Autoignition modeling of natural gas for engine modeling programs: an experimental and modeling study

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Autoignition modeling of natural gas for engine modeling programs: An experimental and modeling study

by

Seref Soylu

A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of
DOCTOR OF PHILOSOPHY

Major: Mechanical Engineering
Major Professor: Jon H. Van Gerpen

Iowa State University
Ames, Iowa
2001

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# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>vii</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>viii</td>
</tr>
<tr>
<td>1. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Statement of Problem</td>
<td>2</td>
</tr>
<tr>
<td>1.2 Objectives</td>
<td>3</td>
</tr>
<tr>
<td>2. LITERATURE REVIEW</td>
<td>4</td>
</tr>
<tr>
<td>2.1 Knock Phenomena</td>
<td>4</td>
</tr>
<tr>
<td>2.2 Knock Detection Techniques</td>
<td>5</td>
</tr>
<tr>
<td>2.2.1 Audible Knock Detection</td>
<td>6</td>
</tr>
<tr>
<td>2.2.2 Detecting Cylinder Pressure Oscillations</td>
<td>7</td>
</tr>
<tr>
<td>2.2.3 Detecting Engine Structure Vibrations</td>
<td>7</td>
</tr>
<tr>
<td>2.2.4 Detecting End-gas Heat Transfer</td>
<td>7</td>
</tr>
<tr>
<td>2.2.5 Gas Ionization Technique</td>
<td>8</td>
</tr>
<tr>
<td>2.3 Characterization of Knock</td>
<td>8</td>
</tr>
<tr>
<td>2.3.1 Characterization of Knock Based on Cylinder Pressure</td>
<td>8</td>
</tr>
<tr>
<td>2.3.1.1 Pressure Data Evaluations</td>
<td>9</td>
</tr>
<tr>
<td>2.3.1.2 Frequency Domain Evaluations</td>
<td>9</td>
</tr>
<tr>
<td>2.3.1.3 Derivative Based Evaluations</td>
<td>11</td>
</tr>
<tr>
<td>2.3.2 Characterization of Knock Based on Engine Structure Vibration</td>
<td>11</td>
</tr>
<tr>
<td>2.4 Effect of Engine Operating Conditions on Knock</td>
<td>13</td>
</tr>
<tr>
<td>2.4.1 Spark Timing</td>
<td>13</td>
</tr>
<tr>
<td>2.4.2 Inlet Pressure and Compression Ratio</td>
<td>14</td>
</tr>
<tr>
<td>2.4.3 Inlet and Coolant Temperatures</td>
<td>14</td>
</tr>
<tr>
<td>2.4.4 Engine Speed</td>
<td>14</td>
</tr>
<tr>
<td>2.4.5 Equivalence Ratio and EGR</td>
<td>14</td>
</tr>
<tr>
<td>2.4.6 Cycle by Cycle Cylinder Pressure Variations</td>
<td>15</td>
</tr>
<tr>
<td>2.5 Effect of Fuel Structure on Knock</td>
<td>15</td>
</tr>
</tbody>
</table>
2.5.1 Paraffins
2.5.2 Olefins
2.5.3 Napthenes and Aromatics
2.5.4 Octane Number
2.5.5 Octane Test
2.5.6 Fuel Sensitivity
2.6 Natural Gas Engines
2.6.1 Compression Ignition Natural Gas Engines
2.6.2 Spark Ignition Natural Gas Engines
2.7 The Influence of Natural Gas Composition on Combustion
2.7.1 Ignition Characteristics of Methane and Higher Alkanes
2.7.2 Knock Rating of Natural Gas and Methane Number
2.8 End-Gas Chemical Kinetics
2.9 Global Reactions
2.10 Autoignition Modeling in SI Engines
2.10.1 Global Models
2.10.1.1 Empirical ignition delay correlation
2.10.1.2 Shell Model
2.10.1.3 Reduced Model
2.10.2 Detailed Chemical Kinetic Models
3. EXPERIMENTAL APPARATUS AND PROCEDURE
3.1 Experimental Setup
3.2 Techniques for Accurate Cylinder Pressure Data Collection
3.3 Cylinder Pressure Data Collection Procedure
4. ANALYSIS OF COMBUSTION
4.1 Development of Two-zone Thermodynamic Model
4.1.1 Formulation of the Model
4.2 Flame Initiation and Propagation Periods
4.3 Effect of Equivalence Ratio, Propane Ratio, and Manifold Absolute Pressure on Burned-Mass Fraction and Burning Rate
4.4 Effects of Equivalence Ratio, Propane Ratio, and Manifold Absolute Pressure on Burned and Unburned Mixture Temperatures 60

4.5 Summary 71

5. ANALYSIS OF KNOCK 75

5.1 Occurrence and Intensity of Knock 75

5.2 Cycle-by-cycle Variations of KOCA and KI 85

5.3 Effects of Equivalence Ratio, Propane Ratio, and Spark Timing on Mean values of KOCA and KI 96

5.4 Summary 98

6. DEVELOPMENT OF THE AUTOIGNITION MODEL 103

6.1 Introduction 103

6.2 Model Development 104

6.3 Steepest-Ascent Method for Optimization of the Model 108

6.4 Optimization of the Model 109

6.5 Accuracy in Model’s Prediction of KOCA 115

6.6 Summary 116

7. GOVERNING EQUATIONS FOR ZERO-DIMENSIONAL AND MULTIDIMENSIONAL MODELS 118

7.1 Zero-Dimensional Two-Zone Model 118

7.2 Multi-Dimensional Model 120

7.2.1 The Governing Equations 120

8. RESULTS AND DISCUSSIONS 128

8.1 Sensitivity Study 128

8.2 Parametric Study 132

8.3 Summary 149

9. CONCLUSIONS AND RECOMMENDATIONS 153

9.1 Advantages and Disadvantages of the Model 153

9.2 Conclusions 154

9.3 Recommendations for Future Work 155

APPENDIX 157

REFERENCES 163
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ABSTRACT

The stringent exhaust emission regulations of Environmental Protection Agency has forced engine manufacturers to develop alternative combustion systems and clean alternative fuels. Lean-burn natural gas engines are attracting increasing attention as a desirable alternative, especially for stationary applications. In-cylinder pollution formation in these engines is significantly lower than that of diesel engines. However, the thermal efficiency and power density of lean-burn natural gas engines must be improved to be considered as an alternative to diesel engines. The higher octane number of methane, which is the dominant component of natural gas, allows the engines to be turbocharged and have higher compression ratio than conventional spark ignited engines. However, seasonal and regional variation in natural gas composition, which cause natural gas to have lower octane number, is the biggest constraint for the most efficient design of these engines. Under these conditions, building a competitive natural gas engine is not possible with conventional methods and requires costly engine tests. One alternative to costly engine testing is analytical engine modeling. However, conventional engine modeling tools do not properly include end-gas autoignition and multi-dimensional engine modeling codes coupled with detailed chemical kinetic codes such as KIVA-CHEMKIN combination may not be preferred by engine designers. This dissertation describes a new autoignition model that does not require extensive computational resources (2-dimensional computations from intake valve closing to exhaust valve opening take generally less than 5 minutes with a 333 MHZ personal computer), is easily portable to various computational environments, is easy to use and the accuracy is compatible with the accuracy of other subroutines of the models. It also considers variation of natural gas composition due to propane addition. Computation results show that the knock occurrence crank angle can be predicted within 2 degrees CA when the model is coupled to a Zero-Dimensional engine model, which was also developed for the present work. The results with the model incorporated into a Multi-Dimensional model (KIVA) are also promising. KIVA was able to predict if the engine was going to knock or not and also gave trends in the knock intensity.
1. INTRODUCTION

Since the invention of Otto's first four-stroke engine, the development of the spark-ignition engine has achieved a high level of success. In the early years, increasing engine power and engine working reliability were the most important goals for engine designers. Within the past decade, however, the regulation of exhaust emissions and the inevitable decline of petroleum resources have brought increased attention to alternative fuels.

In order to be accepted as an alternative fuel, an engine using the fuel must have power and torque at least close to that of traditionally fueled engines and have lower emissions. Currently, lean-burn natural gas engines are gaining some acceptance (especially for stationary applications) due to their lower emissions and acceptable brake mean effective pressure (BMEP). Natural gas has several advantages as an engine fuel. It burns relatively clean and with fewer deposits than gasoline, which leads to longer engine life. Besides a reduction of the usual exhaust emissions (carbon monoxide (CO), hydrocarbons (HC), nitrogen oxides (NOx), and particulates), natural gas also reduces the emissions of carbon dioxide (CO₂), by 26% due to its high hydrogen content [1,2,3]. Cold start enrichment and vaporization of the fuel prior to burning are not required for natural gas as they are in the case of liquid fuels. Cold-start enrichment is one of the most important sources of CO emission in gasoline-fueled engines. The typical octane number of natural gas is over 120, which allows engines to be operated at higher compression ratios. This provides the efficiency needed for acceptance as a heavy-duty engine fuel.

Natural gas is a mixture of gases consisting primarily of methane, other light hydrocarbons, and very small amounts of higher hydrocarbons and inerts. The light hydrocarbons include ethane, propane, and butane. Natural gas composition varies depending on its source and on geological and biological factors. Further, during periods when demand is high, some local companies add a mixture of propane and air in quantities ranging from 20 to 50 percent of the overall volume [4,5]. At this high level of propane and inerts, methane may not dominate the properties of natural gas. In particular, the octane number may change significantly. It is well known that natural gas is resistant to knock and the presence of propane in the natural gas generally has an adverse effect on the knock
resistance of the fuel. Variation in the octane number of the fuel may cause serious damage to the engine unless the engine design and operating variables are set so that the octane number variations can be tolerated. Optimization of the engine design and operating variables requires extensive engine tests even for a natural gas with constant composition. If variations in the gas composition are also included in the optimization, the engine testing cost increases markedly.

Mathematical engine models are one alternative to costly engine tests if properly employed. The models can be classified from simple Zero-Dimensional thermodynamic models to sophisticated Multi-Dimensional models coupled to detailed chemical kinetic mechanisms such as the KIVA-CHEMKIN combination. If Multi-Dimensional models coupled with detailed chemical kinetic mechanisms are employed for engine design, a large number of configurations need to be considered and extensive computational resources are needed. To keep computer utilization within practical limits, it is imperative that the model be no more complex than absolutely needed. In the present project, a simple autoignition model has been developed for natural gas engines that can be incorporated in both Zero-Dimensional and Multi-Dimensional models. The accuracy of the model is expected to be compatible with the accuracy of the other subroutines. In addition, extensive computational resources are not required when incorporated into Multi-Dimensional codes.

1.1 Statement of Problem

Five years ago, during a meeting with John Deere engineers in Waterloo, Iowa natural gas engine engineers complained that natural gas composition was changing season by season and also region by region in the U.S. and this variation was damaging their natural gas engines. After that meeting we started a project to determine the best knock sensor location on the engine so that the knock control system could sense the engine knock reliably. Research on natural gas engines was initiated with that project at Iowa State University and continued with another project which was the examination of the variations of the knock-limited engine operation map caused by the addition of propane to the natural gas. In this project it was observed that the addition of propane to the natural gas was initiating
intense knock that is harmful to the engine. Two years ago, in another meeting with John Deere engineers, they noted that the experimental optimization of engine design and operating variables was very expensive, especially if the fuel composition was changing. Analytical engine modeling tools such as the KIVA-CHEMKIN combination are difficult to use and require extensive computational resources. If these programs are not properly tuned, then their accuracy is limited, also. Therefore, engines are usually designed conservatively so that the variation in fuel composition can be tolerated but this approach lowers thermal efficiency of the engines. It was also discussed that having a cycle simulation program that included a simple but accurate autoignition model to predict the KOCA at various operating conditions with varying fuel composition would reduce the cost significantly. The present work was started to address this need.

1.2 Objectives

The main objective of the present work was to build an autoignition model that would improve the predictive capabilities of overall engine simulation programs when included with them. The accuracy of the autoignition model needed to be compatible with the other subroutines of the engine model and could not require extensive computational resources if incorporated into Multi-Dimensional models. The autoignition model was developed to predict knock in a lean-burn natural gas engine and includes the effects of variations of fuel composition and operating conditions. The model was validated with data collected from a John Deere 6076 lean-burn natural gas engine utilizing natural gas with propane added up to 15% by mass. The specific objectives of the present work can be summarized as follows:

1. Develop an understanding of the phenomenon causing the knock.
2. Examine knock detection and characterization techniques
3. Examine the combustion characteristics of the engine at different operating conditions such as varying equivalence ratios, ignition timing, manifold absolute pressure and propane ratio of the natural gas.
2. LITERATURE REVIEW

This chapter provides the necessary background information for this dissertation. This chapter starts with an explanation of the knock phenomenon and continues with knock detection techniques and characterization of knock. Then, the effects of engine operating condition and fuel structure on knock are reviewed, and knock rating methods for liquid and gaseous fuels are explained. After reviewing some background information on natural gas engines, autoignition-modeling attempts to date are described.

2.1 Knock Phenomena

Knock is the sound that results from an intense vibration of the gases in the combustion chamber that forces the combustion chamber walls to vibrate and thus transmit the sound through the engine structure. Because of the complexity of the phenomena, there have been three different theories that are discussed as the source of knock:

1. Detonation theory: This theory postulates that the spark ignited flame front accelerates to supersonic velocities in the end-gas region and hence produces shock waves [6].
2. Flame acceleration theory: This theory postulates that knock results from rapid burning of the reactants by the spark ignited flame [7,8,9].
3. Autoignition theory: This theory postulates that the end-gas is autoignited at one or more zones when the temperature and pressure reach a critical level [7,10,11,12].

The most commonly accepted of knock is end-gas autoignition. The end-gas is a mixture of fuel, air, and residual gases ahead of the propagating flame front. The variables that control end-gas autoignition are temperature, pressure, compression time, fuel composition, and equivalence ratio. The chemical reaction between the fuel and the air starts as soon as they are mixed. During the intake and the beginning of the compression stroke, the reaction rates are very low due to the low temperature and pressure. After the spark plug ignites the mixture, the flame travels across the combustion chamber. During this period the end-gas is
further compressed by expansion of the burned part of the mixture which raises the temperature and pressure to the critical point where the end-gas autoignites.

The autoignition of the end-gas occurs when the energy released by the chemical reaction is larger than the heat lost to the surroundings. If the end-gas chemical energy release is sufficiently rapid, and a sufficient amount of end-gas is involved, intense pressure waves are created and knock is observed. Even shock waves can be observed with autoignition if a sufficient amount of end-gas is involved in the reaction [11]. The creation of pressure waves by autoignition of the end-gas is explained by the fact that the reaction, if it takes place with sufficient rapidity, will take place at nearly constant volume (because of the inertia of the gases, the instantaneous reaction can be considered to be a constant volume reaction) [13]. Such a reaction will result in high local pressures, and the end-gas will subsequently expand rapidly sending a pressure wave across the chamber. This pressure wave will be reflected from the walls and a wave pattern of a type predictable by acoustic theory will be established quickly.

The impact of knock depends on its intensity and duration. Trace knock has no deleterious effect on engine performance or durability. In fact, trace knock may be desirable if it increases the speed of combustion at a point in the cycle when the flame speed is decreasing [7,13]. Heavy knock, however, can lead to extensive engine damage. Extremely high pressure pulses of up to 180 bar in the 5-10 kHz frequency range can be created locally in the end gas region [13]. High local pressure in the combustion chamber causes the gases to vibrate and scrub the chamber walls. This action reduces the boundary layer thickness and allows increased heat loss to the chamber walls and higher surface temperatures. These temperatures can weaken the cylinder materials. Heavy knock can easily lead to gradual erosion of regions of the combustion chamber.

2.2 Knock Detection Techniques

Knock is a limiting factor for the compression ratio of spark ignited engines (SI engines) and it constrains their operating variables. Spark ignited engines have been designed conservatively thereby avoiding modes of operation that might result in knock. The
conservative design of the engines causes lower thermal efficiency than the maximum possible. However, in the last decade the improved reliability of knock control systems makes it possible to obtain the maximum possible thermal efficiency at all times regardless of variations in fuel quality and environmental conditions. The detection of the onset of knock and the evaluation of its intensity is therefore an important issue in engine and fuel development. The ability of a knock control system to isolate and quantify the knock signal should not be dependent on speed, load, engine temperature, or other variables. Several knock detection techniques have been proposed and used for knock detection [14,15,16,17].

1. Audible knock detection.
2. Detecting cylinder pressure oscillations induced by knock.
3. Detecting engine structure vibrations induced by knock.
4. Detecting end-gas heat transfer.
5. Gas ionization techniques.

These techniques are described in more detail below.

2.2.1 Audible Knock Detection

The audible knock detection method is crude but it is the easiest method of knock detection. A highly experienced operator can detect knocking combustion and many other abnormal operating conditions by listening to the engine either on the road or in a laboratory. The major drawback with this approach is that it results in qualitative measures. Especially when dealing with borderline knock, these qualitative measurements may vary between trained operators [15,16,17]. The same operator may have different perceptions on different days and varying sensitivities. Even if an operator has a high level of accuracy and consistency, it may be difficult to determine which cylinder is knocking by this technique. At high engine speeds, there is considerable background noise from engine components, as well as from road and wind conditions. Under these conditions the reliability of audible knock detection can be questionable.
2.2.2 Detecting Cylinder Pressure Oscillations

This technique allows direct measurements of the primary effects of the autoignition and detailed investigation of the combustion. This is the most prevalent approach for laboratory tests of engine and fuel developments. However, the necessity of one pressure transducer for each cylinder and the high cost of the pressure transducers limit the use of this knock detection method to laboratory research.

2.2.3 Detecting Engine Structure Vibrations

This is the most prevalent approach for knock detection and control in mass-produced engines. The high frequency pressure oscillations in the combustion chamber induced by knock are transmitted through to the engine structure, thus causing vibrations that can be detected by means of an accelerometer installed on the engine block. With this technique, several cylinders can be controlled by using only one low-cost knock sensor. However, knock induced vibrations must be differentiated from mechanically induced structural vibrations that can occur even during normal combustion. For this reason, knock sensor location must be chosen carefully as the background noise may saturate the knock signal, especially at high speeds. Dues et al. [15] has reported that the location must meet the following requirements.

1. Mechanically stiff locations centrally located on the lower portion of the engine.
2. A position away from noise generating components, such as valve train accessory drives.
3. A location between two cylinders is better than on cylinder center lines because of increased stiffness.
4. Limited exposure to harsh environment and high temperatures.
5. Manufacturability, process flow, and serviceability must also be considered.

2.2.4 Detecting End-gas Heat Transfer

As a consequence of knock the heat transfer to the combustion chamber wall increases due to pressure oscillations and flame impingement in the combustion chamber. Lu et al. [16] observed that knock induced pressure oscillations and heat flux oscillations are at
the same frequency and in phase. In addition, the maximum heat flux increased almost linearly with the maximum amplitude of the pressure oscillations for pressure oscillations greater than 5 bar. Although knock detection can be achieved through the analysis of the increase in heat transfer that is a consequence of knock, the thermal effects will be quite negligible for borderline knock detection (the maximum amplitude of the pressure oscillations are generally less than 5 bar under light knock conditions). For this reason this method may not be applicable for borderline knock detection.

2.2.5 Gas Ionization Technique

The spark plug can be used as an ionization probe by supplying a DC (Direct Current) voltage after ignition and measuring the corresponding current. If there is knocking combustion, a sharp increase in ionization is expected which causes a small current to flow across the spark plug gap. However, some concerns regarding the correlation between ion-current and cylinder pressure, have prevented these methods from being widely used [16].

2.3 Characterization of Knock

Knock detection and characterization techniques have not been standardized. As a result, there are a variety of techniques to characterize knock. Puzinauskas et al. [17] has stated that an ideal characterization method should be computationally fast and indicate knock severity with physically familiar quantities.

Most widely used knock detection and control systems focus on cylinder pressure data and engine structure vibration data. The following sections describe the detection and characterization techniques that are based on cylinder pressure and structure vibration.

2.3.1 Characterization of Knock Based on Cylinder Pressure Data

Since the end-gas autoignition produces strong pressure waves during knock, examination of the cylinder pressure provides valuable information for characterization of knock. Simple pressure data, frequency domain, and derivative-based evaluations for the characterization of knock are typical methods within this category.
2.3.1.1 Pressure Data Evaluations

Because of the sharp pressure oscillations that generally follow the onset of knock, the simplest way to detect and characterize knock is to determine the crank angle of the first pressure peak, which is called the knock occurrence crank angle (KOCA), and the maximum amplitude of the pressure oscillations, which is called the knock intensity (KI).

Another popular method to determine the KOCA and the KI is to use band-pass filtered pressure data in a predetermined time window. This window generally starts at top dead center (TDC) and ends at 50 degrees after TDC. The knock is expected to occur during this period. The range of the band-pass filter is determined based on the knock frequencies of the engine, which can be determined from spectral analysis of knocking pressure data. With this method, knock induced pressure oscillations are isolated from background noise to get a clear knock signal. The KOCA is characterized by the first pressure oscillation and the KI is characterized by the maximum amplitude of the oscillations. The integral of the pressure oscillations and the integral of the squared pressure oscillations are other popular methods to characterize the KI [18].

Another method to characterize the KOCA, which uses cylinder pressure data, is the burn-rate analysis method. Knock normally occurs in the latter part of the combustion processes, usually well after the maximum burn rate point where the burn rate is decreasing with crank angle. It has been observed that the burn rate always increases substantially when knock occurs [19,20]. The CA where the burn-rate increases substantially is characterized as the KOCA.

2.3.1.2 Frequency Domain Evaluations

Knock is associated with high frequency pressure oscillations that occur immediately after end-gas autoignition. Since the amplitudes of these pressure oscillations are generally small compared to the average pressure, they are often modeled as acoustical pressure waves. Draper [21] explained the origin of the high frequency pressure oscillations in the combustion chamber in terms of acoustical cavity resonance. Assuming a rigid-walled cylindrical cavity with plane ends, circumferential, radial and axial cavity resonant frequencies can be computed by using the following equation [22].
\[ F_R = c \sqrt{\left( \frac{\alpha_{m,n}}{B} \right)^2 + \left( \frac{p}{2L} \right)^2} \] (2.1)

where,

\( B \) is the cavity diameter
\( L \) is the cavity length
\( c \) is the speed of sound in the gas
\( m, n, p \) are integers denoting circumferential, radial and axial mode numbers, respectively. These numbers can be 0, 1, 2, 3, ...

\( \alpha_{m,n} \) corresponds to different circumferential and radial mode numbers. The values of \( \alpha_{m,n} \) for a few modes are shown in Table 2.1.

Since the knock occurs in a short duration near TDC where the axial length of the combustion chamber cavity is 10 or more times smaller than bore, the contribution of the axial mode can usually be neglected. The circumferential and radial cavity resonance frequencies then can be determined from Equation 2.2.

\[ F_R = c \frac{\alpha_{m,n}}{B} \] (2.2)

Draper [21] has pointed out that there is an excellent match between the calculated and measured knock frequencies. Since there is a distinct difference between the frequency spectrum of cylinder pressures during knocking and non-knocking combustion, the amplitudes of the signals at the knock frequencies can be used to quantify the knock intensity. Haghgooie [23] defined the knock intensity to be the integral of the frequency spectrum of the knock signal from 0 to 20 kHz.

<table>
<thead>
<tr>
<th>Mode</th>
<th>( \alpha_{10} )</th>
<th>( \alpha_{20} )</th>
<th>( \alpha_{00} )</th>
<th>( \alpha_{30} )</th>
<th>( \alpha_{40} )</th>
<th>( \alpha_{11} )</th>
<th>( \alpha_{50} )</th>
</tr>
</thead>
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<td>( \alpha_{m,n} )</td>
<td>0.5861</td>
<td>0.9722</td>
<td>1.2194</td>
<td>1.3373</td>
<td>1.6924</td>
<td>1.6969</td>
<td>2.0419</td>
</tr>
</tbody>
</table>
2.3.1.3 Derivative Based Evaluations

The rapid change of pressure data during end-gas autoignition is commonly used for determination of KOCA and KI, originating with the ASTM-CFR method for rating fuel octane quality. When an engine is knocking lightly the pressure trace will be affected only slightly. However, if the first derivative of the pressure is examined, the disturbance will be greatly magnified because the slope will change dramatically from a large positive to a large negative value. Valtadoros [24] detected knock occurrence by examining two cylinder pressure data points at a time. When the rate of pressure rise (bar/degree CA) exceeded a certain threshold, then the first of these two data points was judged to be the KOCA and the percentage of cycles that knock was characterized as the KI. Another method used to determine KI is the integrated first derivative of the knocking pressure data [25].

Checkel et al. [26] pointed out that it can be desirable in some cases for knocking combustion analysis to use relatively low frequency data acquisition systems. If such a system has a sampling frequency less than the Nyquist criteria (Sampling frequency must be 2 times higher than the knock resonance frequency), knock resonant frequencies may not be measured correctly. Techniques based on the pressure oscillations may fail in this condition. To overcome this problem, a third derivative knock detection method based on the fundamental shape of the pressure curve rather than high frequency oscillations was developed [27,28]. Checkel et al. [26] explained that this technique is a measure of the rate of change from positive curvature to negative curvature in the pressure trace at the time of a pressure peak. An abrupt pressure increase followed by a narrow pressure peak is the fundamental visual characteristic by which knocking pressure traces differ from non-knocking traces. This technique is a quantitative measure of this visual characteristic. Typically, the third derivative of the pressure signal is evaluated at points over a range of ± 2 degree CA around a pressure peak. The maximum negative value of the third derivative is then used as a knock indicator.

2.3.2 Characterization of Knock Based on Engine Structure Vibration

This is the most widely used approach to detect and control knock on production engines. It is well known that knocking combustion pressure oscillations force the engine
structure to vibrate at the same frequencies and these vibrations can be used in a knock control strategy [29-33]. Unfortunately, the structure vibrates at many different frequencies at different amplitudes even during non-knocking conditions, which is called background noise. The structural vibrations induced by intake and exhaust valve closing and piston slaps from adjacent cylinders must be examined carefully. They may cause a false knock detection since they may appear at the same time that knock appears in a cycle. Some of the background noise may be in the same frequency range as the knock induced structural vibrations. The common techniques used to isolate the knocking signal from the background noise are:

1. Identification of the knock induced structural vibration frequencies which can be determined by comparison of the knocking and non-knocking structural frequency spectrum or from theory [29].

2. Looking for higher harmonics of the knock induced structural vibrations since background noise generally has lower frequencies [32].

3. Gating and band pass filtering of the knock sensor signal.

Since the knock is expected to occur in a short period of the cycle (from TDC to 50 degrees after TDC), gating the signal eliminates most of the background noise. The band-pass filtered knock signal is very similar to band-pass filtered pressure data and the same strategies are used which include determination of the maximum amplitude of the vibration data, the integral of the vibration oscillations, and the integral of the squared vibration oscillations (vibration energy). Other approaches to characterize KI are the integration of the rectified knock sensor signal [31] and characterization of KI in the frequency domain of the knock signal [23,29,30]. It has been observed that the frequency spectrum of the engine structure does have several peaks at knocking conditions which correspond to the knocking frequencies of the engine. The integration of the amplitudes of these peaks can characterize the knock intensity.
2.4 Effect of Engine Operating Conditions on Knock

Because of the knock-limited compression ratio, the thermal efficiency of SI engines is lower than for diesel engines. Oppenheim [34] proposed that changing the combustion process of SI engines by replacing moving flames with homogenous and simultaneous combustion would diminish the limitation imposed by the knock-limited compression ratio. These engines would have much higher compression ratio and thus higher thermal efficiency. With current technology, dramatic changes to the combustion process of SI engines is not possible, but careful design of the combustion chamber and operating variables of SI engines allow marked increase of the thermal efficiency. The tendency to knock in a SI engine depends on end-gas state variables, the time of compression to this state, and the fuel's knock resistance. The end-gas state is primarily affected by engine design details and operating conditions which are collectively known as the mechanical octane number. A fuel's chemical knock resistance is determined by its octane number. Taylor [35] examined the effect of engine operating condition and design on the knock tendency of SI engines in detail. These effects are described below.

2.4.1 Spark Timing

End-gas pressure and temperature increase with advanced timing although the end-gas compression time, which is the time period from bottom dead center to the autoignition of the end-gas, decreases. The tendency to knock is promoted by an increase of end-gas temperature and pressure and is reduced by a reduction in compression time. Except for extreme spark advance, the increasing pressure and temperature effects always dominates the reduced time effect and the tendency to knock increases with advancing timing. Obert [13] pointed out that the octane requirement of the engine decreases much faster than does engine power with retard of spark. A spark retard that gives two percent reduction in power at 1500 rpm corresponds to a reduction in full load octane requirement of six numbers. Therefore, the benefits of high compression ratio can be obtained at part loads by slightly sacrificing full load power.
2.4.2 Inlet Pressure and Compression Ratio

It is very obvious that any increase in inlet pressure and compression ratio necessarily increases the knock tendency, because the peak pressure increases along with the end-gas pressure and temperature. Taylor [35] observed that the value of the end-gas temperature at borderline knock is the same with variations of any of these variables.

2.4.3 Inlet and Coolant Temperatures

Increases in inlet and coolant temperatures increases the end-gas temperature at a given pressure, thus increasing the tendency to knock. This tendency is even higher with sensitive fuels. The sensitivity will be discussed later.

2.4.4 Engine Speed

The effect of changes in engine speed on the knock tendency of an engine is dependent on how other operating variables are controlled. When speed effects are under consideration, it is usual to hold the inlet air and coolant temperatures and the air/fuel ratio constant. Timing is also adjusted for MBT timing (minimum timing advance for maximum brake torque). Even under these conditions the effect of speed on knock tendency is complex. Increasing the speed decreases the compression time and thus decreases the knocking tendency. On the other hand, compression temperature increases with speed (due to less time for heat transfer) even if the inlet temperature is held constant. In addition, changes in engine speed usually change the volumetric efficiency and the peak pressure changes in the same direction with the volumetric efficiency [35].

2.4.5 Equivalence Ratio and EGR

Changes in equivalence ratio cause changes in the flame speed, the mixture temperature, and the preflame reaction time of the end-gas. The lower the reaction time, the higher the tendency to knock. Slightly rich mixtures are generally favorable mixtures for knocking tendency. Variation of compression temperature and pressure with air/fuel ratio is complex because of changes in heat transfer, induction work, and the cooling effect of the
fuel. The reaction time of the end-gas is the predominant factor that determines the change in knocking tendency with equivalence ratio [35].

Exhaust gas recirculation (EGR) reduces the tendency to knock due to the increased end-gas preflame reaction time although unburned mixture temperature increases due to increased residual gas fraction. Cooled EGR can be an effective way to reduce knock tendency.

2.4.6. Cycle by Cycle Cylinder Pressure Variations

If an engine's operating map is designed for a specific average peak pressure, then the cycles that have higher peak pressures may knock with increasing intensity as the peak pressure increases. Therefore, any increases in the degree of cyclic variation will increase the percentage of knocking cycles. Generally an engine with less cyclic variations can tolerate a higher compression ratio with the same fuel [18,35].

2.5 Effect of Fuel Structure on Knock

As mentioned earlier, the tendency to knock depends also on the antiknock quality of the fuel. The knock resistance of a hydrocarbon varies enormously depending on its molecular size and structure. The molecular size and structure of a fuel varies widely depending on the source of the crude petroleum and refining methods. The various hydrocarbons that make up petroleum fuels can be classified based on the number of carbon atoms and the structure of the molecules.

2.5.1 Paraffins

Paraffin hydrocarbons only involve carbon-carbon single bonds. Therefore, these hydrocarbons are also called saturated hydrocarbons. Paraffins are also called alkanes. A paraffin can have a continuous chain of carbon atoms, which is called a normal paraffin (n-paraffin), or a branched chain of carbon atoms, which is called an iso-paraffin. The general chemical formula for this series is \( C_nH_{2n+2} \), where \( n \) is the number of carbon atoms.
The knocking tendency of paraffins increases with increasing length of the carbon chain. Iso-paraffins have a lower tendency to knock since they have shorter chain lengths [36, 37].

### 2.5.2 Olefins

Olefin hydrocarbons involves carbon-carbon double bonds, and therefore these compounds are called unsaturated. Olefins contain fewer hydrogen atoms than paraffins. Olefins are also called *alkenes*. The general formulas for olefins are $C_nH_{2n}$ for one double bond and $C_nH_{2n-2}$ for two double bonds.

Olefins with one double bond have little antiknock effect; two or three double bonds generally result in appreciably less knocking tendency. Ethylene ($C_2H_4$), and propylene ($C_3H_6$) are exceptions to this rule and the knocking tendency of these compounds is much higher than the corresponding saturated hydrocarbons [36, 37].

### 2.5.3 Napthenes and Aromatics

Napthenes are characterized by a ring structure. The general formula for napthenes is $C_nH_{2n}$. The knocking tendency of napthenes is significantly greater than the corresponding size aromatic. Aromatics contain benzene rings. Replacing one or more of the hydrogen atoms of the benzene molecule with an organic radical forms various other aromatic compounds. Two or more benzene rings can also combine with each other. Multiple bonds generally reduce the knocking tendency of the compound appreciably. Long side chain attached to the basic ring structure increases the knocking tendency in both groups of fuels [36, 37].

### 2.5.4 Octane Number

Current automotive fuels are blends of a large number of individual hydrocarbon compounds from all of the hydrocarbon classes: paraffins, napthenes, olefins, and aromatics. Determination of the knock tendency of this complex fuel is an important research topic. This property is characterized by the fuel’s *octane numbers* (ON). It determines whether or not a fuel will knock in a given engine under given operating conditions. The higher the
octane number the greater the resistance to knock. The octane number scale is based on two hydrocarbons which define the limits of the scale. By definition, n-heptane (n-C\textsubscript{7}H\textsubscript{16}) has an ON of zero and iso-octane (C\textsubscript{8}H\textsubscript{18}; 2,2,4-trimethylpentane) has an octane number of 100. These hydrocarbons were chosen because normal heptane had the greatest tendency to knock and iso-octane had the greatest resistance to knock compared with any of the gasolines available at the time the scale was established. Blends of these two hydrocarbons define the knock resistance of intermediate octane numbers. For example, a blend of 10 percent n-heptane and 90 percent iso-octane has an octane number of 90. An unknown fuel’s octane number is determined by measuring what blend of these two hydrocarbons matches the fuel’s knock resistance.

2.5.5 Octane Test

The two most commonly used octane rating methods are the Research method (ASTM D-2699) and the Motor method (ASTM D-2700) [13]. These tests are carried out in a standardized single cylinder engine. The engine used for these tests was developed by the Cooperative Fuel Research Committee in 1931 and is known as the CFR engine. The specifications of the engine are given in Table 2. The compression ratio can be varied from 3 to 30 while the engine is operating, with a mechanism that raises or lowers the cylinder and cylinder head assembly relative to the crankcase. A special valve mechanism maintains a constant clearance with vertical adjustment of the head. The engine is equipped with multiple-bowl carburetors so that the blend of the two reference fuels (blends of iso-octane and n-heptane) and the fuel being rated can be placed in separate bowls. By using a selector valve, the engine can be operated on either of the fuels. The engine operating conditions of the research and motor methods are given in Table 3. The test conditions are chosen to be representative of the engine operating range where knock is most severe. The air/fuel ratio of the engine is adjusted for maximum knock with the test fuel. The compression ratio is then raised to produce knock of a standardized intensity, as measured with a magnetostrictive knock detector. The level of knock intensity obtained with the test fuel is compared with the knock intensity of two blends of the reference fuels. The knock intensity of one of the blends must be higher and the other one must be less than the test fuel. The difference between the
octane numbers of the blends must not be more than two. The octane number of the test fuel is then determined by linear interpolation between the knock meter scale readings for the two reference fuels and their octane numbers. For fuels above an octane number of 100, the knock resistance of the fuel is determined by comparison with of iso-octane that includes a certain amount of the antiknock additive, tetraethyl lead. The following formula is used to calculate the effect of tetraethyl lead on the octane number of iso-octane.

\[
ON = 100 + 28.28T / [1.0 + 0.736T + (1.0 + 1.472T - 0.035216T^2)^{1/2}] 
\]

where \( ON \) is the octane number and \( T \) is milliliters of tetraethyl lead per U.S. gallon [36].

Table 3. Operating conditions for research and motor methods [36].

<table>
<thead>
<tr>
<th></th>
<th>Research Method</th>
<th>Motor method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet temperature</td>
<td>52 °C</td>
<td>149 °C</td>
</tr>
<tr>
<td>Inlet pressure</td>
<td>Atmospheric</td>
<td></td>
</tr>
<tr>
<td>Coolant temperature</td>
<td>100 °C</td>
<td></td>
</tr>
<tr>
<td>Engine speed</td>
<td>600 rev/min</td>
<td>900 rev/min</td>
</tr>
<tr>
<td>Ignition timing</td>
<td>13 ° BTDC (constant)</td>
<td>19-26 ° BTDC (varies with compression ratio)</td>
</tr>
<tr>
<td>Air/fuel ratio</td>
<td>Adjusted for maximum knock intensity</td>
<td></td>
</tr>
<tr>
<td>Humidity</td>
<td>0.0036-0.0072 kg/kg dry air</td>
<td></td>
</tr>
</tbody>
</table>
2.5.6 Fuel Sensitivity

Except for the primary reference fuels, almost all fuels show a difference between their research and motor octane numbers. The motor method is considered to have more severe operating conditions than the research method (higher intake air temperature, higher speed). Therefore, the motor octane number is usually lower than the research octane number. The numerical difference between these octane numbers is called the fuel sensitivity. The fuel sensitivity varies with the structure of the fuel. The primary reference fuels (mixtures of iso-octane and n-heptane), by definition have zero sensitivity. Since the primary reference fuels (PRF) are paraffins, we would expect other paraffins to have little or no sensitivity. Gasolines with high percentages of paraffins do generally show low sensitivity [13,36]. However, olefins and aromatics have high sensitivity.

2.6 Natural Gas Engines

Natural gas engines have been drawing increasing attention as transportation and stationary application engines in the past few decades due to their lower emissions and the availability of natural gas at low cost from domestic supplies in the U.S. In addition, current legislation encourages manufacturing and use of natural gas engines due to their lower emissions, especially particulate and NOx emissions, when compared to diesel engines. Depending on the method of utilization of the natural gas, these engines can be classified as compression ignition natural gas engines and spark ignition natural gas engines.

2.6.1 Compression Ignition Natural Gas Engines

Although natural gas has many advantages as an engine fuel, it is not suitable as a compression ignition engine fuel due to its high autoignition temperature. There are some serious attempts to develop engines that utilize natural gas alone as a compression ignition engine fuel, but these engines are not yet marketable [38]. In order to use natural gas as a compression ignition engine fuel the combustion must be initiated either by the assistance of another fuel that has a low autoignition temperature, such as diesel fuel, or by a hot surface in the combustion chamber. If the combustion is initiated with the assistance of diesel fuel,
which is one of the most common approaches, this engine is generally called a dual-fuel engine. The dual-fuel engine is a convenient diesel engine of the compression ignition type in that most of the energy release, and hence power, comes from the combustion of natural gas, while the diesel fuel is used as an ignition source. The main aim of dual-fuel operation is to minimize the use of the diesel pilot fuel required for initiation of combustion and to maximize its replacement by the gaseous fuel for economic reasons and better emissions. The addition of natural gas into the intake manifold, called fumigation, or injection of the natural gas directly into the cylinder provides extra power. The operating range is restricted by the diesel ignition delay associated with light load operation and the knock associated with high load operation.

Hot surface assisted compression ignition of natural gas has been drawing serious attention recently. In this application, natural gas is injected directly into the cylinder near the end of compression stroke close to a hot surface. This hot surface is generally a glow plug with a temperature range of 1200-1400 K \[39\]. The most important advantages of this system are high specific power and thermal efficiency without the limitation of knock.

2.6.2 Spark Ignition Natural Gas Engines

These engines operate in a similar fashion to gasoline engines except that the fuel and fuel system are different. These engines can be further classified as stoichiometric and lean-burn natural gas engines.

2.6.2.1. Stoichiometric Natural Gas Engines

Stoichiometric natural gas engines operate with their equivalence ratio close to or somewhat higher than 1.0. Engine-out NOx emissions tend to be fairly high for these engines, but are controllable through the use of a three-way catalyst and/or EGR. This approach provides the maximum power output for a given engine displacement. Most gasoline-fueled engines converted to natural gas use a stoichiometric mixture. Such engines may be either bi-fuel (can use either natural gas or gasoline) or dedicated to natural gas. Since natural gas has a high octane number, the compression ratio of these engines can be
increased to overcome the power loss due to the lower volumetric energy content of a natural gas-air mixture.

Although gasoline-fueled engines converted to natural gas can use a stoichiometric mixture without any problems, diesel engines converted to stoichiometric natural gas have some limitations. The main limitation is that the converted engine is desired to have similar torque and power output as the diesel engine. This in turn means that high BMEP (brake mean effective pressure) levels are needed to ensure adequate power and driveability. Typical diesel engines in the 10-12 liters range are turbocharged, with rated speeds around 2100 rpm and achieve BMEP ratings of 14 bar at peak torque and 11.5 bar at rated speed [40]. These ratings are achievable with stoichiometric natural gas engines, but supercharging is required. However, to approach these BMEP ratings with stoichiometric natural gas is not a simple matter because of the high thermal loads on the cylinder head and exhaust system. These higher thermal loads result from increased fueling levels (due to increased equivalence ratio compared to diesel engines) and a longer burn period. The lower compression ratio (compared to diesel engines) also increases the temperature of the exhaust gas. Besides high thermal loading, end-gas autoignition places another limit on engine operation. The two limits of knock and thermal load result in conflicting requirements for ignition timing. At low BMEP levels there is a large scope to advance the start of combustion before knock occurs. As the BMEP level increases, the allowable range for advancing and retarding the ignition timing is limited by knock and exhaust gas temperature. There is also a similar effect with compression ratio, where an increase in compression ratio is limited by knock, while a decrease in compression ratio raises the exhaust temperature.

2.6.2.2. Lean-Burn Natural Gas Engines

Lean-burn natural gas engines have received much more attention than stoichiometric engines due to their comparative simplicity, better thermal efficiency, and higher knock-limited BMEP capabilities. It is well known that NOx emissions are a strong function of equivalence ratio and NOx emissions decrease dramatically with lean mixtures beyond equivalence ratios of 0.7. Lean-burn natural gas engines can operate with equivalence ratios as lean as 0.6 and guarantee NOx emissions below current regulations without exhaust
aftertreatment. In addition to NOx control, this lean operation provides reduced exhaust gas temperatures, leading to improved valve life and engine durability. Since the knock resistance of lean mixtures is higher than that of stoichiometric mixtures, lean-burn engines can have higher compression ratios and hence, higher thermal efficiencies. The thermodynamic properties of lean mixtures provide another advantage that improves thermal efficiency due to increased specific heat ratio \( \frac{C_p}{C_v} \). Lean-burn engines commonly attain full-load thermal efficiencies very close to that of diesel engines.

To avoid excessive smoke, diesel engines are designed to run at rather lean mixtures, with equivalence ratios typically in the range of 0.50-0.65 at full power. Therefore, diesel engines are well-adapted to lean-burn operation on natural gas, and can often match their diesel power rating. Although lean-burn engine efficiency is comparable to diesel engine efficiency, there are some limitations that effect the performance and emissions of the engine. The limit of lean combustion in a spark ignition engine is reached when cycle-to-cycle variations during combustion become excessive. This happens because the spark can no longer ignite the mixture reliably, or the flame initiation period (FIP) is very long. Low and unstable flame propagation speed and flame quenching are other factors that produce cycle by cycle variation. With natural gas, the lean ignition limit commonly occurs at an equivalence ratio of 0.6. Other factors such as turbulence, charge temperature, compression ratio, ignition system, and the design of the combustion chamber all affect the location of the lean limit. Similar to stoichiometric engine operation, as the BMEP level increases, the allowable range for advancing and retarding the ignition timing is limited by knock and exhaust gas temperature. There is also a similar effect with compression ratio, where an increase in compression ratio is limited by knock, while a decrease in compression ratio raises the exhaust temperature.

2.7 The Influence of Natural Gas Composition on Combustion

A typical pipeline natural gas is a mixture of gases containing mainly methane, other hydrocarbons, and inerts. The other hydrocarbons are mostly light including ethane, propane, butane, but very small amounts of higher hydrocarbons are found. The principal
inerts found in natural gas are nitrogen and carbon dioxide. The composition of natural gas depends on geological and biological factors and therefore the gas composition changes depending on its source. Liss and Thrasher [41] have done a detailed study of the chemical and physical properties of natural gas in ten major areas of the U.S. They observed that while there is a seasonal effect in a few locations, the gas composition variations tend to occur randomly with time. The seasonal variation of the gas composition is due to the use of propane/air peak-shaving during the winter. Due to the uneven seasonal gas demand some local distribution companies add a 50/50 mixture of propane and air in quantities ranging from 20 to 50 percent of the overall volume [41,42]. During the peak-shaving period the energy content of the pipeline natural gas remains constant on average but it is chemically different from conventional natural gas. This propane/air peakshaving results in high propane and high inert content. Liss and Thrasher [41] pointed out that the gas composition variations can be as high as 24% for propane, 15% for ethane, and 15% for the combination of nitrogen and carbon dioxide. The specifications of the mean natural gas are given in Table 2.4.

The equivalence ratio of natural gas engines is affected significantly by variations of the gas composition. King [43] states that due to the variations of the gas composition, equivalence ratio variations as high as 12% lean and 6% rich are possible.

<table>
<thead>
<tr>
<th>Table 2.4. Specification of Mean Natural Gas in the U.S. [41].</th>
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<tbody>
<tr>
<td><strong>Methane (Mole %)</strong></td>
</tr>
<tr>
<td><strong>Ethane (Mole %)</strong></td>
</tr>
<tr>
<td><strong>Propane (Mole %)</strong></td>
</tr>
<tr>
<td><strong>C4+ (Mole %)</strong></td>
</tr>
<tr>
<td><strong>CO\textsubscript{2} + N\textsubscript{2} (Mole %)</strong></td>
</tr>
<tr>
<td><strong>Heating Value (MJ/m\textsuperscript{3})</strong></td>
</tr>
<tr>
<td><strong>Wobbe Number (MJ/m\textsuperscript{3})</strong></td>
</tr>
<tr>
<td><strong>Air/Fuel (Mass)</strong></td>
</tr>
<tr>
<td><strong>Specific Gravity relative to air</strong></td>
</tr>
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</table>
This uncertainty in equivalence ratio may deteriorate engine operation. Lean-burn engines are usually heavily turbocharged and the engines operate very close to their knock limit to achieve high BMEP and thermal efficiency in an attempt to match diesel operation. To have NOx emissions under the regulations without exhaust after-treatment is another reason the engines operate very close to their lean limit. Under these conditions, the operating map of these engines is very narrow and very sensitive to variations of equivalence ratio. In addition to equivalence ratio variations, combustion characteristics such as ignition delay, flame propagation speed, and the knock resistance of the mixture may change dramatically with the addition of higher hydrocarbons and inerts [44-47]. Modeling studies have shown that if higher hydrocarbons are mixed with methane, radical species generation is faster than that of methane alone because of the greater reactivity of higher hydrocarbons [48]. Once a radical pool is established, the whole mixture oxidizes more rapidly than methane alone. It has also been observed that for mixtures of methane with both propane and ethane, the ignition behavior is most sensitive to the addition of small fractions of the propane and ethane, and further amounts of the additive have comparatively smaller effects [48]. The higher hydrocarbons are known to have generally higher flame speeds which favors power stability [49,50]. However, knock resistance is deteriorated, which is a serious limitation to BMEP.

Aesoy and Valland [39] observed that 8% propane addition to pure methane reduced its autoignition temperature by approximately 120 K, which increases the knocking tendency. Soylu and Van Gerpen [51] have done a detailed study on the effects of gas composition on the operating map of a lean-burn natural gas engine. It was observed that the occurrence and intensity of knock increases with equivalence ratio, advanced timing, as well as with the propane fraction of natural gas. It has also been observed that when increasing the propane fraction of the mixture, the leaner mixtures were able to achieve the BMEP requirement at all spark timings. It was reasoned that the faster burning rate of propane and the increased mixture mass flow rate (due to the high density of propane) to the engine improves the engine BMEP at lean mixtures.
2.7.1 Ignition Characteristics of Methane and Higher Alkanes

Combustion of hydrocarbons is not the simple process given by \textit{global reactions} such as the following.

\[
\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}
\]

As can be seen from the reaction, a \textit{global reaction} involves only the reactants and the products. From the reactants to the products, depending on the molecular structure of the hydrocarbon, there can be thousands of steps (thousands of elementary reactions). These reactions can be categorized as initiation, propagation, branching, and termination reactions. The rates of these reactions are affected by the temperature, pressure, mixture composition (equivalence ratio and inerts), and the fuel’s molecular structure.

For the combustion of pure methane, the initiation reactions are given by the following reactions [55].

\[
\begin{align*}
\text{CH}_4 + \text{M} & \rightarrow \text{CH}_3 + \text{H} + \text{M} \\
\text{CH}_4 + \text{O}_2 & \rightarrow \text{CH}_3 + \text{HO}_2
\end{align*}
\]

where, \text{M} can be any molecule and is often called a third body. The principal product of the initiation reactions of methane is the radical species \text{CH}_3 via thermal decomposition of methane and H atom abstraction from methane by molecular oxygen. These reactions are slow at the temperatures of the compression period but they are faster at elevated temperatures which explains the high knock resistance of methane in internal combustion engines [52]. The reactions of \text{CH}_3 produce a pool of chain propagating radicals such as \text{OH}, \text{H}, \text{HO}_2, and \text{O} [53,54,55]. These radicals then consume the fuel molecules and intermediates. For saturated hydrocarbons heavier than methane, the reaction is initiated mainly through the breaking of a C-C bond due to the higher bond dissociation energy of the C-H bond. The main reason for the reduced ignition delay observed for longer chain hydrocarbons is the easier breaking of the molecule into smaller intermediates and radicals which accelerates the reaction [55].
As mentioned in the previous section, the variations in the concentrations of heavier hydrocarbons in natural gas have a direct impact on the reactivity of natural gas and its tendency to autoignite in internal combustion engines. This observation was also supported by Aesoy and Valland [39]. They observed that the autoignition delay was reduced by a factor of 2-3 for natural gas when compared to pure methane. This is also consistent with observations made by Khalil [55] who observed that for a typical natural gas (84% methane, 3% ethane, 1.40% propane, 6.88% air, 0.17% CO and C3+) the calculated ignition delay for a stoichiometric mixture in air (at constant volume with an initial temperature of 800 K and pressure of 28 atm. representing engine like conditions) will be 36% of the corresponding time needed for the autoignition of methane under the same conditions.

2.7.2 Knock Rating of Natural Gas and Methane Number

Since the variation of natural gas composition strongly affects the knocking tendency of an engine, the knock rating of natural gas has primary importance for engine designers. As mentioned earlier, the knock resistance of an engine fuel is commonly measured by its octane number. However, this scale is questionable for use with natural gas because natural gas has a much higher octane number than iso-octane. Tetraethyl lead (TEL) can be mixed with iso-octane to measure octane numbers of fuels with octane numbers higher than 100. However, the ASTM standard allows a maximum of 6.0 ml of TEL addition per gallon of iso-octane which increases the octane number up to 120.34. This number still can be well below the octane number of some natural gas mixtures.

Leiker [56] has established the so-called methane number (MN) for the classification of gaseous fuels with respect to their knock sensitivity. Methane, as the most knock resistant alkane molecule, was given an arbitrary methane number value of 100. Hydrogen as a knock sensitive fuel was given the MN of 0. In binary mixtures of hydrogen and methane, the volumetric percentage of methane is equal to the MN of the blend. The MN of any blend can be determined by applying it to a test engine and raising the compression ratio until knock occurs. Then, the engine settings are fixed and the test fuel is replaced by a mixture of methane and hydrogen, where the volumetric percentage of hydrogen is increased until the
same knock intensity as with the test fuel is observed. The volumetric percentage of methane then gives the methane number.

The presence of CO$_2$ in natural gas increases its knock resistance. Therefore, the methane number range was extended to values exceeding 100 by comparing the knock resistance of a given fuel with that of a mixture of methane and CO$_2$. The volumetric percentage of CO$_2$ added to 100 indicates the MN of the mixture.

Kubesh [57] developed a correlation between the motor octane number and the reactive hydrogen/carbon (H/C) ratio of a gaseous fuel mixture. The reactive H/C ratio is defined as the total number of hydrogen atoms divided by the number of carbon atoms in the hydrocarbon components of the fuel (the inerts such as CO$_2$ are not included in the H/C ratio). A polynomial regression was used to fit the data. A third order polynomial was chosen as the best fit to the data based on the $r^2$ value. The equation has a $r^2$ value of 0.995.

$$MON = C_\theta + C_1 \cdot X + C_2 \cdot X^2 + C_3 \cdot X^3$$

where, $X = H/C$ ratio. $C_\theta = -406.14$, $C_1 = 508.04$, $C_2 = -173.55$, and $C_3 = 20.17$.

Kubesh [57] also developed a simple relation between the MN and the MON.

$$MN = 1.624 \cdot MON - 119.1$$

Another knock rating method that was developed especially for large bore natural gas engines is the Normal Butane Number (NBN) by Schaub and Hubbard [58]. The NBN is based on molar blends of methane and normal butane. Normal butane as a pro-knock agent is given a NBN of 100 and methane is given a NBN of 0. Ryan et al.[59] states that the NBN provides the most sensitive scale for knock rating of natural gas.

### 2.8 End-gas Chemical Kinetics

When air-fuel mixture is compressed by a piston and the propagating flame in a SI engine, the pressure raises to approximately 60 bar and the temperature increases to about
1400 K. In this period, the fuel-air mixture is not inert and may undergo preflame reactions. The effects of temperature and pressure are to shift the reaction pathways. If an elementary reaction scheme has been formulated that includes all possible reactions, the new reaction pathways will be correctly followed [60,61,62]. From rapid compression machine, motored engine, and constant volume bomb experiments the temperature regimes of hydrocarbon oxidation have been established [53,54,63,64]. For temperatures below 520 K, the reaction rates are too low to be important for end-gas autoignition. In the regime from 520 K to 670 K, complex phenomena are observed in which an initially slow reaction regime sets the stage for a more rapid reaction (the radical pools are established). Relatively low rates of heat release are typically associated with these initially slow reactions. In the regime between 650 K to 700 K, increases in mixture temperature may actually inhibit the onset of rapid reaction. This phenomenon is especially evident with paraffin fuels and is called a negative temperature coefficient (NTC) [65]. Olefins and aromatics generally don't show NTC behavior. This explains the observation that paraffins reduce the octane parameter called sensitivity while olefins and aromatics do not.

NTC behavior becomes more pronounced at lower pressure, higher temperature, and shorter reaction times. Compared to the research octane rating, the motor octane rating condition shows lower pressures, higher temperatures, and shorter times. Therefore, fuels containing large amount of paraffins have more pronounced NTC behavior under motor rating conditions than under research conditions. Paraffins enhance octane qualities under motor rating conditions, which in turn reduces the sensitivity [65].

For a better understanding of temperature and pressure dependent end-gas kinetics the reactions have been grouped into three temperature regimes by Westbrook et al. [53,54] as follows:

1. Low temperature reactions involving the reactions under 650 K.
2. Intermediate temperature reactions involving the reactions between 700 – 1000 K.
3. High temperature reactions over 1000 K.

The kinetic mechanisms for these three regimes are quite complex. Depending on the fuel's molecular structure, thousands of species and elementary reactions are possible. Because of this complexity, *global mechanisms*, which are generally less than 20 reactions,
are drawing increasing attention. These global mechanisms require calibration with experimental data and hence the model predictions cannot be precise outside of the calibrating experimental conditions. However, global models provide some hope for knock predictions in SI engines when complex fuels are employed.

2.9 Global Reactions

The reaction mechanism of hydrocarbons is so complex that most of the time it is not feasible to consider all of the chemically reacting species and their reaction rates when analyzing end-gas autoignition. Besides, automotive fuels are not a single species. The fuels involve many different hydrocarbon compounds which makes the analysis via elementary reactions almost impossible. To simplify the chemistry it is useful to use a global reaction scheme. However, as mentioned earlier, use of global schemes should be limited to the regimes for which they have been tested.

Westbrook et al. [67,68] have proposed single and two step global rate equations for hydrocarbon combustion. The single step global rate equation is

\[ \text{Fuel} + \alpha \text{O}_2 \rightarrow \beta \text{CO}_2 + \gamma \text{H}_2\text{O} \]

where \( \alpha, \beta, \) and \( \gamma \) are stoichiometric coefficients. The associated global rate equation is

\[ \frac{d[\text{fuel}]}{dt} = -AT^n p^m \exp(-E_a/RuT) [\text{fuel}]^a[\text{O}_2]^b \] (2.5)

where, \( n=m=0 \) for many cases for a specified range \( T \) and \( p \). The exponents \( a \) and \( b \) are related to the reaction order. The exponent \( a \) means that the reaction is \( a \)th order with respect to fuel and \( b \) means the reaction is \( b \)th order with respect to \( \text{O}_2 \). The reaction is \( (a+b) \)th order overall. The exponents \( a \) and \( b \) arise from curvefitting and are given in reference [66]. A more advanced two step reaction mechanism involving CO reaction is given by Westbrook et al. [68] as follows:
\[ \text{Fuel} + \alpha \text{O}_2 \rightarrow \beta \text{CO}_2 + \gamma \text{H}_2\text{O} \]

\[ \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2 \]

And the rate equations are

\[
d[\text{fuel}]/dT = -AN_p^n \exp(-E_a/R_uT) [\text{fuel}]^a[\text{O}_2]^b \tag{2.6}
\]

\[
d[\text{CO}]/dT = -10^{14.6} \exp(-40,000/R_uT) [\text{CO}]^{1.0}[\text{O}_2]^{0.23}[\text{H}_2\text{O}]^{0.50} \\
+ 5.0 \times 10^8 \exp(-40,000/R_uT) [\text{CO}_2] \tag{2.7}
\]

Westbrook et al. [68] stated that the addition of the CO reaction improved the accuracy significantly.

### 2.10 Autoignition Modeling in SI Engines

A primary interest in the modeling of knock is the determination of knock occurrence crank angle in SI engines depending on the operating conditions and fuel. Determination of KOCA is very important as knock constrains the increase of compression ratio and hence the thermal efficiency. Since the widespread use of computers in the 1960s, there has been a large increase in the use of mathematical modeling to improve the overall performance of IC engines. These models are essential for IC engine design, as they can predict the important characteristics of new engines before the engines are actually built and tested. These models typically use submodels to predict the more basic engine processes, such as heat transfer, burning rate, KOCA, and emissions. The submodels can be either empirical or based on fundamental physical and chemical processes. The empirical submodels are usually easier to develop but are often limited, and cannot be applied to new situations with much confidence. Submodels based on fundamental processes should be accurate over a wider range of conditions but can be extremely complex and require detailed information about the engine and gas properties that may not be known. The basic autoignition models that have been developed can be categorized as global models and detailed chemical kinetic models.
Global models tend to be empirically-based and chemical kinetic models tend to more physically-based, especially those using large numbers of elementary reactions.

2.10.1 Global Models

Global models are based on global reaction schemes. They are generally based on curvefitting of experimental data. Therefore, they should only be applied to new situations with great care.

2.10.1.1 Empirical ignition delay correlation

The empirical ignition delay correlation is the most basic approach to predicting end-gas autoignition in SI engines. It is also known as the knock integral approach. In this technique, the details of the reactions are not examined. An ignition delay correlation is derived by matching an Arrhenius function to measured data for the induction period over the relevant end-gas pressure and temperature ranges. This function represents the formation of some reaction intermediate, which is assumed to build up to a critical level. When this critical level is reached, the end-gas is assumed to autoignite. The ignition delay correlation is generally in the form of the following equation.

\[ \tau = A p^n \exp(B/T) \quad (2.8) \]

where \( p \) and \( T \) are the pressure and temperature of the end-gas and \( A, B, \) and \( n \) are curve fitting parameters that depend on fuel properties. It is then assumed that autoignition occurs when

\[ \int_{\tau=0}^{\tau_{\text{ign}}} \frac{dt}{\tau} = 1.0 \quad (2.9) \]

where \( \tau \) is the ignition delay time evaluated at the instantaneous temperature and pressure for the end-gas using Equation (2.8), \( t \) is the elapsed time from the start of the end-gas compression at \( t=0 \), and \( t_{\text{ign}} \) is the time at which autoignition occurs.
Livengood and Wu [69] developed an ignition delay correlation (knock integral) for engine knock. The pressure and temperature histories of a fired engine were used to determine knock onset. N-heptane and a mixture of n-heptane and iso-octane were used as fuels. The ignition delays of these fuels were determined from rapid compression machine experiments. A wide range of operating conditions was covered and a good correlation between the predicted and measured times of knock was observed.

Douadi and Eyzat [70] proposed a method (Four-Octane-Number-Method) to determine the knock resistance of fuels based on the ignition delay concept. The curve fitting parameters were obtained through simple processing of the standard “Research” and “Motor” methods combined with two other methods. The pre-exponential parameter was based on the octane number of the fuel and the end-gas pressure as shown:

$$\tau = 17.68(ON/100)^{1.402} p^{-1.7} \exp(3800/T)$$

(2.10)

where $p$, $T$, and $ON$ are the pressure, temperature, and octane number, respectively. They concluded that the knocking behavior of any engine can be specified by measuring its octane requirement. The method’s predictions were claimed to be within an average accuracy of 0.5 octane point.

By et al. [71] tested four different induction time correlations to predict KOCA. Both two-zone and three-zone combustion models were used to estimate the temperature of the unburned gas from measured pressure data. In the three-zone model, the unburned gas was divided into two zones, an adiabatic core and a boundary layer. The data for both the two-zone and three-zone models show considerable scatter. It is mentioned that the average difference in the predicted and measured mass burned fraction increases with octane number. The results for the two zone model are best for the primary reference fuel (PRF) with an ON of 81.4 while the three-zone model results are best for the PRF with 100 ON.

Wayne et al. [72] also developed an ignition delay correlation to predict KOCA. The model was used to design a late closing intake cam to reduce engine knock during gasoline operation of a bi-fuel engine. Comparison of predicted and measured KOCA was provided on a scatter plot. A slope of unity would be expected and the slope was shown to be 0.96.
2.10.1.2. Shell Model

This model was first developed at the Thornton Research Center at Shell by using a simple degenerately-branched chain oxidation mechanism [73]. The mechanism uses fictitious species and reactions to represent different categories of radicals and stable species. The model is able to simulate the essential phenomena of the two-stage autoignition of alkanes under high pressure and temperature conditions. The model correctly predicts the transition to single stage autoignition at higher temperatures. The model is also able to predict, without any adjustment of the kinetic parameters, the cool-flame (this is a reaction that has very low energy release) and ignition behavior at low pressures. The chemical mechanism consists of five general species: fuel, oxygen, radicals, degenerate branching agent, and intermediates. The term degenerate-branching refers to a type of branching-chain reaction in which chain branching occurs infrequently. However, the reaction rate coefficients for this model have to be adjusted for each fuel to be analyzed, a process which requires extensive experimental testing of each fuel.

Natarajan et al. [74] applied the Shell model to spatially uniform charges in a constant volume bomb and in a rapid compression machine. They observed that the model can predict cool flames of iso-octane and n-heptane in a stirred reactor. They also made an attempt to model knock in SI engines and integrated the low-temperature kinetics model with an existing two-dimensional engine model. The results were found to be realistic.

Hirst et al. [75] reviewed the Shell model and optimized it to give a quantitative prediction of the behavior of selected fuels, using data obtained in a rapid compression machine. They also reviewed some of the areas where the model can be applied. These include run-on (continuation of engine firing after the electrical ignition is shut off), the effects of antiknock agents, the ignition of fuel sprays, and the effects of ignition promoters for diesel engines. They have characterized and developed model parameters to simulate the autoignition behavior of both non-sensitive and sensitive fuels. To obtain a suitable fit for these fuels, experimental data were compared with model predictions over a range of temperatures, pressures, and stoichiometries. The model was coupled to the thermodynamic relationships that determine the physical states of the end-gas. The residual gas fraction was also included. A computer program was developed to integrate the coupled differential
equations (thermodynamic relationships and autoignition model) from the point of closure of
the intake valve to the point of autoignition of the end-gas or, for non-knocking cycles, to the
opening of the exhaust valve. The results of the program were compared with measured
cylinder pressure from a knocking engine. The amplitude of the maximum pressure
oscillations characterized engine knock. KOCA was determined from the first knocking
peak. For each cycle recorded, the KOCA, KI, and the peak pressure were determined. The
average values of these parameters over the cycles gave the knock characteristics for the
given condition. Hirst et al. [75] observed that the standard knock intensity, as given in the
ASTM manual [76], has no meaning in terms of the KOCA and the KI. These parameters
are not the same for each fuel at the guide curve compression ratios (a specific relationship
between compression ratio and ON at standard knock intensity for the PRF), which are
defined by the ASTM manual to give standard knock intensity. However, there is a
relationship between the peak pressure in the cylinder and the octane number at the guide
curve compression ratio. This means that for the specific test condition, fuels with the same
octane number have the same peak cylinder pressure. Comparison of experimental results
and mathematical simulations indicated that the model was very successful at predicting the
KOCA. The deviations from the experimental values of the KOCA were +0.3 ° CA for 100
PRF, +0.5 °CA for 90 PRF and +1.7° CA for 70 PRF for RON test conditions at the guide-
curve compression ratios. A close relationship between the KI and the amount of unburned
mixture at the onset of knock was observed. It was further proposed that the energy release
by the autoignition per unit volume of the combustion chamber can be characterized as a KI
with the assumption that all of the fuel in the end-gas ignites. To see how important it is to
have accurate values for the input parameters in terms of their effect on knock prediction,
deviations of 5-10% were applied to the calculated values, and the effect on the simulation
was evaluated. It was found that the critical parameters were initial pressure and
temperature, the heat-transfer coefficient for the unburned gases, and the pressure
development. Errors of 5-10% in these parameters gave errors of between 1 – 3 degrees in
the prediction of KOCA. However, a 1 degree variation in KOCA will give a 10-25%
change in KI.
2.10.1.3. Reduced Model

As mentioned earlier, detailed chemical kinetic models based on elementary reactions are extremely difficult to build for practical fuels due to the lack of information about all the reactions, chemical species, and rate constants. Therefore, it is necessary to use a reduced reaction mechanism to simulate the complicated chemical processes. The Shell model has been used with some success to model the complicated chemical process, but it must be calibrated for each fuel used and there is no direct correspondence between the model parameters and the elementary reaction rate constants. Cox and Cole [77] refined and expanded the Shell model but some of the reaction constants they needed to fit autoignition data vary by orders of magnitude from currently available fundamental kinetic data. Hu and Keck [78] developed a model similar to that of Cox and Cole. The model has 13 active species and 18 chemical reactions which are the most important rate limiting reactions in describing the process leading to autoignition. Some of the species, including OH, O₂, HO₂, HOOH, and to some extent the fuel RH, are real chemical species, while others, like the alkyl radical R and alkylperoxy radical RO₂, represent families or groups of species [79]. The model contains four fundamental steps of thermokinetic development:

1. Chain initiation
2. Chain propagation
3. Chain branching
4. Chain termination

Hu and Keck [78] applied this model to predict the explosion limit of fuel-air-diluent mixtures compressed by an expanding laminar flame in a constant volume spherical bomb. The fuels that were studied ranged from butane to octane at fuel-air equivalence ratios from 0.8 to 1.3. The explosion pressures and temperatures ranged from 10 to 100 atm. and 650 to 850 K. They observed that the model successfully described a two-stage ignition process in constant volume bombs and rapid compression machines. Hydroperoxide (HO₂) was the most important branching agent in the first stage and hydrogen peroxide (H₂O₂) was the most important branching agent in the second stage. They also found that the simplest and most rational way to include the effects of variations in fuel molecule size and structure in this reduced mechanism was to adjust the equilibrium constant of the isomerization reaction for
the alkylperoxy radical by changing the forward rate constant. The rates of all other
reactions in the model were expected to be relatively insensitive to fuel type and were kept
constant. This provided a convenient means of calibrating the model for different fuels. The
adiabatic core temperature controlled the autoignition process and was recommended for use
in correlating experiment and theory. Comparison of constant volume bomb and rapid
compression machine data showed no observable differences due to compression by a hot
flame front rather than by a cold piston.

Chun et al. [80] applied Hu and Keck’s model to predict the onset of knock in a SI
engine. Experimental data from a large number of individual cycles were generated from a
single cylinder engine over a range of operating conditions where knock occurred. The end-
gas temperature used in the kinetic model was calculated from the measured cylinder
pressure data assuming that knock originated in the part of the end-gas region which was
compressed adiabatically. The model successfully predicted the two-stage autoignition
process. The model prediction of KOCA generally matched well with the measured KOCA
on a cycle-by-cycle basis for a range of fuels (isooctane, PRF, and indolene) and engine
operating conditions. The agreement was least satisfactory when knock occurred close to the
end of the burning process when the end-gas mass fraction was small and its temperature was
not known precisely.

2.10.2. Detailed Chemical Kinetic Models

Detailed Chemical Kinetic models are based on the elementary reactions that occur
during combustion. The chemical kinetic scheme involves elementary reaction steps during
the autoignition which are believed to be the real chemical reactions that occur between the
species. The rate coefficients for each step are determined from published data collected
with shock tubes, stirred reactors, rapid compression machines, motored engines, and
constant volume bombs. Since the rate coefficients are determined based on fundamental
chemical processes, there is no need to adjust any of the rate coefficients depending on the
fuel and application if all of the elementary reactions are known. These models are usually
built in a stepwise manner. Once a mechanism has been established for a simple fuel, a
mechanism for a complex fuel is developed based on the simpler fuel molecules [81-84].
The smallest, most fundamental block in this construction is the reaction mechanism for the oxidation of H₂ and CO. The next step is the mechanism for CH₂O, followed by CH₄ and CH₃OH [81,82,85,86]. This mechanism is more costly in terms of development time and requires more powerful computational resources, but it promises an improved ability to treat such effects as fuel molecular structure, fuel mixture, and the use fuel additives [81,82].

Green et al. [81] studied the chemical aspects of the autoignition of iso-butane experimentally in the Sandia optical research engine and theoretically using computer simulations with a detailed chemical kinetic mechanism. They observed that even with a relatively knock-resistant fuel, iso-butane, there is still a significant amount of fuel breakdown in the end-gas with resulting heat release and temperature increase. They concluded that the cool-flame activities increase the tendency to knock because of energy release rather than the production of reactive intermediate chemical species. Fuels releasing greater amounts of heat during the end-gas compression arrive at the point of autoignition sooner than other fuels, and are more likely to knock. Although relatively small, this energy release results in a more rapid attainment of high temperature ignition.

Westbrook et al. [82] have described the development of detailed chemical kinetic reaction mechanisms for the analysis of autoignition and knocking of hydrocarbon fuels. They have emphasized the chemical kinetic mechanisms of complex hydrocarbons. They have compared the model’s predictions with a series of engine cycles of the Sandia optical research engine that were experimentally investigated by Green et al. [81]. It was observed that the wide ranges of temperature and pressure which are encountered by the end-gases in the combustion chambers requires a comprehensive mechanism for the prediction of KOCA. The reactions and chemical species that are the most important in each temperature and pressure regime are discussed and validated through comparisons with idealized experimental results. They concluded that although the rates of reactions and heat release are relatively low at temperatures below 700 K, they can still influence the time at which autoignition occurs. They suggested that the tendency to knock can be modified by changes in the value of the ignition temperature as well as by changes in the amount of low temperature heat release. The higher octane number of iso-octane than n-heptane was cited as the reason for its lower cool flame activity and somewhat higher ignition temperature.
They found that the knock tendency of a given fuel can be altered by changing either the low temperature heat release, or the ignition temperature, or by changing both parameters, through the use of blending fuels or additives.

Westbrook et al. [87] used a detailed chemical kinetic model to examine the chemical kinetic processes leading to knock in SI engines. The model was applied to C₁ to C₇ paraffinic hydrocarbon fuels and a correlation was developed between the RON and the computed time of ignition for each fuel. The octane number was shown to be dependent on the rates of OH radical production through isomerization reactions. The modeling results showed that OH radicals produced by the RO₂ isomerization process consume some of the fuel which accelerates ignition, but more important, they produce a radical pool and a reactive mixture that is then more rapidly ignited as the end-gas temperature reaches about 900 K. This behavior explains the widely observed trends that long chain hydrocarbons have low octane numbers and knock easily while highly branched fuels are knock resistant. The model showed that compact, highly branched fuels have high knock resistance for two simple reasons. First, the majority of the available H atoms are located at primary sites and are therefore relatively difficult to remove, and second, RO₂ isomerizations must overcome large ring strain energy barriers. The effectiveness of fuel additives as both pro-knock and anti-knock agents is also explained in terms of their impact on the OH radical pool. Additives which increase OH production accelerate ignition and promote knock, while additives which remove OH inhibit knock. Anti-knock agents can act either by retarding low temperature oxidation and chain branching or by inhibiting the higher temperature HO₂⁻ dominated ignition.

Modeling of autoignition in SI engines requires detailed knowledge of the effect of fuel's molecular structure and the engine operating and design variables on autoignition. The purpose of this chapter was to provide information from relevant literature to choose the most efficient approach to developing a model for this project. The autoignition model will be validated with the experimental data from a John Deere 6076 natural gas engine. The next chapter describes the experimental apparatus used to produce the experimental data needed for validation of the model.
3. EXPERIMENTAL APPARATUS AND PROCEDURE

This chapter starts with a presentation of the experimental apparatus that was used for this project. Then, the techniques used for accurate cylinder pressure data acquisition are reviewed. Finally, the data collection procedure used for this project is explained.

3.1 Experimental Setup

Figure 3.1 shows the test set-up which consists of the following equipment:

1. **The Engine**: A John Deere lean-burn, open-loop-controlled, natural gas engine. Table 3.1 shows the specifications of the engine.

2. **The Dynamometer**: A 150 HP General Electric model TLC2544 DC dynamometer. It has both speed and torque control options.

3. **The Flowmeters**:
   a) Air flowmeter: Model 50 MC2-4 Meriam Laminar Flow Element.
   b) Natural gas flowmeter: Dresser 1.5M175 roots meter.
   c) Propane flowmeter: Sharp edged orifice flowmeter that was built in the Internal Combustion Engine Laboratory of Iowa State University. It was calibrated to measure both subsonic and sonic flow rates of propane.

<table>
<thead>
<tr>
<th>Table 3.1 Specifications of the engine.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Model</strong></td>
</tr>
<tr>
<td><strong>Number of cylinders</strong></td>
</tr>
<tr>
<td><strong>Displacement</strong></td>
</tr>
<tr>
<td><strong>Compression ratio</strong></td>
</tr>
<tr>
<td><strong>Valves (intake/exhaust)</strong></td>
</tr>
<tr>
<td><strong>Combustion system</strong></td>
</tr>
<tr>
<td><strong>Engine type</strong></td>
</tr>
<tr>
<td><strong>Aspiration</strong></td>
</tr>
<tr>
<td><strong>Intercooler</strong></td>
</tr>
<tr>
<td><strong>Rated power</strong></td>
</tr>
<tr>
<td><strong>Peak torque</strong></td>
</tr>
</tbody>
</table>
Figure 3.1 Experimental Setup
4. Pressure Transducer: The pressure transducer was a KISTLER-6121 ground-insulated high-temperature pressure sensor designed for cylinder pressure measurements in internal combustion engines. The transducer has a protective plate in front of the diaphragm that reduces the thermal shock error. It is especially suitable for natural gas engines. The ground-insulated design avoids electrical interferences due to ground loops. Table 3.2 shows the specifications of the transducer.

Table 3.2 Pressure transducer specifications

<table>
<thead>
<tr>
<th>Range (bar)</th>
<th>0-250</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibrated partial range (bar)</td>
<td>0-50</td>
</tr>
<tr>
<td>Overload (bar)</td>
<td>300</td>
</tr>
<tr>
<td>Sensitivity (pC/bar)</td>
<td>-14</td>
</tr>
<tr>
<td>Natural Frequency (kHz)</td>
<td>55</td>
</tr>
<tr>
<td>Linearity (%FS)</td>
<td>±0.5</td>
</tr>
<tr>
<td>Operating temperature range (°C)</td>
<td>-50...350</td>
</tr>
</tbody>
</table>

5. Data acquisition board: The data acquisition board was a National Instruments AT-MIO E 16 board. It is a plug and play-compatible multifunction analog, digital, and timing I/O board for the PC AT and compatible computers. This board features 12-bit analog to digital conversion (ADC) with 16 analog inputs, 12-bit digital to analog conversion of voltage outputs, 8 lines of TTL compatible digital I/O, and two 24-bit counter/timers for timing I/O. Table 3.3 shows the input characteristics of the data acquisition board.

Table 3.3 Input characteristics of data acquisition board

<table>
<thead>
<tr>
<th>Number of channels</th>
<th>16 single-ended or 8 differential</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of ADC</td>
<td>Successive approximation</td>
</tr>
<tr>
<td>Maximum sampling rate</td>
<td>100 kSample/s</td>
</tr>
<tr>
<td>Resolution</td>
<td>12 bits</td>
</tr>
</tbody>
</table>
3.2 Techniques for Accurate Cylinder Pressure Data Acquisition

Three important steps to achieve the objective of this project were collecting accurate cylinder pressure data, determination of the cylinder volume, and phasing of the pressure data with respect to the cylinder volume.

With current technology, the most accurate way to measure cylinder pressure is to use a piezoelectric pressure transducer. However, it is still not free of errors. During engine operation, the diaphragm of the transducer is heated by the burned gases which can have temperatures over 2000 K. The temperature of the exposed part of the transducer may rise to a temperature of more than 600 K. At this condition, the measurement has an error due to thermal stress in the transducer. This is called short-term drift. The magnitude and direction (positive or negative) of the error is dependent on both the transducer and the engine operating condition. Short-term drift causes two important problems. First, the calculated indicated mean effective pressure (IMEP) may have a significant error so that the IMEP can be even less than the BMEP. Second, if the transducer does not recover from the thermal strain after the expansion period, the pumping loop measurements may have significant errors [88]. In addition, piezoelectric pressure transducers can only be used for relative pressure measurements. Absolute cylinder pressure has to be known at some point in the cycle. In this experiment it was assumed that the cylinder pressure was equal to the intake manifold absolute pressure at bottom dead center (BDC) before compression.

The cylinder volume of the engine at a given crank angle can be determined from the physical dimensions of the piston and crankshaft if the clearance volume is known accurately. The engine clearance volume given by the engine manual may not be accurate enough for combustion analysis. One way to determine the clearance volume is by disassembling the engine head and displacing a known amount liquid in the clearance volume. However, disassembling of the head may not be possible. The clearance volume can also be measured by filling the volume with a measured amount of engine oil. Another method to determine clearance volume is examining the shape of the log $p$-log $v$ diagram at the motoring condition. The compression process from intake valve closing to TDC can be approximated by a polytropic process as given by Equation 3.1.
\[ PV^n = \text{Constant} \quad (3.1) \]

Accordingly the compression line has to be a straight line with a slope of \(-n\) on a log \(p\)-log \(v\) diagram. Any deviation from the straight line can be attributed to errors such as an error in pressure, clearance volume, or the phasing of the pressure with respect to volume. If the main uncertainty is the clearance volume, it can be determined from the polytropic process approximation. Lancaster et al. [89] described the errors causing deviations from the straight line and can be consulted for further information about the subject.

Motoring data also provides valuable information about the phasing of the cylinder pressure data with respect to cylinder volume. A plot of cylinder pressure versus crank angle in the region of the peak pressure can be used for this purpose. The peak pressure should occur 1 or 2 degrees of crank angle before TDC due to the heat transfer from the gases to the cylinder wall. However 1 degree variations of the phasing may cause significant errors in the IMEP. Lancaster et al. [89] observed that 1 degree CA variations of phasing caused 41% variation of the motoring IMEP.

In this project the following procedures were applied to collect accurate data.

1. Determination of TDC: To determine TDC of the No. 1 cylinder, an apparatus was built consisting of a dial indicator that could reach the top of the piston when it was installed in place of a spark plug. The point where the dial indicator scale changed its direction was determined as TDC.
2. Calibration of pressure transducer: A Kistler charge amplifier was used to convert and amplify the transducer output into voltage. The output of the amplifier was measured by a digital voltmeter as a dead weight tester applied a known pressure to the transducer.
3. Transducer Installation: The transducer was installed in the engine with a tightening torque of 10 Nm as suggested by the manufacturer.
4. Determination of clearance volume: Examination of the motoring data indicated that the clearance volume given by the engine manual was not accurate. Therefore, it was determined using the process explained above with the assumption of a polytropic process. The clearance volume was also measured by filling the combustion chamber with a known amount of engine oil. During this measurement the head was not
disassembled.

3.3 Data collection procedure

One of the objectives of this project was to examine the combustion characteristics of the engine at different operating conditions such as varying propane ratio, equivalence ratio, ignition timing. In order to observe the effect of variation of the operation condition, the cylinder pressure data were collected at the operating conditions shown in Table 3.4. From previous experience the engine was known to knock at these conditions.

Table 3.4 Knocking condition test matrix

<table>
<thead>
<tr>
<th>Propane Ratio</th>
<th>Equivalence Ratio</th>
<th>Ignition Timing (degree BTDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>0.80</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.82</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.84</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.86</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td>5%</td>
<td>0.78</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.80</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.82</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.84</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td>10%</td>
<td>0.76</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.78</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.80</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.82</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td>15%</td>
<td>0.76</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.78</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.80</td>
<td>20,22,24,26</td>
</tr>
<tr>
<td></td>
<td>0.82</td>
<td>20,22,24,26</td>
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</tbody>
</table>
To determine the effect of variation of the ignition timing, the timing was varied from 20, 22, 24, and 26 degrees BTDC while the other operating variables were held constant and the cylinder pressure data was collected from 200 successive cycles at each ignition timing. In addition to Table 3.4, the cylinder pressure data were collected at non-knocking conditions and at variable manifold absolute pressures (MAP). The non-knocking condition test matrix was similar to Table 3.4, but involved only leaner equivalence ratios. The data acquisition board was triggered by a shaft encoder every 0.1 degree CA, which provided a 90 kSample/s sampling frequency, to make sure that the details of the knock signal were captured.
4. ANALYSIS OF COMBUSTION

The background section showed that the combustion characteristics and the knocking tendency of natural gas are significantly affected by the addition of propane. In this chapter, the combustion characteristics of natural gas and natural gas-propane mixtures will be examined for the John Deere 7.6 liter engine. The flame initiation period (FIP), flame propagation period (FPP), and the end-gas state variables are of primary interest in the analysis. In order to examine these characteristics of the fuels a two-zone thermodynamic model will be developed.

4.1. Development of Two-zone Thermodynamic Model

Rassweiler and Withrow [90] observed that the pressure rise due to combustion is proportional to the corresponding increments of the mass-burned fraction of the fuel-air mixture. Their observation showed that it was possible to determine the mass-burn fraction of the mixture without knowledge of the flame shape and propagation speed.

The model developed in this project determines the burned-mass fraction and the state variables of the combustion chamber contents from measured experimental cylinder pressure data. This model was developed based on the model of Krieger and Borman [91].

The model is a zero dimensional two-zone thermodynamic model. Since there is only one independent variable (time or CA) for zero dimensional models, the governing equations are ordinary differential equations. The analysis begins at bottom dead center (-180 degrees CA) where the cylinder contains a mixture of air, fuel, and residual gases. The mixture is then compressed until the initiation of combustion at a specified CA degree (note that the independent variable, CA, is the crank angle and defines the piston position relative to TDC in a cycle). Until the start of combustion, the model is a single zone and undergoes no pre-flame reactions. With the initiation of combustion, the second zone (burned zone) is created. Figure 4.1 shows the burned and unburned zones which are separated by an infinitesimally thin flame front. The burned zone consists of the equilibrium products of combustion and both zones are assumed to be at the same pressure at any CA.
Figure 4.1. Schematic of the combustion chamber and the zones.
It is also assumed that the gases in both zones are ideal gases. The final assumption is that there is no charge leakage or blow-by past the piston. The analysis is finished as soon as the exhaust valve is opened.

4.1.1. Formulation of the Model

During the compression period, the properties of the fuel, air, and residual gas mixture are determined by a FORTRAN subroutine FARG, which was written by Ferguson [92]. This program was modified to include a methane and propane mixture as fuel. The cylinder pressure and its derivative are inputs to the model. The temperature of the unburned mixture is determined by the ideal gas law.

\[ PV = mRT \]  \hspace{1cm} (4.1)

where \( P \) is the pressure within the cylinder, \( V \) is the volume, \( m \) is the mass of the fuel, air, and residual gas mixture, \( R \) is the gas constant of the mixture, and \( T \) is the temperature of the mixture.

The second zone is created after the spark fires and initially is assumed to contain 0.01% of the original mixture burned. The volume of the two zones is equal to the total cylinder volume which is a function of the cylinder geometry and CA. The total volume is conserved:

\[ V = V_b + V_u \]  \hspace{1cm} (4.2)

where the subscript "u" refers to unburned and "b" refers to burned gas.

Total mass is assumed to be constant, since valve leakage and blow-by are neglected. The total mass is conserved:

\[ m = m_u + m_b \]  \hspace{1cm} (4.3)
In each zone, assuming ideal gases and the same pressure, the equation of state must be satisfied.

\[ P = m_b R_b T_b / V_b = m_u R_u T_u / V_u \]  \hspace{1cm} (4.4)

The energy equations were written for the two zones as follows:

\[ \frac{d(m_u u)}{d\theta} = \sum_{i=1}^n \frac{dQ_{ui}}{d\theta} - \frac{P}{d\theta} \frac{dV_u}{d\theta} - \frac{d m_u}{d\theta} h_u \]  \hspace{1cm} (4.5)

\[ \frac{d(m_b u_b)}{d\theta} = \sum_{i=1}^n \frac{dQ_{bi}}{d\theta} - \frac{P}{d\theta} \frac{dV_b}{d\theta} + \frac{d m_u}{d\theta} h_u \]  \hspace{1cm} (4.6)

where \( u \) is the internal energy, \( h \) is the enthalpy, \( Q \) is the heat transfer from the gas to surfaces and \( \theta \) is the crank angle. The heat transfer surfaces are the piston, head, and cylinder walls. Heat exchange across the flame front is ignored. The heat transfer rates for both zones were determined using Annand's heat transfer correlation [93] as if each of the zone filled the entire cylinder. Then, the heat transfer rates were multiplied by the fraction of the cylinder volume that is occupied by the zone. This method of volume-weighting was also preferred by Shapiro and Van Gerpen [94]. The equilibrium properties of the burned mixture were determined using a version of the FORTRAN subroutine PER developed by Olikara and Borman [95]. The equations of the model were integrated from the beginning of the second zone to exhaust valve opening to determine the following variables:

\[ T_u(\theta), T_b(\theta), m_u(\theta), m_b(\theta), V_u(\theta), V_b(\theta) \]

The publicly available computer program, Livermore Solution of Ordinary Differential Equations (LSODE) [96] was used to integrate the differential equations.
4.2 Flame Initiation and Propagation Periods

One of the common uses of the burned-mass fraction curve is the determination of the flame initiation and propagation periods. The flame initiation period is the period in which the growth of the flame kernel has proceeded to a size where the flame front for turbulent propagation is established [97]. Since the transition from FIP to FPP is not marked precisely by a distinct measurable characteristic, it is arbitrarily defined in terms of the burned mass fraction. This fraction typically ranges from 1% to 10%. In this project, FIP was assumed to be the crank angle period from the spark firing to where 1% of the mass has been burned. FPP, which involves the developed-turbulent-flame, is assumed to be the crank angle required for 1% to 90% of the mass to be burned. Figure 4.2 shows the FIP and FPP on a typical burned-mass fraction curve for this engine.

Both FIP and FPP shows significant variations even during stable engine operating conditions. Random fluid motion around the spark plug during the kernel growth period is the major source of the random variations of FIP. This random fluid motion affects the required ignition energy of the kernel by changing the surface-to-volume ratio of the kernel and the heat transfer from the kernel to the surroundings [98]. Borman [98] compared the FIP of fast and slow-burn cycles and found that the FIP is extended for slow-burn cycles, which have lower peak pressures. Pischinger et al. [99] observed that cycles in which the flame kernel is moved further away from the gap center have shorter FIPs. The shorter FIP was related to the smaller contact area (heat transfer area) between the electrodes and the kernel. Cycle-by-cycle variations in the contact area, and thus the heat transfer, were due to variations in the local flow field. When a relatively small electrode was used there was an improvement in the observed cycle-by-cycle variations of FIP [99]. They also claimed that providing a moderate magnitude local velocity that will not quench the kernel in the flow (3-5 m/s) around the spark plug at the spark timing extends the engine's lean operating limits.

The cycle-by-cycle variations of FPP are caused by variations in the burning area [100]. Burning area is affected by the fluid motion in the combustion chamber and it is not
Figure 4.2 Determination of FIP and FPP (Spark Timing = 25 degree CA BTDC)
generally a spherical area. As predicted with Equation 4.8, the mass burning rate is proportional to the flame area.

\[
\frac{dm_u}{dt} = \rho_u V_f A_f
\]  

(4.8)

where \( \rho_u \) is the unburned mixture density, \( V_f \) is the turbulent flame velocity, and \( A_f \) is the flame front area. Cycle-by-cycle variations of the turbulent flame speed are not significant compared to variations of the area [100].

### 4.3 Effects of Equivalence Ratio, Propane Ratio, and Manifold Absolute Pressure on Burned-Mass Fraction and Burning Rate

The model described above can be used along with the measured cylinder pressure to investigate the effects of propane ratio (Prop. R.), equivalence ratio (Eq. R.), ignition timing, and manifold absolute pressure (MAP) on the combustion. The temperature, pressure, equivalence ratio, and fuel type are the factors that affect the laminar flame velocity of a fuel-air mixture. The laminar flame velocity of the mixture has a significant influence on both FIP and FPP.

Figures 4.3 and 4.4 show the effect of the equivalence ratio on the burned-mass fraction and the burning rate curves, respectively. As can be seen from Figure 4.3, lean mixtures shift the burned mass fraction curve to the right where FIP and FPP are longer. This effect is also shown in Figure 4.4, where the mass burning rate is shown to be a strong function of the equivalence ratio. The maximum burning rate of the leanest mixture, with an equivalence ratio of 0.67, is significantly lower than that for the 0.78 equivalence ratio mixture and is shifted to the right approximately 7 degrees. The main reason for the shift with lean mixtures is the lower laminar flame speed of the lean mixtures. It is well known that the laminar flame speed is a maximum for slightly rich mixtures and slows down for both leaner and richer mixtures [101,102]. FIP and FPP for the 0.67 equivalence ratio mixture are 16.7 and 40.3 degrees, respectively. The same periods for the 0.78 equivalence ratio mixture are 12.0 and 32.8
Figure 4.3 Variation burned mass fraction with equivalence ratio
(Spark Timing = 26 degree BTDC, Prop. R. = 0%, MAP = 1.4 bar).
Figure 4.4 Variation mass burning rate with equivalence ratio
(Spark Timing = 26 degree BTDC, Prop. R. = 0%, MAP = 1.4 bar).
degrees, respectively. Although increasing laminar flame speed will decrease both FIP and FPP when the equivalence ratio is increased, the FIP seems to be much more strongly affected by increasing equivalence ratio. When the equivalence ratio is increased from 0.67 to 0.78, the FIP was reduced by 28%, but the FPP was reduced by only 18%. This explains that the influence of the laminar flame velocity on the FIP is much higher when compared to the FPP, which is significantly influenced by the turbulent flame velocity. Similar trends were observed by Rauckis et al. [103].

Figures 4.5 and 4.6 show the effect of ignition timing on the burned-mass fraction and burning rate. As expected, the curves are shifted in the direction corresponding to the change in timing. FIP was reduced 14% when the timing was retarded from 26 degrees to 20 degrees BTDC. The reason for the reduction in the FIP is probably increased laminar flame speed of the mixture and hence increased mixture temperature at retarded timing. As will be seen later in this section, through the end of the compression period, the unburned mixture temperature increases as high as 10 K for 1 degree CA change in the compression period. There were no significant variations in FPP with changing ignition timing.

Figures 4.7 and 4.8 show the effect of intake manifold absolute pressure on the burned-mass fraction and burning rate, respectively. Increased pressures decrease the laminar flame velocity of hydrocarbon fuels [102]. However, as can be seen from Figure 4.8, the maximum burning rate is almost doubled when the MAP is raised from 1.0 bar to 1.6 bar. The reasons for the rise are increased unburned mixture density, the flame speed, and decreased residual fraction with increased MAP. Hires et al. [101] states that although pressure has a slight effect on laminar flame speed, the decreasing residual fraction with the increasing MAP does have significant effect on the increasing burning rate. FIP and FPP for the 1.0 bar curve are 14.5 and 35.5 degrees, respectively. FIP and FPP of the 1.6 bar curve are 13.1 and 29.7 degrees, respectively. When the MAP was raised from 1.0 bar to 1.6 bar, the FIP is reduced 9.6% and FPP was reduced by 16.3%. This indicates that at an equivalence ratio of 0.8 with increasing MAP, the turbulent flame propagation speed increases so that the FPP period reduces much more compared with the FIP, which is mainly governed by the laminar flame speed.
Figure 4.5 Effect of spark timing on burned-mass fraction

(Prop. R. = 0%, Eq. R. = 0.80, MAP = 1.4 bar).
Figure 4.6 Effect of spark timing on mass burning rate

(Prop. R. = 0%, Eq. R. = 0.80, MAP = 1.4 bar).
Figure 4.7 Effect of initial pressure on burned-mass fraction (Prop. R. = 0%, Eq. R. = 0.80, Spark Timing = 26 degree BTDC).
Figure 4.8 Effect of initial pressure on mass burning rate
(Prop. R. = 0\%, Eq. R. = 0.80, Spark Timing = 26 degree BTDC).
Figures 4.9 and 4.10 show the effect of propane addition to natural gas on the burned-mass fraction and burning rate. As mentioned in the background section, the addition of small amounts of propane to methane has a significant effect on the autoignition chemistry of the mixture. As can be seen from Figure 4.9, propane addition causes significant variations to the 90% point although there is no significant variation of the 1% point at the equivalence ratio of 0.82. The FPP is reduced by 10% with the addition of 15% propane. This reduction is due to end-gas autoignition that increases the burning rate significantly.

The effect of end-gas autoignition on the burning rate can be observed clearly in Figure 4.10. In this figure, the burning rate curve that does not involve propane addition is called the reference curve and the CA that all the burning rates are about the same for all the mixtures after TDC is called the reference CA. The reference curve and CA are defined for better explanation of the effect of the autoignition on the burning rate. As the propane fraction of the mixture is increased, the burning rates of the mixtures are increasing before the reference CA. The reason for this is that when increasing the propane fraction of the mixture, the amount of mixture that is involved in the autoignition reaction is increasing. The burning rates are decreasing after the autoignition correspondingly since there is not much mixture left. Since the mass burning rate is so sensitive to pressure variations, it can be used as a knock detection technique as mentioned in the background section. It is also important to mention here that the burning rate and the burned-mass fraction curves were determined from the average of 200 pressure traces. If the curves had been determined from an individual cycle pressure trace, the curves would not be smooth as shown in Figures 4.9 and 4.10. The burning rate curve would have a peak at KOCA and the burned-mass fraction would go to 1 immediately after KOCA.

4.4 Effects of Equivalence Ratio, Propane Ratio, and Manifold Absolute Pressure on Burned and Unburned Mixture Temperatures

The unburned mixture temperature is one of the important factors that affects the tendency to knock. The residual fraction and inlet temperature affect the unburned mixture temperature and the compression history of the mixture. In this project, the residual fraction was assumed
Figure 4.9 Effect of propane ratio on burned-mass fraction
(Eq. R. = 0.82, Spark Timing = 26 degree BTDC, MAP = 1.4 bar).
Figure 4.10 Effect of propane ratio on mass burning rate
(Eq. R. = 0.82, Spark Timing = 26 degree BTDC, MAP = 1.4 bar).
to be 5% and to remain constant for all operating conditions. Since the MAP remains constant for most of the operating conditions in this project, this assumption should be reasonable. The unburned mixture temperature is determined by using the ideal gas law from bottom dead center to the creation of the second zone. It is assumed that the cylinder pressure at bottom dead center is equal to the MAP. This pressure was the reference pressure for the cylinder pressure transducer. This calculated value of the initial unburned mixture temperature is approximately 100 K higher than the mixture temperature in the inlet port at all conditions. The reason for this is heat transfer to the mixture from the cylinder components. The residual gas fraction also contributes to increasing the mixture temperature.

Figure 4.11 shows the effect of the equivalence ratio on the unburned mixture temperature. The accuracy of the temperature is questionable after about 40 degrees CA because there will be very little unburned mixture and it is probably in the crevices and the boundary layer. As can be seen from the figure, increasing the equivalence ratio increased the unburned mixture temperature from bottom dead center (-180 degrees CA) to the exhaust valve opening (120 degree CA). However, during the FPP, which is from approximately -10 to 30 degrees CA, the unburned mixture temperatures show marked increases with equivalence ratio. The temperature of 0.67 and 0.82 equivalence ratio curves at -20 degree CA are 810 K and 840 K, respectively. The temperature difference between the two curves is only 30 degree K. However, the difference at 10 degrees CA is 90 K which is 3 times higher than that at -20 degrees CA. After the start of the combustion, the unburned mixture is compressed by both piston motion and by the expansion of the burned zone. The piston motion remains the same for each case, but higher equivalence ratio increases the flame speed so that the temperature of the burned mixture and the pressure increases with increasing equivalence ratio and hence the unburned mixture is compressed and the temperature is increased correspondingly. Figure 4.12 shows the burned gas temperature from -10 degree CA to exhaust valve opening. As can be seen from the figure, when increasing the equivalence ratio, the burned gas temperature increases and the maximum temperatures for each curve shift through the top dead center (0 degree CA). Another important trend that can be observed from Figure 4.12 is that the temperatures become about
Figure 4.11 Effect of equivalence ratio on unburned mixture temperature
(Prop. R. = 0%, Spark Timing = 26 degree BTDC, MAP = 1.4 bar).
the same at 65 degrees CA and after this CA the temperatures are higher with the lower equivalence ratio mixtures. The probable reason for this is the lower flame speed of the leaner mixtures and hence extended combustion and less work done during expansion leaving more energy in the exhaust gases.

Figure 4.13 shows the effect of MAP on the unburned mixture temperature. As shown in the figure, the temperature at bottom dead center is the highest for the 1.0 bar curve. Increasing the residual gas fraction with lower MAP may have a significant contribution to the unburned mixture temperature at this point. The temperature is especially high during the FPP with the higher MAP, but the difference between the maximum temperatures of 1.6 and 1.0 curves is only 20 degree K. The possible reason for this is the compression effect of the burned mixture. Increased unburned mass density and turbulence in the combustion chamber with increasing MAP increases the flame speed and for this reason the unburned mixture temperature increases. As can be seen from Figure 4.14, the burned mixture temperature is higher with higher MAP from -10 degree CA to 9 degree CA. After 9 degrees CA the temperature of the burned mixture with 1.0 bar is higher than that of 1.3 and 1.6 bar. A possible reason for this, as mentioned earlier, is extended combustion due to the lower flame speed caused by increased residual fraction and decreased turbulence at lower MAP.

Figures 4.15 and 4.16 show the effect of timing on the unburned and burned mixture temperatures. As can be seen from the figures, advanced timing generally increases the maximum temperatures and the maximum temperatures occur closer to top dead center. Advanced timing initiates the combustion earlier and the burned mixture fraction increases when the piston reaches top dead center. As could be seen in Figure 4.5, when the timing was 26 degrees BTDC, the burned mass fraction at top dead center was almost 3 times higher than that of 20 degree BTDC timing. Therefore, the maximum temperature and pressure increase with advanced timings. As can be seen from Figure 4.16, the burned gas temperatures are higher with retarded timings after about 10 degree CA and remain high until the exhaust valve opening due to late combustion. Measurements at the exhaust manifold showed that the mean exhaust gas temperatures were higher with retarded timings, which
Figure 4.12 Effect of equivalence ratio on burned gas temperature
(Prop. R. = 0%, Spark Timing = 26 degree BTDC, MAP = 1.4 bar).
Figure 4.13 Effect of initial pressure on unburned mixture temperature

(Prop. R. = 0%, Eq. R. = 0.80, Spark Timing = 26 degree BTDC).
Figure 4.14 Effect of initial pressure on burned gas temperature
(Prop. R. = 0%, Eq. R. = 0.80, Spark Timing = 26 degree BTDC).
Figure 4.15 Effect of spark timing on unburned mixture temperature
(Prop. R. = 0%, Eq. R. = 0.80, MAP = 1.4 bar).
Figure 4.16 Effect of spark timing on burned gas temperature
(Prop. R. = 0%, Eq. R. = 0.80, MAP = 1.4 bar).
support the model's predictions. Figure 4.5 showed that at 10 degree CA, the burned-mass fraction was 54% for 20 degrees BTDC timing and 72% for 26 degrees BTDC timing. At this CA, the unburned mixture mass fraction was 18% higher with 20 degrees BTDC timing. This explains the higher temperature of the burned mixture after 10 degrees CA with 20 degree timing.

Figures 4.17 and 4.18 show the effect of propane fraction in the unburned mixture on the unburned and burned mixture temperatures, respectively. As can be seen from Figure 4.17, increased propane fraction increases the maximum temperatures, but the variations are not significant. Similarly, the maximum burned mixture temperatures don't have significant variations. However, after 20 degree CA the burned mixture temperatures are higher with lower fractions of propane in the mixtures. As mentioned earlier, increasing propane fraction was associated with increasing intensity of knock and hence the mass burning rate through the end of the FPP. After this period the burning rates with higher propane fraction mixtures were lower. This could be the reason for the lower temperature of the burned mixture after about 20 degree CA. Mean exhaust temperature measurements support these results.

4.5 Summary

In this chapter a two-zone thermodynamic model was developed to examine the combustion characteristics and the end-gas state variables of the natural gas and natural gas-propane mixtures. The following conclusions can be drawn from this chapter.

The variations in the flame initiation and propagation period are the major source of cycle-by-cycle variations of cylinder pressure in a SI Engine. The flame initiation period (FIP) is mostly dependent on the laminar flame speed of the fuel-air mixture while the flame propagation period (FPP) is dependent on the turbulence intensity and the turbulent flame area beside the laminar flame speed of the mixture.

It was observed that both FIP and FPP decrease with increasing equivalence ratio, however FIP is more sensitive to the equivalence ratio than FPP due to strong dependency of the FIP on the laminar flame speed.
Figure 4.17 Effect of propane ratio on unburned mixture temperature
(Eq. R. = 0.82, Spark timing = 26 degree BTDC, MAP = 1.4 bar).
Figure 4.18 Effect of propane ratio on burned gas temperature
(Eq. R. = 0.82, Spark timing = 26 degree BTDC, MAP = 1.4 bar).
While the retarded timing reduces the FIP due to the increase in the unburned mixture temperature at spark fire, increasing the MAP decreases the FPP due to the increasing turbulence intensity.

Addition of propane to natural gas reduces the FPP of the mixture although the FIP is not affected. The possible reason for this is increased tendency to autoignition with the addition of propane to the mixture. The end-gas autoignition strongly increases the burning rate.

The unburned and burned mixture temperature are significantly increasing with equivalence ratio. However, the ignition timing, propane ratio, and MAP don’t influence the temperatures as much as the equivalence ratio does.

In the next chapter the effects of the engine operating variables on the occurrence and intensity of knock will be examined.
5. ANALYSIS OF KNOCK

This chapter starts with an explanation of the knock characterization and detection procedure used for this project. Then, the factors that affect the occurrence and intensity of knock will be examined. After that, the cycle-by-cycle variation of the KOCA and the KI will be examined. Finally, the effects of the engine operating conditions on the mean values of the KOCA and the KI will be presented.

5.1 Knock Detection Procedure and Characterization

During this project, cylinder pressure data were collected from the number 1 cylinder at different conditions, as given in Table 3.4, to determine the effect of operating variables and the propane fraction of the fuel on the knocking characteristics of the engine. Prior to data collection the engine was operated at the rated condition for sufficient time to ensure stable cooling water temperature. Figure 5.1 shows a set of raw cylinder pressure data during a typical knocking condition. Figures 5.2 and 5.3 show the results of low-pass and high-pass filtering of the same raw data. Butterworth filter of the LabView was used for the filtering. Order of the filter was 8. The high-pass filtered knock signal was used to characterize the knock. The crank angle at which the first pressure peak over a threshold value occurs characterizes the KOCA and the maximum amplitude of the knock signal characterizes the KI. A Lab-View program was developed for the detection of knock and the determination of KOCA and KI. Examination of KOCA and KI was possible during data acquisition by using the Lab-View program. The threshold value was determined from the maximum intensity of the non-knocking signals. Since the knock occurred in a period from TDC to 40 degrees ATDC, the threshold intensity was determined in this period. The maximum cylinder pressure was determined from the low-pass filtered pressure data. The cut-off frequency of the high-pass filter was determined as 4,500 Hz. Figure 5.4 shows the frequency spectrum of the cylinder pressure data. As can be seen from the figure there are 4 major peaks over 5,000 Hz. The first peak, which is around 5,500 Hz, is the characteristic frequency of the knock.
Figure 5.1 Knocking condition cylinder pressure data
(Eq. R. = 0.82, Prop. R. = 15%, Spark timing = 26 degree BTDC, MAP = 1.4 bar).
Figure 5.2 Knocking condition low-pass filtered cylinder pressure data (Eq. R. = 0.82, Prop. R. = 15%, Spark timing = 26 degree BTDC, MAP = 1.4 bar).
Figure 5.3 Knocking condition high-pass filtered cylinder pressure data (Eq. $R_\text{e} = 0.82$, Prop. $R_\text{e} = 15\%$, Spark timing = 26 degree BTDC, MAP = 1.4 bar cut-off frequency = 4500 Hz).
Figure 5.4 Frequency spectrum of knocking condition cylinder pressure data from 200 cycles (Eq. R. = 0.82, Prop. R. = 15%, Spark Timing = 26 degree CA, MAP = 1.4 bar).
signal which corresponds to the first circumferential mode of acoustical resonance for this engine. The intensity of knock at this mode is very strong compared to the other modes.

5.2 Occurrence and intensity of knock

The occurrence and intensity of knock is dependent on the energy release from the end-gas and the time of the energy release depends on the time required to establish a radical species pool, which leads to the high energy release chemical reactions. The time period, during which the radical species build-up depends on the temperature, the pressure, the fuel's molecular structure, the equivalence ratio, and the presence of residual gas [79,85,87, 104,105]. Even during the stable operation of an engine, none of these variables are the same for individual cycles at a given piston position in the cycle. The compression history of the end-gas is different for each individual cycle and exact prediction of the compression history of each individual cycle is almost impossible.

Figure 5.5 shows the cylinder pressure traces and the high-pass filtered pressure traces from two consecutive cycles. The high-pass filtered pressure data that is used for indication of the KI is arbitrarily scaled and added to 40 bars for better visualization. The traces start at 14 degrees CA BTDC and end at 30 degrees ATDC. The pressure rise period from 25 bar to 60 bar is 21 degrees CA for the first cycle and 17 degrees CA for the second cycle. When compared to the first cycle the second cycle is a faster burning cycle. The KOCA is 4.9 degrees CA earlier and the KI is also significantly higher for the second cycle. It is well known from the literature that KOCA correlates very well with the individual cycle pressure history [18,19].

The compression process of a cycle starts at the end of the intake process when the cylinder contains fuel, air, and residual gas mixture. The temperature of this mixture is dependent on the mixture inlet temperature, the temperatures of the metal components of the cylinder, and the residual gas fraction. The estimated values of the temperatures of the components and residual gas are given by Chun et al. [19] as:

Piston crown: 480 K to 540 K, Cylinder head: 400 K to 550 K, Cylinder liner: 390 K,
Exhaust valve : around 900 K, Residual gas : around 830 K
First cycle
KOCA = 14.7 degrees CA
KI = 1.17 bar
Xu = 13%

Second Cycle
KOCA = 9.8 degrees CA
KI = 6.2 bar
Xu = 15%

Figure 5.5 Raw and high pass filtered cylinder pressure data from two consecutive cycles.
Due to the different temperatures of the cylinder components, there will be a temperature distribution in the mixture. In addition, the fresh air-fuel mixture may not mix homogeneously with the residual gas and hence there can be a species distribution in the mixture. During the compression period before the spark fires, the cycle-by-cycle variations of cylinder pressure are very low. However, as mentioned in Chapter 4, after the spark fires, the flame initiation period (FIP) and the flame propagation period (FPP) show cycle-by-cycle variations that have a very significant effect on the pressure and temperature history of the end-gas. After the spark fires, the end-gas location varies depending on the fluid motion in the combustion chamber. The area/volume ratio of the end-gas also varies depending on the propagating flame front shape. Due to variations of all these parameters, there will be a temperature and species distribution in the end-gas. Depending on the temperature and species distribution in the end-gas, the regions that have the most favorable conditions for autoignition will release their energy first [11, 104]. The time of energy release from the end-gas depends on the compression history of each individual cycle and this is the source of cycle-by-cycle variations of KOCA.

Figure 5.6 shows the burned-mass fraction and the high-pass filtered pressure data of two consecutive cycles. The KOCAs for the first and the second cycles are 12.4 and 7.2 degrees and the KIs are 3.16 and 9.36 bar, respectively. The cylinder volume at the KOCA is only 9% higher for the first cycle. Although the KOCA is earlier and KI is significantly higher for the second cycle, the unburned-mass fraction (Xu) at KOCA, which is 15%, is only 1% higher than the first cycle. The maximum amount of energy that can be released from the end-gas is limited by the total energy content of the end-gas mixture. However, due to the temperature and species distribution in the end-gas, the entire end-gas may not release its energy instantaneously. Further, as shown in Figure 5.7, the end-gas may be separated in parts and all parts of the end-gas may not autoignite simultaneously. As can be seen from Figure 5.6, the burned-mass fraction of the second cycle shows a step increase at KOCA. This means that most of the end-gas mixture is involved in the autoignition reaction (multiple site autoignition could be occurring) and releases its energy simultaneously. At the moment of spontaneous energy release from the end-gas, a pressure wave will be set up. The
Figure 5.6 Burned mass fraction and high-pass filtered cylinder pressure data for two consecutive knocking cycles.
Figure 5.7 End-gas Configurations (the end gas is dark portion of combustion chamber)
magnitude of the pressure wave, which is directly related to the KI, is dependent on the amount of released energy. The cycle-by-cycle variations in the released energy are the source of the cycle-by-cycle variations in the KI.

5.2 Cycle-by-cycle variations of KOCA and KI

Figure 5.8 shows pressure traces from 200 consecutive cycles. As can be seen from the figure, there are significant differences between the traces during the main combustion period from the CA for spark firing (26 degree BTDC) to 20 degree ATDC. As shown in Figure 5.9 the most frequent maximum pressure is 65 bar, however the maximum pressure varies between 59 bar and 72 bar. This is approximately ±14% variation from the mode and the effect of cycle-by-cycle variations of the pressure on end-gas autoignition probably dominates the fluctuations of other variables. The cycle-by-cycle variation of cylinder pressure is one of the main constraints for the conservative design of the knock-limited compression ratio. If these variations can be reduced, a significant increase in the knock-limited compression ratio can be provided.

Figures 5.10 and 5.11 show the distribution of KOCA and KI for 200 cycles. As can be seen from the figure, KOCA is distributed from 5 to 17 degrees CA although the most frequent crank angles for knock occurrence are varying from 9 to 12 degree CA. KI variations are even broader as the KI is distributed from 1 bar to 14 bar. The most frequent KIs are varying from 1 to 5 bar. Figures 5.12 and 5.13 show the correlation of KOCA and KI with the maximum cylinder pressure. As can be seen from the figures, KOCA correlates fairly well with maximum pressure with a R² of 0.858, however the KI intensity does not correlate very well with an R² of only 0.20. Figures 5.12 and 5.13 prove that the KOCA is strongly dependent on individual cycle pressure history while the KI is not.

Figures 5.14 and 5.15 show the correlation of KOCA and KI with the unburned-mass fraction at KOCA. As can be seen from the figures neither KOCA nor KI correlates with the unburned-mass fraction at KOCA. This is somewhat surprising because it would be expected that the quantity of end-gas would affect the intensity of the knock event. Figures 5.16 and 5.17 show that KI does not correlate well with the end-gas temperature and KOCA, either.
Figure 5.8 Individual cylinder pressure traces from 200 consecutive cycles (Prop. R. = 15%, Eq. R. = 0.82, Spark Timing = 26 degree CA, MAP = 1.4 bar).
Figure 5.9 Distribution of maximum cylinder pressure
(Prop. R. = 15%, Eq. R. = 0.82, Spark timing = 26 degree BTDC, MAP = 1.4 bar).
Figure 5.10 Distribution of KOCA
(Prop. R. = 15%, Eq. R. = 0.82, Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
Figure 5.11 Distribution of KI

(Prop. R. = 15%, Eq. R. = 0.82, Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
Figure 5.12 Correlation between maximum cylinder pressure and KOCA
(Prop. R. = 15\%, Eq. R. = 0.82, Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
Figure 5.13 Correlation between maximum cylinder pressure and KI
(Prop. R. = 15%, Eq. R. = 0.82. Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
Figure 5.14 Correlation of KOCA with the unburned-mass fraction
(Prop. R. = 15%, Eq. R. = 0.82, Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
Figure 5.15 Correlation of KI with the unburned-mass fraction
(Prop. R. = 15%, Eq. R. = 0.82, Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
Figure 5.16 Correlation between end-gas temperature at KOCA and KI
(Prop. R. = 15%, Eq. R. = 0.82, Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
Figure 5.17 Correlation of the KOCA and the KI
(Prop. R. = 15%, Eq. R. = 0.82, Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
It is also known from the literature that individual cycle KIs do not correlate well with parameters such as the unburned-mass fraction, burning rate, KOCA, and end-gas pressure and temperature [19,79]. This poor correlation is attributed to cycle-by-cycle variations of the non-uniform end-gas state, variations in the geometric shape of the end-gas and its location within the combustion chamber. Chun et al. [19] states that due to the non-uniformity of the end-gas only a small portion of the end-gas may autoignite first and the rest of the unburned mixture may autoignite slowly or may not autoignite at all before the propagating flame consumes it.

5.3 Effects of equivalence ratio, propane ratio, and spark timing on mean values of KOCA and KI

Cycle-by-cycle variations of the end-gas compression history, the state variables, and the geometric shape cause a broad distribution of KI and KOCA. Under these conditions, a direct way to study the effects of engine operating variables and propane fraction in the fuel on KI and KOCA is an examination of their effects on the mean values of KI and KOCA. It is known from the literature that the mean values of KI and KOCA correlate well with the engine operating variables such as equivalence ratio and ignition timing [18,19]. Figure 5.18 shows the effects of equivalence ratio and propane fraction of the fuel on the KI. Prop. R. = 0% in the legend indicates that this fuel contains 0% propane in the natural gas. As can be seen from the figure, constant propane lines are not parallel, but a trend can be observed. KI increases with increasing equivalence ratio and propane ratio for all of the four fuel blends. However, when the equivalence ratio was increased from 0.80 to 0.82, the KI did not increase significantly for the 0% propane ratio and 5% propane ratio fuels. A similar trend is again observed with the 0% propane ratio fuel when the equivalence ratio was increased from 0.84 to 0.86. The reason for this behavior is not currently understood.

The increased KI with equivalence ratio can be explained by the fact that increased equivalence ratio causes higher end-gas energy content and end-gas temperature as explained in the previous chapter. Higher temperature probably causes faster reactions in the end-gas that increases the intensity of knock. A second reason is that the time period for establishing
Figure 5.18 Effect of equivalence and propane ratios on the KI

( Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
the radical pool will be shorter with increasing equivalence ratio and this will also cause earlier KOCA. The KI generally increases with earlier KOCA. As can be seen from Figure 5.19, KOCA is consistently earlier with increasing equivalence ratio and also with increasing propane ratio. The reason for earlier KOCA with increasing propane ratio is that the time period for establishing the radical species pool is shorter with the addition of propane to the mixture. As discussed in the background section, autoignition reactions are initiated at lower temperature with the addition of propane. It was also mentioned that the ignition delay is shorter with propane addition.

Figures 5.20 and 5.21 show the effect of ignition timing on KOCA and KI. Advancing the spark timing increases the end-gas pressure and temperature because the end-gas compression by the propagating flame starts earlier and most of the mixture is burned when the combustion volume is relatively smaller. Therefore, advancing the timing means that the end-gas pressure and temperature reach their maximums earlier. This explains why KOCA is earlier and for this reason KI is higher with advanced timing. Figures 5.20 and 5.21 show that retarding ignition timing is an efficient method for avoiding knock.

5.4 Summary

In this chapter the factors that are affecting the occurrence and intensity of the knock were examined. It was observed that the KOCA correlates very well with individual cycle pressure history. Therefore, individual cycle pressure history can be used for autoignition modeling. However, individual cycle KIs do not correlate well with parameters such as the unburned-mass fraction, burning rate, KOCA, and end-gas pressure and temperature. This poor correlation is attributed to cycle-by-cycle variations of the non-uniform end-gas state, variations in the geometric shape of the end-gas and its location within the combustion chamber.

Some other observations from the chapter can be listed as follows:
1. The high-pass filtered pressure data is a convenient way to characterize KI and KOCA.
2. The power spectral density of the knock signal at the first circumferential mode of acoustical resonance frequency, which is 5.5 kHz, is the highest of all modes.
Figure 5.19 Effect of equivalence and propane ratios on the KOCA
(Spark Timing = 26 degree CA BTDC, MAP = 1.4 bar).
Figure 5.20 Effect of spark timing on the KOCA
( Prop. R. = 15%, Eq. R. = 0.82, MAP = 1.4 bar).
Figure 5.21 Effect of spark timing on the KI
(Prop. R. = 15%, Eq. R. = 0.82, MAP = 1.4 bar).
3. The increasing equivalence ratio and propane fraction of the fuel cause earlier KOCA and higher KI.

4. Retarding the ignition timing is an efficient method for avoiding knock.

The next chapter will explain the model that will be developed for this project.
6. DEVELOPMENT OF THE AUTOIGNITION MODEL

The main objective of the present work was to develop an autoignition model for a John Deere 6076 natural gas engine. The model was expected to predict end-gas autoignition when combined with a cycle simulation model. The model needed to be able to handle variations in the equivalence ratio and the propane fractions of the natural gas. The previous chapters explained the methods used to determine the end-gas state variables and experimentally determine the KOCA and KI. In this chapter, the development of the autoignition model will be explained.

6.1 Introduction

Knock is harmful to the engine and audible knock will usually be taken as an indication of poor engine quality to drivers. Therefore, the engine compression ratio is generally designed conservatively to avoid knock. However, in order to increase the market share of an engine, it has to be as efficient as possible and for this reason has to have the highest possible compression ratio. Designing such an engine is challenging and requires extensive engine testing which can be very expensive. Computer models of engine processes are valuable tools for predicting and analyzing engine performance and allow exploration of many engine design alternatives in an inexpensive fashion. Recently, autoignition models have been developed to improve the predictive capabilities of cycle simulation models.

As discussed earlier, the basic autoignition models can be categorized as Global Models and Detailed Chemical Kinetic Models. Global models, which are based on global reaction schemes, are generally based on experimental data. Therefore, they can only be applied to new situations with great care. Detailed chemical kinetic models are based on the elementary reactions that occur during and after pre-flame reactions. The chemical kinetic schemes involve elementary reaction steps that are believed to be the real chemical reactions that occur between the species. Since the rate coefficients are determined based on fundamental chemical processes, there is no need to adjust any of the rate coefficients for different fuels or applications if all of the elementary reactions are known. However,
because of the complexity of petroleum-based engine fuels all of the elementary reactions may not be known. Therefore, even the current detailed chemical kinetics models may need some calibrations [79].

The flow and combustion processes in internal combustion engines are very complex. Accurate prediction of the end-gas thermodynamic state, which is very important for knock prediction, depends on flow dynamics in the intake manifold, heat transfer, and chemical reactions between the species. Modeling of all these processes is possible with multi-dimensional flow codes coupled to detailed chemical kinetic mechanisms. However, multi-dimensional modeling of all these processes from the intake manifold to the exhaust manifold requires extensive computation time and very powerful computers. If these multi-dimensional reactive flow codes require extensive amounts of time, they may not be used by engine designers. These codes are not still perfect and require some tuning with experimental engine data that requires expertise and even more computer time. In addition, engine designers may need model predictions at several initial conditions. If these predictions take extensive amounts of time with multi-dimensional codes, engine designers will prefer to use simple codes. There is a trade off between the accuracy of model predictions and computational time so engine designers must decide which way to proceed. The simplest and fastest way to model engine processes and end-gas autoignition is using a zero-dimensional model with estimated initial conditions at intake valve closing and combining it with a global autoignition model. The most complete and expensive method to model engine processes and end-gas autoignition is coupling a detailed chemical kinetic code to a multi-dimensional flow code such as the KIVA-CHEMKIN combination. It should also be remembered that each subroutine of the model must be compatible with the accuracy of all other subroutines.

### 6.2 Development of the Autoignition Correlation

As mentioned in the previous section, the end-gas autoignition is a complex chemical kinetics process that may involve thousands of elementary reaction steps and species. If all of the reaction steps and rate coefficients were known and very fast computation resources
were available at low cost, the most convenient way to predict the knock occurrence crank angle (KOCA) would be using a detailed chemical kinetics model coupled to a 3 dimensional code such as KIVA or FLUENT. However, lack of knowledge of the elementary reaction steps and rate coefficients and expensive computation time caused by the difficulty of analyzing thousands of equations make global models more useful for engine designers.

In the previous chapter it was observed that the individual cycle pressure history correlates very well with the KOCA. Therefore, by using a global model based on the cylinder pressure history, the KOCA can be predicted from cylinder pressure data. If a global model is developed based on an engine's experimental data, this model can be used for new engines with similar design in a predictive fashion. New developments in internal combustion engines have been evolutionary and radical changes to the combustion processes are not common. The most important parameters for global autoignition models are the pressure and temperature histories of the end-gas and these histories show similarities for most SI engines.

Rapid compression machine experiments are the earliest attempts to develop autoignition correlations for modeling. These machines compress a fuel-air mixture to a high pressure very quickly and keep the mixture at this state until the mixture autoignites. During the time interval from the end of compression to autoignition, the physical state is assumed to be constant and this period is called the ignition delay. The ignition delay time represents the time to establish the radical species pool. Once the radical pool is established these radicals consume fuel molecules very rapidly. The common approach to modeling the ignition delay is fitting an equation, which is usually in the form of an Arrhenius equation, to the experimental data. Equation 6.1 is a typical equation used to correlate the ignition delay time data.

\[
\tau = X_1 P^{X_2} \exp(X_3 Eu/T_u)
\]  

(6.1)

where \(\tau\) is the ignition delay, \(P\) is the pressure, \(T_u\) is the temperature, \(Eu\) is the temperature coefficient. \(X_1, X_2, X_3\) are experimental constants.
In a SI engine, however, the end-gas physical state is not constant. An ignition delay correlation developed from rapid compression machine experiments cannot be applied directly to determine the KOCA of SI engines.

Livengood and Wu [47] proposed a method by which an ignition delay correlation could be used to determine KOCA. The method is known as the knock integral method. It was proposed that a global reaction producing a fictitious species necessary for autoignition could be used to describe the process leading to knock. The global reaction has the following form:

\[
\frac{d[X]}{dt} = f(T_u, p, \Phi, fuel, t) \quad (6.2)
\]

where \([X]\) is the concentration of the fictitious species, \(T_u\) is the end-gas temperature, \(p\) is the pressure, \(t\) is the end-gas compression time, and \(\Phi\) is the equivalence ratio. Equation 6.2 implies that the rate of production of the fictitious species, which leads to autoignition, is a function of the end-gas temperature, pressure, equivalence ratio, fuel type, and the compression time. Further, it is assumed that there is a critical concentration of the species \([X]\) such that when this concentration is reached, the fuel molecules are consumed instantaneously [47]. The critical concentration, \([X_c]\), is constant for a given unburned mixture composition. It is further assumed that

\[
\frac{d\left(\frac{[X]}{[X_c]}\right)}{dt} = g(t / \tau) \quad (6.3)
\]

where \(g\) is a different function from \(f\). Equation 6.3 can be integrated over the autoignition reaction time as follows:

\[
\frac{[X]}{[X_c]} = \frac{\int_{t=\tau_{\text{min}}}^{t_{\tau_{\text{max}}}} g(t / \tau) dt}{\int_{t=\tau_{\text{min}}}^{t_{\tau_{\text{max}}}} 1 dt} = 1 \quad (6.4)
\]
where $t_c$ is the overall reaction time. Unfortunately, the form of function $g$ cannot be obtained from experimental data. However, if it is assumed that the reaction rate does not change with time during a constant state process, then

$$g(t/\tau) = 1/\tau$$  \hspace{1cm} (6.6)$$

and

$$\frac{[X]}{[X_c]} = \int_{t=0}^{t=a} (1/\tau) dt = 1$$  \hspace{1cm} (6.7)$$

If the state-time history of the end-gas and an ignition delay correlation are known, then Equation 6.7 can be integrated to predict the KOCA. Alternatively, if the state-time history of the end-gas and the KOCA are known, then a correlation for the ignition delay time which best fits the experimental data can be developed.

In this project, cylinder pressure data have been collected for different operating conditions of the engine. The KOCA for individual cycles was determined from these measured cylinder pressure data. The unburned mixture temperature was calculated using the two-zone thermodynamic model described in the Chapter 4. The substitution of an Arrhenius type equation such as Equation 6.1 into Equation 6.7 results in Equation 6.8. Equation 6.8 is a non-linear equation and the values of the coefficients $X_i, X_3,$ and $X_j$ that give the best fit to the experimental data can be determined.

$$\int_{t=0}^{t=a} \frac{dt}{X_1 \cdot p(t) \cdot X_2 \cdot \exp(X_3 E_u / T_u(t))} = 1$$  \hspace{1cm} (6.8)$$

A mathematical optimization technique was developed to determine the values of $X_i, X_3,$ and $X_j$ in Equation 6.9 that minimize the sum of the squares (SS) of the deviations between the integral and the theoretical value of the integral, which is 1 at $t_c$. 

N in Equation 6.9 is the number of individual cycles. Different types of autoignition correlations can be matched to the experimental data with this approach and compared for goodness of fit.

### 6.3 Steepest-Ascent Method for Optimization of the Model

There are a wide variety of search methods available in the literature for multivariable systems. In this project the Steepest-Ascent method as outlined by Stoecker [106] was used for optimization of the autoignition correlation. In this method the state point is moved in such a direction that the objective function changes at the greatest favorable rate. The gradient vector, given by Equation 6.10, indicates the direction of the maximum rate of change.

\[
\nabla y = \frac{\partial y}{\partial x_1} i_1 + \frac{\partial y}{\partial x_2} i_2 + \frac{\partial y}{\partial x_3} i_3
\]

where, \( i_1, i_2, \) and \( i_3 \) are unit vectors in the \( x_1, x_2, \) and \( x_3 \) directions, respectively.

The steps in the application of the method are as follows:

1. **Select a trial point:** The trial point should be chosen as near to the optimum as possible. A literature review for the trial point can be the best approach.

2. **Evaluate the gradient:** If analytical derivation is not possible, the partial derivatives can be computed numerically as follows:

\[
\frac{\partial y}{\partial x} = \frac{y(x, ..., x + \Delta x, ..., x) - y(x, ..., x)}{\Delta x}
\]

where, \( \Delta x \) is a small value.
3. **Evaluate the step size**: After guessing a $\Delta x$ for a variable the others can be determined as follows:

$$
\frac{\Delta x_i}{\partial y_i / \partial x_i} = \frac{\Delta x_j}{\partial y_j / \partial x_j} = \frac{\Delta x_k}{\partial y_k / \partial x_k} \tag{6.12}
$$

$\Delta x_i$ indicates the change in $x_i$, but a decision must be made whether to increase $x_i$ by $\Delta x_i$ or to decrease $x_i$. That decision is made by whether a maximization or minimization is being performed. If a minimization is in progress and $\partial y_i / \partial x_i$ is negative $x_i$ must be increased for $y$ to decrease as a result of the move.

3. **How far to move**: Move until reaching a minimum in the direction of gradient. Test it to determine whether the optimum has been achieved, if so, terminate. Otherwise calculate another gradient vector and repeat the steps.

### 6.4 Optimization of the Model

As mentioned earlier, if the physical state of the end-gas and the KOCA are known for individual cycles, then an autoignition correlation for the knock integral model can be developed. Equation 6.13 shows the function which was optimized for this project. Equation 6.13 is the same as Equation 6.9 but the time variable has been replaced by crank angle, CA.

$$
SS = \sum_{i=1}^{N} \left[ \int_{\theta - \pi}^{\theta + \pi} \frac{d\theta}{X_i * P_i(\theta)^*X_j * \exp(X_j E_i / T_i(\theta))} - 1 \right]^2 \tag{6.13}
$$

A FORTRAN program was developed for optimization of the coefficients $X_1$, $X_2$, and $X_3$. Figure 6.1 shows a flow chart of the program. The program starts with reading the trial values of the coefficients and the pressure and temperature data for the individual cycles. The two-zone thermodynamic model provides the unburned zone temperature data. The unburned zone is assumed to be adiabatic when determining the unburned gas temperature.
Although the real engine will have a temperature distribution in the end-gas, the autoignition will be initiated at the most favorable center which considered to be the highest temperature in the end-gas. This temperature will be best estimated by assuming adiabatic conditions. The assumption is assumed to be valid from the initiation of the second zone to the KOCA. The assumption of adiabatic end-gas is common for knock models[19, 79].

The integration is performed from Bottom Dead Center to the experimentally determined KOCA for the cycle. Then, the calculated value of the KOCA is compared to the measured value to determine the square of the error. This computation is repeated for the N individual cycles of the particular engine operating condition and the sum of squares of errors (SS) for all N cycles is computed. If the SS is less than the tolerance, the computation is stopped. Otherwise, the derivatives with respect to $X_1$, $X_2$, and $X_3$ are computed, the direction to move is determined, the adjustments are made to the coefficients $X_1$, $X_2$, and $X_3$, and the SS is computed again. The SS is determined at every move to determine the minimum value of SS for the particular operating condition. Once the minimum is determined and if the minimum is less than the tolerance, the computation is finished for the particular engine operating condition.

Table 6.1 shows 16 different engine-operating conditions for which the optimization was performed along with the optimum values of the coefficients, and the SS per cycle (SSPC). The optimization was performed only for the knocking cycles of two hundred consecutive cycles. As can be seen from the table, the SSPC is generally higher for the operating conditions that have a lower knocking percentage of knocking cycles. At those conditions where the percentage of knocking cycles is low, the equivalence ratio is also leaner. As was seen in Figure 5.19, the mean KOCA is later for leaner mixtures and, as was seen in Figure 5.17, for later KOCAs, the KI is generally lower. One possible reason for the higher SSPC is that the model's prediction of end-gas temperature may not be accurate through the end of combustion and for this reason the correlation does not fit the experimental data well. The actual end-gas temperature may be significantly cooler than the computed adiabatic end-gas temperature through the end of combustion and the adiabatic
START

READ
X_1, X_2, X_3

COMPUTE
SS(X_1, X_2, X_3)

PRINT
X_1, X_2, X_3

SS<TO

yes

no

COMPUTE
\frac{dSS}{dX_1}, \frac{dSS}{dX_2}, \frac{dSS}{dX_3}

\frac{dX_1}{dSS/dX_1} = \frac{dX_2}{dSS/dX_2} = \frac{dX_3}{dSS/dX_3}

choose the dX_i, compute dX_2 and dX_3

X_1 = X_1 + dX_1,
X_2 = X_2 + dX_2,
X_3 = X_3 + dX_3

COMPUTE
SS(X_1, X_2, X_3)

SS<TO

no

yes

PRINT
X_1, X_2, X_3

STOP

Figure 6.1 Flow Chart of the optimization program
Table 6.1 Three variable optimization of the model.

<table>
<thead>
<tr>
<th>Propane Ratio</th>
<th>Equivalence Ratio</th>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
<th>%K. Cycles</th>
<th>SSPC</th>
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<tr>
<td>0%</td>
<td>0.8</td>
<td>1.033</td>
<td>-0.903</td>
<td>7.026</td>
<td>9</td>
<td>5.39</td>
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<tr>
<td>0%</td>
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<td>-0.916</td>
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<td>36</td>
<td>8.29</td>
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<td>0%</td>
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<td>6.979</td>
<td>74</td>
<td>5.05</td>
</tr>
<tr>
<td>0%</td>
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<td>0.992</td>
<td>-0.914</td>
<td>6.983</td>
<td>94</td>
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</tr>
<tr>
<td>5%</td>
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<td>17.78</td>
</tr>
<tr>
<td>5%</td>
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<td>6.982</td>
<td>30</td>
<td>8.62</td>
</tr>
<tr>
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<td>0.986</td>
<td>-0.916</td>
<td>6.978</td>
<td>66</td>
<td>7.92</td>
</tr>
<tr>
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<td>-0.943</td>
<td>6.978</td>
<td>89</td>
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</tr>
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<td>8.63</td>
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<td>6.959</td>
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<td>10%</td>
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<td>6.05</td>
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<tr>
<td>15%</td>
<td>0.76</td>
<td>0.896</td>
<td>-0.880</td>
<td>6.814</td>
<td>8</td>
<td>15.67</td>
</tr>
<tr>
<td>15%</td>
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</tr>
<tr>
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<td>8.30</td>
</tr>
<tr>
<td>15%</td>
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<td>1.012</td>
<td>-0.955</td>
<td>6.923</td>
<td>94</td>
<td>4.72</td>
</tr>
</tbody>
</table>

%K. Cycles = Percentage of knocking cycles in 200 consecutive cycles.
SSPC = Sum of squares of errors per cycle.

assumption is not good for this case. However, the adiabatic end-gas temperature assumption provides better fits for the earlier, more intense knocking cycles which are the most important cycles for borderline knock threshold determination [19, 79]. As can be seen from Table 6.1, the coefficients show variations with the operating conditions. The 3 variable optimization of the model produced 16 different values for each coefficient. To simplify this model, it is desirable to have less than three coefficients ($X_1$, $X_2$, $X_3$) which provides the best fit to the model over a wide operating range of the engine. Therefore, the average value of $X_1$ was chosen as a constant value of $X_1$ for the model and the model was reoptimized for $X_2$ and $X_3$. Then, the average of the $X_2$ values was chosen as a constant value of $X_2$ for the model and the model was re-optimized for $X_3$ only. Table 6.2 shows the results of the single variable optimization of the model. During single variable optimization
the temperature coefficient $Eu$ was changed to 7000 from 1000, for this reason the magnitudes of $X_j$ are lower than that of Table 6.1. As can be seen from the table, the SSPC values do not change significantly between the 3 and the single variable optimization. Now, there are 16 different $X_j$ values to be reduced to a single $X_j$ or to an equation that fits these $X_j$ values.

Figure 6.2 shows the variations of $X_j$ with the equivalence ratio and propane ratio. As can be seen from the figure, $X_j$ is generally higher with leaner mixtures and also with the mixtures that have lower propane ratio. There is one exception to this generalization at the equivalence ratio of 0.78. As can be seen from the figure, the $X_j$ value is lower at this equivalence ratio than that of 0.80 on the 10% propane ratio line. And, the $X_j$ is higher at this equivalence ratio than that of 0.76 on the 15% propane ratio line. The reason for this unexpected trend could be possible variations in room temperature and the manifold absolute

<table>
<thead>
<tr>
<th>Propane Ratio</th>
<th>Equivalence Ratio</th>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_3$</th>
<th>%K. Cycles</th>
<th>SSPC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>0.8</td>
<td>0.9850</td>
<td>-0.887</td>
<td>1.0011</td>
<td>9</td>
<td>5.38</td>
</tr>
<tr>
<td>0%</td>
<td>0.82</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9849</td>
<td>36</td>
<td>8.18</td>
</tr>
<tr>
<td>0%</td>
<td>0.84</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9730</td>
<td>74</td>
<td>4.98</td>
</tr>
<tr>
<td>0%</td>
<td>0.86</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9831</td>
<td>94</td>
<td>5.85</td>
</tr>
<tr>
<td>5%</td>
<td>0.78</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9611</td>
<td>4</td>
<td>16.89</td>
</tr>
<tr>
<td>5%</td>
<td>0.8</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9816</td>
<td>30</td>
<td>8.59</td>
</tr>
<tr>
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<td>0.82</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9800</td>
<td>66</td>
<td>7.95</td>
</tr>
<tr>
<td>5%</td>
<td>0.84</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9684</td>
<td>89</td>
<td>6.97</td>
</tr>
<tr>
<td>10%</td>
<td>0.76</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9767</td>
<td>5</td>
<td>7.22</td>
</tr>
<tr>
<td>10%</td>
<td>0.78</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9648</td>
<td>35</td>
<td>8.63</td>
</tr>
<tr>
<td>10%</td>
<td>0.8</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9679</td>
<td>62</td>
<td>5.45</td>
</tr>
<tr>
<td>10%</td>
<td>0.82</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9584</td>
<td>90</td>
<td>6.10</td>
</tr>
<tr>
<td>15%</td>
<td>0.76</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9648</td>
<td>8</td>
<td>15.67</td>
</tr>
<tr>
<td>15%</td>
<td>0.78</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9667</td>
<td>49</td>
<td>9.44</td>
</tr>
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<td>15%</td>
<td>0.8</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9579</td>
<td>73</td>
<td>8.07</td>
</tr>
<tr>
<td>15%</td>
<td>0.82</td>
<td>0.9850</td>
<td>-0.887</td>
<td>0.9552</td>
<td>94</td>
<td>4.81</td>
</tr>
</tbody>
</table>
Figure 6.2 Variation of $X_3$ with the equivalence ratio and propane ratio

$\{X_1 = 0.985, X_2 = -0.887\}$.
pressure (MAP) between the two experiments which were supposed to be constant. While the equivalence ratio and the propane ratio were changing over a wide range, choosing the average of the \( X_3 \) values produced significant errors. Therefore, it was decided to develop an equation in terms of the equivalence ratios and the propane ratios to correlate the values of \( X_3 \). Equation 6.14 is a somewhat complicated equation with 4 constants. It was desirable to develop an equation that is as simple as possible, however slight variations in \( X_3 \) causes significant variation in the prediction of the KOCA because of the exponent term in the model. Therefore the flexibility provided by Equation 6.14 was preferred.

\[
x_3 = (-0.575 + (a_1*PR+a_2*PR^2))*EQR+(1.456+(b_1*PR+b_2*PR^2))
\]  

(6.14)

\( PR \) is the propane ratio by volume, \( EQR \) is the equivalence ratio, and, the constants determined by minimizing the sum of the squares are:

\[
\begin{align*}
a_1 &= 10.058 & b_1 &= -8.703 \\
a_2 &= -54.053 & b_2 &= 43.615
\end{align*}
\]

6.5 Accuracy in the Model’s Prediction of KOCA

The SSPC in Table 6.2 is a measure of the accuracy of the model but it does not show the difference between the experimental KOCA and the model’s prediction explicitly, in terms of CA. It is desirable to determine the accuracy of the model before incorporating it in a cycle simulation program. In order to determine the accuracy, the model was combined with the two-zone model and the model’s predictions were compared with the experimental KOCA for 16 different engine operating conditions. The two-zone model provided the unburned zone temperature.

Table 6.3 shows the average and standard deviation of the errors in the model’s predictions for the 16 different engine operating conditions. As can be seen from this table, the average error in the predictions is less than 1 degree CA in general and the standard
Table 6.3 Average and standard deviation of errors in KOCA prediction.

<table>
<thead>
<tr>
<th>Propane Ratio</th>
<th>Equivalence Ratio</th>
<th>Percentage of Knocking Cycles</th>
<th>Average, CA</th>
<th>Standard Deviation, CA</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>0.8</td>
<td>9</td>
<td>0.83</td>
<td>2.35</td>
</tr>
<tr>
<td>0%</td>
<td>0.82</td>
<td>36</td>
<td>0.55</td>
<td>2.85</td>
</tr>
<tr>
<td>0%</td>
<td>0.84</td>
<td>74</td>
<td>0.41</td>
<td>2.20</td>
</tr>
<tr>
<td>0%</td>
<td>0.86</td>
<td>94</td>
<td>0.37</td>
<td>2.21</td>
</tr>
<tr>
<td>5%</td>
<td>0.78</td>
<td>4</td>
<td>4.23</td>
<td>7.05</td>
</tr>
<tr>
<td>5%</td>
<td>0.8</td>
<td>30</td>
<td>0.32</td>
<td>2.99</td>
</tr>
<tr>
<td>5%</td>
<td>0.82</td>
<td>66</td>
<td>1.01</td>
<td>2.73</td>
</tr>
<tr>
<td>5%</td>
<td>0.84</td>
<td>89</td>
<td>0.67</td>
<td>2.60</td>
</tr>
<tr>
<td>10%</td>
<td>0.76</td>
<td>5</td>
<td>0.70</td>
<td>3.05</td>
</tr>
<tr>
<td>10%</td>
<td>0.78</td>
<td>35</td>
<td>-0.18</td>
<td>3.12</td>
</tr>
<tr>
<td>10%</td>
<td>0.8</td>
<td>62</td>
<td>0.66</td>
<td>2.29</td>
</tr>
<tr>
<td>10%</td>
<td>0.82</td>
<td>90</td>
<td>0.35</td>
<td>2.46</td>
</tr>
<tr>
<td>15%</td>
<td>0.76</td>
<td>8</td>
<td>1.37</td>
<td>3.86</td>
</tr>
<tr>
<td>15%</td>
<td>0.78</td>
<td>49</td>
<td>1.52</td>
<td>2.78</td>
</tr>
<tr>
<td>15%</td>
<td>0.8</td>
<td>73</td>
<td>0.42</td>
<td>2.88</td>
</tr>
<tr>
<td>15%</td>
<td>0.82</td>
<td>94</td>
<td>0.50</td>
<td>2.16</td>
</tr>
</tbody>
</table>

deviation in the errors is generally less than 3 degrees. For better accuracy, the model could be further tuned for a specific engine operating condition by modifying the model constants if experimental data is available.

6.6 Summary

This chapter has shown that if the state time history of the end-gas and autoignition correlation are known, then the knock integral can be used to predict the KOCA. Alternatively, if the state-time history of the end-gas and the KOCA are known, an autoignition correlation which fits the experimental data can be developed. The Steepest-Ascent method is an effective method for optimization of the autoignition correlation. The optimized correlation described here can predict 95% of the knocking cycles within ±6
degrees of CA. At the engine operating conditions where the percentage of knocking cycles is low, the average and the standard deviation of errors are generally higher. The reason for this is probably inaccurate end-gas temperature prediction of the two-zone model at these conditions.
7. GOVERNING EQUATIONS FOR ZERO-DIMENSIONAL AND MULTI-DIMENSIONAL MODELS

Zero-dimensional models are the most commonly preferred analytical tools for internal combustion engine development. Because of its simplicity, the predictive capability of this type of models are limited. However, if the model is tuned by experimental data for various engine operating conditions the model can simulate engine operating conditions very quickly and accurately. Multi-Dimensional models on the other hand are very sophisticated models and they can provide detailed information about the process both spatially and temporally. They are very powerful tools to determine engine emission formation and are attracting increasing attention as the EPA regulates exhaust emissions with an increasing intensity. The most commonly used multi-dimensional engine modeling code is KIVA, which is a transient reactive flow code. The governing equations for both models are presented in the following sections.

7.1 Zero-Dimensional Two-Zone Model

In section 4.1, a two-zone thermodynamic model for spark ignition engines was developed. That model calculates a mass burning rate from given cylinder pressure data. If the mass-burning rate is given, the equations of the same model can be solved to calculate the cylinder pressure and the model can be used for parametric studies.

The Zero-D model developed in the current project avoids attempting to predict directly the detailed features of turbulent flame propagation. Instead, through an assumed mass burn rate model, the thermodynamic states of both the burned and unburned zones are computed.

Heywood [36] suggests that the mass burning fraction may be represented by a Weibe function as given in Equation 7.1.

\[ x_b = 1 - \exp[-\left(\frac{\theta - \theta_0}{\Delta \theta}\right)^m + 1] \]  

(7.1)
Where $\theta$ is the crank angle, $\theta_0$ is the start of combustion, $\Delta\theta$ is the total combustion duration, $x_b$ is the burned mass fraction, $a$ and $m$ are adjustable parameters which fix the shape of the curve. The model’s adjustable parameters and the combustion duration are determined for various engine operating conditions by matching the derivative of the Wiebe function to the experimental mass burning rate.

As explained in section 4.2, the combustion process in a spark ignition engine progresses in two stages, the flame initiation period (FIP) and the flame propagation period (FPP). The flame initiation period is the period in which the growth of the flame kernel has proceeded to a size where the flame front for turbulent propagation is established. Since the transition from FIP to FPP is not marked precisely by a distinct measurable characteristic, it is arbitrarily defined in terms of the burned mass fraction. This fraction typically ranges from 1% to 10%. In this project, the FIP was assumed to be the crank angle period from the spark firing to where 1% of the mass has been burned.

Simple engine models generally ignore FIP and the combustion may be started with the assumption of up to 10% of the mixture already burned instead of starting combustion model with the time when the spark fires. In the current project, the FIP was modeled by using the single step global reaction scheme of Abraham [107], which is used for conversion of reactants to products. With this model, the time rate of change of species mass fraction due to conversion from one species to another given by

$$\frac{dX_i}{dt} = -\frac{X_i - X_i^*}{\tau}$$ (7.2)

where $X_i$ is the mass fraction of species $i$ and $X_i^*$ is the local and instantaneous thermodynamic equilibrium value of the mass fraction.

The characteristic conversion time $\tau$ for the achievement of equilibrium is assumed to be the sum of the local laminar kinetics time, $\tau_L$, and the turbulent mixing time, $\tau_t$.

$$\tau = \tau_L + \tau_t$$ (7.3)
The present computation only considers the laminar conversion time since the laminar kinetics effects are known to be important during the FIP. The laminar conversion time constants $A_{\text{ign}}$, $n_{\text{ign}}$, and $E_{\text{ign}}$ as shown in Equation 7.4 can be determined by matching the experimentally determined FIP from various operating conditions of the engine.

$$\tau_l = A_{\text{ign}} \cdot T \cdot P^{n_{\text{ign}}} \cdot \exp \left[ 1 + 0.08 \cdot \phi - 1.15 \cdot E_{\text{ign}} / (R_T \cdot T) \right]$$  \hspace{1cm} (7.4)$$

where $\phi$ is the equivalence ratio, $T$ is the temperature, $P$ is the pressure, and the $R_T$ is the universal gas constant.

7.2 Multi-Dimensional Model

The multi-dimensional computations in this project were performed using the computational fluid dynamics code KIVA-3V Release 2 [108]. This model intends to describe the real engine processes by considering temporal and spatial variations of the flow field, temperature, pressure, species composition, and turbulence within the combustion chamber. The code solves the mass, momentum, energy conservation equations, coupled with the $k$-$\varepsilon$ turbulence model in three dimensions as a function of time. The governing equations and the numerical solution method have been discussed in detail by Amsden et al. [109]. The governing equations will be described in the following sections.

7.2.1 The Governing Equations

The governing equations can be used to solve both laminar and turbulent flows. The mass, momentum, and energy equations for two cases differ primarily in the form and magnitude of the transport coefficients (viscosity, thermal conductivity, and species diffusivity), which are much larger in the turbulent case, because of the additional transport caused by turbulent fluctuations. In the turbulent case the transport coefficients are derived.
from a turbulent diffusivity that depends on the turbulent kinetic energy and its dissipation rate. For compactness, the equations are written in vector notation. The unit vectors in the \( x \), \( y \), and \( z \) directions are donated by \( i \), \( j \), and \( k \) respectively. The position vector \( \mathbf{x} \) is given by:

\[
\mathbf{x} = xi + yj + zk \tag{7.5}
\]

the vector operator \( \nabla \) is given by:

\[
\nabla = i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z} \tag{7.6}
\]

and the fluid velocity vector \( \mathbf{u} \) is given by:

\[
\mathbf{u} = u(x, y, z, t) i + v(x, y, z, t) j + w(x, y, z, t) k \tag{7.7}
\]

where \( u \), \( v \), and \( w \) are the \( x \), \( y \), and \( z \) components of the velocity vector and \( t \) is the time.

The continuity equation for species \( m \) is given by:

\[
\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}) = \nabla \cdot \left( \rho D \nabla \left( \frac{\rho_m}{\rho} \right) \right) + \rho_m^\prime + \rho \delta_{m1} \tag{7.8}
\]

where \( \rho_m \) is the mass density of species \( m \), \( \rho \) is the total mass density. Fick's law of diffusion is assumed with a single diffusion coefficient \( D \). The \( \rho_m^\prime \) is a source term due to chemical reactions and \( \rho \delta_{m1} \) is a source term due to the spray. Species 1 is the species of which the spray droplets are composed, and \( \delta \) is the Dirac delta function. Summation of Equation 7.8 over all species gives the total fluid density as follows:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \rho^\prime \tag{7.9}
\]
The momentum equation for the mixture is given by:

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\frac{1}{a^2} \nabla P - \mathcal{A}_n \nabla \left( \frac{2}{3} \mathbf{p} \mathbf{k} \right) + \nabla \cdot \mathbf{\tau} + F + \rho g \quad (7.10)
\]

where \( P \) is the fluid pressure. The dimensionless quantity "\( a \)" is used in conjunction with the Pressure Gradient Scaling (PGS) method. This is a method for enhancing the computational efficiency in low MACH number flows, where the pressure is nearly uniform. \( \mathcal{A}_n \) is zero in laminar calculations and unity for turbulent calculations. \( \mathbf{\tau} \) is the viscous stress tensor in Newtonian form. \( F \) is the rate of momentum gain per unit volume due to the spray and \( g \) is the specific body force constant.

The internal energy equation is given by:

\[
\frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho \mathbf{u} I) = -\rho \nabla \cdot \mathbf{u} + \left( 1 - \mathcal{A}_n \right) \nabla \cdot \mathbf{\tau} - \nabla \cdot \mathbf{J} + \mathcal{A}_n \rho \varepsilon + Q^c + Q^* \quad (7.11)
\]

where \( I \) is the specific internal energy, exclusive of chemical energy. The heat flux vector \( \mathbf{J} \) is the sum of contributions due to heat conduction and enthalpy diffusion.

\[
\mathbf{J} = -K \nabla T - \rho D \sum_m h_m \nabla \left( \frac{\rho_m}{\rho} \right) \quad (7.12)
\]

where \( K \) is the conduction coefficient, \( T \) is the temperature, and \( h_m \) is the specific enthalpy of species \( m \). \( Q^c \) and \( Q^* \) are the source terms due to chemical heat release and spray interactions, respectively.

Two additional transport equations to solve for the turbulent kinetic energy and its dissipation rate are given by:

\[
\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} k) = \nabla \cdot (\rho \nabla D \nabla k) - \rho \varepsilon + P \quad (7.13)
\]
and
\[
\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho \mathbf{u} e) = \nabla \cdot \left( \rho \sigma D \nabla e \right) + C_{\varepsilon} \rho \frac{\varepsilon}{k} - C_{\varepsilon} \rho e \varepsilon : + C_{\varepsilon} \rho e \nabla \cdot \mathbf{u} \tag{7.14}
\]
where
\[
P = \rho D \left[ 2 (\nabla \cdot \mathbf{u})^2 + (\nabla \cdot \mathbf{u} + \nabla \cdot \mathbf{u}^T)^2 - \frac{2}{3} (\nabla \cdot \mathbf{u})^2 \right] - \frac{2}{3} \rho k \nabla \cdot \mathbf{u} \tag{7.15}
\]
and the conventional turbulence model constants used were as follows:
\[
C_{\varepsilon} = 1.45, \quad C_{\omega} = 1.92, \quad C_{\omega} = -1.0, \quad \sigma_k = 1.0, \quad \text{and} \quad \sigma_{\varepsilon} = 0.7
\]
Near a wall the \(k-\varepsilon\) equation becomes as follows:
\[
k = C_u \varepsilon^4 = \frac{C_u}{u_L} \frac{\tau_u}{\rho \varepsilon} \tag{7.16}
\]
\[
\varepsilon = \frac{C_u}{k} \frac{k^{3.5}}{y} \tag{7.17}
\]
where the assumptions of quasi-steadiness, low Mach number, and high Reynolds number have been made.

The computations were started at intake valve closure (IVC). The gas temperature, pressure, and species density were assumed to be uniform throughout the chamber at IVC. The amount of residual mass fractions was estimated to be 5%. The initial mixture temperature was adjusted so that the experimental mass flow rate could be matched.

Turbulence was initialized using the equations of Grasso et al. [110] as follows:
\[
k_{\text{IVC}} = 0.165 U_i^2 \tag{7.18}
\]
\[
\varepsilon_{\text{IVC}} = 0.055 U_i^2 / A_i^{0.5} \tag{7.19}
\]
where $U_i$ and $A_i$ are the average values of the intake-flow velocity and the valve-open area during the intake period. These quantities were estimated from the valve lift, trapped mass, and the valve specifications.

The wall heat flux model of KIVA is a modified version of the model of Launder and Spalding [111]. The equations are given as follows:

\[
Q_w = \frac{\rho U_i c_i}{Pr_i} F (T - T_w),
\]

where

\[
F = \begin{cases} 
\frac{R'}{Pr_i RPR} & \text{if } R' \geq 11.05 \\
(1/\kappa) \ln R' + B + 11.05(Pr_i RPR - 1) & \text{if } R' \leq 11.05 
\end{cases}
\]

\[
F = 1.0 \quad \text{if } R' \leq 11.05
\]

where

\[
R' = \frac{c_{nu}^{0.25} k^{0.5} y}{v_l}
\]

where $v_l$ is the laminar kinematic viscosity of air, $Pr_i$ is the laminar Prandtl number, $\kappa$ is the Karman’s constant, $RPR$ is the reciprocal of the turbulent Prandtl number, and $T_w$ is the wall temperature. The gas temperature $T$, turbulent kinetic energy $k$, and the distance from the wall $y$ are evaluated at the midpoint of the face that lies opposite the wall face of the computational call next to the wall.

The state relations are assumed to be those of an ideal gas mixture as follows:
\[ P = R_n T \sum_m \left( \rho_m / W_m \right) \]  

(7.24)

\[ l(T) = \sum_m (\rho_m / \rho) I_m(T) \]  

(7.25)

\[ c_p(T) = \sum_m (\rho_m / \rho) c_{pm}(T) \]  

(7.26)

\[ h_m(T) = l_m(T) + R_n T / W_m \]  

(7.27)

where \( R_n \) is the universal gas constant; \( W_m \) is the molecular weight of species \( m \). \( I_m(T) \) is the specific internal energy of species \( m \) and \( c_{pm}(T) \) is the specific heat of species \( m \) are taken from the JANAF tables [112].

The chemical reactions occurring in the system are symbolized by

\[ \sum_m a_{mr} \chi_m \rightleftharpoons \sum_m h_{mr} \chi_m \]  

(7.28)

where \( a_{mr} \) and \( h_{mr} \) are the integral stoichiometric coefficients for reaction \( r \).

There are two types of chemical reactions: those that proceed kinetically and those that are assumed to be in equilibrium. Kinetic reaction \( r \) proceeds at a rate \( \dot{\omega}_r \) given by

\[ \dot{\omega}_r = k_{fr} \prod_m \left( \rho_m / W_m \right)^{amr} - k_{hr} \prod_m \left( \rho_m / W_m \right)^{hm} \]  

(7.29)

\( amr \) and \( hmr \) do not have to be equal to the stoichiometric coefficients so that empirical reaction orders can be used. The coefficients \( k_{fr} \) and \( k_{hr} \) are assumed to be of a generalized Arrhenius form as follows:

\[ k_{fr} = A_{fr} T^{qfr} \text{EXP}(\frac{-E_{fr}}{T}) \]  

(7.30)
and

\[ k_{lr} = A_{lr} T^{e_{lr}} \exp(-E_{lr} T) \tag{7.31} \]

The rates of equilibrium reactions are implicitly determined by the constraint conditions given by

\[ \prod (\rho_{m} \dot{W}_{m})^{b_{m}} = K_{r}^{'}(T) \tag{7.32} \]

where \( K_{r}^{'}(T) \) is the concentration equilibrium constant that has the following form:

\[ K_{r}^{'}(T) = \exp(A_{r} \ln T + B_{r} / T + C_{r} + D_{r} T + E_{r} T^{2}) \tag{7.33} \]

where \( T_{\text{at}} = T/1000 \text{ K} \).

If the reaction rates, \( \omega_{r} \), determined for either the kinetic or equilibrium reactions then the chemical source term in the species continuity equation is given by

\[ \rho_{m}^{'} = W_{m} \sum_{r} (b_{mr} - a_{mr}) \omega_{r} \tag{7.34} \]

and the chemical heat release term in the energy equation is given by

\[ Q^{r} = \sum_{r} Q_{r} \omega_{r} \tag{7.35} \]

where \( Q_{r} \) is the negative of the heat of reaction at absolute zero and given by

\[ Q_{r} = \sum_{m} (a_{mr} - b_{mr}) (\Delta h_{m}^{r}) \tag{7.36} \]
and $\Delta h_i^*$ is the heat of formation of species $m$ at absolute zero.

In this chapter, the governing equations for both the Zero-D model and the Multi-D models were presented. In the next chapter a sensitivity and parametric study will be conducted using both of the models.
8. RESULTS AND DISCUSSION

This chapter involves two main sections. The first part discusses the sensitivity of the models to variations of the initial conditions and a model tuning constant. It is beneficial to study the relative effects of uncertainties in the input parameters and the model constant on the predictions. The second section presents a parametric study. In this section, the autoignition model, which was developed in Chapter 6, will be incorporated with the models and a parametric study will be performed to determine the knock-limited operating conditions of the engine.

8.1 Sensitivity Study

To determine the sensitivity of both models to variations in the initial conditions, the experimental engine cylinder pressure data will be simulated using both the Zero-Dimensional (Zero-D) and Multi-Dimensional (Multi-D) models for a baseline condition. Then the model's response to variations in the input parameters will be observed. To save computer time, the multi-dimensional computations will be performed in 2-dimensions. Table 8.1 shows the matrix for the sensitivity study. In the baseline condition, the model tuning constants were tuned so that the deviation between the simulated and measured cylinder pressure trace is a minimum.

The tuning constants for the Zero-D model are the Wiebe function constants $\Delta \theta$, $a$, and $m$ and the ignition model constants $A_{\text{ig}}, n_{\text{ig}}$, and $E_{\text{ig}}$. The constants for the Multi-D model are the turbulence constant (CAPA) and the pre-exponential factor for the kinetic reaction $A_0$.

Figure 8.1 shows the measured and simulated pressure traces for the baseline condition. As can be seen from the figure, the Zero-D model can be tuned so that the measured data can be simulated very well. However, the Multi-D simulation, although tuned for the best match, still shows significant deviation from the measured data. The maximum cylinder pressure is almost 20% higher for the Multi-D simulation than that of the measured. The possible reason for such a high deviation is KIVA's chemical kinetic model for
Table 8.1 shows the matrix for sensitivity study.

<table>
<thead>
<tr>
<th>Conditions</th>
<th>Mixture temp. at IVC</th>
<th>Mixture press. at IVC</th>
<th>Turbulence factor, CAPA</th>
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</thead>
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</table>

Combustion. It is a single step oxidation model, which converts fuel and oxygen to carbon dioxide and water. The real combustion process would be much more complex than a single step mechanism, therefore the accuracy will be limited but under some conditions it can be satisfactory. It is generally recommended by KIVA users that the kinetic chemistry subroutine CHEM be replaced with a more sophisticated model. It is generally agreed that the single step reaction mechanism either predicts the burning rate to be too fast or too slow depending on the pre-exponential factor [108, 113, 114]. It is also suggested that the optional mixing-controlled combustion model can be used to mitigate the dependency on the pre-exponential factor. If the mixing-controlled combustion model is chosen, the burning rates are computed by the kinetic and the mixing-controlled models and the maximum is chosen as the burning rate.

The estimated mixture temperature at intake valve closing (IVC) depends on the estimated values for the residual mass fraction. Although the amount and temperature of the residuals could be estimated, there is uncertainty in determining these quantities. It will be very useful to determine sensitivity of the models to the initial conditions. In this project, the residual mass fraction was estimated to be 5% of the mass flow rate. Figures 8.2 and 8.3 show the effect of initial mixture temperature on both the Zero-D and Multi-D model predictions. As can be seen from Figure 8.2, higher initial temperatures increase the peak pressures. The reasons for the higher peak pressures with the higher temperature are probably increased fuel conversion rate for the Multi-D model and shorter FIP for the Zero-D
Figure 8.1 Comparison of measured and simulated cylinder pressure traces at baseline condition (Comp. R. = 10.5, Prop. R. = 0%, Eq. R. = 0.82, MAP = 1.4 bar).
Figure 8.2 Sensitivity of the models on higher initial temperatures.
Any increase in temperature during ignition significantly increases the laminar flame speed which makes the FIP shorter. Figure 8.3 shows the effect of lower initial temperatures on the model generated pressure traces. As can be seen from the figures the peak pressures are lower than that of the baseline. However, the Multi-D model shows a stronger dependency on the temperature when compared to the Zero-D model.

Determination of cylinder pressure at IVC may also involve significant error. It is generally assumed that the cylinder pressure at IVC is equal to the intake manifold pressure. However, because of the dynamics in the intake manifold the pressures may not be equal. Figures 8.4 and 8.5 show the effect of initial pressure on the model predictions. As can be seen from the figures, the model predictions have similar trends. The higher the initial pressure the higher the maximum pressures.

As mentioned earlier, the mixing controlled combustion model is used to improve the predictive capability of KIVA. The mixing controlled combustion model of Magnussen et al. [115] was modified by Amsden [108] for the current version of KIVA. It produces a dependency of the turbulent flame speed on the square root of the turbulent kinetic energy, $k$, and with no dependence on the dissipation, $\epsilon$. The model has two tuning parameters, CAPA and CAPB. CAPA relates to the turbulent reaction rate. The range of CAPA is from near unity for heavy diesel fuels to 100 for hydrogen. It is generally recommended that CAPA is best chosen by experimental comparison and then held constant for similar operating conditions. CAPB is set to 0.5 within KIVA and it should not require modifications [108]. Figure 8.6 shows the effect of CAPA on the predicted cylinder pressure. As can be seen from the figure, increasing CAPA increases the burning rate and the peak pressure is higher.

### 8.2 Parametric Study

The objective of the present work was to develop a global autoignition model that could be incorporated into engine simulation models to determine knock-limited engine operating conditions. Knock limitation provides a realistic constraint as compression ratio and turbo-charging are increased in a SI engine. Therefore, it is imperative to incorporate
Figure 8.3 Sensitivity of the models on lower initial temperatures.
Figure 8.4 Sensitivity of Multi-D model on initial pressure.
Figure 8.5 Sensitivity of the Zero-D model on initial pressures.
Figure 8.6 Sensitivity of Multi-D model on tuning parameter CAPA.
autoignition models with analytical engine models. In this section, the autoignition model which is developed in Chapter 6 will be incorporated with both the Zero-D and Multi-D models and a parametric study will be performed to determine the effect of engine operating parameters on KOCA and Kl. The following operating conditions will be studied.

- Equivalence ratio
- Propane ratio in natural gas
- Spark timing
- Compression ratio
- Initial conditions

As mentioned earlier the individual cycle Kl does not correlate well with the engine operating parameters although KOCA does. However, the maximum possible Kl can be modeled as if all the end-gas releases its chemical energy in very short time at the time of KOCA and the rise in the cylinder pressure can be characterized as the Kl.

For the Zero-D model it is assumed that the end-gas is standard air and all the end-gas energy is released at constant volume. The Kl model can be formulated as follows:

\[ Q_{auto} = m_{end\text{-gas}} c_v (T - T_u) \]  \hspace{1cm} (8.1)

\[ P = \frac{T}{T_u} P_u \]  \hspace{1cm} (8.2)

where \( Q_{auto} \) is the energy released from the end-gas, \( m_{end\text{-gas}} \) is the mass of the end-gas, \( c_v \) is the specific heat at constant volume, \( T \) is the mixture temperature after autoignition, \( T_u \) is the end-gas temperature before autoignition, and the \( P \) is the pressure after autoignition.

For the Multi-D model, the pre-exponential factor of the forward reaction rate is arbitrarily multiplied by 100 after the KOCA so that the burning rate can be increased similar to the burning rate of autoignition.
These Kl modeling methods are very simple way to model Kl intensity and both intensity magnitudes and cylinder pressure traces can be significantly different from real cylinder pressure during and after the knock. However, the trends in the maximum possible Kl with variations of engine operating conditions can be observed, which provide some useful information to the engine designers.

With the established KOCA and Kl model, it is possible not only to investigate if knock is observed with changing operating and design parameters, but also to evaluate their effects on the Kl. It may also show how much various individual operating and design parameters can be adjusted to reduce the engine autoignition tendency. In addition, the present model can be used in a predictive fashion to search for better combinations of the engine operating and design variables beyond the availability of experimental data. Manipulating changes in the operating and design parameters to avoid knock while enhancing engine performance is a reality with the present work without performing extensive experimental engine testing.

Figure 8.7 shows the Zero-D model predictions for KOCA and Kl with variations in equivalence ratio. As can be seen from the figure, whether or not the end-gas autoignites depends strongly on equivalence ratio. It is confirmed by measured cylinder pressure data that if the equivalence ratio is 0.74, autoignition is not observed at this operating condition of the engine. It is also observed from the measured cylinder pressure data that if the equivalence ratio is 0.82, the average autoignition for 200 consecutive cycles is observed at 13 degrees CA after TDC. As can be seen from the figure, the KOCA prediction of the model is 13.8 degrees CA after TDC if the equivalence ratio is 0.82, which is only a 0.8 degree CA deviation from the measured data.

Figure 8.8 shows the Multi-D model predictions for KOCA and Kl at the same engine operating conditions. As can be seen from the figure, autoignition is observed only if the equivalence ratio is higher than 0.74. KOCA predictions are not as accurate as those of the Zero-D model. As shown earlier, the Multi-D model predictions of maximum cylinder pressure are significantly higher than the measured data. This can be the reason for the earlier prediction of KOCA. Another reason for the earlier KOCA prediction of the Multi-D model could be the method of KOCA determination. With the Multi-D model, all of the
Figure 8.7 Zero-D model predictions of the KOCA and KI at various equivalence ratios 
(Comp. R. = 10.50, Prop. R. = 0%, Spark Timing = 26 degree CA, MAP = 1.4 bar).
Figure 8.8 KOCA and KI predictions of the Multi-D model at various equivalence ratios (Comp. R. = 10.50, Prop. R. = 0%. Spark Timing = 26 degree CA. MAP = 1.4 bar).
unburned cells were checked for autoignition and the fictitious species concentration is updated for every unburned cell at every crank angle until two neighboring cell’s fictitious species concentration reaches the critical value. After the two neighboring cell’s fictitious species reach the critical value the forward reaction rate coefficient is updated to the autoignition condition for all the cells. In the Zero-D model case, only the unburned zone temperature is used for determination of autoignition. It is possible that some local cells can have higher temperatures than the zone-averaged temperature of the Zero-D model. KI intensity predictions of the Multi-D model are also promising. KI is higher for the equivalence ratio of 0.82 because KOCA is very early, therefore the unburned mass fraction is significantly higher than that of the 0.78 case.

Season by season and region by region variations of the natural gas composition is the biggest constraint on the thermal efficiency of natural gas engines. The engine designer must consider all the variations in gas composition while determining the engine compression ratio and the initial conditions at IVC. The main objective of the current project was to develop an autoignition model that would be responsive to variations in the natural gas composition. Such a model could significantly improves the predictive capability of engine modeling tools to design the most efficient natural gas engines. Figure 8.9 shows the Zero-D model predictions for KOCA and KI with variations in the propane ratio of natural gas. As can be seen from the figure the autoignition model is responsive to variations in the propane ratio. If the propane ratio in the natural gas increases, KOCA is earlier. The measured KOCA are 10.2, 10.6, and 12.0 degree CA for propane ratio 15%, 10%, and 5%, respectively. The predicted KOCA for the same conditions are 10.3, 11.7, and 12.50. The current model is not only responsive to the variations in natural gas composition but also can predict KOCA within 1 degree CA.

Since the KIVA standard combustion model does not support a chemical kinetic mechanism for natural gas. variations in natural gas composition were not studied using KIVA.

Spark timing is one of the important engine operating parameters for the designer. The end-gas temperature is strongly dependent on the timing and therefore, any retardation in the timing decreases the end-gas temperature. Knock control systems generally retard the
Figure 8.9 KOCA and KI predictions of Zero-D model at various propane ratios in natural gas (Compression ratio = 10.5, Eq. R. = 0.82, Spark timing = 26 degrees BTDC, MAP = 1.4 bar).
spark timing to prevent heavy knock. Figure 8.10 shows the spark timing response of the Zero-D model. As can be seen from the figure, the KI is reduced with retarded timings. KOCA prediction of the model at 26 degree CA timing is very accurate with a deviation of 0.5 degree CA. However at 20 degree CA, there should not be an autoignition. The reason for this could be inaccuracy of the determination of end-gas temperature at retarded timings. During the optimization process of the autoignition model, it was assumed that the unburned zone compression was adiabatic. Figure 8.11 shows the spark timing response of the Multi-D model at the same initial conditions as the Zero-D model. As can be seen from the figure, the 26 degrees CA timing is predicted to be almost 10 degree earlier than was measured but the 20 degrees CA timing case does not predict autoignition, which is correct.

The initial mixture temperature is one the most important operating parameters that influences the onset of knock. If the initial temperature is increased, the unburned gas temperature is also increased therefore, the reaction rate in the end-gas increases, which leads to earlier autoignition with higher KI. Figures 8.12 and 8.13 show the initial temperature response of the Zero-D and Multi-D models. As can be seen from the figures, both of the models agree that there is no autoignition if the initial temperature is 440 K. If the initial temperature is increased, the KOCA is advanced with increasing KI. However, the KOCA prediction is about 3 degree CA earlier for the Multi-D model than the Zero-D.

Even spark ignited engines can be turbocharged to improve the power density of the engines. However, an after-cooler must be used to decrease the initial temperature. Increasing the intake pressure increases the mass flow rate and also the peak cylinder pressure. Any increase in the cylinder pressure will also increase end-gas temperature, which increases the knock tendency. Figures 8.14 and 8.15 show the initial pressure response of the Zero-D and Multi-D models. As can be seen from the figures, the KI is increased with increasing initial pressure for both of the models. However, the KOCA is retarded with increasing initial pressure for the Multi-D model and the autoignition is not observed for lower initial pressure. The reason for this inconsistency is under investigation. The effect of compression ratio on engine thermal efficiency is very well known. If end-gas autoignition had not been a constraint the compression ratio of SI engines would be as high as that of diesel engine. The autoignition model’s prediction capability at various
Figure 8.10 KOCA and KI predictions of the Zero-D model at various spark timings
(Comp. R. = 10.5, Eq. R. = 0.82, Prop. R. = 0%, MAP = 1.4 bar).
Figure 8.11 KOCA and KI predictions of the Multi-D model at various spark timings
(Comp. R. = 0.78, Eq. R. = 0.82, Prop. R. = 0%, MAP = 1.4 bar).
Figure 8.12 KOCA and K1 predictions of the Zero-D model at various initial temperatures (Comp. R. = 10.5, Eq. R. = 0.82, Spark Timing = 26 degree CA, MAP = 1.4 bar).
Figure 8.13 KOCA and KI predictions of the Multi-D model at various initial temperatures (Comp. R. = 10.5, Eq. R. = 0.82, Spark Timing = 26 degree CA, MAP = 1.4 bar).
Figure 8.14 KOCA and KI predictions of the Zero-D model at various initial pressures
(Comp. R. = 10.5. Eq. R. = 0.82. MAP, Prop.R. = 0%).
Figure 8.15 KOCA and KI predictions of the Multi-D model at various initial pressures
(Comp. R. = 10.5. Eq. R. = 0.82. Prop. R. = 0%).
compression ratios was also investigated. It is well known that increasing the compression ratio increases the end-gas temperature and therefore the tendency to knock increases. If the initial mixture temperature is decreased using an after-cooler, higher compression ratios can still be attained. As mentioned earlier, the present models are useful for investigation of various engine operating parameters such as initial conditions, fuel composition, spark timing, and the compression ratio on engine performance. Figures 8.16 and 8.17 shows KOCA and KI predictions of the models at various compression ratios. As can be seen from the figures both of the models agree that autoignition is not observed if the compression ratio is 10.50 at the given engine operating conditions. However, the maximum cylinder pressure CA is somewhat different for the two models. The cylinder pressure is a maximum at 18 degrees CA ATDC for the multi-D model which is 5 degrees CA later than that of the Zero-D model. If the compression ratio is raised to 11.50 the Multi-D model predicts trace autoignition at 16 degrees CA ATDC while Zero-D model does not predict any autoignition. Both of the models agree that autoignition is observed if the compression ratio is raised to 12.5. However, the cylinder pressure traces show significant differences for both models. First of all, the KOCAs are significantly different. The Zero-D model predicts KOCA at 20 degrees CA after TDC while the Multi-D model predicts KOCA at 13 degrees CA after TDC. The reason for this inconsistency is probably the simplified combustion model of the KIVA.

8.3 Summary

The autoignition model, which was developed in Chapter 6, was incorporated in both Zero-D and Multi-D models and a parametric study was conducted to determine the knock-limited engine operating and design variables. It was shown that the Zero-D model’s cylinder pressure trace and KOCA predictions show perfect agreement with experimental measurements. The Multi-D results are also promising. The model was able to predict whether or not knock will be observed and also trends in the KI.
Figure 8.16 KOCA and KI predictions of the Zero-D model at various compression ratios (Prop. R. = 0%, Eq. R. = 0.82, Spark Timing = 26 degree CA, MAP = 1.4 bar).
Figure 8.17 KOCA and KI predictions of the Multi-D model at various compression ratios (Prop. R. = 0\%, Eq. R. = 0.82, Spark Timing = 26 degree CA, MAP = 1.4 bar).
Multi-D computations were performed using a 333 Mega Hertz personal computer. The 2-D computations from intake valve closing to exhaust valve opening were generally less than 5 minutes.

Zero-D model was able to predict KOCA accurately if the fuel composition is changing with propane addition to the natural gas. This model can be used for combustion phasing of homogeneous charge compression ignition of natural gas. The model can predict the correct amount of propane to be added to the natural gas for proper combustion phasing.
Chapter 9: Conclusions and Recommendations

In this chapter, both the advantages and the disadvantages of the developed autoignition model will be discussed and then conclusions from the project will be given. Then recommendations for future work will be provided.

9.1 Advantages and Disadvantages of the Model

This project started with a literature review. Then experimental cylinder pressure data were collected at various engine operating conditions to analyze natural gas combustion at different fuel compositions. After that, a simple but accurate (the accuracy is compatible with other subroutines of the models) autoignition model was developed, optimized, and validated with experimental data. Finally, the autoignition model was coupled to both the Zero-D and Multi-D models to improve the predictive capabilities of those models. The greatest advantage of the autoignition model is that it can be coupled to analytical engine modeling tools easily and does not require extensive computational resources. Because of its simplicity tuning of the model is also very easy, if required. The disadvantage of the model is that does not provide any information about the chemical kinetics of the end-gas. Rather it assumes that a fictitious species is building up until a critical value and then the end-gas autoignites.

If a detailed chemical kinetic model, which is very costly to build and operate, had been coupled to the models, the accuracy gained from the model would possibly be decreased by the uncertainties of the initial conditions at IVC. It is likely that the model would still assume that the mixture at the IVC is homogenously mixed, the pressure is equal to the manifold pressure, and the temperature would be calculated from estimated residual mass fractions. It was mentioned earlier that it is essential that all of the subroutines of the models should have accuracies that are compatible with each other. Otherwise the accuracy gained from one particular subroutine would be lessened by the uncertainties of the others. On the other hand, there is nothing wrong if one subroutine of the model is more accurate than the others. However, if that particular subroutine requires extensive computational
resources and make the analysis extremely difficult, then engine designers will not use such an analytical tool for their engine development.

9.2 Conclusions

This dissertation started with a literature review to develop an understanding of the autoignition phenomenon and to develop an autoignition sub-model for engine modeling programs. Then, the combustion characteristics of natural gas and natural gas-propane mixture were examined. After that the knock occurrence crank angle and knock intensity were characterized and the factors that affect the occurrence and intensity of knock were examined. After that a simple but accurate autoignition model that can handle variations in the equivalence ratio and the propane fraction of the natural gas was developed (the accuracy of the model is compatible with the subroutines of the engine modeling programs). Finally, the autoignition model was incorporated with the Zero-Dimensional model, which was developed for this dissertation, and the Multi-Dimensional model, which was developed by Los Alamos National Laboratory, and a parametric study conducted to determine knock limited operating conditions of the engine.

The followings are the conclusions that can be drawn from this dissertation.

1. The variations in the flame initiation and propagation period are the major source of cycle-by-cycle variations of cylinder pressure in a SI Engine. The flame initiation period (FIP) is mostly dependent on the laminar flame speed of the fuel-air mixture while the flame propagation period (FPP) is dependent on the turbulence intensity and the turbulent flame area beside the laminar flame speed of the mixture. It was observed that both FIP and FPP decrease with increasing equivalence ratio, however FIP is more sensitive to the equivalence ratio than FPP due to strong dependency of the FIP on the laminar flame speed. It was also observed that the addition of propane to natural gas reduces the FPP of the mixture although the FIP is not affected. The possible reason for this is increased tendency to autoignition with the addition of propane to the mixture. The end-gas autoignition strongly increases the burning rate.
2. KOCA correlates very well with individual cycle pressure history. Therefore, individual cycle pressure history can be used for autoignition modeling. However, individual cycle KIs do not correlate well with parameters such as the unburned-mass fraction, burning rate, KOCA, and end-gas pressure and temperature. This poor correlation is attributed to cycle-by-cycle variations of the non-uniform end-gas state, variations in the geometric shape of the end-gas and its location within the combustion chamber.

3. It was shown that if the state time history of the end-gas and autoignition correlation are known, then the knock integral can be used to predict the KOCA. Alternatively, if the state-time history of the end-gas and the KOCA are known, an autoignition correlation, which fits the experimental data, can be developed. At the engine operating conditions where the percentage of knocking cycles is low, the average and the standard deviation of errors are generally higher. The reason for this is probably inaccurate end-gas temperature prediction of the two-zone model at these conditions.

4. It was shown that the Zero-D model's cylinder pressure trace and KOCA predictions show excellent agreement with experimental measurements. The Multi-D results are also promising. The model was able to predict whether or not knock will be observed and also trends in the KI. Zero-D model was able to predict KOCA accurately if the fuel composition is changing with propane addition to the natural gas. This model can be used for combustion phasing of homogeneous charge compression ignition of natural gas. The model can predict the correct amount of propane to be added to the natural gas for proper combustion phasing.

9.3 Recommendations for Future Work

1. The chemical kinetic subroutine of KIVA should be modified to improve the combustion predictions and to improve the predictive capability of the code if the fuel is a mixture of hydrocarbons.

2. The Zero-D model was able to predict the KOCA accurately if the fuel composition is changing with propane addition to the natural gas. This model can be used for combustion
phasing of a homogeneous-charge compression ignition of natural gas. The model could predict the right amount of propane to be added to the natural gas for correct combustion phasing.

3. This model was validated with experimental data from John Deere 6076. The predictive capability of the model can be tested with experimental data from other engines, also.
APPENDIX

Engine data for various engine operating conditions.
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AFR = Air flow rate (kg/hour)  
NGFR = Natural gas flow rate (kg/hour)  
PFR = Propane flow rate (kg/hour)  
MFR = Mixture flow rate per cycle per cylinder (kg/cyc-cyl)  
MAP = Manifold absolute pressure (bar)  
BMEP = Brake mean effective pressure (bar)  
COT = Coolant out temperature (F)  
EGT = Exhaust Gas Temperature (F)  
MIT = Mixture inlet temperature (F)  
AIT = Air inlet temperature (F)  
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| pr5e82t26 | 361.32 | 16.702 | 0.884 | 0.00140  | 393.73 | 0.345 | 1.4  | 195 | 86 | 195 | 1095 | 8.72 |
| pr5e84t26 | 356.47 | 16.874 | 0.917 | 0.00139  | 393.22 | 0.34  | 1.39 | 195 | 86 | 196 | 1103 | 8.77 |

| pr5e84t24 | 356.47 | 16.874 | 0.917 | 0.00139  | 393.22 | 0.34  | 1.39 | 195 | 86 | 196 | 1103 | 8.77 |
| pr5e84t22 | 364.99 | 17.265 | 0.916 | 0.00142  | 405.61 | 0.343 | 1.41 | 195 | 83 | 195 | 1129 | 9.01 |
| pr5e84t20 | 369.61 | 17.464 | 0.908 | 0.00144  | 409.65 | 0.343 | 1.4  | 197 | 83 | 195 | 1137 | 9.06 |

| pr10e76t26 | 376.83 | 15.434 | 1.689 | 0.00146  | 385.02 | 0.347 | 1.42 | 192 | 83 | 192 | 1064 | 8.57 |
| pr10e78t26 | 370.94 | 15.477 | 1.74  | 0.00144  | 386.05 | 0.346 | 1.4  | 195 | 85 | 195 | 1078 | 8.61 |
| pr10e80t26 | 365.62 | 15.749 | 1.753 | 0.001419 | 389.14 | 0.343 | 1.42 | 195 | 85 | 195 | 1087 | 8.66 |
| pr10e82t26 | 367.88 | 16.099 | 1.81  | 0.00143  | 399.65 | 0.345 | 1.39 | 196 | 83 | 196 | 1096 | 8.86 |

<p>| pr10e82t24 | 367.88 | 16.099 | 1.81  | 0.00143  | 399.65 | 0.345 | 1.39 | 196 | 83 | 196 | 1096 | 8.86 |
| pr10e82t22 | 363.64 | 16.016 | 1.792 | 0.00141  | 394.39 | 0.342 | 1.41 | 193 | 82 | 192 | 1114 | 8.75 |
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