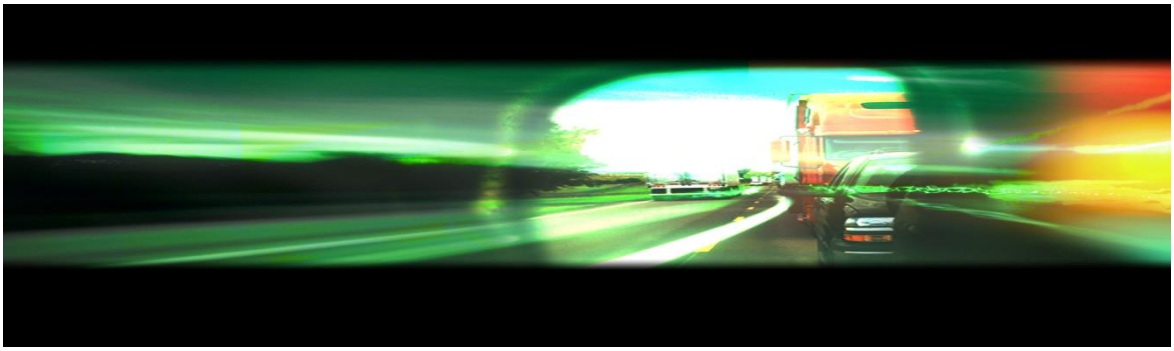
PROGRESS IN CATALYTIC IGNITION FABRICATION, MODELING AND INFRASTRUCTURE:

(Part 1) Catalytic Ignition Studies

Final Report



TranLIVE

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February 2014

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16. Abstract

Progress was made in measuring the temperature coefficient of thermal resistance. Thermal shielding improved results at high temperatures. Convective mixing was implemented to improve low temperature results. The temperature coefficient of thermal resistance is needed to measure the catalyst temperature at which surface reactions initiate.

A separate report was prepared on the development of a multi-zone engine model simulated using MATLAB software.

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EXECUTIVE SUMMARY

Platinum has been recognized as a viable combustion catalyst for use in transportation engines operating at fuel-lean conditions. Its change in electrical resistance with temperature has been used to measure light-off temperatures and rates of heat generation for various fuel-oxygen mixtures at the University of Idaho. In an attempt to maximize the surface area for these reactions to occur, platinum-coated nanosprings have been manufactured. A reliable method of determining an effective temperature-dependent temperature coefficient of resistance ($\alpha(T)$) for the nanosprings assembly has been developed and verified using pure platinum. Measured values of $\alpha(T)$ for platinum were matched against literature data at 373 and 1100 K. A linear fit was assumed for the gap between these temperatures; measurements made with platinum at intermediate temperatures were in good agreement. Using the same methodology, $\alpha(T)$ for the nanosprings assembly will be determined, which will allow for further research of the nanosprings in catalytic combustion.

DESCRIPTION OF PROBLEM

Catalytic igniters allow for lower ignition temperatures of lean mixtures in homogeneous charge, catalytically-assisted compression ignition engines. These systems have been the subject of much research at the University of Idaho, including both real-world setups to measure the power output and emissions of catalytic engines [Cherry, 1992; Cordon, 2002, 2006, 2008; Olberding, 2005], and laboratory setups to explore the catalytic effects of platinum and platinum-rhodium wires with various fuels [Elgan, 2012; Gibson, 2009; Leichliter, 2010; Lounsbury, 2007; McGary, 2011; Mehaffey, 2011]. Increasing the surface area of the wire increases its effectiveness as a catalyst, as shown with previous experiments in which the wire was coiled within the testing apparatus. For a greater increase in surface area, platinum-coated nanospring wire created at the University of Idaho will be used in coming research [McIlroy, 2001, 2004; Morton, 1999; Timalsina, 2010; Wang, 2006; Zhang, 2003]. This research requires the ability to measure the temperature of the wire to find the temperature at which surface reactions initiate, as well as the heat caused by these reactions. Knowing the temperature-dependent coefficient of thermal resistance, $\alpha(T)$, allows for the calculation of temperature from known voltage and current values.

To determine $\alpha(T)$ of the nanospring wire, a method had to be verified using known values. Literature data was found for platinum at 273-373 K and 1100-1900 K, and a linear fit was assumed for the gap. An experimental setup was constructed, and platinum wires were tested to establish proper procedure.

APPROACH AND METHODOLOGY

The relationship between temperature and electrical resistance can be described by

$$R(T) = R_a[1 + \alpha(T)(T - T_a)]$$

where R_a is the resistance at ambient temperature T_a [Scorzoni, 2004]. A single value for α(T) for 273-373 K is given in the literature as 0.0039 K^{-1} [Butler, 1957]. Glazkov [1985] gives an equation for α(T) for 1100-1900K as follows:

$$\left(\frac{1}{R_{273}}\right) * \left(\frac{dR}{dT}\right) = A + BT + \left(\frac{C}{T^2}\right)\exp\left(-\frac{H}{kT}\right)$$

where A = 4.21E-3 K^{-1}, B = -1.08E-6 K^{-2}, C = 3.78E7 K, H = 1.6 eV, and k is the Boltzmann constant [Glazkov, 1985]. If α(T) was a constant, and if the reference resistance was taken at T_a = 273 K, the left hand side of the second equation would equal α(T) in the first equation. This second definition of α(T) [$\alpha(T) = (1/R_{273})*(dR/dT)$] was used. Between 1100 and 1200 K, Glazkov's equation approaches linear. This linearity was extended to 273 K to serve as the expected values for measurements.

For the heating element, a Thermolyne furnace (350 cubic inch, SSP, 120 V, Model F48025-60) was chosen. Short lengths of 127 µm-diameter platinum wire were tested in a four-wire resistance test (Figure 1). The steady current connections were placed outside of the voltage-measuring connections to eliminate contact resistance errors [Kreider, 2009]. The four wires used to supply current and measure voltage were run through the vent on the top of the furnace. The back wall of the furnace was modified with two steel plates to secure a propeller shaft near the furnace's thermocouple. Figure 2 shows this modification, as well as the 2.5" model boat propeller that was run by a flex-cable motor to promote mixing within the furnace. A metal propeller was chosen to withstand the heat of the furnace and did not off-gas. Stainless steel foil was used as radiation shielding and stood between the exposed furnace coils and both the tested wire and furnace's thermocouple.

A Labview program controlled the current output and measurement timing of a Keithley 2440 5A SourceMeter (Figure 3). Measurements were taken with 0.1 amp current, 0.5 seconds apart for ten seconds with a four-second current head-start to avoid spikes. The reference temperature and resistance were taken before all other measurements; ambient temperature was 293-295 K. To remain well within the various temperature limits of all materials involved, a maximum temperature of 1000 K was chosen, and the oven was run to 993 K. To promote consistency and to reduce the effects of radiation, the oven was allowed to cool to 973 K before the first measurement was taken. The oven was then reheated to 993 K and allowed to cool to 973 K five times to condition the wire such that the change in resistance between successive measurements was less than 0.75%. No imaging or other testing has been done to discover what physical changes occur during this conditioning phase, but hypotheses include changing grain boundaries. After these five resistance measurements at 973 K, the oven was allowed to cool without periods of reheating, and further data points were taken approximately every 20 K down to 593 K.

FINDINGS; CONCLUSIONS; RECOMMENDATIONS

It was found that the resistance of the wire changed with successive runs to 993 K. Table 1 shows a representative sample of 973 K measurements (taken March 10). Between each pair of measurements, the oven was reheated to 993 K. Percent difference is calculated using the last measurement as the true value.

The fifth measurement taken at 973 K showed a change of only 0.56% for this particular wire, so the wire was deemed sufficiently conditioned and the oven was allowed to cool for further testing.

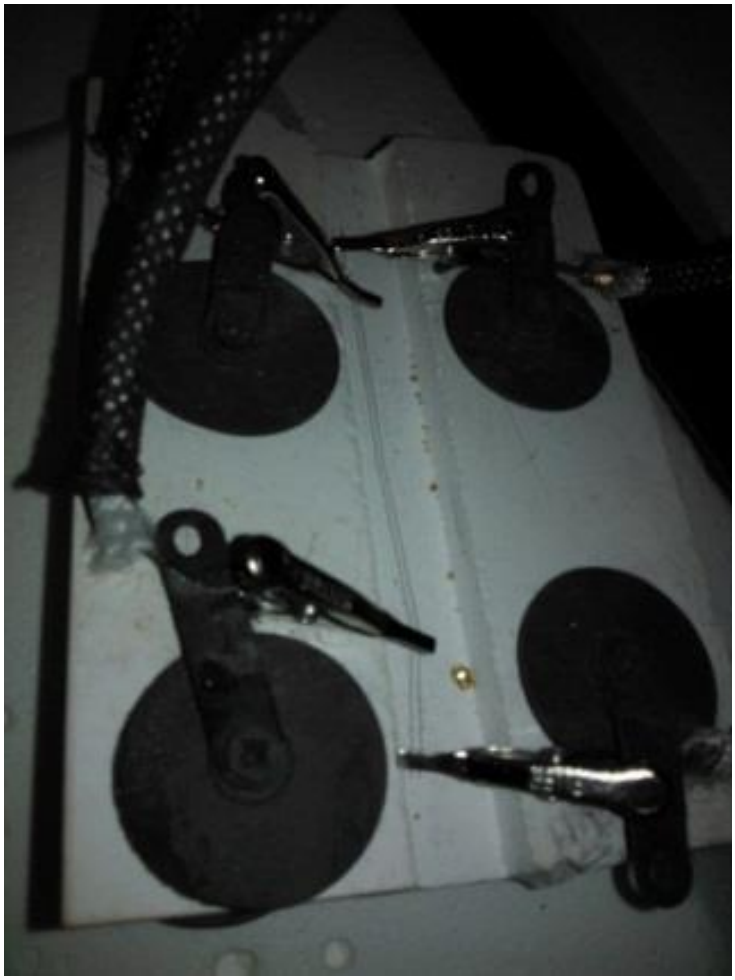

Figure 1: Four-wire setup.

Figure 2: Setup inside furnace (sans shielding).

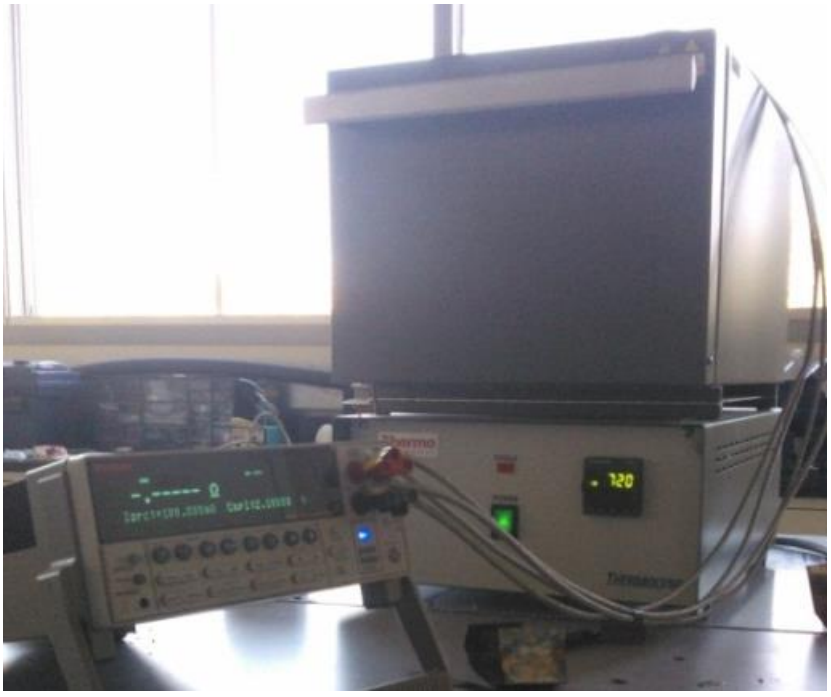

Figure 3: SourceMeter to furnace.

Table 1: Changes in Pt Resistance with Conditioning

% Difference in Successive Max Temp Runs		
Temp (K)	Resistance (Ω)	% Difference
973	0.971032143	4.734943
973	0.991634524	2.713705
973	1.004665143	1.435310
973	1.013548143	0.563826
973	1.019295190	

Figure 4 shows the α(T) of several runs versus the temperature compared to the linear approximation and literature data. The literature data was taken with a reference temperature of 273 K, which accounts for some of the difference shown. Figure 5 shows the α(T) of the same runs calculated with an estimated reference resistance corresponding to 273 K. Figure 6 shows this same data condensed into an average value with error bars of 1.96 standard deviations.

Using the estimated reference resistance, the data appears close to the assumed linear approximation for the range 593-833 K. The data is somewhat more curved than the assumed linear approximation. At higher temperatures, deviations from expected values may be due to insufficient radiation shielding or conditioning. Too few data points at lower temperatures do not allow definite conclusions to be made for that range.

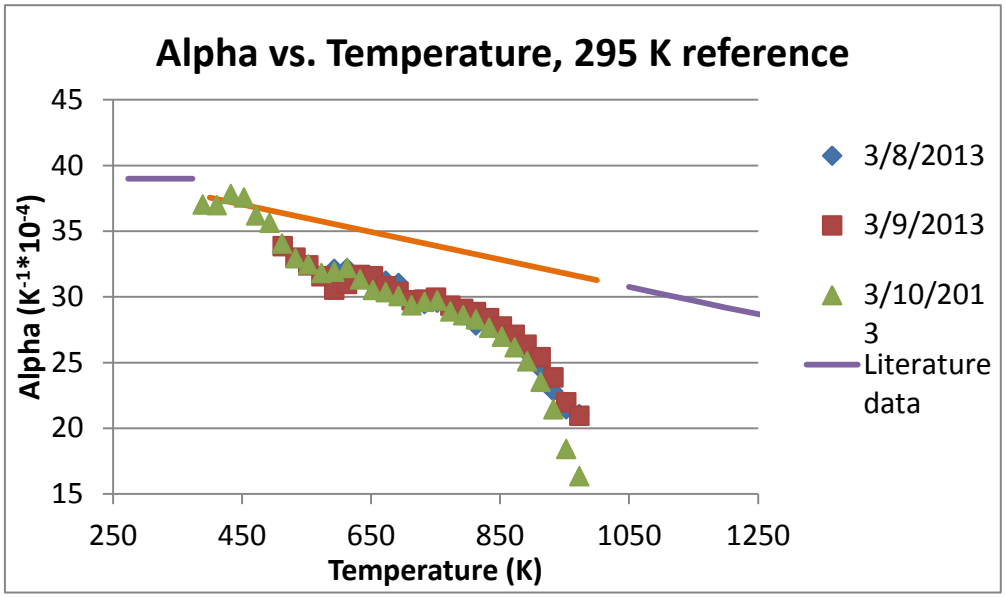

Figure 4: α as a function of temperature, 295 K reference.

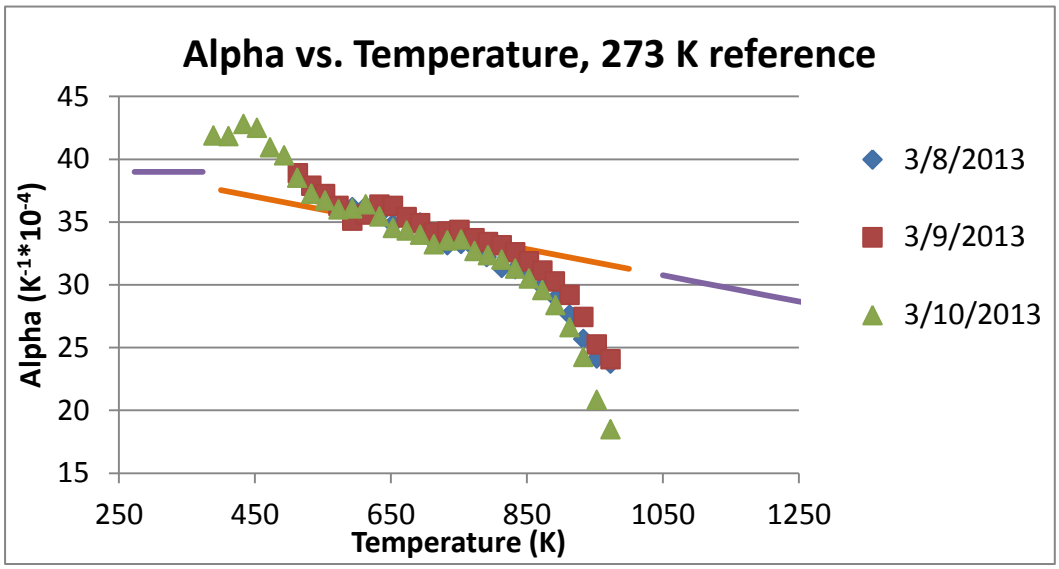

Figure 5: α as a function of temperature, 273 K reference.

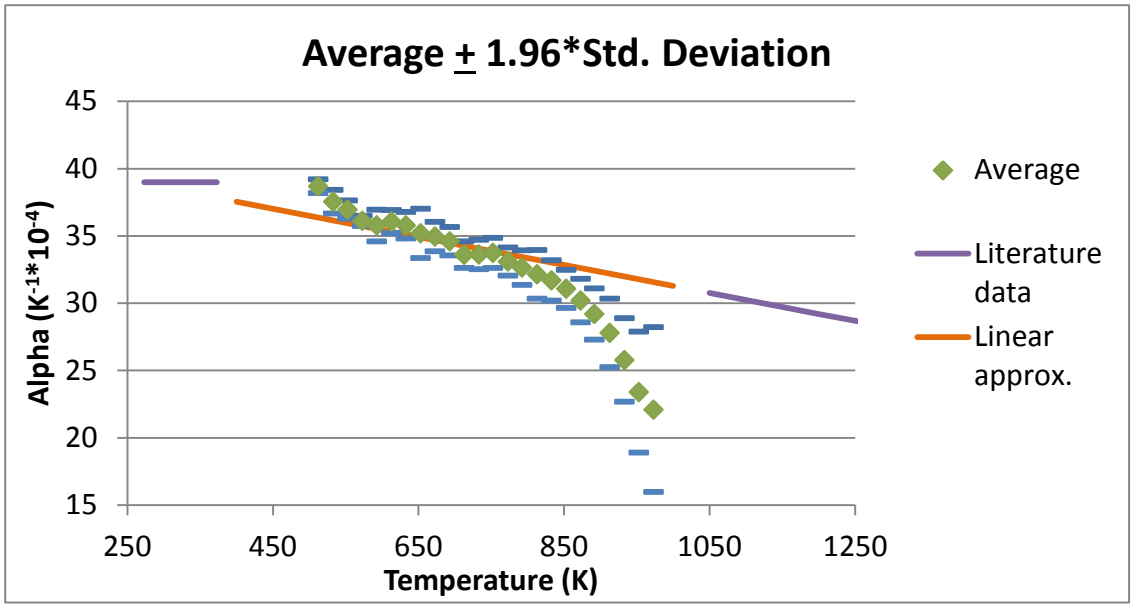

Figure 6: Average α with error bars, 273 K reference.

In summary, for the range 593-833 K, the current method outputs a reasonable approximation of α(T), within two standard deviations. At lower temperatures and higher temperatures, however, the values deviate from the expected. Further testing is required to address this issue before research on nanospring wires may begin. These conclusions are based on an estimated reference resistance corresponding to 273 K; testing to determine this value is required for accurate data.

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APPENDIX

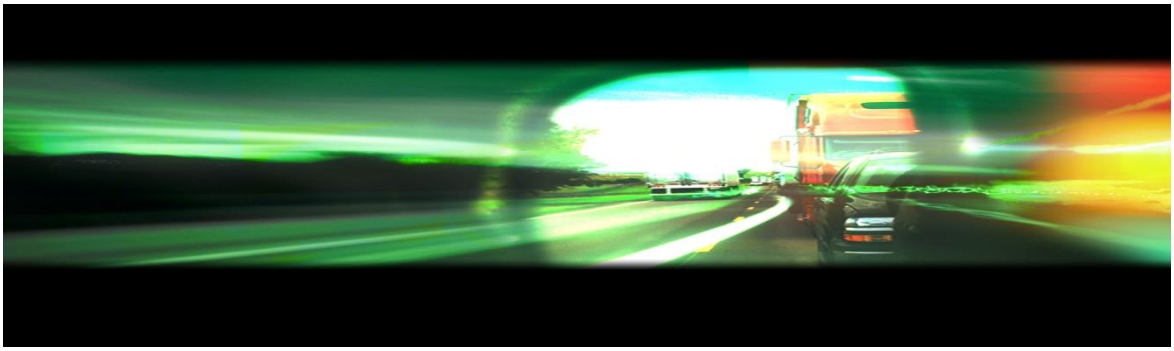
The following is a publication that resulted from this research:

Quinn, C., Steciak, J., Budwig, R., Beyerlein, S., "Measuring the Coefficient of Thermal Resistance of Nanospring Combustion Catalysts," *ASME Publication* IMECE13-64912, 2013.

PROGRESS IN CATALYTIC IGNITION FABRICATION, MODELING AND INFRASTRUCTURE:

(Part 2) Development of a Multi-Zone Engine Model Simulated using MATLAB Software

Final Report



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February 2014

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7. Author(s) Cuddihy, J., Beyerlein, S.		8. Performing Organization Report No. N14-09B
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16. Abstract A mathematical model was developed for the purpose of providing students with data acquisition and engine modeling experience at the University of Idaho. In developing the model, multiple heat transfer and emissions models were researched and compared before being implemented in the final model. It was decided that empirical methods would be used to predict engine performance facets due to their simplicity, and would be later modified, or adjusted, to fit the test results.		
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EXECUTIVE SUMMARY

A mathematical model was developed for the purpose of providing students with data acquisition and engine modeling experience at the University of Idaho. In developing the model, multiple heat transfer and emissions models were researched and compared before being implemented in the final model. It was decided that empirical methods would be used to predict engine performance facets due to their simplicity, and would be later modified, or adjusted, to fit the test results.

In an attempt to improve the accuracy of the MATLAB (Matrix Laboratory) model, specific heats were modeled as a function of temperature, friction effects were modeled as a function of engine speed (RPM), valve opening and closing was included, and emissions predictions were included based on a two-zone approach. Although the model is in the process of being validated, preliminary comparisons with engine manufacturer's data has shown promising results.

DESCRIPTION OF PROBLEM

Each summer, the University of Idaho offers an internal combustion engines course in which students learn about spark-ignition and compression-ignition engines, road load modeling, and numerical engine modeling. During the summer of 2013, this model was incorporated into students' final projects as a means of calculating engine performance under different operating conditions. Students were required to simulate brake specific fuel consumption (BSFC) maps and analyze pressure and temperature characteristics of a given engine.

In the summer of 2014, students will use this model in the internal combustion engines course to compare theoretical and analytical data on a GM 4.3L V6 engine. This will include a procedure by which students can manipulate the Vibe function using a known pressure trace. Students will then be able to compare a set of MATLAB outputs and the known engine outputs for accuracy.

Students will also be able to grow familiar with numerical simulations and data acquisition. This model will use many empirical methods to calculate friction losses and emissions. Students will be able to see overall predictions, and through the observation of the relative contributions of each sub-category (such as heat transfer, exhaust gas recirculation (EGR), etc.), they will be able to see where errors may accrue in a numerical model.

This model will also be helpful for the future development of engine and emissions models centered on competition-based vehicles at the University of Idaho, such as the formula hybrid car. A simple engine performance and emissions model will assist students in evaluating the overall effect of changing performance parts. Instead of using a trial and error method of increasing performance, students will have analytical results to justify the purchasing of new parts. With increasingly stringent emissions rules in these competitions, an emissions prediction model becomes increasingly important.

APPROACH AND METHODOLOGY

Developing a Single-Zone Engine Model

The simplest approaches in engine modeling treat the cylinder contents as a single fluid or zone [1]. The single-zone model views the burned and unburned gases, residual gases, and unburned hydrocarbons within the cylinder as a single, ideal gas with uniform pressure; in single-zone models, the single ideal gas is considered to be air. This section will outline the methodology used to implement a modified, single-zone model to predict engine performance.

Single-zone models typically use the Vibe function to represent the chemical, or gross, energy release as a function of crank angle [2]. The Vibe function has a characteristic "S-shape" and is defined as follows:

$$\mathbf{X_{b(\theta)} = 1 - exp\left[-a\left(\frac{\theta(i)-\theta_o}{\theta_b}\right)^{k+1}\right]} \qquad \textbf{(Equation 1)}$$

where **a** and **k** are adjustable constants (5 and 2 are commonly used values), $\boldsymbol{\theta(i)}$ is the instantaneous crank angle, $\boldsymbol{\theta_o}$ is the spark angle at the start of combustion, and $\boldsymbol{\theta_b}$ is the burn duration. The burn profile is engine specific, and the constants **a** and k can be adjusted to tune the profile to a specific engine or application.

The ideal gas law and the first law of thermodynamics form the basis for the single-zone engine model. The ideal gas law is defined as:

$$\mathbf{PV = mRT} \qquad \textbf{(Equation 2)}$$

where **P** is the pressure of an ideal gas, **V** is the volume of the gas, **m** is the mass of the gas, **R** is the universal gas constant, and **T** is the mean gas temperature. The cylinder gas volume, **V**, in a combustion engine can be related to the engine geometry as a function of crank angle [2]:

$$\mathbf{V(\theta) = V_c + \frac{\pi B^2}{4}(l + a - s)} \qquad \textbf{(Equation 3)}$$

where **B** is the cylinder bore, **l** is the connecting rod length, **a** is the crank radius, **s** is the distance between the crank axis and the piston pin axis, and $\mathbf{V_c}$ is the clearance volume, which is defined as:

$$\mathbf{V_c} = \left(\frac{\mathbf{V_d}}{\mathbf{C_r - 1}}\right) \qquad \textbf{(Equation 4)}$$

where $\mathbf{V_d}$ is the displaced cylinder volume, and $\mathbf{C_r}$ is the compression ratio. A diagram of these variables is included in Figure 1.

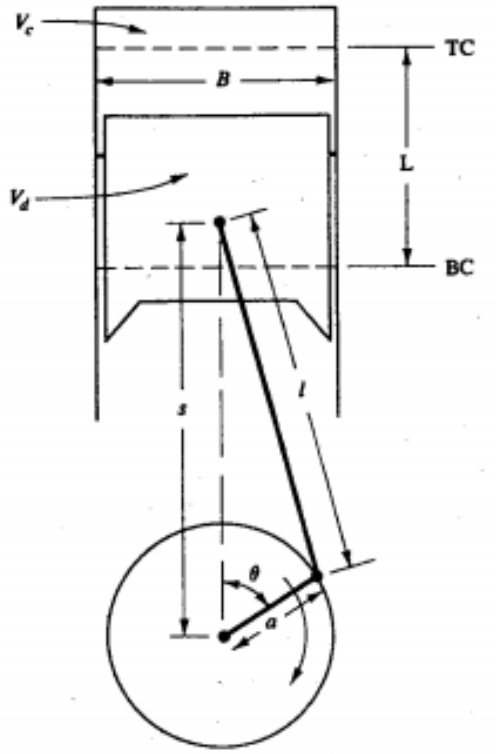

Figure 1: A diagram of engine geometry variables [2].

In differentiating equation 2 with respect to **dθ**, the following expression is obtained:

$$\frac{\mathbf{dP}}{\mathbf{d\theta}} = \left(-\frac{\mathbf{P}}{\mathbf{V}}\right)\left(\frac{\mathbf{dV}}{\mathbf{d\theta}}\right) + \left(\frac{\mathbf{P}}{\mathbf{T}}\right)\left(\frac{\mathbf{dT}}{\mathbf{d\theta}}\right) \qquad \textbf{(Equation 5)}$$

where **P**, **V**, and **T** are instantaneous values that are modeled relative to the engine's crank angle. The same process can be applied to the first law of thermodynamics, which is expressed as:

$$\Delta U = Q - W \qquad \text{(Equation 6)}$$

where Q is the total energy transferred into the system, W is the work transferred out of the system, and ΔU is the change in internal energy within the system. In differentiating equation 6 with respect to $d\theta$, equation 7 can be obtained:

$$\frac{dU}{d\theta} = \frac{dQ}{d\theta} - \frac{dW}{d\theta} = mC_v\left(\frac{dT}{d\theta}\right) \qquad \text{(Equation 7)}$$

where C_v is the specific heat of the combustion chamber gas. Upon dividing the specific heat by the universal gas constant, and using η_c (the combustion efficiency) and LHV (the lower heating value of the supplied fuel) we come up with equation 8, which gives us the change in temperature as a function of crank angle:

$$\frac{dT}{d\theta} = T(\gamma - 1)\left[\left(\frac{1}{PV}\right)\left(\frac{dQ}{d\theta}\right) - \left(\frac{1}{V}\right)\left(\frac{dV}{d\theta}\right)\right] \qquad \text{(Equation 8)}$$

The heat input from the fuel can be used to find the change in pressure as a function of crank angle. The heat input from the fuel is defined as [3]:

$$Q_{in} = \eta_c LHV\left(\frac{1}{AF_{ac}}\right)\left(\frac{P}{RT}\right)V_d \qquad \text{(Equation 9)}$$

where AF_{ac} is the actual air fuel ratio. Lastly, the change in pressure is defined as:

$$\frac{dP}{d\theta} = \left(\frac{-\gamma P}{V}\right)\left(\frac{dV}{d\theta}\right) + \left(\frac{\gamma - 1}{V}\right)Q_{in}\frac{dX_b}{d\theta} + (\gamma - 1)\left(\frac{1}{V}\right)\left(\frac{dQ_w}{d\theta}\right). \qquad \text{(Equation 10)}$$

Equation 10 is the basis for a numerical model that can be used to simulate engine performance.

Using a Pressure Trace to Modify the Vibe Function

The accuracy of an engine simulation is highly dependent on the in-cylinder burn profile. The previously defined Vibe function constants (equation 1) can produce moderately accurate results for a given platform under given circumstances, but a method for curve-fitting the Vibe function to an engine's pressure trace should be included in this model.

A method of deriving the mass fraction burned as a function of experimental cylinder pressure describes the incremental change in pressure across known crank increments as:

$$\Delta P = \Delta P_v + \Delta P_c \qquad \text{(Equation 11)}$$

where ΔP_v is the incremental change in pressure due to piston motion and ΔP_c is the incremental change in pressure due to combustion. In employing the polytropic relationships, the incremental change in pressure due to piston motion is defined as:

$$\Delta P_v = P(i)\left[\left(\frac{V(i)}{V(i+1)}\right)^n - 1\right] \qquad \text{(Equation 12)}$$

where n represents a polytropic index, and $P(i)$ and $V(i)$ are the pressure and volume at known crank positions. With these known values, the mass fraction burned is then defined as:

$$x_b(\theta) = \frac{\Sigma_0^i \Delta P_c^*}{\Sigma_0^{N_{tot}} \Delta P_c^*} \qquad \text{(Equation 13)}$$

where N_{tot} is the total number of increments. The mass burn fraction is a parameter that can be dynamically measured using an in-cylinder pressure transducer while the engine is being tested on a dynamometer. With the known mass fraction burned profile, the constants of the Vibe function can then be modified to produce matching profiles. As such, test data from the engine will be used to fine tune the parameters in the Vibe function.

Developing a Variable Specific Heats Ratio Model

Because of the large temperature gradients in an internal combustion engine cycle, a variable specific heats ratio was desired for the current engine model. It was found that numerous specific heats ratio models exist and the accuracy of these models depended highly on the complexity of the corresponding computer code. It was decided that a curve-fit polynomial method would be used to model the specific heats ratio as a function of in-cylinder temperature.

This polynomial method was developed in 1966 by Krieger and Borman for combustion processes such as those involving iso-octane and other fuels [4]. The Krieger and Borman method models changes in internal energy through the use of ideal gas constant "correction factors" corresponding to changes in temperature (based on a given reference temperature). Through a series of derivations, the specific heats ratio as a function of temperature can be obtained through the use of this method. The derivation of the polynomial method and corresponding polynomials can be found in Appendix A.

Modeling Engine Friction

Friction losses vary significantly from engine to engine and can be introduced through bearing components and pistons, along with the process of driving engine accessories [5]. Engine friction losses can be very difficult to model without known engine data and can vary based on engine coolant and oil temperatures, ambient conditions, and engine speed and throttle settings [5]. Although friction losses are difficult to predict, they can be estimated based on general engine trends such as the number of rolling element bearings and the engine displacement. For this model, plain engine bearings were assumed, and a process suggested by Blair was used to estimate friction mean effective pressure (fmep) losses [6]. It should be noted that an engine's actual friction data can be obtained and updated in this model by modifying a few lines of MATLAB code. However, the current method being described was implemented so that this model could be used on a variety of theoretical or actual engines to predict performance without limiting the model to a specific application.

Various researchers such as Heywood and Blair [2][6] have used general linear equations to predict fmep losses as a function of RPM. Although this method only provides ballpark estimations of the friction losses, this provides a starting point at which a numerical simulation can begin. According to Blair [6], the linear fmep loss equation is defined as:

$$\mathbf{fmep} = \mathbf{a} + \mathbf{b}(\mathbf{L})(\mathbf{RPM}) \qquad \textbf{(Equation 14)}$$

where **a** and **b** are constants that vary depending on the engine type, **L** is the stroke [m] of the engine, and RPM is the engine speed $\left[\frac{\text{rev}}{\text{min}}\right]$. For a spark-ignition engine with plain internal bearings, Blair [6] has assumed different forms of the fmep loss equations based on the engine displacement ($(\mathrm{V_d} > 500\ c\mathrm{m}^3)$ and $(\mathrm{V_d} < 500 c\mathrm{m}^3)$ respectively):

$$\mathbf{fmep} = \mathbf{100000} + \mathbf{350}(\mathbf{L})(\mathbf{RPM}) \qquad \textbf{(Equation 15)}$$

$$\mathbf{fmep} = \mathbf{100000} + \mathbf{100}(\mathbf{500} - \mathbf{V_d}) + \mathbf{350}(\mathbf{L})(\mathbf{RPM}). \qquad \textbf{(Equation 16)}$$

The provided, respective fmep losses are in units of [Pa].

Formulation of a Two-Zone Model

Two-zone engine models are closely related to the equations that were derived in the single-zone model. The bulk-system pressure, mass burned fraction, and bulk-system volume can be described using equations 1, 3, and 10. However, the two-zone model considers a burned and unburned ideal gas region in the combustion chamber thus allowing for more accurate heat transfer and emissions predictions.

Burned and Unburned Cylinder Masses

The development of a two-zone engine model can begin with the modification of the Vibe function to include unburned and burned regions. In order to determine the unburned mass at bottom-dead-center, the following three relationships can be used [6]:

$$\mathbf{m_a = \rho_a V_d} \qquad \textbf{(Equation 17)}$$

$$\mathbf{m_f = \frac{m_a}{AF_{ac}}} \qquad \textbf{(Equation 18)}$$

$$\mathbf{m_c = m_a + m_f} \qquad \textbf{(Equation 19)}$$

where $\mathbf{m_a}$ is the mass of air contained within the cylinder, $\boldsymbol{\rho_a}$ is the density of air, $\mathbf{m_f}$ is the mass of fuel contained within the cylinder, and $\mathbf{m_c}$ is the total mass contained within the cylinder.

Burned and Unburned Volumes and Temperatures

With known unburned and burned masses, the corresponding volumes can be obtained. Blair [6] suggests using the polytropic relations and the known pressure-trace to define the unburned and burned volumes. The unburned volume is defined in a discretized form as:

$$\mathbf{V_u(i) = \left(\frac{m_u(i)V_u(i-1)}{m_u(i-1)}\right)\left(\frac{P(i)}{P(i-1)}\right)^{-\frac{1}{\gamma_u(i)}}} \qquad \textbf{(Equation 20)}$$

where $\boldsymbol{\gamma_u(i)}$ is the specific heats ratio as a function of crank angle in the unburned-gas region. The polynomials method, which is explained in detail in Appendix A, can be used to define the specific heats ratio as a function of crank angle. The assumption that only unburned gases are contained within the cylinder before the spark advance $\boldsymbol{(\theta_0)}$ should also be taken into consideration.

It was previously mentioned that two-zone models split the single-zone model into two zones or regions. In order for the two-zone model to work, the ideal gas assumption has to continue to each constituent zone where the burned and unburned temperatures are defined in a discretized form as:

$$\mathbf{T_b(i)} = \frac{\mathbf{P(i)V_b(i)}}{\mathbf{m_b(i)R(i)}} \quad \textbf{(Equation 21)}$$

$$\mathbf{T_u(i)} = \frac{\mathbf{P(i)V_u(i)}}{\mathbf{m_u(i)R(i)}} \quad \textbf{(Equation 22)}$$

where the bulk-system pressure can be used (since pressure is constant throughout the combustion chamber) and $\mathbf{R(i)}$ is the fluid specific gas constant (air in this case). The fluid specific gas constant can be found using the polytropic method described in Appendix A.

Burned and Unburned Areas

This model neglects heat transfer between the burned and unburned zones and doesn't delve into geometric positioning of the flame front, so assumptions need to be made in reference to the burned and unburned areas. According to Rakopoulos and Michos [7], the unburned and burned areas are defined as:

$$\mathbf{A_u(i)} = \mathbf{A(i)}\left(\mathbf{1} - \left(\mathbf{X_b(i)}\right)^{\frac{1}{2}}\right) \quad \textbf{(Equation 23)}$$

$$\mathbf{A_b(i)} = \mathbf{A(i)}\left(\frac{\mathbf{X_b(i)}}{\left(\mathbf{X_b(i)}\right)^{\frac{1}{2}}}\right) \quad \textbf{(Equation 24)}$$

where $\mathbf{X_b(i)}$ is the mass fraction burned as a function of crank angle. $\mathbf{A(i)}$ is the instantaneous cylinder area in contact with combustion chamber gases and is defined as:

$$\mathbf{A(i)} = \mathbf{A_{ch}} + \frac{\pi \mathbf{B}^2}{2} + \pi \mathbf{B}(\mathbf{l} + \mathbf{a} - \mathbf{s(i)}) \quad \textbf{(Equation 25)}$$

where $\mathbf{A_{ch}}$ is the surface area of the cylinder heat [m^2], **B** is the cylinder bore [m], **l** is the connecting rod length [m], **a** is the crank radius [m], and $\mathbf{s(i)}$ is the instantaneous distance between the crank axis and the piston pin axis [m]. For the purpose of this model, the surface area of the cylinder head was assumed to be the same as the cross-sectional area of the piston even though the area was known to be slightly larger due to the head curvature. The crank radius can be assumed to be half of the length of the stroke, while $\mathbf{s(i)}$ is defined as:

$$s(i) = a(\cos\theta) + (l^2 - a^2 \sin^2\theta)^{\frac{1}{2}} \quad \text{(Equation 26)}$$

Although this method doesn't account for heat transfer between zones and assumes a surface area of the cylinder head, it can be shown to be physically consistent because the fractional heat transfer between the burned gas and the cylinder wall is always highest in the burned region [7].

Selecting and Developing a Computer Program

In selecting a computer program to develop the multi-zone model in, EES (engineering equation solver) and MATLAB were carefully considered. EES was initially considered and experimented with because of its ability to effectively calculate fluid properties from a built-in database. It was theorized that the accuracy of a zone-based engine model could be drastically improved with EES because of the on-hand fluid properties.

With the complexity of the given model, EES struggled mightily in the iteration process. It was found that EES could work its way through the most basic single-zone model, but it took careful selection of initial guesses and proved to be very clunky. Although EES didn't work very well on its own, it was found that there are ways of communicating between EES and MATLAB. One could use a call function in the MATLAB program to call fluid properties (or likewise).

Although the built-in fluid properties in EES would have been handy, MATLAB proved to be more than sufficient. Building functions and loops within MATLAB proved to be much easier than in EES and even the most complex code ran very quickly.

The MATLAB Interface

The MATLAB program was set up through the use of a script. Because the program required so many equations, functions were only used in a couple scenarios; this was because it was determined that functions would only add to the complexity of the code. The MATLAB code was broken into the following sub-sections:

1. Engine and atmospheric inputs.

2. Pre-allocation of array and matrix components inside and outside of the main loop.
3. Fuel inputs and combustions efficiencies.
4. Instantaneous engine characteristics (i.e. volume as a function of crank angle).
5. Combustion chamber fluid properties and valve opening and closing.
6. Two-zone calculations and the variable specific heats ratio model.
7. The simulation of EGR.

The purpose of these sub-sections and how the MATLAB code works will be explained in the following sections.

Engine and Atmospheric Inputs

The MATLAB code began with known engine inputs. The bore, stroke, connecting rod length, number of cylinders, compression ratio, and operating characteristics were defined in lines 12-25 of the MATLAB script. Figure 2 shows an image of the corresponding block of MATLAB code that contained the known engine inputs.

```
%Engine Inputs
Load = 1;           %Engine Load (Affects Inlet Pressure)
RPM = 4500;         %Revolutions Per Minute [1/min]
L = .08839;         %Stroke of Engine [m]
B = .1016;          %Bore of Engine [m]
l = .0935;          %Length of Engine Connecting Rod [m]
N_cyl = 6;          %Number of Cylinders [unitless]
C_r = 9.1;          %Compression Ratio [unitless]
N_r = 2;            %Number of Revolutions Per Power Stroke
theta_b = 60;       %Combustion Burn Duration [degrees]
theta_0 = 156;      %Crank Angle At Start of Combustion [degrees]
theta_f = theta_0+theta_b; %Final Comb. Angle [degrees]
IVC = 0;            %Time [degrees] when Intake Valve Closes
EVO = 330;          %Time [degrees] when Exhaust Valve Opens
```

Figure 2: Engine inputs in the MATLAB model.

An add-on for this model optimized the spark advance based on a given burn duration (~60° for initial iterations) and known outputs.

The model then calculated engine parameters based on the previously defined inputs and geometric constraints. This block of code calculated the cross-sectional area of the piston, the

surface area of the cylinder head within the combustion chamber, the displaced cylinder volume, the crank radius length, and the clearance and bottom-dead-center volumes. The block of code then used an if-then statement to predict engine friction losses based on the displaced volume, RPM, and engine stroke. Figure 3 shows lines 29-52 of the MATLAB script, which calculated these engine parameters.

```
%Engine Calculations Based On Previous Inputs
%Assumes Average Surface Area In Which Heat Transfer Occurs

A_p = (pi/4)*B^2;               %Cross Sectional Piston Area [m^2]
A_ch = A_p;                     %Cylinder Head Surface Area (in chamber)
V_d = N_cyl*A_p*L;              %Displaced Volume Of Engine [m^3]
N = RPM/60;                     %Converts RPM to RPS [1/s]
S_bar_p = 2*L*N;                %Calculates Mean Piston Speed [m/s]
a = L/2;                        %Calculates Crank Radius (1/2 stroke)[m]
V_TDC = (V_d/(C_r-1))/N_cyl;    %Calculates Clearance Volume [m^3]
V_BDC = (V_d/N_cyl)+V_TDC;      %Cyl. Volume At BDC [m^3]

%_____________________________________________________________________


%Calculating Losses Due To Friction
%fmep (obtained from Blair) Based On Displacement, RPM

if V_d>500*10^(-6)
    fmep=(100000+350*L*RPM)*10^(-3);
end
if V_d<500*10^-6
    fmep=(100000+100*(500-V_d*10^(-6))+350*L*RPM)*10^(-3);
end
```

Figure 3: Engine calculations based on engine inputs.

The model specified the atmospheric inputs in lines 82-88 and used several of these inputs throughout the main loop to simulate EGR, the opening and closing of valves, and other physical phenomena. Atmospheric pressure was reduced to simulate operating conditions in Moscow, Idaho, and a temperature of 350[K] was chosen to represent the cylinder wall temperature, per the suggestion of Stone [5]. An initial inlet temperature of 300[K] was then specified in line 106; with the initial inlet temperature being placed in the main loop because of EGR, and an if-then statement that corrected the inlet temperature as a function of iterations.

Pre-allocation of Array and Matrix Components

Through experimentation and displayed MATLAB errors, it was found that pre-allocating arrays and matrices drastically improved the program efficiency. Pre-allocated arrays and

matrices were used outside of the main loop to specify initial conditions (such as the cylinder volume at the beginning of the cycle) and to specify the overall size of the matrix or array. This prevented MATLAB from re-sizing the array or matrix with each iteration, thus decreasing the overall calculation time. Arrays and matrices were also used inside of the main loop to assist in the simulation of EGR; in order for the EGR simulation to work correctly, the program had to run two times with only the starting gas temperature and fluid characteristics of the gases being changed. The pre-allocation of arrays and matrices was used to set all other arrays and matrices to their initial values. The pre-allocation of arrays and matrix components was specified in lines 54-66 and 117-169.

Fuel Inputs and Combustion Efficiency

The fuel, stoichiometric air-fuel ratio, and combustion efficiency inputs were placed in lines 70-80 of the MATLAB script. A lower heating value (LHV) of 44.6$\left[\frac{\text{MJ}}{\text{kg}}\right]$ was used per the suggestion of Stone [5], and a maximum combustion efficiency of .95 was selected based on intuition and the curve-fitting of given engine information. The actual combustion efficiency was then calculated using an empirical method developed by Blair [6]. The fuel and combustion efficiency inputs can be observed in Figure 4.

```
%Fuel Inputs/Efficiencies

AF_ratio_stoich = 15.09;    %Theoretical Air Fuel Ratio
lambda = 1;                 %Excess Air Coefficient
AF_ratio_ac = lambda*AF_ratio_stoich; %Actual Air Fuel Ratio
LHV = 44.6e6;               %Lower Heating Value Of Fuel Mixture [J/kg]
eta_combmax = .95;          %Assumed MAX COmb. Efficiency

%Predicts Combustion Efficiency (Reference To Blair)

eta_comb=eta_combmax*(-1.6082+4.6509*lambda-2.0764*lambda^2);
```

Figure 4: Fuel and combustion efficiency inputs.

Instantaneous Engine Characteristics

The instantaneous engine characteristics were calculated within the main loop of the MATLAB script, which fell between lines 103-366. The main loop was broken into two sub-

loops that served different functions. The loop with a specified index (k = 1:2) served as the EGR simulation, while the loop with a specified index (i = 2:360) calculated all instantaneous engine features. Fluid properties, array pre-allocations, and temperature corrections factors were placed between the first and second sub-loops, that way, all fluid and gas properties were updated as a function of EGR.

Combustion Chamber Fluid Properties and the Opening and Closing of Valves

In the second sub-loop, the combustion chamber volume, instantaneous heat transfer area and overall heat transfer, Vibe function, and all other instantaneous engine characteristics were calculated. Lines 176-191 calculated geometric properties such as the instantaneous cylinder volume; these lines also calculated the viscosity, thermal conductivity, and other instantaneous combustion chamber gas properties. The Vibe function and fuel-mass contained within the cylinder were calculated in lines 202-209 and can be observed in Figure 5 where an if-then statement was used to specify the mass-fraction burned as being zero until the cycle reached the spark advance.

```
if theta(i)<theta_0
     X(i)=0;
 else
 X(i) = 1-exp(-5*((theta(i)-theta_0)/theta_b)^3);
 if theta(i) < theta_f
       M_F(i) = V(theta_0-1)*rho(theta_0-1)/(lambda*AF_ratio_ac);
 end
end
```

Figure 5: The Vibe function.

Lines 218-235 were reserved for heat transfer properties and lines 239-254 simulated the opening and closing of intake and exhaust valves, respectively. The empirical models for predicting heat transfer were incorporated, and the simulated opening and closing of intake and exhaust valves was assumed to be instantaneous, in that the gas dynamics and valve-lift profile were not considered. The opening and closing of the valves can be observed in Figure 6.

```
if IVC< theta(i)
    DT(i)=T(i-1)*(gamma(i-1)-1)*((1/(P(i-1)*V(i-1)))*DQ(i)...
        -(1/V(i-1))*DV(i));
    DP(i)=(-P(i-1)/V(i-1))*DV(i)+(P(i-1)/T(i-1))*DT(i);
    P(i) = P(i-1)+DP(i);
end
if EVO < theta(i)
    P(i) = P_atm;
end
if 200 < theta(i)
  if P(i)<=P_atm
    P(i)=P_atm;
  end
end
```

Figure 6: Valve opening and closing statements.

It can be seen that this script includes a statement referencing 200 crank angle degrees. Upon the opening of the exhaust valve, the cycle pressure is set equal to atmospheric pressure, but in part load scenarios, the cycle pressure can become negative relative to atmospheric pressure before the exhaust valve opens. To prevent negative cycle pressure, an if-then statement was created for all crank degrees past 200, where 200 degrees was arbitrarily chosen.

Two-zone Calculations and the Variable Specific Heats Ratio Model

Lines 257-282 were reserved for two-zone calculations such as the burned and unburned masses, volumes, temperatures, and areas, while much of the rest of the second sub-loop was occupied by variable specific heats ratio and other combustion gas calculations. The two-zone calculations used variables from the single-zone calculations such as the bulk gas pressure and the mass fraction burned to calculate two-zone characteristics. Lines 310-355 used coefficients that were defined in lines 93-99 to calculate the specific heats ratio as a function of combustion chamber gas temperature; where the coefficients were defined outside of the main loop because they were unchanging, therefore, less information within the main loop resulted in a more efficient MATLAB simulation. Appendix A provides a detailed derivation of the variable specific heats ratio model.

THE SIMULATION OF EGR

Line 290 calculates the residual fraction of exhaust gases within the combustion chamber based on polytropic relationships and line 365 calculates a corrected temperature based on the volumetric ratios of residual and inlet gases. The calculations are placed on different lines because of the constantly updating temperatures as a function of crank angle. The first sub-loop iterates twice with the first iteration assuming inlet gas properties equal to atmospheric properties, while the second iteration used the corrected temperature to update the inlet gas properties. This results in reduced peak pressures and temperatures, and in turn, NO_x emissions.

FINDINGS; CONCLUSIONS; RECOMMENDATIONS

Ongoing and future research using a motorcycle engine equipped with high speed in-cylinder pressure data acquisition will be used to validate the current MATLAB model, and many of the empirical predictions used in the current model will be modified to create a model that predicts the motorcycle's performance to the highest degree of accuracy. At this point in time the model has been simulating a GM 4.3L V6 engine. Although the results are preliminary, the simulated output, shown below in figures 7 and 8, agrees nicely with values typical for that engine. Figure 7 shows the temperatures in the unburned and burned zones as part of the two-zone model. We see that the temperatures in the burned zone do not exist until after ignition (~160° crank angle), and the peak temperature of the burned zone is slightly below 3000 K, which is typical flame temperature for a gasoline engine. The burned zone temperature decreases to around 1500 K prior to the exhaust valve opening, which is also a typical value for this type of engine.

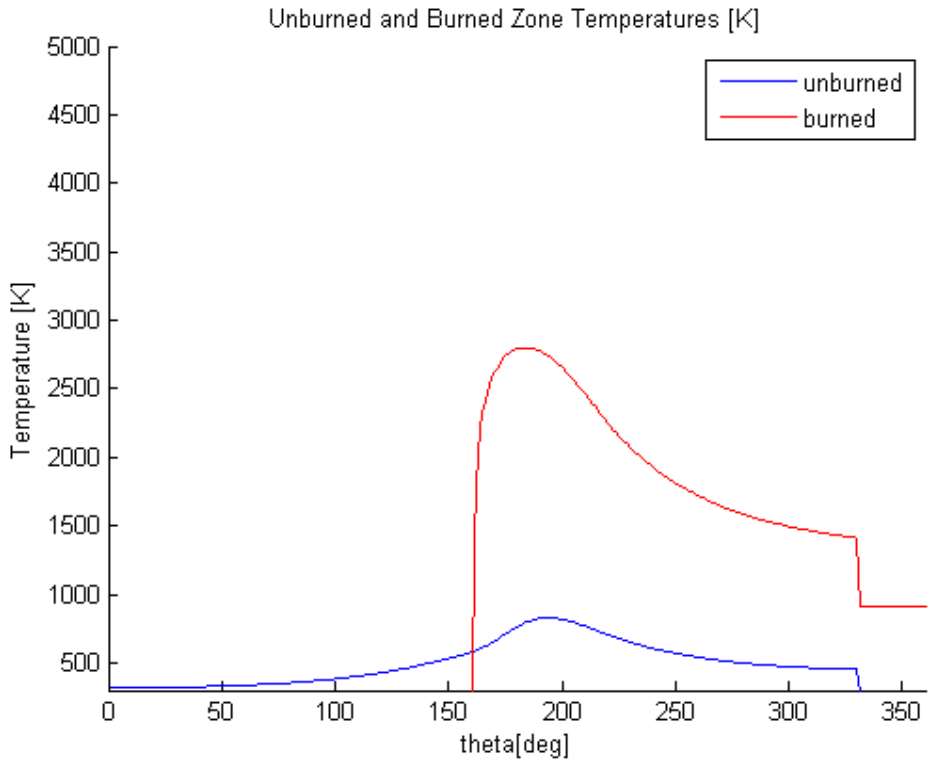

Figure 7: Burned and unburned zone temperatures on a V6 engine.

Figure 8 shows several calculated engine parameters as a function of crank angle. The blue line shows in-cylinder pressure. We expect this to have a maximum pressure at around 190-200° crank angle, and to have a value between 3500-5000 kPa. The simulated results fall within these ranges of typical values. The green line represents cumulative power output. This is the net power output as a function of crank angle. At the end of the cycle the model is predicting around 200 kW of power output, which is about what we would expect from a GM 4.3L V6 engine at full load.

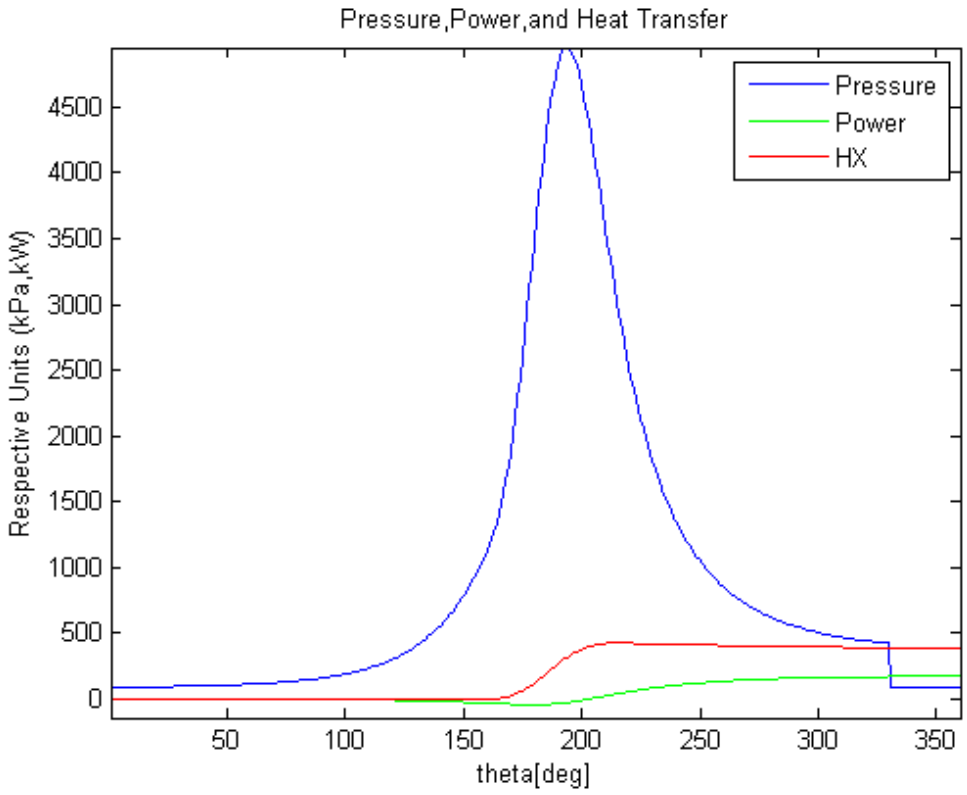

Figure 8: Predicted pressure, power, and heat transfer on V6 engine.

APPENDIX

A: Derivation of the Polynomial Method

Table of Coefficients

$\mathbf{a_1}$ .692	$\mathbf{a_2}$ 39.17e-06	$\mathbf{a_3}$ 52.9e-09	$\mathbf{a_4}$ -228.62e-13
$\mathbf{a_5}$ 227.58e-17	$\mathbf{b_o}$ 3049.33	$\mathbf{b_1}$ -5.7e-03	$\mathbf{b_2}$ -9.5e-05
$\mathbf{b_3}$ 21.53e-09	$\mathbf{b_4}$ -200.26e-14	$\mathbf{C_u}$ 2.32584	$\mathbf{C_r}$ 4.186e-03
$\mathbf{d_o}$ 10.41066	$\mathbf{d_1}$ 7.85125	$\mathbf{d_3}$ -3.71257	$\mathbf{e_o}$ -15.001e03
$\mathbf{e_1}$ -15.838e03	$\mathbf{e_3}$ 9.613e03	$\mathbf{f_o}$ -.10329	$\mathbf{f_1}$ -.38656
$\mathbf{f_3}$ .154226	$\mathbf{f_4}$ -14.763	$\mathbf{f_5}$ 118.27	$\mathbf{f_6}$ 14.503
$\mathbf{r_o}$ -.2977	$\mathbf{r_1}$ 11.98	$\mathbf{r_2}$ -25442	$\mathbf{r_3}$ -.4354

Constants as a Function of Temperature:

$$A(T) = a1T + a2T2 + \ldots + a5T5$$

$$B(T) = b0 + b1T + \ldots + b4T4$$

Constants as a Function of Lambda (Excess Air Coefficient):

$$D(\lambda) = d0 + d1\lambda - 1 + d3\lambda - 3$$

$$E(T,\lambda) = e0 + e1\lambda - 1 + e3\lambda - 3$$

Constant as a Function of Temperature, Pressure, and Lambda:

$$F(T,p,\lambda) = (f_0 + f_1\lambda - 1 + f_3\lambda - 3 + f_4 + f_5\lambda - 1\ T)\ln(f_6 p)$$

Correction Factors for Internal Energy and the Gas Constant were Found to be:

$$ucorr(T,p,\lambda) = C_u \exp(D(\lambda) + E(T,\lambda) + F(T,p,\lambda))$$

$$\mathrm{Rcorr}(T, p, \lambda) = C_r \exp\left(r_o \ln(\lambda) + \frac{r_1 + \frac{r_2}{T} + r_3 \ln(f_6 P)}{\lambda} \right)$$

The Internal Energy as a Function of Temperature, Pressure, and Lambda was Found to be:

$$u(T, p, \lambda) = A(T) - B(T)\,\lambda + \mathrm{ucorr}(T, p, \lambda)$$

The Ratio of Specific Heats was then Found to be:

$$\gamma = \frac{cp}{cv} = 1 + \frac{R}{C_v}$$

B: Two-zone MATLAB Code Using Annand's Method

```
%University Of Idaho Engine Simulation
%Uses "Two Zone" Combustion Analysis With Variable Specific Heats Ratios
%Only Models The Compression And Expansion Strokes
%_____________________________________________________________________

clear all;
close all;
clc;

%_____________________________________________________________________

%Engine Inputs
Load = 1;            %Engine Load (Affects Inlet Pressure)
RPM = 4500;          %Revolutions Per Minute [1/min]
L = .08839;          %Stroke of Engine [m]
B = .1016;           %Bore of Engine [m]
l = .0935;           %Length of Engine Connecting Rod [m]
N_cyl = 6;           %Number of Cylinders [unitless]
C_r = 9.1;           %Compression Ratio [unitless]
N_r = 2;             %Number of Revolutions Per Power Stroke
theta_b = 60;        %Combustion Burn Duration [degrees]
theta_0 = 156;       %Crank Angle At Start of Combustion [degrees]
theta_f = theta_0+theta_b; %Final Comb. Angle [degrees]
IVC = 0;             %Time [degrees] when Intake Valve Closes
EVO = 330;           %Time [degrees] when Exhaust Valve Opens

%_____________________________________________________________________

%Engine Calculations Based On Previous Inputs
%Assumes Average Surface Area In Which Heat Transfer Occurs

A_p = (pi/4)*B^2;                %Cross Sectional Piston Area [m^2]
A_ch = A_p;                      %Cylinder Head Surface Area (in chamber)
V_d = N_cyl*A_p*L;               %Displaced Volume Of Engine [m^3]
N = RPM/60;                      %Converts RPM to RPS [1/s]
S_bar_p = 2*L*N;                 %Calculates Mean Piston Speed [m/s]
a = L/2;                         %Calculates Crank Radius (1/2 stroke)[m]
V_TDC = (V_d/(C_r-1))/N_cyl;     %Calculates Clearance Volume [m^3]
V_BDC = (V_d/N_cyl)+V_TDC;       %Cyl. Volume At BDC [m^3]

%_____________________________________________________________________

%Calculating Losses Due To Friction
%fmep (obtained from Blair) Based On Displacement, RPM

if V_d>500*10^(-6)
    fmep=(100000+350*L*RPM)*10^(-3);
end
if V_d<500*10^-6
    fmep=(100000+100*(500-V_d*10^(-6))+350*L*RPM)*10^(-3);
end
```

```
%Initial Preallocation Of Matrices (Second Preallocation In Loops Needs To
%Be Included (Do Not Delete)
V(1:360)=zeros;DV(1:360)=zeros;rho(1:360)=zeros;mu(1:360)=zeros;
C_k(1:360)=zeros;C_R(1:360)=zeros;X(1:360)=zeros;M_F(1:360)=zeros;
DX(1:360)=zeros;Re(1:360)=zeros;Nus(1:360)=zeros;h_g(1:360)=zeros;
DQ_w(1:360)=zeros;DQ(1:360)=zeros;Q(1:360)=zeros;DT(1:360)=zeros;
DP(1:360)=zeros;P(1:360)=zeros;T(1:360)=zeros;W_dot(1:360)=zeros;
W(1:360)=zeros;T_indicated(1:2)=zeros;Q_dot(1:360)=zeros;u(1:360)=zeros;
du(1:360)=zeros;cv(1:360)=zeros;m_b(1:360)=zeros;m_u(1:360)=zeros;
V_u(1:360)=zeros;V_b(1:360)=zeros;T_u(1:360)=zeros;T_b(1:360)=zeros;
A_u(1:360)=zeros;A_b(1:360)=zeros;DT_u(1:360)=zeros;gamma_u(1:360)=zeros;
u_u(1:360)=zeros;du_u(1:360)=zeros;cv_u(1:360)=zeros;DQ2(1:360)=zeros;
DQ_w2(1:360)=zeros;Q2(1:360)=zeros;

%_____________________________________________________________________

%Fuel Inputs/Efficiencies

AF_ratio_stoich = 15.09;    %Theoretical Air Fuel Ratio
lambda = 1;                 %Excess Air Coefficient
AF_ratio_ac = lambda*AF_ratio_stoich; %Actual Air Fuel Ratio
LHV = 44.6e6;               %Lower Heating Value Of Fuel Mixture [J/kg]
eta_combmax = .95;          %Assumed MAX COmb. Efficiency

%Predicts Combustion Efficiency (Reference To Blair)

eta_comb=eta_combmax*(-1.6082+4.6509*lambda-2.0764*lambda^2);

%Atmospheric Inputs

P_atm = 92500;
P_BDC = Load*P_atm;      %Inlet Pressure[Pa] Moscow,ID
R_air = 287;             %Gas Constant For Air [J/kg-K]
gamma(1:360) = 1.4;      %Preallocate Gamma Array (sets initial value)
T_w =350;                %Assumed Wall Temperature (Reference Stone)
%_____________________________________________________________________

%Polynomials Used To Calculate Gamma As A Function Of RPM

a_1 = .692;     a_2 = 39.17e-06;    a_3 = 52.9e-09; a_4 = -228.62e-13;
a_5 = 277.58e-17;b_0 = 3049.33;  b_1 = -5.7e-02; b_2 = -9.5e-05;
b_3 = 21.53e-09;b_4 = -200.26e-14;c_u = 2.32584;  c_r = 4.186e-03;
d_0 = 10.41066; d_1 = 7.85125;  d_3 = -3.71257;e_0 = -15.001e03;
e_1 = -15.838e03;   e_3 = 9.613e03;f_0 = -.10329;  f_1 = -.38656;
f_3 = .154226;  f_4 = -14.763;  f_5 = 118.27;   f_6 = 14.503;
r_0 = -.2977;   r_1 = 11.98;    r_2 = -25442;   r_3 = -.4354;

%_____________________________________________________________________

R=R_air/1000;
for k = 1:2
%Corrects Temperature Based On Exhaust Gas Residuals
```

```
if k==1
    T_BDC = 300;            %Assumed Inlet Temperature [K]
else
    T_BDC=T_corr;
end

%Calculate Mass of Air In Cylinder/ Mass Of Fuel Based On AFR
rho_a = P_atm/(R_air*T_BDC);    %Air Density kg/m^3
m_a = rho_a*V_d;                %Mass of Air In Cylinder [kg]
m_f = m_a/AF_ratio_ac;          %Mass Of Fuel In Cylinder [kg]
m_c = m_a+m_f;                  %Mass In Cylinder

%Specifying Initial Conditions For Loops
%DV,DX,etc. Are Relative To Change In Theta (i.e. DV/Dtheta)

theta(1:360)=zeros; %Starting Crank Angle [deg]
V(1:360)=zeros;     %Preallocate Volume Array
V(1)=V_BDC;         %Starting Combustion Chamber Volume [m^3]
DV(1:360) = zeros;  %Preallocate Change In Volume Array
DV(1) = 0;          %Specifying Initial Change In Volume [m^3}
P(1:360)=P_BDC;     %Preallocate Pressure Array
DP(1:360) = zeros;  %Specifying Initial Change In Pressure
T(1:360)=zeros;     %Preallocate Temperature Array
T(1) = T_BDC;       %Inlet Temperature [K]
T_u(1)=T_BDC;       %Initial Unburned Temperature[K]
DT(1:360) = zeros;  %Specifying Initial Change In Temperature
DT_u(1:360)=zeros;  %Preallocate Change In Unburned Temperature
gamma(1)=1.4;       %Initial Gamma Input
gamma_u(1)=1.4;     %Initial Gamma Input
X(1:360) = 0;       %Preallocate Mass Burn Array
DX(1:360) = zeros;  %Preallocate Change In Mass Burn Fraction [unitless]
DQ(1:360) = zeros;  %Preallocate Heat Release Array
DQ2(1:360)=zeros;   %Preallocate Two Zone Heat Release Array
Q(1:360)=zeros;     %Preallocate Heat Array
Q2(1:360)=zeros;    %Preallocate 2 zone Heat Array
M_F(1:360) = 0;     %Preallocate Mass In Comubstion Chamber Array
rho(1:360) = zeros;    %Preallocates Ideal Gas Law array
rho(1) = P(1)/(R_air*T(1)); %Initial Value Ideal Gas Array
mu(1:360)=zeros;     %Preallocate Viscosity Array
mu(1)=7.457*10^(-6)+4.1547*10^(-8)*T_BDC-7.4793*10^(-12)*T_BDC^(2);
C_k(1:360)=zeros;   %Preallocate Thermal COnductivity Array
C_k(1) = 6.1944*10^(-3)+7.3814*10^(-5)*T_BDC-1.2491*10^(-8)*T_BDC^(2);
C_R(1:360) = zeros; %Preallocate Radiation Coefficient Array
C_R(1) = 4.25*10^(-09)*((T(1)^4-T_w^4)/(T(1)-T_w)); %Initial Rad. Coeff
Re(1:360)=zeros;    %Preallocate Reynolds Value Array
Re(1)=rho(1)*S_bar_p*B/mu(1); %Initial Reynolds Value
Nus(1:360)=zeros;   %Preallocating Nusselt Number Array
Nus(1)=.49*Re(1)^(.7);  %Initial Nusselt Number
h_g(1:360)=zeros;   %Preallocate Heat Transfer Coefficient Array
h_g(1)=C_k(1)*Nus(1)/B; %Initial Heat Transfer Coefficient
s(1:360)=zeros;     %Preallocates Distance Crank/Piston Axes Array
s(1) = -a*cosd(theta(1))+sqrt(l^2 - a^2*sind(theta(1))^2);%Initial Val.
W(1:360) = zeros;   %Preallocate Work Array
W_dot(1:360) = zeros; %Preallocate Power Array
T_indicated(1:360) = zeros; %Preallocate Torque Array
```

```
Q_dot(1:360) = zeros; %Preallocate Heat Transfer Array
u(1:360) = zeros;    %Preallocate Internal Energy Array
du(1:360) = zeros;   %Preallocates Change In Internal Energy Array
cv(1:360) = zeros;   %Preallocates Heat Capacity Array
DQ_w(1:360)=zeros;   %Preallocate Convective Heat Loss Array
DQ_w2(1:360)=zeros; %Preallocate Convective Heat Loss Array 2 zone
m_b(1:360)= zeros;   %Preallocate mass burned array
m_u(1:360)=m_c;      %Preallocate unburned mass array
V_u(1:360)=zeros;    %Preallocate unburned Volume Array
V_u(1) = V(1);       %Initial Unburned Volume

%_____________________________________________________________________________
theta=1:360;

for i = 2:360

    %Specifies Distance Between Crank/Piston Axes As A Function Of theta
    s = -a*cosd(theta(i))+sqrt(l^2 - a^2*sind(theta(i))^2);
    %Specifies Volume As A Function Of Crank Angle
    V(i) = V_TDC +((pi/4)*B^2)*(l + a - s);
    %Specifies Change In Volume As A Function Of Crank Angle
    DV(i) = V(i)-V(i-1);
    %Calculates Density As A Function Of Crank Angle
    rho(i) = P(i-1)/(R_air*T(i-1));
    %Calculates Viscosity As A Function Of Temperature
    mu(i)=7.457*10^(-6)+4.1547*10^(-8)*T(i-1)-7.4793*10^(-12)*T(i-1)^(2);
    %Calculating Instantaneous Thermal Conductivity of Cylinder Gas
    C_k(i) = 6.1944*10^(-3)+7.3814*10^(-5)*T(i-1)-1.2491*10^(-8)*T(i-
1)^(2);
    %Calculating The Radiation Heat Transfer Coefficient
    C_R(i) = 4.25*10^(-09)*((T(i-1)^4-T_w^4)/(T(i-1)-T_w));
    %Instantaneous Suface Area (For Heat Transfer)
    A = A_ch + A_p + pi*B*(l+a-s);
    if i<=2
        A_u=A;
    end

%_____________________________________________________________________________

    %Specifies Mass Fraction Burn As A Function Of Crank Angle (Weibe
Fcn.)
    %Also Specifies Mass Of Fuel In Combustion Chamber As A Function Of
    %Theta

       if theta(i)<theta_0
            X(i)=0;
        else
        X(i) = 1-exp(-5*((theta(i)-theta_0)/theta_b)^3);
        if theta(i) < theta_f
              M_F(i) = V(theta_0-1)*rho(theta_0-1)/(lambda*AF_ratio_ac);
        end
       end

%_____________________________________________________________________________
```

```
    %Specifies Change In Mass Fraction Burn As A Function Of Crank Angle
    DX(i) = X(i) - X(i-1);

%_____________________________________________________________________

    %Incorporating The Annand Method To Predict Heat Transfer
    %Calculating Reynolds Number
    Re(i)=rho(i)*S_bar_p*B/mu(i);
    %Calculating Nusselt Number (constant=.26 two stroke, .49 4 stroke)
    Nus(i)=.49*Re(i)^(.7);
    %Calculating Heat Transfer Coefficient Using Annand Method
    h_g(i)=C_k(i)*Nus(i)/B;
    %Calculates Convective Losses Into Wall As A Function Of Crank Angle
    DQ_w(i) = (h_g(i)+C_R(i))*A*(T(i-1)-T_w)*(60/(360*RPM));
    DQ_w2(i) = ((h_g(i)+C_R(i))*A_b(i-1)/N_cyl*(T_b(i-1)-T_w)...
        +(h_g(i)+C_R(i))*A_u(i-1)/N_cyl*(T_u(i-1)-T_w))*(60/(360*RPM));
    %Calculates Change In Heat Transfer (total) As A Function Of Crank
    %Angle
    DQ(i) = eta_comb*LHV*M_F(i)*DX(i)-DQ_w(i);
    DQ2(i) = eta_comb*LHV*M_F(i)*DX(i)-DQ_w2(i);
    %Calculates Total Heat Transfer (Per Cycle)
    Q(i) = Q(i-1)+DQ(i);
    Q2(i) = Q2(i-1)+DQ2(i);

%_____________________________________________________________________

    %Specifies Pressure and Temperature Increases Between Intake Valve
    %Closing and Exhaust Valve Opening
    if IVC< theta(i)
        DT(i)=T(i-1)*(gamma(i-1)-1)*((1/(P(i-1)*V(i-1)))*DQ(i)...
            -(1/V(i-1))*DV(i));
        DP(i)=(-P(i-1)/V(i-1))*DV(i)+(P(i-1)/T(i-1))*DT(i);
        P(i) = P(i-1)+DP(i);
    end
    if EVO < theta(i)
        P(i) = P_atm;
    end
    if 200 < theta(i)
      if P(i)<=P_atm
        P(i)=P_atm;
      end
    end
%_____________________________________________________________________

    %Calculate Burned, Unburned Mass Fractions
    m_b(i) = m_b(i-1)+DX(i)*m_c;     %Burned Mass
    m_u(i) = m_u(i-1)-DX(i)*m_c;     %Unburned Mass
    %Calculating Burned, Unburned Volumes
    if theta(i)<=theta_0
        V_u(i)=N_cyl*V(i);
    end
    if theta(i)>theta_0
    V_u(i)=((m_u(i)*V_u(i-1))/m_u(i-1))*(P(i)/P(i-1))^(-1/gamma_u(i-1));
```

```
    end
    V_b(i)=N_cyl*V(i)-V_u(i);
    if V_b(i)<0
        V_b(i)=0;
    end
    %Calculating Burned, Unburned Temperatures
    T_u(i)=P(i)*V_u(i)/(m_u(i)*R*1000);
    if theta(i) <= theta_0+4
        T_b(i)=0;
    end
    if theta(i)>theta_0+4
        T_b(i)=P(i)*V_b(i)/(m_b(i)*R*1000);
    end

    %Calculate Unburned, Burned Areas Based On Volume Ratio
    A_u(i)=A*(1-sqrt(X(i)));
    A_b(i)=A*(X(i)/sqrt(X(i)));
    DT_u(i)=T_u(i)-T_u(i-1);

%_____________________________________________________________________

    %Returns Temperature Values To Beginning Of Loop
    %Assumes Temperature Drops Back To ATM Temp After Exhaust Is Extracted
    T(i) = T(i-1)+DT(i);
    %Calculate The Residual Gas Fraction
    %Assume A Polytropic Constant Of 1.3
    R_frac = (1/C_r)*(P_BDC/P(EVO))^(1/1.3);
    %Calculates Cylinder Work [J] As A Function Of Crank Angle
    %Treats Atmospheric Pressure As Reference State
    W(i) = W(i-1)+(P(i)-P_atm)*DV(i);
    %Calculates Power [kW] As A Function Of Crank Angle
    W_dot(i)=(N_cyl*W(i)*N/N_r)/1000;
    %Indicated Mean Effective Pressure
    imep = W_dot(360)*N_r*1000/(V_d*1000*N);
    %Calculates Torque[N*m] As A Function Of Crank Angle
    T_indicated(i) = (W_dot(i)*1000)/(2*pi*N);
    %Calculates Heat Loss [kW] As A Function Of Crank Angle
    Q_dot(i) = (N_cyl*Q(i)*N/N_r)/1000;

%_____________________________________________________________________

    % The Following Section Of Code Calculates An Updated Value Of Gamma
    % Using The "Polynomial Method" Developed By Krieger-Borman
    % User Of This Code Must Be Careful Because Accuracy Of This Method
    % Drops As The Fuel Mixture Becomes Increasingly Rich

    %Calculates A,B Factors For Following Block Of Code
    A_t = a_1*T(i)+a_2*T(i)^2+a_3*T(i)^3+a_4*T(i)^4+a_5*T(i)^5;
    A_tu = a_1*T_u(i)+a_2*T_u(i)^2+a_3*T_u(i)^3+a_4*T_u(i)^4+a_5*T_u(i)^5;
    B_t = b_0+b_1*T(i)+b_2*T(i)^2+b_3*T(i)^3+b_4*T(i)^4;
    B_tu = b_0+b_1*T_u(i)+b_2*T_u(i)^2+b_3*T_u(i)^3+b_4*T_u(i)^4;
    %Calculates Factor "D" As A Function Of lambda
    D_lambda = d_0 + d_1*lambda^(-1)+ d_3*lambda^(-3);
    %Calculates Factor "F" As A Function Of Temperature,lambda
```

```
    E_TLambda = (e_0 + e_1*lambda^(-1)+ e_3*lambda^(-3))/T(i);
    E_TLambdau = (e_0 + e_1*lambda^(-1)+ e_3*lambda^(-3))/T_u(i);
    F_TPLambda = (f_0 + f_1*lambda^(-1) + f_3*lambda^(-3) + ...
        ((f_4 + f_5*lambda^(-1))/T(i)))*log(f_6*P(i));
    F_TPLambdau = (f_0 + f_1*lambda^(-1) + f_3*lambda^(-3) + ...
        ((f_4 + f_5*lambda^(-1))/T_u(i)))*log(f_6*P(i));
    %Calculates Correction Factor For Internal Energy
    u_corr = c_u*exp(D_lambda +E_TLambda + F_TPLambda);
    u_corr_u=c_u*exp(D_lambda +E_TLambdau + F_TPLambdau);
    %Calculates Internal Energy As A Function Of Crank Angle
    u(i) = A_t - B_t/lambda + u_corr;
    u_u(i) = A_tu - B_tu/lambda + u_corr_u;
    %Calculates Change In Internal Energy
    du(i) = u(i) - u(i-1);
    du_u(i) = u_u(i) - u_u(i-1);
    %Calculates Heat Capacity "C_v" As A Function Of Crank Angle
    cv(i) = du(i)/DT(i);
    cv_u(i)=du_u(i)/DT_u(i);
    %Calculates Correction Factor For "R" Value As A Function Of Crank
    %Angle
    R_corr = c_r*exp(r_0*log(lambda) + (r_1+r_2/T(i) + ...
        r_3*log(f_6*P(i)))/lambda);
    R_corr_u = c_r*exp(r_0*log(lambda) + (r_1+r_2/T_u(i-1) + ...
        r_3*log(f_6*P(i)))/lambda);
    %Calculates Actual "R" Value
    R = .287 + .020/lambda + R_corr;
    R_u = .287 + .020/lambda + R_corr_u;
    %Calculates Actual Gamma Value And Returns To Beginning Of Code
    gamma_u(i)=1+R_u/cv_u(i);
    gamma(i) = 1 + R/cv(i);
        if gamma(i)<1.2
            gamma(i)=1.4;
            gamma_u(i)=1.4;
        end

    if theta(i)>=EVO
        gamma(i)=1.4;
        gamma_u(i)=1.4;
    end
%_____________________________________________________________________

    %Calculate Temperature Of Exhaust Based On Polytropic Relations
    if EVO < theta(i)
    T(i)=T(EVO)*(P_BDC/P(EVO))^((gamma(i)-1)/gamma(i));
    T_b(i)=T_b(EVO)*(P_BDC/P(EVO))^((gamma(i)-1)/gamma(i));
    end
end
%Calculates A Corrected Inlet Temperature Based On EGR
T_corr = R_frac*T(360)+(1-R_frac)*T_BDC;
end
%_____________________________________________________________________

%Specified Outputs (On Matlab Screen)
W_dot_indicated=W_dot(360);
bmep = imep-fmep;
```

```
W_dot_ac = (bmep*V_d*1000*N/(N_r*1000));

%Calculated Mechanical Efficiency (Based On Previous Inputs)
eta_m = bmep/imep;   %Calculates Mechanical Efficiency

%_____________________________________________________________________

%Calculates Brake Specific Fuel Consumption
m_ta = P_BDC*V_d/(R_air*T_BDC);        %Calculate Trapped Air In Cylinder
eta_v = (m_ta)/(1.2*V_d);                    %Volumetric Efficiency
m_dot_a = 1.2*V_d*N*eta_v/N_r;               %Mass Flow Air
m_dot_f = m_dot_a/AF_ratio_ac;               %Mass Flow Fuel
BSFC = (m_dot_f*1000*3600)/(W_dot_ac);  %BSFC [g/kW*h]
eta_f = 3600/(BSFC*(LHV*10^(-6)));           %Arbitrary Efficiency

%_____________________________________________________________________

%Specifies Conditions For Minimum and Maximum Plot Values
v_min = min(V); v_max = max(V);
p_min = min(P); p_max = max(P);
w_min = min(W_dot); w_max = max(W_dot);
T_min = min(T); T_max = max(T);
Q_min = min(Q_dot); Q_max = max(Q_dot);
Tmin = min(T_indicated); Tmax = max(T_indicated);

%_____________________________________________________________________

%Plot Statements

figure(1)
plot(theta,X)
title('Mass Fraction Burned Vs. Theta')
xlabel('theta[deg]')
ylabel('Mass Fraction Burned (%)')
axis([0 360 -.1 1.1])

figure(2)
plot(theta,V)
title('Volume Vs. Crank Angle')
xlabel('theta[deg]')
ylabel('Volume [m^3]')
axis([0 360 v_min v_max])

figure(3)
plot(theta,P/1000)
title('Cylinder Pressure Vs. Crank Angle')
xlabel('theta[deg]')
ylabel('Pressure [kPa]')
axis([0 360 p_min/1000 p_max/1000])

figure(4)
plot(theta,T)
title('Cylinder Temperature Vs. Crank Angle')
```

```
xlabel('theta[deg]')
ylabel('Temperature [K]')
axis([0 360 T_min T_max])

figure(5)
plot(theta,P/1000,'b')
title('Pressure,Power,and Heat Transfer')
hold on;
plot(theta,W_dot,'g')
plot(theta,Q_dot,'r')
legend Pressure Power HX
xlabel('theta[deg]')
ylabel('Respective Units (kPa,kW)')
axis([1 360 w_min-100 p_max/1000])

figure(6)
plot(theta,T,'g')
xlabel('theta[deg]')
ylabel('Temperature [K]')
title('Bulk, Unburned, and Burned Temperatures [K]')
hold on;
plot(theta,T_u,'b')
plot(theta,T_b,'r')
legend Bulk Unburned Burned
axis([0 360 300 5000])
```

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