convexity

The function derived for computation of initial estimation of mole fractions is checked for concavity and convexity.

Methane CH_4 is selected as a fuel.

Equivalence ratio is taken to be one.

It is assumed that the product species are at temperature 2225.565 K and pressure at 101325 Pa.

Putting in the values of C_{10} , n , C_9 , m , r and X_{13} from software(this work) in equation 3.93:

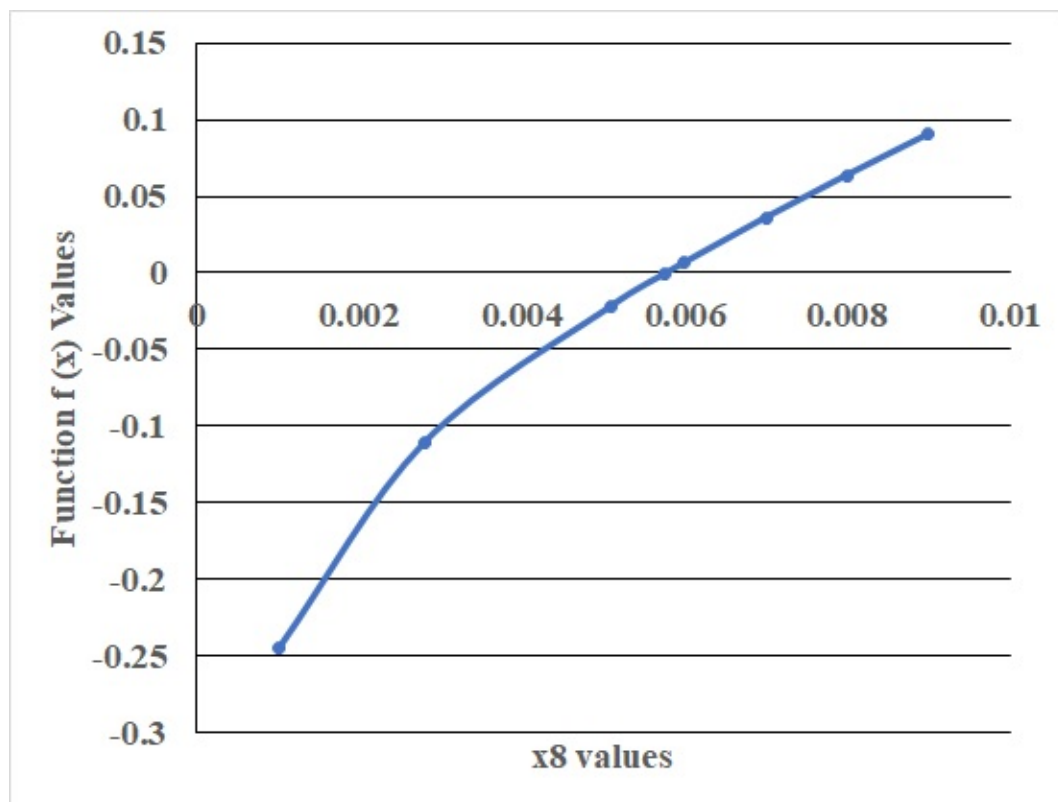
$$f(x) = \frac{282.793x_8^{1/2} + 1}{1 + 141.3965x_8^{1/2}} + \frac{1493.956x_8^{1/2}}{1 + 746.9781x_8^{1/2}} + 21.0495x_8 - 4.002 = 0 \quad (5.3)$$

Putting in different values of x_8 and evaluating $f(x)$ by equation 5.3. Also first derivative and second derivative computed from MATLAB software [25] of equation 5.3 is given in table 5.8:

x_8	$f(x)$	$f'(x)$	$f''(x)$
0.001	-0.24495	134.6974	-155240
0.0028	-0.1103	48.2156	-1.3696×10^4
0.00509980	-0.0216	32.6299	-3.2513×10^3
0.005760	-6.6469×10^{-4}	30.7754	-2.4237×10^3
0.006	0.0067	30.2217	-2.1961×10^3
0.007	0.0359	28.3973	-1.5124×10^3
0.008	0.0636	27.1099	-1.0941×10^3
0.009	0.0902	26.1610	-821.9052

TABLE 5.8: Function values at different x_8

Plot of function $f(x)$ with different values of x_8 is shown in figure 5.8. From table 5.8, the values of second derivative of function $f(x)$ are negative. Therefore the function is concave, as is clear from the plot 5.2. Also the function $f(x)$ would never diverge because the concave function curve is passing through zero y-axis.

FIGURE 5.2: Function values $f(x)$ at different x_8

5.4 Case 2 : Equilibrium Combustion for Iso-Octane

In this case study steadiness burning of Iso Octane is discussed. Outcome parameters are computed and validated against Borman Numerical Scheme.

Fuel C_8H_{18}

Equivalence Ratio: $F=1$

Temperature: $T=3000K$

Pressure: $P=101325Pa$

The table below shows percentage error between this work and borman algorithm for iso-octane. The percentage error for mixture enthalpy is -0.00383 . The percentage error for mixture specific heat is -0.0000388 . The percentage error for specific heat ratio is 0.00208 . The percentage error for mixture molecular weight is 0.0000762 . The percentage error between this work and borman work for moles of fuel per mole of products is 0 .

Properties	This Work	Borman Values	% Error (a-b)/a*100
Mixture Enthalpy (J/kg)	2494904.56258	2495000	-3.83×10^{-3}
Mixture Specific Heat $C_p(J/kg - K)$	5150.528	5150.53	-3.88×10^{-5}
Specific Heat Ratio C_p/C_v	1.105123	1.1051	2.08×10^{-3}
Mixture Molecular Weight ($kg/kmol$)	26.24072	26.2407	7.62×10^{-5}
Moles of fuel per mole of products	0.01432578	0.01432578	0

TABLE 5.9: Calculated Combustion products Properties

Mole Fraction	This Work (a)	Borman values (b)	% Error (a-b)/a*100
<i>H</i>	0.02314756	0.02314757	-4.32×10^{-5}
<i>O</i>	0.019161654	0.01916166	-3.13×10^{-5}
<i>N</i>	1.1309959×10^{-5}	1.131×10^{-5}	0
<i>H₂</i>	0.02162772	0.02162772	0
<i>OH</i>	0.02910304	0.02910304	0
<i>CO</i>	0.07537333	0.07537334	-1.33×10^{-5}
<i>NO</i>	0.01697829	0.01697829	0
<i>O₂</i>	0.029031	0.02903127	-9.30×10^{-4}
<i>H₂O</i>	0.08117902	0.08117902	0
<i>CO₂</i>	0.0392329	0.03923293	-7.65×10^{-5}
<i>N₂</i>	0.66515384	0.66515385	-1.50×10^{-6}

TABLE 5.10: Validation of Species Mole Fraction Results

5.5 Case 3 : Equilibrium Combustion for CH_4 Methane

In this case study steadiness burning of Methane is discussed. Outcome parameters are computed and validated against Borman Numerical Scheme and NASA CEA Code.

Fuel CH_4

Equivalence Ratio: F=1

Temperature: T=3000K

Pressure: P=101325Pa

Pressure: P=1 atm

Properties	This Work	Borman Values (b)	% Error (a-b)/a*100
Mixture Enthalpy (J/kg)	2566143.4625	2566000	5.59×10^{-3}
Mixture Specific Heat $C_p(J/kg - K)$	5592.01	5592.01	0
Specific Heat Ratio C_p/C_v	1.1027046	1.1027	4.17×10^{-4}
Mixture Molecular Weight ($kg/kmol$)	25.335066	25.3351	-1.34×10^{-4}
Moles of fuel per mole of products	0.0871099	0.08710993	-3.44×10^{-5}

TABLE 5.11: Calculated Combustion products Properties

Table below shows the percentage error between this work and NASA Chemical Equilibrium Analysis code. The percentage error for all the mixture properties are in the range from -2.97 to 0.453.

Properties	This Work	NASA CEA (b)	% Error (a-b)/a*100
Mixture Enthalpy (J/kg)	2566143.4625	2561470	1.82×10^{-1}
Mixture Specific Heat $C_p(J/kg - K)$	5592.01	5566.7	4.53×10^{-1}
Specific Heat Ratio C_p/C_v	1.1027046	1.1355	-2.97
Mixture Molecular Weight ($kg/kmol$)	25.335066	25.344	-3.53×10^{-2}
Moles of fuel per mole of products	0.0871099	-	-

TABLE 5.12: Validation of Combustion Products Properties with NASA CEA Code

Mole Fraction	This Work (a)	Borman values (b)	% Error (a-b)/a*100
<i>H</i>	0.027874	0.02787461	-2.19×10^{-3}
<i>O</i>	0.0182657	0.01826570	0
<i>N</i>	1.1158×10^{-5}	0.00001116	0
<i>H₂</i>	0.031363	0.03136299	3.19×10^{-5}
<i>OH</i>	0.03340759	0.03340759	0
<i>CO</i>	0.0582217	0.05822169	1.72×10^{-5}
<i>NO</i>	0.015967	0.01596704	-2.51×10^{-4}
<i>O₂</i>	0.02637987	0.02637988	-3.79×10^{-5}
<i>H₂O</i>	0.1122157	0.11221577	-6.24×10^{-5}
<i>CO₂</i>	0.02888	0.02888825	-2.86×10^{-2}
<i>N₂</i>	0.6474053	0.64740531	-1.54×10^{-6}

TABLE 5.13: Validation of Species Mole Fraction Results

Table below shows the percentage error between this work and NASA CEA Code.

Mole Fraction	This Work (a)	NASA CEA (b)	% Error (a-b)/a*100
<i>H</i>	0.027874	0.02762	9.11×10^{-1}
<i>O</i>	0.0182657	0.01826	3.12×10^{-2}
<i>N</i>	1.1158×10^{-5}	0.00001	0
<i>H₂</i>	0.031363	0.03091	1.44
<i>OH</i>	0.03340759	0.03342	-3.71×10^{-2}
<i>CO</i>	0.0582217	0.05836	-2.38×10^{-1}
<i>NO</i>	0.015967	0.01535	3.86
<i>O₂</i>	0.02637987	0.02638	-4.93×10^{-4}
<i>H₂O</i>	0.1122157	0.11293	-6.37×10^{-1}
<i>CO₂</i>	0.02888	0.02882	2.08×10^{-1}
<i>N₂</i>	0.6474053	0.64793	-8.10×10^{-2}

TABLE 5.14: Validation of Species Mole Fraction Results

5.6 Case 4 : Constant Volume Combustion for Iso-Octane

This case study deals with the computation of the Constant Volume Adiabatic Flame properties for specific fuel, equivalence ratio and reactant properties. Using Newtons method

$$T_{n+1} = T_n - \frac{U(T_n) - U_r}{(\partial U / \partial T)_n} \quad (5.4)$$

Fuel C_8H_{18} Equivalence Ratio: F=1.0

Final(Product) Temperature (Guess): T=2000K

Reactant Temperature: TREAC=556K

Reactant Pressure: PREAC=755885Pa

Enthalpy of Reactant (KJ/Kmol of fuel): HREAC=-614070

Moles of Reactants (kmol/kmol of fuel): XNREAC=72.60

Molecular weight of Reactants (kg/kmol): XMREAC=29.980

Properties	This Work	Borman Values (b)	% Error (a-b)/a*100
Constant Volume Flame Temperature [k]	2572.46	2572.46	0
Pressure (Pa)	3699071	3699070	2.70×10^{-5}
Mixture Enthalpy (J/kg)	318264.376	318300	-1.12×10^{-2}
Mixture Specific Heat $C_p(J/kg - K)$	2100	2100.05	-2.38×10^{-3}
Specific Heat Ratio C_p/C_v	1.17715	1.1772	-4.25×10^{-3}
Mixture Molecular Weight (kg/kmol)	28.34	28.3445	-1.59×10^{-2}
Moles of fuel per mole of products	0.0154743026	0.01547430	1.70×10^{-5}

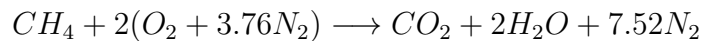
TABLE 5.15: Constant Volume Combustion Products Properties

Mole Fraction	This Work (a)	Borman Values (b)	% Error (a-b)/a*100
H	0.0002890	0.00028907	-2.42×10^{-2}
O	0.00024217	0.00024217	0
N	7.88625×10^{-8}	0.00000008	0
H_2	0.0026112	0.00261124	-1.53×10^{-3}
OH	0.0033582	0.00335819	2.98×10^{-4}
CO	0.0134	0.01340202	-1.51×10^{-2}
NO	0.0041044	0.00410448	-1.95×10^{-3}
O_2	0.00516278	0.00516279	-1.94×10^{-4}
H_2O	0.1348338	0.13483385	-3.71×10^{-5}
CO_2	0.1103924	0.11039240	0
N_2	0.72560	0.72560373	-5.14×10^{-4}

TABLE 5.16: Validation of Species Mole Fraction Results

5.7 Case 5 : Constant Volume Combustion for Methane

In this case study a comparison is made between Analytical Calculation and UVFlame software. For the chemical Reaction:



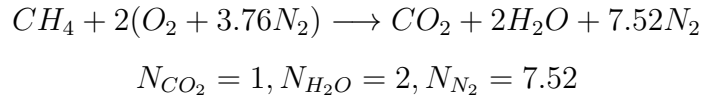
5.7.1 Complete Combustion (no dissociation) Adiabatic Flame Temperature at Constant Volume (Methane)

Assumptions:

- Comprehensive Burning (no detachment), i.e. the outcome combination contains only CO_2, N_2 and H_2O .

- The outcome combination enthalpy is assessed using constant specific heats gaged at 1200K ($0.5(T_i + T_{ad})$), where T_{ad} is predicted to be about 2100 K)

Compound Combination Arrangement:



Species	Enthalpy of Formation @ 298K	Specific Heat @ 1200 K
CH_4	-74831	
CO_2	-393546	56.21
H_2O	-241845	43.87
N_2	0	33.71
O_2	0	

TABLE 5.17: Enthalpy & Specific Heat for Species at 1200K

$$H_{react} - H_{prod} - R_u(N_{react}T_{init} - N_{prod}T_{ad}) = 0$$

$$\sum_{react} N_i \bar{h}_i - \sum_{prod} N_i \bar{h}_i - R_u(N_{react}T_{init} - N_{prod}T_{ad}) = 0$$

Substituting numerical values, we have

$$H_{react} = (1)(-74831) + 2(0) + 7.52(0) = -74831 kJ$$

$$H_{prod} = (1)[-393546 + 56.21(T_{ad} - 298)] + (2)[-241845 + 43.87(T_{ad} - 298)] +$$

$$(7.52)[0 + 33.71(T_{ad} - 298)]$$

$$H_{prod} = -877236 + 397.5(T_{ad} - 298) kJ$$

And

$$R_u(N_{react}T_{init} - N_{prod}T_{ad}) = 8.315(10.52)(298 - T_{ad})$$

Where $N_{react}=N_{prod}=10.52$ kmol

Reassembling and solving for T_{ad} yields

$$T_{ad} = 2889K$$

Adiabatic flame temperature for constant volume is calculated analytically

$$T_{ad} = 2889K$$

5.7.2 Constant Volume Combustion Present Work Validation with Borman Code & NASA Code (Methane)

Adiabatic Flame Temperature for constant volume is calculated using UVFlame software as

Number of Carbon Atom = 1 Number of Hydrogen Atom = 4

Equivalence Ratio = 1 Product Temperature (guess) = 2000K

Reactant Temperature = 298K Reactant Pressure = 101325Pa

Enthalpy of Reactant = -74874.93 KJ/kmol(fuel)

Moles of Reactants = 10.52 Molecular Weight of Reactants = 27.62 kg/kmol

Adiabatic Flame Temperature at Constant Volume $T_{ad}=2587.72K$

Adiabatic Flame Temperature Calculated using NASA CEA $T_{ad} = 2592.12 K$

Properties	This Work	Borman Values	% Error (a-b)/a*100
Constant Volume Flame Temperature [K]	2587.72	2587.72	0
Pressure (Pa)	892100.45	892100	5.04×10^{-5}
Mixture Enthalpy (J/kg)	442402.82	442400	6.37×10^{-4}
Mixture Specific Heat $C_p(J/kg - K)$	2497.178	2497.18	-8.01×10^{-5}
Specific Heat Ratio C_p/C_v	1.1584	1.1584	0
Mixture Molecular Weight (kg/kmol)	27.2413	27.2413	0
Moles of fuel per mole of products	0.093664	0.09366413	-1.39×10^{-4}

TABLE 5.18: Constant Volume Combustion Products Properties

Properties	This Work (a)	NASA CEA (b)	% Error (a-b)/a*100
Constant Volume Flame Temperature [K]	2587.72	2592.12	-1.70×10^{-1}
Pressure (Pa)	892100.45	894280	-2.44×10^{-1}
Mixture Enthalpy (J/kg)	442402.82	433110	2.10
Mixture Specific Heat C_p (J/kg - K)	2497.178	2482	6.08×10^{-1}
Specific Heat Ratio C_p/C_v	1.1584	1.1734	-1.29
Mixture Molecular Weight (kg/kmol)	27.2413	27.573	-1.22
Moles of fuel per mole of products	0.093664	-	-

TABLE 5.19: Constant Volume Combustion Products Properties

Table below shows the percentage error between this work and borman algorithm.

Mole Fraction	This Work (a)	Borman Values (b)	% Error (a-b)/a*100
H	0.000967	0.00096738	-3.93×10^{-2}
O	0.0006388	0.0006388	0
N	1.8034×10^{-7}	0.00000018	0
H_2	0.0062164	0.00621648	-1.29×10^{-3}
OH	0.0063166	0.00631661	-1.58×10^{-4}
CO	0.0169497	0.01694969	5.90×10^{-5}
NO	0.00499719	0.00499719	0
O_2	0.0075215	0.00752149	1.33×10^{-4}
H_2O	0.177467	0.17746979	-1.57×10^{-3}
CO_2	0.0767144	0.07671444	-5.21×10^{-5}
N_2	0.7022	0.70220794	-1.13×10^{-3}

TABLE 5.20: Comparison of Species Mole Fraction Results

Mole Fraction	This Work (a)	NASA CEA (b)	% Error (a-b)/a*100
<i>H</i>	0.000967	0.00098	-1.34
<i>O</i>	0.0006388	0.00066	-3.32
<i>N</i>	1.8034×10^{-7}	0	0
<i>H₂</i>	0.0062164	0.00623	-2.19×10^{-1}
<i>OH</i>	0.0063166	0.00644	-1.95
<i>CO</i>	0.0169497	0.01734	-2.30
<i>NO</i>	0.00499719	0.00484	3.15
<i>O₂</i>	0.0075215	0.00767	-1.97
<i>H₂O</i>	0.177467	0.17853	-5.99×10^{-1}
<i>CO₂</i>	0.0767144	0.07718	-6.07×10^{-1}
<i>N₂</i>	0.7022	0.70013	2.95×10^{-1}

TABLE 5.21: Validation of Species Mole Fraction Results

5.8 Case 6 : Present Work Validation with other References

The Visual Basic Code was validated with various researches on calculating Adiabatic Flame Temperature. Following are the list of work conducted by different authors:

5.8.1 A Lean Pre Mixed Combustor and Conventional Combustor By Honegger

Figure 5.3 express a diagram of a conventional and lean-premixed combustor. The fuel is expected to be pure methane. The universal knowledge of a Dry Low NOx (DLN) combustor is to produce a carefully diverse lean fuel and air combination before entering the burning cylinder of the stationary turbine locomotive. The lean blend generates a comparatively small flame temperature, which yields lesser

quantities of NO_x. Supposing the combination is too lean that is near to the lean blow out margin, the fuel to air fraction has to be maintained constant within thin boundaries. This is also essential due to additional restraint. The lesser burning temperature inclines to create an elevated cluster of outcomes linked to imperfect burning, for instance carbon monoxide (CO) and unburned hydrocarbons. The requirement to handle the fuel to air fraction strictly produces dissimilar reduced load performance when relating stationary turbines with conventional combustors and DLN locomotive.

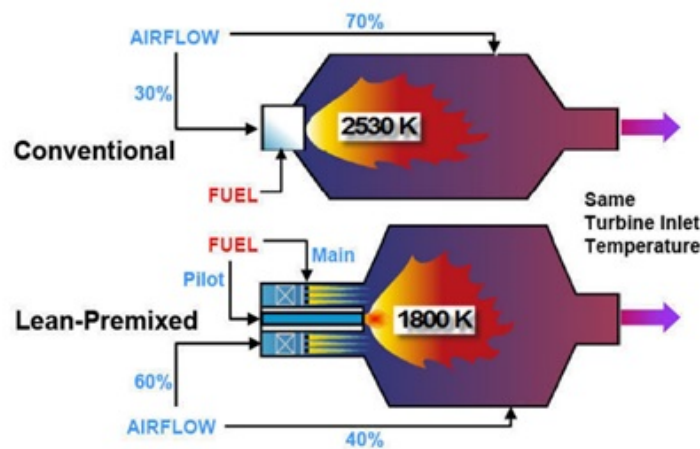


FIGURE 5.3: Conventional & Lean Premixed Combustor [31]

At confident stages of reduced load, DLN engines typically supply some quantity of air from the compressor exit straight into the exhaust section. Considering the airflow for any two shaft engines is lessened at reduce load, the decline in flow of air is larger for a conventional combustion engine than for a DLN engine (Kurz, et al. 2003 [32]). Honegger (2004) [31] used equivalence ratios, and the stoichiometric coefficient with chemical reaction coefficients in a lean, pre-mixed combustor to determine the adiabatic temperature, assuming, thereby, a complete combustion, in a plug-flow reactor (PFR).

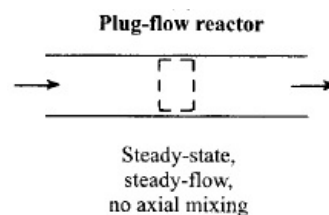


FIGURE 5.4: Plug flow Reactor [24]

Author	Method of Computation	T_{ad} Values
Honegger (2007)-KANSAS STATE UNIVERSITY	A lean Premixed Combustor in a Plug-Flow Reactor (PFR)	1800 K
Honegger (2007)-KANSAS STATE UNIVERSITY	A Conventional Combustor in a Plug-Flow Reactor (PFR)	2530 K

TABLE 5.22: Adiabatic Temperature Values By Honegger [31]

5.8.2 Computation of Laminar and Turbulent Combustion

Strong burning inside a little space is modeled by concept of premixed flames. This is the situation in domestic appliances and spark ignition locomotives. Additional case for non-premixed combustion are Diesel combustors, where a liquid fuel spray is inserted into the compressed hot air inside the cylinder. Huge burning devices such as heaters, on the contrary, function with non-premixed settings through diffusion flames.

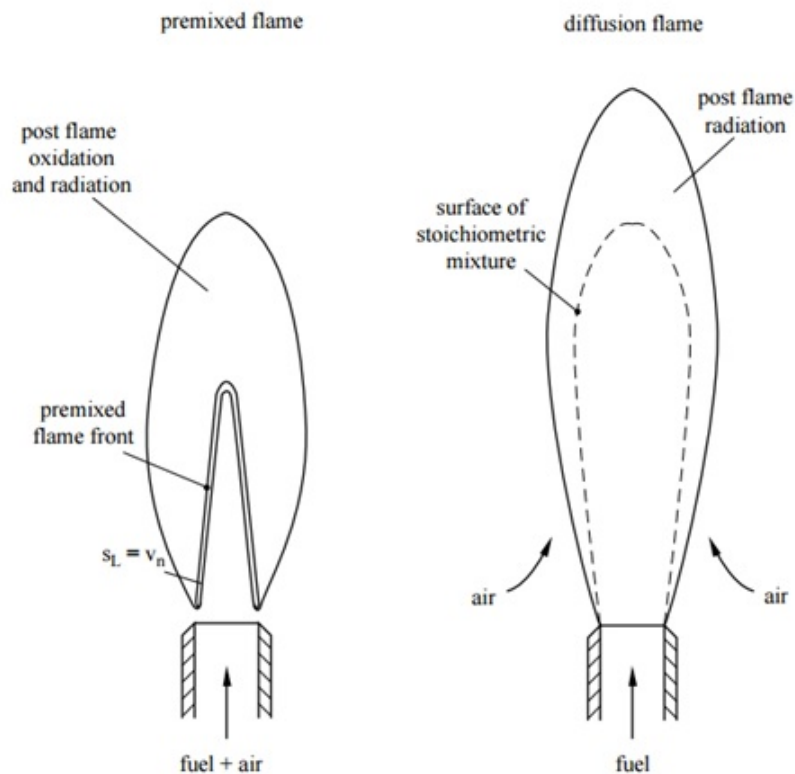


FIGURE 5.5: Premixed flame and Diffusion flame [33]

Subsequently the premixing of bulky weight of fuel and air signifies a thoughtful security issues.

From time to time burning is incompletely pre-combined in order to have a improved control over flame steadiness and contaminants.

This is also a situation in air breathing constant pressure combustors, boilers or in stratified charge spark ignition locomotives.

Peters, (1992) [33] used inputs of the mole fraction of the species i , mass of species i , the mass fraction of elements, the mixture fraction, the stoichiometric blend fraction and the fuel-air equivalence ratio. They arrived at the stoichiometric flame temperature T_{st} , for some hydrocarbon-air mixtures, for some stoichiometric fractions. They arrived also at the adiabatic flame temperatures for fuel supply less than stoichiometric for methane, acetylene and propane flames as a relation to equivalence ratios.

Fuel	Z_{st}	T_{st} [k]
CH_4	0.05496	2263.3
C_2H_6	0.05864	2288.8
C_2H_4	0.06349	2438.5
C_2H_2	0.07021	2686.7
C_3H_8	0.06010	2289.7

TABLE 5.23: Stoichiometric mixture fractions and stoichiometric flame temperatures for some fuels [33]

Table below shows the adiabatic temperature values computed by peters.

Author	Method of Computation	T_{ad} Values
N. Peters (1992)- Aachen-Germany	RWTH Inputs of the mole fraction the stoichiometric mixture, etc	2263.3K 2686.7K

TABLE 5.24: Adiabatic Temperature Values By N.Peters [33]

5.8.3 Adiabatic Flame Temperature Computation for Gas-Turbine Combustors at 1.4 Equivalence Ratio

The paper [34] certify a feature of adiabatic flame temperature numerical processing in a conventional burning locomotive. The scheme employed registered enthalpy matching model and matched the inflow with outflow energy in the burning cylinder. Axial compressor released air at a temperature of 620 K and a pressure of 5.92 atm (6 bars). Analyzing the exhaust gas components that are taking out the output energy with the adiabatic temperature, it was possible to graphically determine the flame temperature.

Author	Method of Computation	T_{ad} Values
I. E. Douglas E. Ufot, B. T. Lebele-Alawa (2011)- European Journal of Scientific Research	Enthalpy – computations with conventional combustor at an equivalent ratio of 1.4	2620 K

TABLE 5.25: Adiabatic Temperature Values By Ufot, Lebele and Douglas [34]

The adiabatic flame temperature (T_{ad}) was computed as 2620K.

5.8.4 NASA CEA Chemical Equilibrium Analysis Code

Equivalence Ratio = 1.4

Temperature T = 620 K

Pressure P = 600,000 Pa

Pressure P = 6 bars

From NASA CEA Code

$$T_{ad} = 2169.96K$$

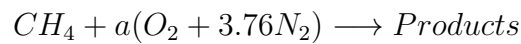
5.8.5 Present Work-2020 Capital University of Science & Technology

Equivalence Ratio = 1.4

Temperature T = 620 K

Pressure P = 600,000 Pa

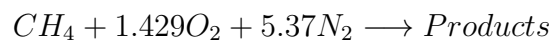
The combustion equation is:



Where

$$a = \frac{x+y/4}{F} = \frac{(1+4/4)}{1.4} = 1.429$$

Thus



The reactants enthalpy (per mole of fuel) is then

$$\begin{aligned} H_{react} &= \overline{h_{f,CH_4}} + 1.429\overline{\Delta h_{s,O_2}} + 5.37\overline{\Delta h_{s,N_2}} \\ H_{react} &= -74831 + 1.429(9254) + 5.37(8905) \\ H_{react} &= -13787.184 \text{ KJ/kmol}_{(Fuel)} \end{aligned}$$

From HPFlame Software

$$T_{ad} = 2200 \text{ K}$$

5.8.6 Validation Summary

Authors	Method of Computation	T_{ad} Values
Honegger (2007)- KANSAS STATE UNIVERSITY	A lean Premixed Combustor in a Plug-Flow Reactor (PFR)	1800 K
Honegger (2007)- KANSAS STATE UNIVERSITY	A Conventional Combustor in a Plug-Flow Reactor (PFR)	2530 K
N. Peters (1992)- RWTH Aachen-Germany	Inputs of the mole fraction the stoichiometric mixture etc	2263.3K 2686.7K
I. E. Douglas E. Ufot, B. T. Lebele-Alawa (2011) – European Journal of Scientific Research	Enthalpy computations with conventional combustor at an equivalent ratio of 1.4	2620 K
NASA CEA Chemical Equilibrium Analysis Code	Schemes are employed to reduce either the Helmholtz or Gibbs energies, link to atom balance limitations	2169.96 K
Present Work	Mole Fractions-Gas Constant-Enthalpy-Internal Energy-Partial derivatives of mole fractions, enthalpy, internal energy with reference to Equivalence Ratio, Pressure and Temperature	2200 K

TABLE 5.26: Validation Summary

Table 5.26 above can be put up from Authors of T_{ad} as validation for the method used in the present work. It is fascinating to record from Table 5.26, that the outcome of T_{ad} matches well with the values by other authors.

5.9 Case 7 : Determination of Constant Volume Flame Temperature (Propane)

The code UVFlame is used to determine Constant Volume Adiabatic Flame Temperature of a stoichiometric propane-air combination guessing reactants at 298K, no detachment of the outcomes, and constant specific heats evaluated at 298K. It is assumed that reaction takes place considering ideal gas and product dissociation.

$$C_3H_8 + 5(O_2 + 3.76N_2) \longrightarrow Products$$

$$H_R = (1)[\overline{h_{f,C_3H_8}^O} + \Delta h_{s,C_3H_8}] + 5[\overline{h_{f,O_2}^O}] + 5(3.76)[\overline{h_{f,N_2}^O} + \Delta h_{s,N_2}]$$

$$H_R = -103848 kJ/kmol_{C_3H_8}$$

$$N_R = 1 + 5(4.76) = 24.8 kmol$$

$$MW_R = \frac{(1)44.096 + 23.8(28.85)}{24.8} = 29.465$$

Output From UVFlame:

Constant Volume Adiabatic Flame Computation for Itemized Fuel

Number of atoms of carbon in propane fuel = 3.0

Number of atoms of hydrogen in propane fuel = 8.0

Number of atoms of oxygen in propane fuel = 0.0

Number of atoms of nitrogen in propane fuel = 0.0

Propane fuel equivalence ratio = 1.0

Propane fuel outcome temperature (K) (Estimate) = 2500

Propane fuel temperature of the reactants (K) = 298.1

Propane fuel pressure of the reactants (Pa) = 101325.0

Propane fuel reactants enthalpy (kJ/kmol fuel) = -1013848.0

Propane fuel number of reactants moles (kmol/kmol fuel) = 24.800

Propane fuel reactants molecular weight (kg/kmol) = 29.465

FLAME TEMPERATURE & BURNING OUTCOMES PROPERTIES

Propane combustion constant volume flame temperature [K] = 2631.53

Propane combustion outcome pressure [Pa] = 0.946107E+06

Propane combustion product enthalpy [J/kg] = 0.5593E+06

Propane combustion product specific Heat C_p [J/kg-K] = 0.255109E+04

Propane combustion specific heat ratio C_p/C_v = 1.1531

Propane combustion outcome molecular weight [kg/kmol] = 27.8520

Propane combustion mole of fuel per mole of outcomes = 0.03809654

The amount fractions of the outcome species are:

H:0.00104322

O:0.00083162

N:0.00000026

H_2 :0.00538231

OH:0.00664940 CO:0.02220778

NO:0.00594248 O_2 :0.00910174 H_2O :0.14315753

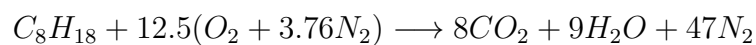
CO_2 :0.09208184 N_2 :0.71360183

5.10 Case 8 : Iso Octane Comparison of Analytical and Present Work Results (Constant Pressure Combustion)

Assumptions:

- Comprehensive Burning (no detachment), i.e. the outcome blend contains only CO_2, N_2 and H_2O .
- The outcome combination enthalpy is forecast using constant specific heats assessed at 1350K ($\approx 0.5(T_i + T_{ad})$), where T_{ad} is estimated to be about 2400K)

Combination Arrangement:



$$N_{CO_2} = 8, N_{H_2O} = 9, N_{N_2} = 47$$

Species	Enthalpy of Formation @ 298K	Specific Heat @ 1350K
C_8H_{18}	-208447	
CO_2	-393546	57.00
H_2O	-241845	45.50
N_2	0	34.2
O_2	0	

TABLE 5.27: Enthalpy & Specific Heat for Species at 1200K

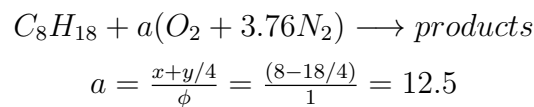
First Law:

$$\begin{aligned}
 H_{react} &= \sum_{react} N_i \bar{h}_i = H_{prod} = \sum_{prod} N_i \bar{h}_i \\
 H_{react} &= (1)(-208447) + 12.5(0) + 47(O) = -208447kJ \\
 H_{prod} &= \sum N_i [h_{f,i}^{\bar{O}} + \bar{C}_{p,i}(T_{ad} - 298)] \\
 H_{prod} &= (8)[-393546 + 57.00(T_{ad} - 298)] + (9)[-241845 + 45.5(T_{ad} - 298) + \\
 &\quad (47)[0 + 34.2(T_{ad} - 298)]
 \end{aligned}$$

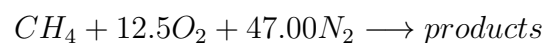
Linking H_{react} to H_{prod} and cracking for T_{ad} reveals

$$T_{ad} = 2367K$$

Using HPFlame software:



Thus



The inflow enthalpy (per mole of fuel) at that point

$$H_{\text{reac}} = \overline{h_{fCH_4}^O} + 12.5\Delta\overline{h_{sO_2}} + 47.0\Delta\overline{h_{sN_2}}$$

$$H_{\text{reac}} = -208447 \text{ KJ/Kmol}(\text{fuel})$$

Number of atoms of carbon in iso octane fuel = 8.0

Number of atoms of hydrogen in iso octane fuel = 18.0

Number of atoms of oxygen in iso octane fuel = 0.0

Number of atoms of nitrogen in iso octane fuel = 0.0

Iso octane fuel equivalence ratio = 1.0

Iso octane fuel outcome temperature (K) (Estimate) = 3000

Iso octane fuel pressure of the reactants (Pa) = 101325.0

Iso octane fuel reactants enthalpy (kJ/kmol fuel) = -208447

FLAME TEMPERATURE & BURNING OUTCOMES PROPERTIES

Iso octane combustion constant pressure flame temperature [K] = 2275.33

Iso octane combustion product enthalpy [J/kg] = -113798

Iso octane combustion product specific Heat C_p [J/kg-K] = 2284.79

Iso octane combustion specific heat ratio C_p/C_v = 1.1633

Iso octane combustion outcome molecular weight [kg/kmol] = 28.33

Iso octane combustion mole of fuel per mole of outcomes = 0.0154668

The amount fractions of the outcome species are:

H:0.000468 O:0.000338 N:2.53E-08

H_2 :0.003055 OH:0.003202 CO:0.0136306

NO:0.0026083 O_2 :0.006283 H_2O :0.1343

CO_2 :0.1101 N_2 :0.72599

T_{ad} (HPFlame)=2275.33K

T_{ad} (Analytical)=2367K

Chapter 6

Results and Discussions

Three codes named “HPFlame”, “TPEquil” and “UVFlame” are written to compute adiabatic flame temperature, species mole fractions and other mixture thermodynamic properties.

Full equilibrium model algorithm is implemented in the codes (present work). This work is an extension of Borman and Olikara Algorithm [35] [36]. The codes (this work) are written in System International Units with variable composition of air. The codes (this work) solve for twelve species (H , OH , O , H_2 , N , CO , NO , H_2O , CO_2 , O_2 , Ar , N_2) which was formulated by Borman and Olikara [1]. “HPFlame” code calculates combustion products properties at constant pressure. “UVFlame” code calculates combustion products properties at constant volume. “TPEquil” code calculates combustion mixture properties at equilibrium conditions. Flowcharts (main program) are drawn for constant pressure combustion, constant volume combustion and combustion at equilibrium conditions. Codes are written in Microsoft Visual Basic.Net software with modern user interface and robust object oriented language. All the three codes are validated with Borman code [1], NASA Chemical Equilibrium Analysis Code [12] and other international reputed reports [31] [33] [34].

Case 1 deals with the validation of constant pressure combustion of methane against BORMAN algorithm and NASA Chemical Equilibrium Analysis Code. There is a minor difference between flame temperature calculated theoretically,

this work and NASA CEA Code. It is observed that percentage error for flame temperature between this work and Borman work is $-2.01\text{E-}04$; for mixture enthalpy is $-1.78\text{E-}02$; for mixture specific heat is $7.69\text{E-}05$; for specific heat ratio is $-2.16\text{E-}03$; for mixture molecular weight is $-1.48\text{E-}04$; for moles of fuel per mole of products is $-4.64\text{E-}05$.

The percentage error for flame temperature between this work and NASA work is $-1.38\text{E-}02$; for mixture enthalpy is $1.45\text{E-}01$; for mixture specific heat is $-2.46\text{E-}01$; for specific heat ratio is $-5.16\text{E-}01$; for mixture molecular weight is $5.27\text{E-}03$.

The percentage error for species H between this work and Borman work is $-1.71\text{E-}03$; for species O is 0; for species N is 0; for species H_2 is 0; for species OH is 0; for species CO is $-9.99\text{E-}05$; for species NO is $-1.24\text{E-}04$; for species O_2 is $-1.09\text{E-}04$; for species H_2O is $-5.88\text{E-}08$; for species CO_2 is $-1.19\text{E-}05$; for species N_2 is 0.

The percentage error for species H between this work and NASA work is $-2.67\text{E+}00$; for species O is $-1.51\text{E+}00$; for species N is 0; for species H_2 is $6.05\text{E-}01$; for species OH is $-5.86\text{E-}01$; for species CO is $-7.93\text{E-}01$; for species NO is $5.80\text{E+}00$; for species O_2 is $4.39\text{E-}01$; for species H_2O is $-8.93\text{E-}02$; for species CO_2 is $-6.50\text{E-}02$; for species N_2 is $-2.41\text{E-}03$.

Case 2 deals with the validation of equilibrium combustion of iso-octane between this work and Borman work. The percentage error for mixture enthalpy between this work and Borman work is $-3.83\text{E-}03$; for mixture specific heat is $-3.88\text{E-}05$; for specific heat ratio is $2.08\text{E-}03$; for mixture molecular weight is $7.62\text{E-}05$; for mole of fuel per mole of outcomes is 0.

The percentage error for species H between this work and Borman work is $-4.32\text{E-}05$; for species O is $-3.13\text{E-}05$; for species N is 0; for species H_2 is 0; for species OH is 0; for species CO is $-1.33\text{E-}05$; for species NO is 0; for species O_2 is $-9.30\text{E-}04$; for species H_2O is 0; for species CO_2 is $-7.65\text{E-}05$; for species N_2 is $-1.50\text{E-}06$.

Case 3 deals with the validation of equilibrium combustion of methane between this work, Borman work and NASA work. The percentage error of mixture enthalpy between this work and Borman work is $5.59\text{E-}03$; for mixture specific heat

is 0; for specific heat ratio is 4.17E-04; for mixture molecular weight is -1.34E-04; for moles of fuel per mole of products is -3.44E-05.

The percentage error of mixture enthalpy between this work and NASA work is 1.82E-01; for mixture specific heat is 4.53E-01; for specific heat ratio is -2.97E+00; for mixture molecular weight is -3.53E-02.

The percentage error for species H between this work and Borman work is -2.19E-03; for species O is 0; for species N is 0; for species H_2 is 3.19E-05; for species OH is 0; for species CO is 1.72E-05; for species NO is -2.51E-04; for species O_2 is -3.79E-05; for species H_2O is -6.24E-05; for species CO_2 is -2.86E-02; for species N_2 is -1.54E-06.

The percentage error for species H between this work and NASA work is 9.11E-01; for species O is 3.12E-02; for species N is 0; for species H_2 is 1.44E+00; for species OH is -3.71E-02; for species CO is -2.38E-01; for species NO is 3.86E+00; for species O_2 is -4.93E-04; for species H_2O is -6.37E-01; for species CO_2 is 2.08E-01; for species N_2 is -8.10E-02.

Case 4 deals with the validation of constant volume combustion of Iso-Octane of this work and Borman work. The percentage error between this work and Borman work for flame temperature is 0; for pressure is 2.70E-05; for mixture enthalpy is -1.12E-02; for mixture specific heat is -2.38E-03; for specific heat ratio is -4.25E-03; for mixture molecular weight is -1.59E-02; for moles of fuel per mole of products is 1.70E-05.

The percentage error for species H between this work and Borman work is -2.42E-02; for species O is 0; for species N is 0; for species H_2 is -1.53E-03; for species OH is 2.98E-04; for species CO is -1.51E-02; for species NO is -1.95E-03; for species O_2 is -1.94E-04; for species H_2O is -3.71E-05; for species CO_2 is 0; for species N_2 is -5.14E-04.

Case 5 deals with the validation of constant volume combustion of methane between theoretical work, Borman work and NASA CEA work. It is observed that the difference is less for this work and NASA CEA code. The percentage difference

between this work and Borman work for Constant Volume Flame Temperature is 0; for pressure is 5.04E-05; for mixture enthalpy is 6.37E-04; for mixture specific heat is -8.01E-05; for specific heat ratio is 0; for mixture molecular weight is 0; for moles of fuel per mole of products is -1.39E-04.

The percentage error between this work and NASA CEA work for constant volume flame temperature is -1.70E-01; for pressure is -2.44E-01; for mixture enthalpy is 2.10E+00; for mixture specific heat is 6.08E-01; for specific heat ratio is -1.29E+00; for mixture molecular weight is -1.22E+00.

The percentage error for species H between this work and Borman work is -3.93E-02; for species O is 0; for species N is 0; for species H_2 is -1.29E-03; for species OH is -1.58E-04; for species CO is 5.90E-05; for species NO is 0; for species O_2 is 1.33E-04; for species H_2O is -1.57E-03; for species CO_2 is -5.21E-05; for species N_2 is -1.13E-03.

The percentage error for species H between this work and NASA CEA work is -1.34E+00; for species O is -3.32E+00; for species N is 0; for species H_2 is -2.19E-01; for species OH is -1.95E+00; for species CO is -2.30E+00; for species NO is 3.15E+00; for species O_2 is -1.97E+00; for species H_2O is -5.99E-01; for species CO_2 is -6.07E-01; for species N_2 is 2.95E-01.

Case 6 deals with the validation of this work with other international reputed sources. A research carried out for calculation of adiabatic flame temperature of a lean premixed combustor in a plug flow reactor by Honegger at KANSAS State University shows a value of 1800 K. A similar research for a conventional combustor in a plug flow reactor conducted by Honegger at KANSAS State University calculates a value of adiabatic flame temperature to be 2530 K. A research conducted by N. Peters at Aachen Germany using stoichiometric mixture method computes adiabatic flame temperature for methane 2263.3 K. Douglas, Ufot and Lebele-Alawa computes adiabatic flame temperature of 2620 K at an equivalence ratio of 1.4. NASA CEA Chemical Equilibrium Analysis Code calculates adiabatic flame temperature using techniques to lessen either the Helmholtz or Gibbs

energies to be 2169.96K. Present work works on the principle of optimize algorithm and adiabatic flame temperature is calculated to be 2200 K. In summary it is observed that the results of N. Peters, NASA CEA Code and Present work are similar.

Case 7 deals with the computation of constant volume adiabatic flame temperature for propane using UVFlame (This work). It is observed that constant volume flame temperature is found to be 2631.53 K.

It is observed that case 8 comparing Analytical and Present Work results for iso-octane shows little difference. The adiabatic flame temperature computed by HPFlame (This work) code is 2275.33 K and that computed analytically is 2367 K.

Chapter 7

Conclusion and Future Work

In conclusion a code is written in Microsoft Visual Basic to calculate mole fractions of 12 species and their derivatives with reference to equivalence ratio, pressure and temperature. The code gives a robust calculation of Specific Gas constant of mixture (R), enthalpy per unit mass (h) and internal energy per unit mass (u). The code also calculates derivatives of Specific Gas Constant, enthalpy and internal energy with reference to equivalence ratio, pressure and temperature. The code has the option to deal with variable air properties. The codes can be used for combustion analysis of Turbojet and Ramjet engine as well as for Spark Ignition Engine.

The methods of computing adiabatic flame temperature for both constant pressure and constant volume combustion using numerical technique is focused in this thesis. Also equations are discussed that computes combustion products mole fractions and partial derivatives of these twelve mole fractions with reference to equivalence ratio, pressure and temperature. Coding technique are discussed that computes mixture enthalpy, mixture specific heat, specific heat ratio, outcome compounds molecular weight and moles of fuel per mole of outcomes. In step one, several different computing method are studied to compute adiabatic flame temperature for stoichiometric condition, fuel lean and fuel rich condition. Full equilibrium model for solving twelve combustion product species as well as NASA CEA

Chemical Equilibrium Analysis code for solving four hundred species are assessed. The important species are listed as: *Ag, AL, ALBr₃, ALCL₃, ALF₃, CaH₂, CaI₂, CaO, Ca(OH)₂, CaS, Ga, GaBr₃, GaCL₃, GaF₃GaI₃, LiBO₂, LiBr, LiCL, LiF, LiH, Na₂S, Na₂SO₃, Na₂SO₄, Na₃ALF₆, Na₅AL₃F₁₄, SnBr₂, SnBr₄, SnCL₄, SnF₂, CH₃OH, C₂H₅OH, C₆H₆, C₆H₅NH₂, C₆H₁₄, C₇H₈, C₇H₁₆, C₈H₁₈, H₂O₂, Jet – A, Zr, ZrC, ZrN, ZrO₂.*

In step two, commercially available Microsoft software was studied for the design of robust user interface and code. For that reason code is written in Microsoft Visual Basic.Net software. In step three, three different codes by the name “HPFlame”, “UVFlame” and “TPEquil” are written for the computation of constant pressure combustion, constant volume combustion and combustion products at equilibrium conditions. Flowcharts are designed of the main program for all of the three codes. Main program is a sequence of code for iteration and calling subroutines. For constant pressure combustion the code calls for subroutine TABLES () to assess thermodynamic tables and then iteration is performed to update combustion adiabatic flame temperature at constant pressure and call subroutine for computing of mole fractions and partial differential of amount fractions with reference to equivalence ratio, pressure and temperature.

The codes written by present work may be enhanced by introducing chemical kinetics (Rate of change of combustion species mole fractions with time). This is a subject of professionally written CHEMKIN software that is a part of ANSYS library. Different reaction mechanisms for different hydrocarbon fuels are available in databases. The future work would focus on the export of the CHEMKIN reaction mechanism file to Computational Fluid Dynamics Software. Grid is generated for any two dimensional combustor geometry. The analysis is carried out by Computational Fluid Dynamics Combustor module. Grid can also be generated for any three dimensional combustor geometry and analysis can be performed by any three dimensional computational fluid dynamics software. A combustor 3D prototype is required to validate the results of computational fluid dynamics software with experimentation. The above mentioned future work is the underline of the PhD Studies.

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Appendix A

Appendix A Programs User Interface

A.1 HPFlame User Interface

The screenshot displays the HPFLAME software interface. It features a menu bar with 'File' and 'Help'. The main area is divided into three sections: INPUT, OUTPUT, and MOLE FRACTION. Each section contains several input fields with numerical values.

INPUT			
Number of carbon atoms	1	Equivalence Ratio	0.9
Number of Hydrogen atoms	4	Temperature (K)	2000
Number of Oxygen atoms	0	Pressure (Pa)	101325
Number of Nitrogen atoms	0	Enthalpy of reactants (KJ/Kmol fuel)	155037

OUTPUT			
Flame Temperature (K)	2455.62596178486	Mixture Enthalpy [J/kg]	482649.882076978
Mixture Specific Heat Cp [J/kg-K]	2737.09214144688	Specific Heat Ratio Cp/Cv	1.14585619197051
Mixture Molecular Weight [kg/kmol]	27.365676118787	Moles of Fuel per mole of products	0.08519283250158

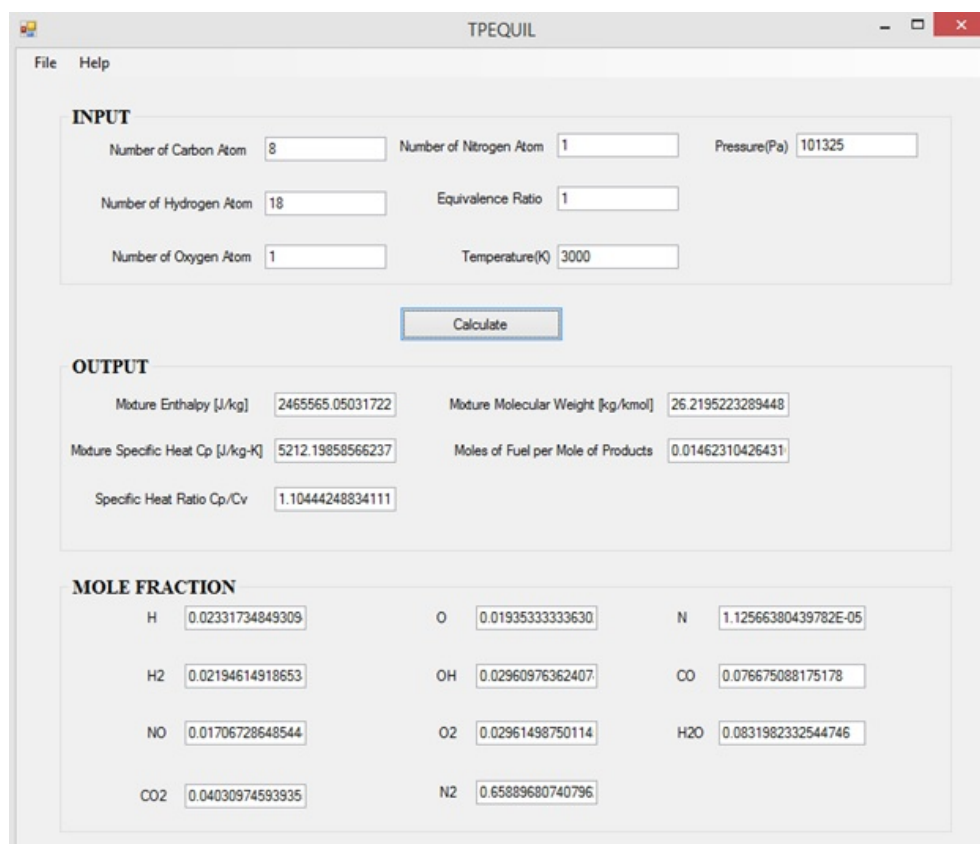
MOLE FRACTION					
H	0.00147476133536	O	0.00171529393234	N	1.61592885054483E-07
H2	0.00515289841755	OH	0.00901984095887	CO	0.0137222307119145
NO	0.00687640112028	O2	0.02218718755066	H2O	0.159985465567294
CO2	0.07147060178967	N2	0.70839515881246		

FIGURE A.1: HPFlame User Interface

Listing of a sample program which calculates Constant Pressure Adiabatic Temperature is given above.

A.2 TPEquil User Interface

Listing of a sample program which computes combustion products equilibrium composition and properties for temperature, pressure, specified fuel and equivalence ratio is given below.



The screenshot shows the TPEquil user interface with the following data:

INPUT					
Number of Carbon Atom	8	Number of Nitrogen Atom	1	Pressure(Pa)	101325
Number of Hydrogen Atom	18	Equivalence Ratio	1		
Number of Oxygen Atom	1	Temperature(K)	3000		

Calculate

OUTPUT			
Mixture Enthalpy (J/kg)	2465565.05031722	Mixture Molecular Weight (kg/kmol)	26.2195223289448
Mixture Specific Heat Cp (J/kg-K)	5212.19858566237	Moles of Fuel per Mole of Products	0.01462310426431
Specific Heat Ratio Cp/Cv	1.10444248834111		

MOLE FRACTION					
H	0.02331734849309	O	0.01935333333630	N	1.12566380439782E-05
H2	0.02194614918653	OH	0.02960976362407	CO	0.076675088175178
NO	0.01706728648544	O2	0.02961498750114	H2O	0.0831982332544746
CO2	0.04030974593935	N2	0.65889680740796		

FIGURE A.2: TPEquil User Interface

A.3 UVFlame User Interface

Listing of a sample program which computes the adiabatic flame temperature, equilibrium composition and properties of the products of combustion for adiabatic constant volume combustion with specified fuel composition, equivalence

ratio, reactant enthalpy and initial pressure and temperature is given below.

The screenshot displays the UVFLAME software interface, which is organized into three main sections: INPUT, OUTPUT, and MOLE FRACTION. Each section contains various numerical input and output fields.

INPUT

Number of Carbon Atom	8	Equivalence Ratio	1	Enthalpy of Reactant per Kmol Fuel(KJ/kmol)	293579
Number of Hydrogen Atom	18	Product Temperature(K)	2000	Moles of Reactants (kmol/kmol of fuel)	60.5
Number of Oxygen Atom	0	Reactant Temperature(K)	556	Mol Wt of Reactants(kg/kmol)	30.261
Number of Nitrogen Atom	0	Reactant Pressure(Pa)	755885		

OUTPUT

Constant Volume Flame Temperature [K]	2804.29097691776	Specific Heat Ratio Cp/Cv	1.15770693817899
Pressure [Pa]	4104802.35411609	Mixture Molecular Weight [kg/kmol]	28.1057406879287
Mixture Enthalpy [J/kg]	837168.096054107	Moles of Fuel per Mole of Products	0.01534396720309
Mixture Specific Heat Cp [J/kg-K]	2456.93962397269		

MOLE FRACTION

H	0.000897742625369531	O	0.000820793201436839	N	4.79675277774945E-07
H2	0.00477240256415115	OH	0.00691967027418681	CO	0.024658657908081
NO	0.00766022527508912	O2	0.00906548684866983	H2O	0.12941459592406
CO2	0.0980930797166926	N2	0.717696867038147		

FIGURE A.3: UVFlame User Interface