Computer Simulation of an Internal Combustion Engine

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Commonly used symbols, subscripts, and abbreviations

1. Symbols

- \(a\) Crank radius
- \(A_c\) Clearance volume
- \(A_t\) Effective flow area
- \(A_p\) Port area
- \(A_v\) Valve cross sectional area
- \(A_w\) Exposed total cylinder area
- \(b_o\) Cylinder bore
- \(c_o\) Sound speed
- \(C_f\) Flow coefficient
- \(C_p\) Specific heat at constant pressure
- \(C_v\) Specific heat at constant volume
- \(d\) Diameter
- \(D\) Diameter
- \(h\) Specific enthalpy
- \(h\) Height
- \(h_g\) Heat transfer coefficient
- \(k\) Turbulent kinetic energy
- \(l\) Connecting rod length
- \(m\) Mass
- \(m_r\) Residual mass
- \(\dot{m}\) Mass flow rate respective to time
- \(\dot{m}\) Mass flow rate respective to angle
- \(N\) Crankshaft rotational speed
- \(P\) Pressure
- \(\dot{P}\) Power
- \(\dot{Q}\) Heat transfer rate respective to time
- \(\dot{Q}\) Heat transfer rate respective to angle
- \(r\) Radius
- \(r_c\) Compression ratio
- \(R_c\) Connecting rod/stroke length
s   Stroke  
T   Temperature  
u   Specific internal energy  
U   Internal energy  
V   Velocity  
     Speed  
     Cylinder volume  
V_c  Clearance volume  
V_d  Displacement volume  
W   Work transfer  
x   Mass fraction  
x_r  Residual mass fraction  
θ   Crank angle  
ρ   Density  
ω_s  Angular velocity  

2. Subscripts  

b   Burned gas  
c_r  Crevice  
e   Exhaust  
f   fuel  
i   Intake  
L   Laminar  
u   Unburned  
v   valve  
w   wall  
o   Reference value  
     Stagnation value  

3. Notation  

~   Value per second  
^   Value per angle  
.   Moment after the spark
4. Abbreviations

<table>
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<tr>
<th>Abbreviation</th>
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<tr>
<td>BC</td>
<td>Bottom-center crank position</td>
</tr>
<tr>
<td>ICE</td>
<td>Internal Combustion Engine</td>
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<tr>
<td>TC</td>
<td>Top-center crank position</td>
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Abstract

My end course project was performed in the exchange program between Faculdade de Engenharia da Universidade do Porto (FEUP) and the University of Maryland, Baltimore County (UMBC).

The project was proposed by Dr. Christian von Kerczek (CVK) who developed a thermodynamic engine model for which a computer program had been written for its implementation.

The computer simulation was developed and implemented numerically by way of a “Scilab”. However, heat transfer, Q (Q=0), was left out which results somewhat artificially in an "adiabatic engine". Also the combustion model used was based on a somewhat simple formulation. It was assumed that burned and unburned gases were homogeneously mixed and burning rate was a constant. Based on CVK work, my work has added heat transfer and a two zone combustion model that separates the action of the burned and unburned gases during the combustion. The boundary of these zones was then determined by a turbulence flame speed model.

In both of these cases, there exist well developed empirical models, and the main objective of my work was to understand and adjust these models and implement them within the theoretical model and the computer program developed by CVK.

This work contains a complete description of the theoretical framework employed by CVK as well as the modifications and implementation of heat transfer and combustion model by me.

The result of my project is a computer simulation which may be used to obtain some fairly good estimates of engine performance. These estimates are most useful for understanding basic engine performance as well as assessing modifications as regards valve sizing, spark advance and various fuels. A particularly useful application is to do a compressor/turbine engine matching for turbocharging.

The report is based on and extends a prior, informal, report by CVK.
Objectives

The main propose of my work:

- Complete the program with the heat transfer model and insert the correct modifications to perform a simulation of a non adiabatic engine;
- Add a new combustion model, replacing the existing one used in the initial program. The new combustion model would take into account the turbulence in the cylinder and would then allow the variation of burn duration (which is fixed in the simple model used) to vary with engine speed.

Despite this, I also had to understand the existing computer simulation implemented by CVK and the theoretical concepts behind it.
Introduction

This report presents the Thermodynamics theory describing the main physical phenomena occurring inside a spark ignition four stroke (4S) internal combustion engine (ICE) while it is running at steady speed (constant revolutions per minute, rpm). The mathematical form of the Thermodynamic theory is developed and implemented numerically by way of a “Scilab” computer program. The result is an ICE computer simulation. This computer simulation may be used to obtain some fairly good estimates of engine performance in which the main effects of compression ratio, sparks timing, some aspects of valve timing, valve sizing, and fuel types, over a range of engine speeds.

Of course not every detail of ICE performance can be accounted for, but depending on the physical details incorporated and their relative importance, many of the most important performance characteristics can be determined to a reasonable degree of accuracy. This report does not deal with any structural or mechanical aspects of an ICE beyond those of the basic geometric features relevant to the containment and external manifestations of the Thermodynamics processes occurring in the engine. These thermodynamic processes are idealized to a certain degree in order to reduce the complexity at this stage of development of the engine simulation.

The simulation is based on the standard configuration of a reciprocating piston in a cylinder closed at one end, the cylinder 'head'. The piston is connected to a crank by way of a connecting rod that protrudes out the opposite open end of the cylinder and connects to a crank. Figure 1 is a schematic diagram of one cylinder of an ICE. The resulting reciprocating motion of the piston imparts a rotation to the crank. This basic slider-crank mechanism (the piston being the slider) transmits power generated by a working fluid, or gas, in the space enclosed by the piston, cylinder and cylinder head, to whatever is connected to crank. The crank is also geared to a camshaft that operates the valves in the cylinder head that periodically open and close to expel or inhale the working gases. Most ICE's have multiple cylinders operating in unison on a common crankshaft. The processes that occur are essentially identical for each cylinder so that the analysis need be done for only one cylinder. The ICE performance is then simply the number of cylinders times the input/output for a single cylinder.
The ICE Thermodynamics analysis is based on the following primary assumptions. All thermodynamics processes are assumed to be internally reversible. The working medium (fuel and air mixtures) is assumed to be an ideal gas with constant specific heats. The equations of state for the burned and unburned media are derived on the basis of equilibrium chemistry. The gas exchange process is based on quasi-steady compressible flow through an orifice.

Further secondary assumptions and idealizations are discussed in the formulation of the thermodynamics model in the next chapters.
Chapter 1- Internal Combustion Engine

1.1. The Basic ICE Mechanism

The piston cylinder-crank mechanism (the slider-crank) is shown schematically in Figure 2. This figure indicates how the up and down motion of the piston turns the crank. The space enclosed by the piston and the cylinder is the main concern here. This is where the latent energy of the fuel-air mixture is released by combustion (oxidized) to produce the sensible energy, which drives the piston. The top of the cylinder enclosure contains an intake and exhaust valve which open and close at appropriate moments of the engine cycle to allow escape of burned gases and ingestion of fresh fuel-air mixture.

![Figure 2 - A four-stroke spark ignition cycle.](image)

The basic engine performance cycles are controlled by the crank rotation. The crank rotation in turn moves the piston up and down, thus varying the volume \( V \) of the space enclosed by the piston and cylinder. This varying volume is the primary controlling factor of the sequence of thermodynamic events occurring in the piston-cylinder space. Henceforth this space will be referred to simply as the cylinder.

The crank rotation is measured in terms of the rotation angle \( \theta \) shown in Figure 3.
At $\theta=0 \left(2n\pi\right)$ the piston is at the bottom-most point in its travel. This point is called bottom center, BC. The cylinder volume $V(\theta)$ can be shown, by an analysis of the slider-crank mechanism to be,

$$v(\theta) = V_m \left(\frac{1}{r_c} + \frac{1}{2} \left(1 - \frac{1}{r_c}\right) \left(1 + \cos(\theta) + R_c - \sqrt{R_c^2 - \sin^2(\theta)}\right)\right)$$  \hspace{1cm} (1.1)

In formula (1.1), $V_m$ is the (maximum) volume in the cylinder at BC, $R_c$ is the ratio of connecting rod length to $s$, where $s=stroke$, and $r_c$ is the compression ratio $\frac{V_m}{V_c}$, where $V_c$ is the (minimum) volume of the cylinder at top center (TC) or $\theta=\pi \left(2(n-1)\pi\right)$. $V_c$ is called the clearance volume and $V_d = V_m - V_c$ is the “displacement” volume, the usual measure of engine capacity or, more commonly, engine size.

The calculation of the instantaneous volume equation (1.1) is discussed in “Appendix A.1”.

Using $V_m$ as an input variable, some other variables such as the $V_c$, $V_d$, bore (bo) and stroke (s) have to be calculated in order to proceed. It was assumed that the bore was equal to the stroke in order to simplify some equations and to use the minimum ones possible,

$$V_d = \frac{\pi}{4} b^2 s$$  \hspace{1cm} (1.2)
\[
\frac{V_d}{V_c} = r_c - 1
\]  
(1.3)

\[
V_c = \frac{V_m}{r_c}
\]  
(1.4)

\[
h_c = \frac{4 \times V_c}{\pi \times b_o}
\]  
(1.5)

assuming that the shape of the clearance volume is a cylinder with diameter \( b_o \) and height, \( h_c \) (Figure 4).

![Figure 4 – Basic geometry of the internal combustion engine](image)

The exposed total cylinder area \( A_w(\theta) \) is the sum of the cylinder clearance area and the displacement area,

\[
A_w = A_d + A_c
\]  
(1.6)
\[ A_w = \frac{v - V_c}{bo/8} + A_c \]  

(1.7)

and

\[ A_c = \pi \times bo \times h_c + \frac{\pi}{2} bo^2 \]  

(1.8)

The operation of the valves is synchronized to the motion of the piston by way of gear or chain drives from the crankshaft. This is not shown in Figure 2. There will be no need for a description of this mechanism here since it will not be made use of. For the present it is only necessary to describe the valve configuration and actual motion of the valves as a function of the crank angle \( \theta \). This will be reserved for the chapter on the gas exchange process in order to keep the exposition simple at this stage. The function, of \( \theta \), describing the motion of the valves is given as part of the basic engine specifications utilized in this study. The camshaft and valve actuation mechanism must then be designed to realize this valve motion function. For this the reader is referred to books on engine and mechanism design given in the bibliography.
1.2. The Equations of State of the Working Gases

This gaseous mixture is assumed to be an ideal gas, albeit with different equations of state in the unburned and burned states. The equations of state of the unburned (subscript u) and burned (subscript b) are derived on the basis of combustion equilibrium chemistry and the coefficients of the thermodynamic properties are given in Reference 1. These two thermodynamic laws apply to the gaseous fuel-air mixture in the cylinder. The linearized versions of the equations are used here. For illustrative purpose the fuel used here is CH$_4$ with an equivalence ratio of 1 and whose properties are very similar to gasoline. During the process of combustion the cylinder contains a mixture of the unburned and burned fuel-air. The mixture is quantified by the burned to total mass ratio $x = \frac{m_b}{m}$, where $m = m_b + m_u$. The equations of state for each of the gases is

\[ PV_u = m_u * R_u * T \]  
\[ u_u = C_v u * T + h_f u \]  
\[ PV_b = m_b * R_b * T \]  
\[ u_b = C_v b * T + h_f b \]

then, if the gases are homogeneously mixed,

\[ PV = m * (x R_b + (1 - x) R_u) * T = mRT \]  
\[ U = m * u = m * (x * C_v_b + (1 - x) * C_v_u) * T + x * h_f b + (1 - x) * h_f u \]

CVK utilized the homogeneously mixed charge described by equations (1.13) and (1.14), where

\[ \frac{dx(t)}{dt} \] is an empirically determined burning rate.

One of the main aims of this study is to implement a more realistic combustion model in which unburned and burned gases remain separated, i.e., a “two zone” model.
1.3. Thermodynamics and Mathematical Model of the Engine

The engine operates in a two-cycle (4 stroke) mode. Each cycle consists of a complete rotation, through an angle of $2\pi$, of the crank. The first cycle is called the power cycle in which both valves are closed and the power of the engine is produced. This cycle consists of the compressions stroke roughly from $\theta=0$ to $\theta=\pi$, in which the fuel-air mixture in the cylinder is compressed, followed by the expansion stroke, roughly from $\theta=\pi$ to $\theta=2\pi$, in which the main positive engine work is done. The second cycle is called the gas exchange cycle in which the burned gases from the expansion stroke are expelled (exhaust stroke, $\theta=2\pi$ to $\theta=3\pi$) and fresh fuel-air is ingested (intake stroke, $\theta=3\pi$ to $\theta=4\pi$).

These two cycles are completely described by the main two laws of thermodynamics governing the unburned and burned fuel-air mixture in the cylinder. The two laws are the Conservation of Mass,

$$\frac{dm}{dt} = \dot{m}_i - \dot{m}_e$$  \hspace{1cm} (1.15)

and the Conservation of Energy (1st Law of Thermodynamics),

$$\frac{dU}{dt} = \dot{Q} - \dot{W} + \dot{H}_i - \dot{H}_e$$  \hspace{1cm} (1.16)

Here $m$ is the mass of burned plus unburned fuel-air mixture in the cylinder at any instant of time $t$, $\dot{m}_i$ and $\dot{m}_e$ are the mass flow rates into and out the cylinder, respectively, $\dot{Q}$, $\dot{W}$, $\dot{H}_i$, and $\dot{H}_e$ is the heat rate into or out of the cylinder, the work rate into or out of the cylinder, the enthalpy flow rate into the cylinder, and the enthalpy flow rate out the cylinder respectively.

In the application of these equations to the analysis of the engine cycles at constant speed (constant crank angular velocity, $\omega$), it is the most convenient to transform time $t$ to angle $\theta$ by the equation $\omega \ dt = d \theta$. Then the time derivatives in equations (1.15) and (1.16) are replaced by angle derivatives and the ~ over symbols is replaced by ^ over the symbols to signify that rates are with respect to angle instead of time. Then,
\[ \frac{dm}{d\theta} = \dot{m}_i - \dot{m}_e \]  \hspace{2cm} (1.17)

\[ \frac{dU}{d\theta} = \dot{Q} - \dot{W} + \dot{H}_i - \dot{H}_e \]  \hspace{2cm} (1.18)
Chapter 2 - Power Cycle

This chapter presents the thermodynamics theory describing the main physical phenomena occurring inside an ICE.

The thermodynamic models of the four movements, or strokes, of the piston before the entire engine firing sequence is repeated, are described in this chapter and chapter 3.

2.1. Introduction

In this cycle, the valves are closed so there is no mass exchange and it is where the main power of the engine is produced.

This cycle consists in a complete rotation which is characterized by two stages:

(a) Compression stage - roughly from \( \theta = 0 \) to just before the spark plug goes off,

\[ \theta_s = 0.88 \pi \]

in which the fuel-air mixture in the cylinder is compressed. The value of \( \theta_s \) given is typical. All engines start combustion before TC \( (\theta = \pi) \). This called spark advance.

(b) Combustion stage - roughly from \( \theta_s \) to just before exhaust valve opens,

\[ \theta_{cvo} = 2 \pi - \delta \]

where \( \delta > 0 \) depending on some factors, such as the flame speed and piston speed. Combustion begins during compression and most expansion.

In the beginning of this cycle, the cylinder and the combustion chamber are full of the low pressure fresh fuel/air mixture and residual (exhaust gas), as the piston begins to move, the intake valve closes. With both valves closed, the combination of the cylinder and combustion chamber form a completely closed vessel containing the fuel/air mixture. As the piston is pushed to the TC, the volume is reduced and the fuel/air mixture is compressed during the compression stroke.

As the volume is decreased because of the piston's motion, the pressure in the gas is increased, as described by the laws of thermodynamics.

Sometime before the piston reaches TC of the compression stroke, the electrical contact is opened. The sudden opening of the contact produces a spark in the combustion chamber which ignites the fuel/air mixture. Rapid combustion of the fuel releases heat, and produces exhaust gases in the combustion chamber. Because the intake and exhaust valves are closed, the combustion of the
fuel takes place in a totally enclosed (and nearly constant volume) vessel. The combustion increases
the temperature of the exhaust gases, any residual air in the combustion chamber, and the
combustion chamber itself. From the ideal gas law, the increased temperature of the gases also
produces an increased pressure in the combustion chamber. The high pressure of the gases acting
on the face of the piston cause the piston to move to the BC which produces work.

Unlike the compression stroke, the hot gas does work on the piston during the expansion stroke.
The force on the piston is transmitted by the piston rod to the crankshaft, where the linear motion of
the piston is converted to angular motion of the crankshaft. The work done on the piston is then used
to turn the shaft, and to compress the gases in the neighboring cylinder’s compression stroke.

As the volume increase during the expansion, the pressure and temperature of the gas tends to
decrease once the combustion is completed.

2.2 Compression stage

2.2.1 Thermodynamic Model of the compression stage

During this stage, the energy balance on the in-cylinder gas is,

\[
\frac{dU}{d\theta} = \dot{Q} - \dot{W}
\]  

(2.1)

As both valves are closed there is no mass exchange so

\[
\frac{dm}{d\theta} = \dot{m}_i = \dot{m}_e = 0
\]  

(2.2)

After the algebraic manipulation shown in “Appendix A.2” equation (2.1) becomes,

\[
\frac{dT}{d\theta} = \frac{\dot{Q}}{m*A} - (xR_b + (1-x)R_u) \frac{T}{AV} \frac{dV}{d\theta} - \frac{\Delta CvT + \Delta hf}{A} \frac{dx}{d\theta}
\]  

(2.3)

where the quantity  
\[
A = x*\Delta Cv + Cv_u
\]

At this stage, the mass of gases in the cylinder is primarily unburned. However, there is a small
amount of burned gas, called residual gases \( m_r \) which remains after the exhaust stroke. These
gases are homogeneously mixed, where \( x = \frac{m_r}{m} \). Thus equations (1.13) and (1.14) do apply for this part of the cycle.

2.2.2 Heat transfer

Heat transfer plays an important role inside an ICE because it affects the engine performance, efficiency, and emissions.

“The peak burned gas temperature in the cylinder of an internal combustion engine is of order 2500K. Maximum metal temperatures for the inside of the combustion chamber space are limited to much lower values by a number of considerations, and cooling for the cylinder head, cylinder, and piston must therefore be provided. These conditions lead to heat fluxes to the chamber walls that can reach as high as 10 MW/m\(^2\) during the combustion period.”[1]

In regions of high heat transfer, it is necessary to estimate it in order to avoid thermal stresses that would cause fatigue cracking in the engine's materials (“temperatures must be less than about 400°C for cast iron and 300°C for aluminum alloys”[1])

The critical areas due to the heat transfer inside an ICE are the engine's piston which is exposed to the gases at the combustion chamber and exhaust system that contains the exhaust valve which is exposed to the exhaust gases that flow past it at high velocities (making for good heat transfer).

For a given mass of fuel within the cylinder, higher heat transfer to the combustion chamber walls will lower the average combustion gas temperature and pressure, and reduce the work per cycle transferred to the piston. Thus specific power and efficiency are affected by the magnitude of engine heat transfer.

The source of the heat flux is not only the hot combustion gases, but also the engine friction that occurs between the piston rings and the cylinder wall which will not be contained in this work. Heat transfer due to the friction is negligible.

“The maximum heat flux through the engine components occurs at fully open throttle and at maximum speed. Peak heat fluxes are on the order of 1 to 10 MW/m\(^2\). The heat flux increases with increasing engine load and speed. The heat flux is largest in the center of the cylinder head, the exhaust valve seat and the center of the piston. About 50% of the heat flow to the engine coolant is through the engine head and valve seats, 30% through the cylinder sleeve or walls, and the remaining 20% through the exhaust port area.”[3]
Therefore, heat transfer is a very important parameter in an engine because it is required for a number of important reasons, including engine’s performance and efficiency, material temperature limits, lubricant performance limits, emissions, and knock (see appendix B.1).

a) Heat transfer modeling

In the previous equations, the differential heat transfer is represented by $\dot{Q}$.

The differential heat transfer $\dot{Q}$ to the cylinder walls can be calculated if the instantaneous average cylinder heat transfer coefficient $h_g(\theta)$ and engine speed $N (= \text{rpm})$ are known.

The average heat transfer rate at any crank angle $\theta$ to the exposed cylinder wall at an engine speed $N$ is determined with a Newtonian convection equation:

$$
\dot{Q} = h_g(\theta) A_w(\theta)(T(\theta) - T_w)/N \tag{2.4}
$$

The cylinder wall temperature $T_w$ is the area-weighted mean of the temperatures of the exposed cylinder wall, the head, and the piston crown. The heat transfer coefficient $h_g(\theta)$ is the instantaneous averaged heat transfer coefficient. At this stage, the exposed cylinder area $A_w(\theta)$ is the sum of the cylinder bore area, the cylinder head area and the piston crown area, assuming a flat cylinder head.

b) Heat transfer coefficient

The instantaneous heat transfer coefficient, $h_g(\theta)$ during the power cycle depends on the gas speed and cylinder pressure, which change significantly during the combustion process.

There are two correlations that are used to get the heat transfer coefficient, the Annand and the Woschni correlation. However, to compute the heat transfer coefficient it was used an empirical formula for a spark ignition engine given in Han et al. (1997),

$$
h_g = 687 * P^{0.75} * U^{0.75} * bo^{-0.25} * T^{-0.465} \tag{2.5}
$$
with some slightly modifications.

The units of \( h_g \), \( P \), \( U \), \( b \) and \( T \) are \( \text{W/m}^2\text{K} \), \( \text{kPa} \), \( \text{m/s} \), \( \text{m} \) and \( \text{K} \), respectively.

The heat transfer coefficient can also be obtained using the averaged heat transfer coefficient correlation of C. F. Taylor ("The Internal Combustion Engine in Theory and Practice", MIT Press, 1985),

\[
\frac{h \times b}{k} = 10.4 \times m^{(3/4)} \left( \frac{U \times b}{V \times \mu} \right)^{(3/4)}
\]

(2.6)

where \( k \) is gas thermal conductivity and \( \mu \) the gas kinematic conductivity.

However, this formula can be manipulated into the form,

\[
h_g = C' \times P^{0.75} \times U^{0.75} \times b^{0.25} \times T^{-0.75}
\]

(2.7)

Formula (2.5) differs from this only by the coefficient \( C' \) and the power of \( T \). We have found that the value of \( C'=300 \) along with the power of \( T \) in formula (2.6) seems to be more reasonable.

\[
h_g = 300 \times P^{0.75} \times U^{0.75} \times b^{-0.25} \times T^{-0.465} / 1000
\]

(2.8)

Note that the unit used for energy in the "Scilab" simulation was kJ, so, equation (2.8) was divided by 1000 to get everything in the same units.

In equation (2.8), \( U \) is an empirical piston speed and calculated using the equation,

\[
U = 0.494 \times \overline{Up} + 0.73 \times 10^{-6} \times (PdV + VdP)
\]

(2.9)

where

\[
\overline{Up} = \frac{(2 \times N \times S)}{60}
\]

(2.10)

is the actual piston speed. It is very unclear what the last term, \( (PdV + VdP) \), in equation (2.9)
means. Since the coefficient of this term is very small, we left it out.

### 2.3. Combustion stage

In the power cycle chemical combustion commences with spark ignition at the point $\theta_s$ of crank angle just before BC on the compression stroke, $\theta_s = 0.88*\pi$.

The combustion processes that occur in an ICE are very complex and there are many types of models which can describe it. The combustion model used by CVK was based on a single zone homogeneously mixed burning mass with a constant burning rate. This is a model with empirical burning rates that does fairly well, but does not capture true combustion rates.

We now introduce a somewhat more sophisticated combustion model. In the one zone model firstly used, the rate of combustion is assumed to be proportional to crank angle. This is the main assumption we would like to remove. It is well known that the combustion rate has its own dynamics and does not follow crank angle. The combustion rate depends on the dynamics of the gas motion inside the cylinder, especially the turbulence level. As engine speed increases, the turbulence level increases and thus combustion rate increase, but it does not increase at the same rate as engine speed. In order to capture this effect and assess its impact on engine performance we now develop a two zone combustion model. The model used consists in a two zone analysis of the combustion chamber which contains an unburned and burned gas region separated by a turbulent flame front. The flame front progresses at a turbulent flame speed. The turbulence model used that determines the flame speed is given in [2].

#### 2.3.1 Combustion modeling

In an ICE the fuel and air are mixed together in the intake system, inducted through the intake valve into the cylinder, where mixing with residual gas take place, and then compressed. Under normal operating conditions, combustion is initiated towards the end of the compression stroke at the spark plug by an electric discharge. Following inflammation, a turbulent flame develops, propagates through this premixed fuel, air, burned gas mixture until it reaches the combustion chambers walls, and then extinguishes.

From this description it is plausible to divide the combustion process into three distinct phases:

1. Spark ignition
2. Combustion development
(3) Combustion termination
The understanding of each of these phases will be developed next.

(1) Spark Ignition

Ignition is treated as an abrupt discontinuity between the compression and burn stages with the
instantaneous conversion of a specified mass fraction \( f \) of the reactants to products. This produces
the unburned and burned zone, each assumed to be homogeneous and hence characterized by its
own single state.

Using the 1\textsuperscript{st} law equation for burned gas developed later in this section

\[
M_b^* C_{v_b} \frac{dT_b^*}{dt} = \dot{Q}_b - P \frac{dV_b^*}{dt} + M_b^*(C_{p_u} T_u^* - C_{v_b} T_b^* + h_{f_u} - h_{f_b})
\] (2.11)

integrate it over a small time interval \( \Delta t \) (or \( \Delta \vartheta \)). Then by use of the mean value theorem, one
obtains (see “Appendix A.3”),

\[
\ddot{T}_b = \frac{1}{C_{v_b}} \left( C_{p_u} T_u + \| \Delta h_f \| - \frac{P \dot{V}_b}{M_b^*} \right)
\] (2.12)

where the “double dots” represent the moment right after the spark goes on, \( \vartheta_s + \varepsilon \). \( \ddot{T}_b \) is the
initial value of the temperature in the burned zone right after spark.

(2) Combustion development

After the ignition, useful combustion chamber design information can be generated with simple
geometric models of the flame. Usually, the surface which defines the leading edge of the flame can
be approximated by a portion of the surface of a sphere. Thus the mean burned gas front can also be
approximated by a sphere. However, in this study we are mainly interested in overall performance and
not in detailed combustion chamber design. Hence we will use a simplified model of the combustion
chamber and flame front.

a) Engine combustion Chamber Design
There are a large number of options for the ICE chamber design which includes cylinder head and piston crown shape, spark plug location, size and number of valves, and intake port design. The design of these important parts of the ICE revolves around issues such as chamber compactness, surface/volume ratio, flame travel length, the fuel mixture motion and more important the burning velocity.

It is known, that the combustion chamber design which increases the burning velocity, favors the engine performance. When the fuel burning process takes place faster, occupies a shorter crank angle interval at a given engine speed, produces less heat transfer (due to lower burned gas temperatures) and increases efficiency.

Illustrations of each of the most commons examples ICE chamber shapes which produces a “fast burn” will be given next (Figure 5),

![Illustrations](image)

Figure 5 – Example of common internal combustion engine chambers: (a) hemispherical chamber; (b) wedge shaped chamber; (c) bathtub chamber; (d) bowl & piston with flathead on the right. [6]
In the scilab's program it was assumed that the combustion chamber was the simplest possible, so the piston is flat on top, the location of the spark plug is in the middle of the cylinder between the valves and the combustion chamber has a cylindrical geometry. Using this shape and knowing that the combustion reaction is so quick, it is possible to assume that the mean burned gas front can also be approximated by a cylinder instead by a sphere without committing significant errors as regards overall performance.

b) Combustion chamber considerations

Assuming that the burned zone is a cylinder of height, \( h \) and radius, \( r \) at any instant of \( \theta \) and using the model which consists in a two zone analysis of the combustion chamber which contains an unburned and burned gas region separated by a turbulent flame front (Figure 6),

![Figure 6 – Sketch of the front shape of the combustion chamber](image)

It is possible to predict how the radius, \( r \) is going to change during the flame travel, assuming a linear distribution as it will be explained next. The variation of the burned radius due to the change of the crank angle can be expressed by the approximation (Figure 7),
where \( R = \frac{b_0}{2} \), and \( \theta_d \) is the angle \( \theta \) at which the burned gas cylinder reaches the engine cylinder wall. \( \theta_d \) is determined by the flame speed \( \hat{V}_f \) (in terms of angular rates).

Then,

\[
\begin{align*}
\frac{dr}{d\theta} = 0 & \quad \text{for} \quad \theta < \theta_s \\
\frac{dr}{d\theta} = \hat{V}_f (\theta - \theta_s) \quad \text{and} \quad \frac{dr}{d\theta} = \hat{V}_f & \quad \text{for} \quad \theta_s < \theta < \theta_d \\
\frac{dr}{d\theta} = 0 & \quad \text{for} \quad \theta > \theta_d
\end{align*}
\]  

The flame speed \( \hat{V}_f \) is given by the turbulence model. See “Appendix A.4” for mathematical development.

Being \( h = h(\theta) \) the height from piston, at any instant of \( \theta \), to the top of the cylinder, comes

\[
h = \frac{v}{(\pi * R^2)}
\]  

where \( v \) is the total volume of the cylinder.

The burned and unburned volume and mass are easy to predict, now that \( r \) and \( h \) are known.

The burned volume is,

\[
V_b = \pi * h * r^2
\]  

so
\[ V_b = \frac{1}{R^2} v^* r^2 \]  

(2.16)

and its derivative

\[ \frac{dV_b}{d\theta} = \frac{1}{R^2} r^2 \frac{dv}{d\theta} + \frac{2 v^* r}{R^2} \frac{dv}{d\theta} \]  

(2.17)

the unburned volume comes,

\[ V_u = v - V_b \]  

(2.18)

Finally, assuming that \( m_b \) is proportional to \( V_b \), it is possible to say,

\[ \frac{m_b}{m} = \frac{V_b}{v} \]  

(2.19)

then, the burned mass is

\[ m_b = \frac{m}{v} V_b \]  

(2.20)

its derivative

\[ \frac{dm_b}{d\theta} = m^* \left( \frac{1}{v} \frac{dV_b}{d\theta} - \frac{V_b}{v^2} \frac{dv}{d\theta} \right) \]  

(2.21)

and the unburned mass is

\[ m_u = m - m_b \]  

(2.22)

and its derivative

\[ \frac{dm_u}{d\theta} = - \frac{dm_b}{d\theta} \]  

(2.23)

c) Thermodynamic model

The energy balance on the unburned zone is

\[ \frac{dU_u}{dt} = \dot{Q}_u - P \frac{dV_u}{dt} - \dot{M}_b \ast h_u \]  

(2.24)
where \( \frac{dm_u}{dt} = \dot{M}_u = -\dot{M}_b \), \( \dot{M}_u \) is the mass transfer rate to the unburned zone and \( \dot{M}_b \) is the mass transfer rate to the burned zone; \( \dot{Q}_u \) is the heat transfer rate from the unburned zone to the walls; \( P \) is the pressure in the cylinder; \( V_u \) the unburned volume; and \( U_u \) is the total internal energy in the unburned zone.

After the algebraic manipulation explained in "Appendix A.5" this equation becomes,

\[
M_u \cdot C_v u \frac{dT_u}{dt} = \dot{Q}_u - P \frac{dV_u}{dt} + \dot{M}_b \cdot (C_v u - C_p u) \cdot T_u
\]  

(2.25)

The energy balance for the burned zone is

\[
\frac{dU_b}{dt} = \dot{Q}_b - P \frac{dV_b}{dt} + \dot{M}_b \cdot h_u
\]  

(2.26)

where \( \frac{dm_b}{dt} = \dot{M}_b \); where \( \dot{Q}_b \) is the heat transfer rate from the burned zone to the walls; \( V_b \) and \( U_b \) are the volume and internal energy of the burned zone. The mass balances are

\[
\dot{M}_b = \frac{dM_b}{dt}
\]  

(2.27)

and

\[
\dot{M}_u = \frac{-dM_b}{dt}
\]  

(2.28)

where \( M_b \) and \( M_u \) are the zone masses.

After the algebraic manipulation explained in "Appendix A.6" equation (2.26) becomes,

\[
M_b \cdot C_v b \frac{dT_b}{dt} = \dot{Q}_b - P \frac{dV_b}{dt} + \dot{M}_b \cdot (C_p u \cdot T_u - C_v b \cdot T_b + h_f u - h_f b)
\]  

(2.29)

(3) Combustion termination

The end of the combustion occurs when the flame front reaches the walls of the cylinder,
If the end of the combustion process is progressively delayed by retarding the spark timing, or decreasing the flame speed by decreasing the piston speed, the peak cylinder pressure occurs later in the expansion stroke and is reduced in magnitude. These changes reduce the expansion stroke work transfer from the cylinder gases to the piston.

2.3.2 Turbulence characteristics

The flow processes in the engine cylinder are turbulent. In turbulent flows, the rates of transfer and mixing are several times greater than the rates due to molecular diffusion. This turbulent flow is produced by the high shear flow set up during the intake process and modified during compression. It leads to increased rates of heat, mass transfer and flame propagation, so, is essential to the satisfactory operation of the ICE.

This section explains the structure of the turbulent engine flame in the combustion process, as it develops from the spark discharge and the speed at which it propagates across the combustion chamber.

The turbulence model is based on equations that describe the evolution of turbulence in a fluid where the density is a function only of time. For details see [2].

The turbulence kinetic energy per unit mass, \( k \) is described by,

\[
\frac{dk}{dt} = P - D + \frac{1}{M_c} (I - E - k \frac{dM_c}{dt})
\]  

(2.30)

During the burn stage the turbulence energies of the burned and unburned gases are tracked together using the above equation with just the P and D terms,

\[
\frac{dk}{dt} = P - D
\]  

(2.31)

because during the combustion there is no mass transfer, so \( \frac{dM_c}{dt} = 0 \) and \( I \) and \( E \) are
functions of \( \frac{dM_c}{dt} \).

The term \( P \) is the turbulence energy production rate per unit mass and is modeled by,

\[
P = F_p \frac{A_W}{v} \left( \frac{1}{3} \right) \frac{1}{2} k \frac{dv}{v \, dt}
\]

where the first term accounts for turbulence production due to the strain in the shear flow on the walls and the second the effects of compression.

D is the turbulence energy dissipation rate per unit mass and is modeled by,

\[
D = F_d \frac{kV_f}{v^{(1/3)}}
\]

The coefficients \( F_p \) and \( F_d \) are parameters that can be set by reference to experiments. To get the respective values for each term, the Engine Simulation Program (ESP) which is available in the Internet at the site “http://esp.stanford.edu/” was referenced.

Using the turbulence equation and the next two equations, it is possible to estimate \( V_f \) which is the velocity of the flame front relative to the unburned gases,

\[
k = \frac{V_i^2}{2}
\]

and

\[
V_f = V_L + C_f * V_i
\]

where \( V_i \) is the turbulence velocity in the unburned zone, \( V_L \) is the specified laminar flame speed and \( C_f \) is a specified coefficient, approximately unity. The value for \( V_L \) was obtained from the ESP.

After having the \( V_f \) estimated, it is possible to make a realistic approximation to the real variation of the burned radius. Knowing that,

\[
\frac{dr}{dt} = V_f
\]
and \( dt = \frac{1}{w} d \theta \) comes,

\[
\frac{dr}{d \theta} = \frac{V_f}{w}
\]  

(2.37)

Finally, the real variation of the burned radius due to the change of the crank angle when \( \theta_s < \theta < \theta_d \) can be expressed by the next equation,

\[
r = \frac{V_f}{w} (\theta - \theta_s)
\]  

(2.38)

and

\[
\frac{dr}{d \theta} = \frac{V_f}{w} \quad \text{for} \quad \theta_s < \theta < \theta_d
\]  

(2.39)

2.3.3 Heat Transfer

The heat transfer model used in this report is the same as before. However, since we are using the two zone combustion model, during the development of the combustion, different quantities of heat are released from the burned and unburned zone.

Applying the Newtonian convection equation,

\[
\dot{Q} = h_g(\theta) A_w(\theta) (T(\theta) - T_w) / N
\]  

(2.40)

The only thing that will change in this two zone combustion model are the exposed burned and unburned areas as shown in figure 8.

Figure 8 – Areas evolution during the combustion

Unburned Area

Burned Area
The exposed burned area varies in function of the burned radius,

\[ A_{wb} = \pi * r^2 \quad (2.41) \]

the exposed unburned area comes,

\[ A_{wu} = A_w - A_{wb} \quad (2.42) \]

Finally, the heat transfer equation for the burned zone is,

\[ \hat{Q}_{wb} = -h_g * A_{wb} * (T_b - T_w) / N \quad (2.43) \]

where,

\[ h_g = 300 * P^{0.75} * U^{0.75} * b_0^{-0.25} * T_b^{-0.465} / 1000 \quad (2.44) \]

and the heat transfer equation for the unburned zone is,

\[ \hat{Q}_{wu} = -h_g * A_{wu} * (T_u - T_w) / N \quad (2.45) \]

where,

\[ h_g = 300 * P^{0.75} * U^{0.75} * b_0^{-0.25} * T_u^{-0.465} / 1000 \quad (2.46) \]

where the units of \( h_g, P, U, b \) and \( T \) are kW/m²K, kPa, m/s, m and K, respectively. The piston speed, \( U \) is given by equations (2.9) and (2.10).

2.4. Completely burned gas expansion

The burning stage lasts until the piston has progressed beyond TC, but ends before the piston has descended to the point of \( \theta = \theta_{evo} \) near BC. The expansion from the end of combustion to \( \theta_{evo} \) involves completely burned gas.
2.4.1 Thermodynamic equation of burned gas expansion

During this stage, the energy balance on the in-cylinder gas is,

\[ \frac{dU}{d\theta} = \dot{Q} - \dot{W} \]  (2.47)

As both valves are closed there is no mass exchange so

\[ \frac{dm}{d\theta} = \dot{m}_i = \dot{m}_e = 0 \]  (2.48)

After the algebraic manipulation shown in “Appendix A.7” comes,

\[ \frac{dT}{d\theta} = \frac{\dot{Q}}{\dot{m} \Delta C_v} - R_b \frac{T}{\Delta C_v V} \frac{dV}{d\theta} \]  (2.49)

2.4.2 Heat Transfer

At this stage, the heat release rate at any crank angle \( \theta \) to the exposed cylinder wall at an engine speed \( N \) is determined with a Newtonian convection equation,

\[ \dot{Q} = h_g(\theta) A_w(\theta) (T(\theta) - T_w)/N \]  (2.50)

The heat transfer coefficient \( h_g(\theta) \) is the instantaneous averaged heat transfer coefficient and \( A_w \) is the exposed cylinder area.

The instantaneous heat transfer coefficient during the expansion stage is estimated in the same way as the heat transfer coefficient in the compression stage.

\[ h_g = 300 \times P^{0.75} \times U^{0.75} \times b_o^{-0.25} \times T_b^{-0.465} / 1000 \]  (2.51)
where the units of $h_0$, $P$, $U$, $b$ and $T$ are kW/m$^2$K, kPa, m/s, m and K, respectively. The piston speed, $U$ is given by equations (2.9) and (2.10).
Chapter 3 – Gas exchange cycle

This cycle deals with the fundamentals of the gas exchange process, intake and exhaust and the valves mechanism in a four stroke internal combustion engine, called the gas exchange cycle. Only a brief explanation about the thermodynamics state and gas flow rate will be given.

This cycle is called the gas exchange cycle because it is where the burned gases from the expansion stroke are expelled (exhaust stroke, \( \theta = \theta_{evo} \approx 2\pi \) to \( \theta = 3\pi \)) and fresh fuel-air is ingested (ingested stroke, \( \theta_{ivo} \) to \( \theta = 4\pi \)).

This cycle is also described by the main two laws of thermodynamics governing the unburned and burned fuel-air mixture in the cylinder.

The gas exchange process is based on a “perfect valve timing”. In perfect valve timing the exhaust valve closes exactly when the cylinder pressure drops below exhaust system pressure, but after TC at \( \theta = 3\pi \). Then both valves remain closed while the piston descends (expanding the cylinder volume) until the cylinder pressure reaches the intake system pressure, which is less than the exhaust pressure for unsupercharged engines.

3.1. Valve action

Valves allow the gas exchange to occur. Valve opening and closing control is called valve timing. The valves action occurs for the following values of \( \theta \),

- exhaust valve opens (evo) at \( \theta = \theta_{evo} = 2\pi - \pi/9 \);
- exhaust valve closes (evc) at \( \theta = \theta_{evc} = 3\pi \);
- intake valve opens (ivo) at \( \theta = \theta_{ivo} \) determined by intake pressure;
- intake valve closes (ivc) at \( \theta = \theta_{ivc} = 4\pi \).

3.1.1 Geometry

The valves are driven by a cam that rotates at half the speed of the crankshaft.

The valve flow area depends on valve lift and the geometric details of the valve head, seat and stem.
Curtain area = $\pi \times D \times l$ \hspace{1cm} (3.1)

and

Port area = $\frac{1}{4} \pi (D^2 - d^2)$ \hspace{1cm} (3.2)

where $l = l(\theta)$ is the valve lift, D the port diameter and d the stem diameter.

It can be written mathematically as,

$$A_v = \min(\pi D l(\theta), \frac{1}{4} \pi (D^2 - d^2))$$ \hspace{1cm} (3.3)

The valve lift, $l(\theta)$ is usually a curve that looks like figure 9,

![Figure 9 - Typical exhaust valve timing diagram](image)

Approximating this curve by the formula,

$$l(\theta) = \frac{l_m}{2} (1 - \cos(\theta))$$ \hspace{1cm} (3.4)

where $l_m$ is the maximum valve lift and usually

$$l_m > \frac{(D^2 - d^2)}{4D}$$ \hspace{1cm} (3.5)
3.1.2 Isentropic flow thought an orifice

From the gas dynamics, the isentropic flow through an orifice is given by,

\[ \dot{m} = \rho_o \cdot C_f \cdot A_v \cdot c_o \cdot \left( \frac{2}{k-1} \left( \frac{P_v}{P_o} \right)^{\frac{2}{k}} - \left( \frac{P_v}{P_o} \right)^{\frac{k+1}{k}} \right)^{\frac{1}{2}} \]  

(3.6)
as long as,

\[ \frac{P_o}{P_v} < \left( \frac{P_o}{P_v} \right)_{cr} = \left( \frac{k+1}{k} \right)^{\frac{k}{k+1}} \]  

(3.7)

if

\[ \frac{P_o}{P_v} \geq \left( \frac{P_o}{P_v} \right)_{cr} \]  

(3.8)

then

\[ \dot{m} = \dot{m}_{cr} = \rho_o \cdot C_f \cdot A_v \cdot c_o \cdot \left( \frac{2}{k+1} \right)^{\frac{k+1}{2(k+1)}} \]  

(3.9)

When

\[ \frac{P_o}{P_v} \leq \left( \frac{P_o}{P_v} \right)_{cr} \]

the flow is "choked". This means that the flow right at the orifice (the valve passage) is "sonic". At this condition only \( \dot{m}_{cr} \) (=constant) can pass through the valve passage regardless of how small we make \( \frac{P_v}{P_o} \) (see figure 10). Note that \( P_o \) is the upstream pressure (stagnation pressure) and \( P_v \) is the downstream (static pressure – just "behind" valve).
Figure 10 – Isentropic flow through an orifice

For an ideal gas,

\[ \rho_o = \frac{P_o}{R \cdot T_o} \quad (3.10) \]

and \( c_o \) is the speed of sound,

\[ c_o = \sqrt{kRT_o} \quad (3.11) \]

Note that the speed of sound goes up with the upstream temperature. And note that the upstream for exhaust is the cylinder temperature and the upstream for intake is the manifold temperature which is much less than cylinder temperature. That is why exhaust valve is smaller than intake valve.

The non-ideal effects are accounted by introducing a flow coefficient \( C_f \), which is here assumed to be \( C_f \approx 0.40 \).

3.2. Exhaust stage

The configuration of the exhaust system plays an important role for a good engine performance.

The exhaust system typically consists of an exhaust manifold, exhaust pipe, often a catalytic converter for emission control, and a muffler or silencer. My study concerns only with the exhaust stroke which proceeds the power stroke cycle.

At the end of the power stroke, the piston is located at the bottom center, \( \theta = 2\pi \). Heat that is left over from the power stroke is now transferred to the water in the water jacket until the pressure approaches atmospheric pressure. The exhaust valve is then opened by the cam on the rocker arm to begin the exhaust stroke.

The purpose of the exhaust stroke is to clear the cylinder of the spent exhaust in preparation for
another ignition cycle. As the exhaust stroke begins, the cylinder and combustion chamber are full of
exhaust products at low pressure. Because the exhaust valve is open, the exhaust gas is pushed past
the valve and exits the engine.

3.2.1 Thermodynamics Model of the Exhaust stage

As it was said, this stroke is also described by the main two laws of thermodynamics. The energy
balance for the exhaust stroke is,

$$\frac{dU}{d\theta} = \dot{Q} - \dot{W} - H_e$$

(3.12)

As the intake valve is closed there is no mass exchange through it so \( \dot{m}_i = \dot{H}_i = 0 \) and as the
exhaust valve is opened comes \( \frac{dm}{d\theta} = -\dot{m}_e \).

After the algebraic manipulation shown in “Appendix A.8” comes,

$$\frac{dT}{d\theta} = \frac{\dot{Q}}{m*V_b} - \frac{R_b*T}{(V*V_b)} \frac{dV}{d\theta} - \frac{\dot{m}_b}{m} \frac{R_b*T}{C_{y_b}}$$

(3.13)

3.2.2 Heat transfer

At this stage, the heat release rate at any crank angle \( \theta \) to the exposed cylinder wall at an engine
speed \( N \) is determined with a Newtonian convection equation,

$$\dot{Q} = h_{gg}(\theta) A_w(\theta)(T(\theta) - T_w)/N$$

(3.14)

The heat transfer coefficient \( h_{gg}(\theta) \) is the instantaneous averaged heat transfer coefficient and is the
exposed cylinder area.

The instantaneous heat transfer coefficient during the expansion stage is estimated in the same
way as the heat transfer coefficient in the compression stage.
\[ h_g = 300 \times P^{0.75} \times U^{0.75} \times b^{0.25} \times T_b^{-0.465} / 1000 \]  

(3.15)

where the units of \( h_g \), \( P \), \( U \), \( b \) and \( T \) are kW/m\(^2\)K, kPa, m/s, m and K, respectively. The piston speed, \( U \) is given by equations (2.9) and (2.10).

### 2.3. Intake stage

The exchange cycle ends with the intake stroke as the piston is pulled towards the crankshaft (to the bottom center position, BC) as the intake valves opens and fuel (unburned gas) and air are drawn past it and into the combustion chamber and cylinder from the intake manifold located on top of the combustion chamber. The exhaust valve is closed and the electrical contact switch is open. The fuel/air mixture is at a relatively low pressure (near atmospheric). At the end of the intake stroke, the piston is located at the bottom center position, ready to begin the power cycle.

Intake manifolds consisting of plenums (separated spaces containing air at a pressure greater than atmospheric pressure) and pipes are usually required to deliver the inlet air charge from some preparation device such as an air cleaner or compressor.

#### 3.3.1 Thermodynamics Model of the Intake stage

Using the main two laws of thermodynamics, the energy balance for the intake stroke is,

\[ \frac{dU}{d\Theta} = \hat{Q} - \hat{W} + \dot{H}_i \]  

(3.18)

As the exhaust valve is closed there is no mass exchange trough it so \( \dot{m_e} = \dot{H}_e = 0 \) and as the intake valve is opened comes \( \frac{dm}{d\Theta} = \dot{m}_i \).

After the algebraic manipulation shown in “Appendix A.9” comes,

\[ \frac{dT}{d\Theta} = \frac{\hat{Q}}{\dot{m} \times C_{vu}} - \frac{R_u \times T}{V \times C_{vu}} \frac{dV}{d\Theta} + \frac{\dot{m}_u}{\dot{m} \times C_{vu}} \left( C_{pu} \times T_u - C_{vu} \times T \right) \]  

(3.19)
3.3.2 Heat transfer

The heat transfer model for the intake is the same as it was explained for the exhaust process.

Note that in the intake process the heat transfer can be neglected, when comparing it to the heat released in the exhaust and combustion stages.
As it was said, the computer simulation was implemented by way of “Scilab” computer program. “Scilab” is a scientific software for numerical computations, and it is currently used in educational and industrial environments around the world. This program can be found freely in the following website: http://www.scilab.org/

The ICE computer simulation developed is called CycleComQC (see appendix C.1) and the original one developed by CVK is called CycleCom (see appendix C.2).

CycleComQC Inputs

The values of the input parameters used in this simulation can be found in the tables below.

**Engine data:**

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<tr>
<th>Parameter</th>
<th>Value</th>
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<tr>
<td>Compression ratio</td>
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<td>Maximum cylinder volume</td>
<td>Vm</td>
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**Exhaust valve data:**

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<tr>
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<td>Exhaust valve max lift</td>
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Intake-exhaust  state

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<th>Pi</th>
<th>100</th>
<th>K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake pressure</td>
<td>Pi</td>
<td>100</td>
<td>K</td>
</tr>
<tr>
<td>Exhaust pressure</td>
<td>Pe</td>
<td>150</td>
<td>K</td>
</tr>
<tr>
<td>Intake temperature</td>
<td>Ti</td>
<td>320</td>
<td>K</td>
</tr>
</tbody>
</table>

Unburned fuel-air equation of state, CH₄:

<table>
<thead>
<tr>
<th></th>
<th>Ru</th>
<th>0.2968</th>
<th>kJ/kgK</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uf-air gas constant</td>
<td>Ru</td>
<td>0.2968</td>
<td>kJ/kgK</td>
</tr>
<tr>
<td>Cp for uf-air</td>
<td>Cpu</td>
<td>1.022</td>
<td>kJ/kgK</td>
</tr>
<tr>
<td>Specific heat ration for uf-air</td>
<td>ku</td>
<td>1.409</td>
<td>/</td>
</tr>
<tr>
<td>Zero degree enthalpy of uf-air</td>
<td>hfu</td>
<td>-692.0</td>
<td>kJ/kg</td>
</tr>
<tr>
<td>Cv for uf-air</td>
<td>Cvu</td>
<td>0.725</td>
<td>kJ/kgK</td>
</tr>
</tbody>
</table>

Burned fuel-air equation of state, CH₄:

<table>
<thead>
<tr>
<th></th>
<th>Rb</th>
<th>0.2959</th>
<th>kJ/kgK</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bf-air gas constant</td>
<td>Rb</td>
<td>0.2959</td>
<td>kJ/kgK</td>
</tr>
<tr>
<td>Cp for bf-air</td>
<td>Cpb</td>
<td>1.096</td>
<td>kJ/kgK</td>
</tr>
<tr>
<td>Specific heat ration for bf-air</td>
<td>kb</td>
<td>1.370</td>
<td>/</td>
</tr>
<tr>
<td>Zero degree enthalpy of bf-air</td>
<td>hfb</td>
<td>-3471.0</td>
<td>kJ/kg</td>
</tr>
<tr>
<td>Cv for bf-air</td>
<td>Cvb</td>
<td>0.800</td>
<td>kJ/kgK</td>
</tr>
</tbody>
</table>
Turbulence coefficients:

| Parameters set by reference to experiments | \( F_d \) | 0.03 | / |
| Parameters set by reference to experiments | \( F_p \) | 0.05 | / |
| Coefficient set by reference to experiments | \( C_f \) | 0.4 | / |
| Laminar flame speed | \( V_L \) | 0.04 | m/s |
Results/Discussion

The single zone with homogeneously mixed burned and unburned gases developed by CVK is called the single zone adiabatic model. I have added heat transfer to this model and it will be called the single zone heat transfer model so first the results obtained from the single zone heat transfer model simulation program (see appendix C.3.) are discussed. After that, it is discussed the main simulation program and how the power, efficiency and heat transfer vary with the engine speed and how this have influence on the engine performance. Another point explained is the turbulence model and how it affects the combustion stage.

As illustration an engine with a compression ratio of 11, total volume of 55 cm$^3$, using methane (CH$_4$) which properties are very similar to gasoline and setting the engine to run at 6000rpm was obtained the following results for the heat transfer model,

![Temp vs theta](image)

Figure 11 - Temperature vs crank angle diagram for a four stroke engine running at 6000rpm
Figure 12 - P-V diagram for a four stroke engine running at 6000rpm

Figure 13 - Work vs Volume diagram for a four stroke engine running at 6000rpm
In order to compare the performance of an adiabatic engine with a non-adiabatic engine, the following results were obtained,

<table>
<thead>
<tr>
<th>RPM</th>
<th>Power (kW)</th>
<th>Efficiency (%)</th>
<th>Work (kJ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000</td>
<td>14.81</td>
<td>0.49</td>
<td>0.59</td>
</tr>
<tr>
<td>4000</td>
<td>16.32</td>
<td>0.47</td>
<td>0.49</td>
</tr>
<tr>
<td>5000</td>
<td>16.60</td>
<td>0.46</td>
<td>0.40</td>
</tr>
<tr>
<td>6000</td>
<td>16.22</td>
<td>0.43</td>
<td>0.32</td>
</tr>
<tr>
<td>7000</td>
<td>15.57</td>
<td>0.41</td>
<td>0.27</td>
</tr>
<tr>
<td>8000</td>
<td>14.84</td>
<td>0.39</td>
<td>0.22</td>
</tr>
</tbody>
</table>

Figure 14 – Variation of the power, efficiency and work with the engine speed (rpm) for an adiabatic engine

<table>
<thead>
<tr>
<th>RPM</th>
<th>Power (kW)</th>
<th>Efficiency (%)</th>
<th>Work (kJ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000</td>
<td>12.40</td>
<td>0.40</td>
<td>0.50</td>
</tr>
<tr>
<td>4000</td>
<td>13.79</td>
<td>0.38</td>
<td>0.41</td>
</tr>
<tr>
<td>5000</td>
<td>14.05</td>
<td>0.37</td>
<td>0.34</td>
</tr>
<tr>
<td>6000</td>
<td>13.66</td>
<td>0.35</td>
<td>0.27</td>
</tr>
<tr>
<td>7000</td>
<td>13.00</td>
<td>0.32</td>
<td>0.22</td>
</tr>
<tr>
<td>8000</td>
<td>13.58</td>
<td>0.34</td>
<td>0.20</td>
</tr>
</tbody>
</table>

Figure 15 – Variation of the power, efficiency and work with the engine speed (rpm) for a non-adiabatic engine

As we can see, the heat loss affects the engine performance. As we were expecting, the power, efficiency and the work drops when we have a non-adiabatic engine. In a non-adiabatic engine the temperature and pressure is smaller than in an adiabatic engine due to the greater heat losses which represents work that cannot be done.

Note that as the engine speed increases, the work drops off because the amount of gas burned goes down. At high engine speed the burn gas exchange is restricted by the flow through the valves. In particular the exhaust gases can not be completely expelled. Hence the amount of intake gases is reduced. Also the work required for pumping of the intake and exhaust, especially exhaust is greatly increased.
The results from the last version of the CycleComQC are the followings,

<table>
<thead>
<tr>
<th>RPM</th>
<th>Power (kW)</th>
<th>Efficiency (%)</th>
<th>Qt (kW)</th>
<th>Work (kJ)</th>
<th>Qw (kW/rad)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000</td>
<td>8.90</td>
<td>40.0%</td>
<td>-10.60</td>
<td>0.534</td>
<td>-0.636</td>
</tr>
<tr>
<td>3000</td>
<td>13.52</td>
<td>43.1%</td>
<td>-14.98</td>
<td>0.541</td>
<td>-0.599</td>
</tr>
<tr>
<td>4000</td>
<td>17.89</td>
<td>47.2%</td>
<td>-19.03</td>
<td>0.537</td>
<td>-0.571</td>
</tr>
<tr>
<td>5000</td>
<td>21.85</td>
<td>52.1%</td>
<td>-22.79</td>
<td>0.524</td>
<td>-0.547</td>
</tr>
<tr>
<td>6000</td>
<td>25.24</td>
<td>57.4%</td>
<td>-26.21</td>
<td>0.505</td>
<td>-0.524</td>
</tr>
<tr>
<td>7000</td>
<td>27.55</td>
<td>62.8%</td>
<td>-28.91</td>
<td>0.472</td>
<td>-0.496</td>
</tr>
<tr>
<td>8000</td>
<td>27.93</td>
<td>67.5%</td>
<td>-30.05</td>
<td>0.419</td>
<td>-0.451</td>
</tr>
<tr>
<td>9000</td>
<td>26.71</td>
<td>69.7%</td>
<td>-29.75</td>
<td>0.356</td>
<td>-0.397</td>
</tr>
<tr>
<td>10000</td>
<td>24.38</td>
<td>68.8%</td>
<td>-28.43</td>
<td>0.293</td>
<td>-0.341</td>
</tr>
<tr>
<td>11000</td>
<td>21.38</td>
<td>65.1%</td>
<td>-26.52</td>
<td>0.233</td>
<td>-0.289</td>
</tr>
<tr>
<td>12000</td>
<td>18.04</td>
<td>59.1%</td>
<td>-24.29</td>
<td>0.180</td>
<td>-0.243</td>
</tr>
</tbody>
</table>

Comparing this values for the final program with the ones obtained in heat transfer model, we conclude that the values for the efficiency are to high. For 6000rpm, the efficiency result obtained for this final simulation doing Q=0 is 77%. This cannot be correct because it exceeds Carnot efficiency which is only approximately 60%. This confirms that something is wrong with the basic two zone model we have developed. However, we will show the results obtained by this model.
As expected, the power rises and falls with rpm, but the peak occurs for 8500rpm which is much too high. Also the peak power is much too large.

When we have heat loss in an engine, occurs a reduction in its temperature and pressure which represents work that cannot be done leading to lower values of power.
Analising the figure 18 and the efficiency values obtained for an non-adiabatic engine (figure 16), we see that the combustion model is not correct in the simulation program. In fact, as expected the efficiency drops for a non-adiabatic engine. However, and as it was said, for an adiabatic engine running at 6000rpm the efficiency is 77% which is impossible to occur because even the Carnot Cycle does not have so high efficiency.

After some experiences with the program, CVK and I conclude that something is wrong with the pressure calculation which is leading to high values of work and efficiency.

From figure 19 we can say that the peak of total heat transfer occur for 9000rpm. As the engine speed is increasing the heat transfer also increase because the temperature and pressure in the chamber are also increasing. However, after 9000rpm, the heat transfer start to decrease due to the decrease of the temperature in the chamber because the amount of fresh gas decreases due to restricted gas exchange process as explained before.

Note as the engine speed increases, the heat loss per cycle and the work drops off because the amount of gas burned goes down. As it was said, at high engine speed the gas exchange process is more and more restricted.
As it was expected, the temperature peak occurs for the combustion stage, when the spark goes off. Looking to the average temperature curve, the temperature peak occurs for 4 rad, but this is due
to the fact that in the unburned curve there is a small glitch when the unburned mass goes to zero (the temperature increase which in a real engine is wrong). This problem is occurring due to some restrictions that were implemented for the combustion stage.

Figure 22 – P-V diagram for a four stroke engine running at 6000rpm

The pressure increases with the movement of the piston from the BC position to the TC position. The peak pressure occurs when the piston is in the TC position. In this position, the spark already went off and we are in the middle of the combustion stage. The pressure starts to drop when the piston start the descending movement to the BC position, where the exhaust valve will open. Note that with the increase of the piston speed, the peak pressure gets smaller.

We can see that the pressure peak here is considerably higher (5200kPa) than the 4200kPa of the single zone model with heat transfer (figure 12). The single zone model is much more realistic for typical engines. This shows that the approximation we have made for the pressure calculation is not accurate.
As we can see from figure 23, the main work produced in an engine occurs in the combustion and expansion stage. The high temperature of the gases during the combustion also leads to high pressure. This high pressure of the gases will act on the face of the piston causing it to move from TC (minimum volume) to the BC (maximum volume) in which produces the main work. In the intake stage, the work is also positive, however it can be neglected.
Figure 24 - Heat transfer coefficient vs crank angle diagram for a four stroke engine running at 6000rpm

Figure 25 – Heat transfer vs crank angle diagram for a four stroke engine running at 6000rpm
Figures 24 and 25 represent the results from the heat transfer model. As we were expecting in both curves the peaks occur for the combustion stage in which the temperature hits the higher values. Note that the values for the heat transfer are negative because this heat represents the heat losses in the engine.

![Turbulence vs Theta graph](image)

**Figure 26 – Turbulence vs crank angle diagram for a four stroke engine running at 6000rpm**

![Flame speed vs Theta graph](image)

**Figure 27 – Flame speed vs crank angle diagram for a four stroke engine running at 6000rpm**

Figures 26 and 27 represent the results from the combustion model in which is taken into account the turbulence in the cylinder.

The main objective of this model was to watch the variation of burn duration with the engine speed. In real engines, the mixture burning and the flame speed are strongly influenced by engine speed.
When the engine speed increases, the flame speed also increases. However, the burning rate throughout the combustion process increases, thought not quite, as rapidly as engine speed leading to higher crank angle intervals.

In the CycleComQC, the objective was to implement one turbulence model that represent this variation, however the results were not quite the ones expected. As we can see from the figures 26 and 27 the variation of the turbulence is proportional to the piston speed. From this we can conclude, that the turbulence model used were not the most accurate. The increase in the engine speed leads to a proportional increase in the flame speed and the combustion duration stays constant. The net effect is not much different from CvK's essentially constant burning rate. The turbulence model used was approximated from Lumley's model. This should be corrected in a future effort.
Concluding remarks

The fundamentals principles which govern internal combustion engine design and operations were well developed and implemented using the “Scilab” computer program. All the objectives proposed were achieved. For the heat transfer model the results obtained were quite good. However, the results obtained from the last simulation where it was added the heat transfer model plus the combustion model were not the ones expected. As mentioned previously, the model used was oversimplified, thus leading to quantitatively erroneous results although the results were qualitatively correct.

We can conclude that treating the combustion model CVK developed is simpler than the one developed during this project and leads to the good results. However, the CycleComQC is more realistic because it presents a non-adiabatic engine, and the two zone model inside the combustion chamber which takes into account the turbulence inside it. However, some of the details need to be improved in order to give quantitatively more accurate results.

We have concluded that the main difficulty is the pressure approximation. It is felt that with a little more time the pressure calculation can be improved by a new model that we have developed.
Bibliography

Appendix A

Mathematical and thermodynamic manipulations

A.1. Equation 1.1

Figure 23 - Sketch of the slider crank model of piston-cylinder geometry

When

\[
\begin{align*}
\theta = 0 &: y(\theta) = &l - \frac{s}{2} \\
\theta = \pi &: y(\pi) = &l + \frac{s}{2}
\end{align*}
\]

\[
y(\theta) = l \cdot \cos(\varphi) - \frac{s}{2} \cdot \cos(\varphi)
\]

\[
l \cdot \sin(\varphi) - \frac{s}{2} \cdot \sin(\varphi) = \sin(\varphi) = \frac{s}{2l} \cdot \sin(\varphi)
\]

and

\[
\cos(\varphi) = \sqrt{1 - \sin^2(\varphi)}
\]

comes,

\[
\cos(\varphi) = \sqrt{1 - \left(\frac{s}{2l}\right)^2 \sin^2(\varphi)}
\]

so

\[
y(\theta) = l \sqrt{1 - \left(\frac{s}{2l}\right)^2 \sin^2(\theta)} - \frac{s}{2} \cos(\theta)
\]
Finally,

\[ V(\theta) = \frac{\pi}{4} b o^2 (y(\theta) - l + \frac{s}{2}) \]

A.2. Equation 2.3

Energy Balance for the compression stage:

\[
\frac{dU}{\theta} = \dot{Q} - \dot{W}
\]

\[
\frac{dm}{\theta} = \dot{H}_i = \dot{H}_e = 0
\]

- Total internal energy (U):

\[
U = m \left[ x(C_v_b * T + h_f_b) + (1-x)(C_v_u * T + h_f_u) \right]
\]

and its derivative

\[
\frac{dU}{d\theta} = m \left[ \frac{dx}{d\theta} (C_v_b * T + h_f_b) + x(C_v_b \frac{dT}{d\theta}) - \frac{dx}{d\theta} (C_v_u * T + h_f_u) + (1-x)(C_v_u \frac{dT}{d\theta}) \right]
\]

\[
= \frac{dU}{d\theta} = m \left[ ((C_v_b - C_v_u) * T + h_f_b - h_f_u) \frac{dx}{d\theta} + x(C_v_b - C_v_u) + C_v_u \frac{dT}{d\theta} \right]
\]

where \( \Delta h_f = h_f_b - h_f_u \) and \( \Delta C_v = C_v_b - C_v_u \)

- Power output to the piston (W):

\[
\delta W = PdV
\]

so

\[
\delta \dot{W} = P \frac{dV}{d\theta}
\]

assuming ideal gas behavior,

\[ PV = mRT \] then,
\[ P = \frac{mRT}{V} \] where \[ R = xR_b + (1 - x)R_u \]

Finally,

\[ \delta \dot{W} = m(xR_b + (1 - x)R_u) \frac{T}{V} \frac{dV}{d\theta} \]

- Energy balance equation:

\[ \frac{dU}{d\theta} = \dot{Q} - \dot{W} \text{ comes} \]

\[ m*(x*\Delta Cv + Cv_u) \frac{dT}{d\theta} = \dot{Q} - m(xR_b + (1 - x)R_u) \frac{T}{V} \frac{dV}{d\theta} - m*(\Delta Cv*T + (hf_u - hf_b)) \frac{dx}{d\theta} \]

where \[ A = x*\Delta Cv + Cv_u \]

Finally,

\[ \frac{dT}{d\theta} = \frac{\dot{Q}}{m*A} - (xR_b + (1 - x)R_u) \frac{T}{AV} \frac{dV}{d\theta} - \frac{\Delta Cv*T + \Delta hf}{A} \frac{dx}{d\theta} \]

A.3. Equation 2.12

Calculation of the spark ignition equation using the “Mean Value theorem of Calculus”:

Using the following general equation which it will be explained in this appendix,

\[ M_b*CV_b \frac{dT_b}{dt} = \dot{Q}_b - P \frac{dV_b}{dt} + \dot{M}_b*(Cp_u*T_u - Cv_b*T_b + hf_u - hf_b) \]

and applying the “Mean Value theorem of calculus” comes,

\[ \int_\epsilon M_b*CV_b \frac{dT_b}{d\theta} d\theta = \int_\epsilon \dot{Q}_b d\theta - \int_\epsilon P \frac{dV_b}{d\theta} d\theta + \int_\epsilon \dot{M}_b*(Cp_u*T_u - Cv_b*T_b + hf_u - hf_b) d\theta \]

where \( \epsilon \) represents \([\theta, \theta + \epsilon]\) and
\[ \int_c \dot{Q}_b \, d\theta = 0 \ ; \\
\int_c P \frac{dV_b}{d\theta} \, d\theta = P(\theta_s)(V_b(\theta_s + \epsilon) - V_b(\theta_s)) = P(\theta_s) V_b(\theta_s + \epsilon) \]

\[ \int_c \frac{dM_b}{d\theta} (C_{p_u} T_u - C_{v_b} T_b + h_{f_u} - h_{f_b}) \, d\theta = (C_{p_u} T_u(\theta_s) - C_{v_b} T_b(\theta_s))(M_b(\theta_s + \epsilon) - M_b(\theta_s)) + (h_{f_u} - h_{f_b})(M_b(\theta_s + \epsilon) - M_b(\theta_s)) \]

Knowing that

\[ M_b(\theta_s) = 0 \]
\[ \dot{M}_b = M_b(\theta_s + \epsilon) > 0 \ , \]

\[ \int_c M_b \cdot C_{v_b} \frac{dT_b}{d\theta} \, d\theta = M_b(\epsilon) \cdot C_{v_b}(T_b(\theta_s + \epsilon) - T_b(\theta_s)) \]

Replacing the integrals in equation comes,

\[ M_b(\epsilon) \cdot C_{v_b}(T_b(\theta_s + \epsilon) - T_b(\theta_s)) = -P(\theta_s) V_b(\theta_s + \epsilon) + (C_{p_u} T_u(\theta_s) - C_{v_b} T_b(\theta_s))(M_b(\theta_s + \epsilon) - M_b(\theta_s)) + (h_{f_u} - h_{f_b})(M_b(\theta_s + \epsilon) - M_b(\theta_s)) \]

and knowing that

\[ T_b(\theta_s) = T_u \ , \quad T_b(\theta_s + \epsilon) = \ddot{T}_b \quad \text{and} \quad V_b(\theta_s + \epsilon) = \ddot{V}_b \]

\[ C_{v_b}(\ddot{T}_b - T_u) = (C_{p_u} T_u(\theta_s) - C_{v_b} T_u) + (h_{f_u} - h_{f_b}) - P(\theta_s) \frac{\ddot{V}_b}{M_b} \]

\[ C_{v_b} \ddot{T}_b = C_{v_b} T_u + C_{p_u} T_u - C_{v_b} T_u + (h_{f_u} - h_{f_b}) - P(\theta_s) \frac{\ddot{V}_b}{M_b} \]

Finally,

\[ \ddot{T}_b = \frac{1}{C_{v_b}} \left( C_{p_u} T_u + [(h_{f_u} - h_{f_b}) - P(\theta_s) \frac{\ddot{V}_b}{M_b}] \right) \]
A.4. Equation 2.13

Calculation of the burned radius, \( r \) assuming a “linear distribution”,

\[
 r (\theta) = a \theta + b
\]

Boundary conditions:

i. \( r (\theta_s) = 0 \)

ii. \( r (\theta_d) = R \) where \( R = \frac{b_0}{2} \)

it comes,

i. \( r (\theta_s) = 0 \Rightarrow 0 = a \theta_s + b \Rightarrow b = -a \theta_s \)

ii. \( r (\theta_d) = R \Rightarrow R = a \theta_d + b \Rightarrow R = a \theta_b - a \theta_s \Rightarrow a = \frac{R}{\theta_d - \theta_s} \)

Replacing \( a \) and \( b \) in equation comes,

\[
 r (\theta) = \frac{R}{\theta_d - \theta_s} \theta - \frac{R}{\theta_d - \theta_s} \theta_s,
\]

\[
 r (\theta) = \frac{R}{\theta_d - \theta_s} (\theta - \theta_d)
\]

A.5. Equation 2.25

The energy balance on the unburned zone is described by

\[
 \frac{dU_u}{dt} = \dot{Q}_u - P \frac{dV_u}{dt} - \dot{M}_b h_u
\]

applying to it some thermodynamic concepts and algebraic manipulation comes:

- Unburned Internal Energy and its derivative
\[ U_u = M_u \left( C_{v_u} T_u + h_{f_u} \right) \]

and its derivative is

\[
\frac{dU_u}{dt} = \frac{dM_u}{dt} \left( C_{v_u} T_u + h_{f_u} \right) + M_u C_{v_u} \frac{dT_u}{dt}
\]

- Expressing the unburned enthalpy as

\[ h_u = C_{p_u} T_u + h_{f_u} \]

Replacing in the main energy balance equation comes

\[
M_u C_{v_u} \frac{dT_u}{dt} = \dot{Q}_u - P \frac{dV_u}{dt} + \dot{M}_b \left( C_{p_u} T_u + h_{f_u} \right) + \dot{M}_b \left( C_{v_u} T_u + h_{f_u} \right)
\]

and finally

\[
M_u C_{v_u} \frac{dT_u}{dt} = \dot{Q}_u - P \frac{dV_u}{dt} + \dot{M}_b \left( C_{v_u} - C_{p_u} \right) T_u
\]

A.6. Equation 2.29

The energy balance on the burned zone is described by

\[
\frac{dU_b}{dt} = \dot{Q}_b - P \frac{dV_b}{dt} + \dot{M}_b h_u
\]

applying to it some thermodynamic concepts and algebraic manipulation comes:

- Burned internal energy and its derivative

\[ U_b = M_b \left( C_{v_b} T_b + h_{f_b} \right) \]

and its derivative is

\[
\frac{dU_b}{dt} = \frac{dM_b}{dt} \left( C_{v_b} T_b + h_{f_b} \right) + M_b C_{v_b} \frac{dT_b}{dt}
\]
Expressing the burned enthalpy as
\[ h_b = h_u \]
Substituting in the main energy balance equation on the burned zone comes
\[ M_b \cdot C_v b \frac{dT_b}{dt} = \dot{Q}_b - P \frac{dV_b}{dt} + \dot{M}_b (C_p u \cdot T_u + hf_u) - \dot{M}_b (C_v b \cdot T_b + hf_b) \]
and finally
\[ M_b \cdot C_v b \frac{dT_b}{dt} = \dot{Q}_b - P \frac{dV_b}{dt} + \dot{M}_b (C_p u \cdot T_u - C_v b \cdot T_b + hf_u - hf_b) \]

A.7. Equation 2.49

Energy Balance for completely burned gas expansion:
\[ \frac{dU}{\theta} = \dot{Q} - \dot{W} \]
\[ \frac{dm}{\theta} = \dot{H}_i = \dot{H}_e = 0 \]

- Total internal energy (U):
\[ U = \dot{m} \cdot [x \cdot (C_v b \cdot T + hf_b) + (1-x) \cdot (C_v u \cdot T + hf_u)] \]
and its derivative
\[ \frac{dU}{d\theta} = \dot{m} \cdot [x \cdot (C_v b \cdot T + hf_b) + x \cdot (C_v b \cdot \frac{dT}{d\theta}) - \frac{dx}{d\theta} \cdot (C_v u \cdot T + hf_u) + (1-x) \cdot (C_v u \cdot \frac{dT}{d\theta})] \]
\[ = \frac{dU}{d\theta} = \dot{m} \cdot [((C_v b - C_v u) \cdot T + hf_b - hf_u) \frac{dx}{d\theta} + (x \cdot (C_v b - C_v u) + C_v u) \frac{dT}{d\theta}] \]

where \( \Delta hf = hf_b - hf_u \) and \( \Delta C_v = C_v b - C_v u \)

- Power output to the piston (W):
\[ \Delta W = PdV \]
so

\[ \delta \dot{W} = P \frac{dV}{d\theta} \]

assuming ideal gas behavior,

\[ PV = mRT \quad \text{then,} \]

\[ P = \frac{mRT}{V} \quad \text{where} \quad R = xR_b + (1 - x) R_u \]

Finally,

\[ \delta \dot{W} = \dot{m}(xR_b + (1 - x) R_u) \frac{T}{V} \frac{dV}{d\theta} \]

- Energy balance equation:

\[ \frac{dU}{d\theta} = \dot{Q} - \dot{W} \quad \text{comes} \]

\[ \dot{m}(x \Delta C_v + C_{V_u}) \frac{dT}{d\theta} = \dot{Q} - \dot{m}(xR_b + (1 - x) R_u) \frac{T}{V} \frac{dV}{d\theta} - \dot{m}(\Delta C_v \ast T + (h_f_b - h_f_u) \frac{dx}{d\theta}) \]

where \( A = x \Delta C_v + C_{V_u} \)

Finally and since \( x = 1 \),

\[ \frac{dT}{d\theta} = \frac{\dot{Q}}{\dot{m} \ast \Delta C_v} - R_b \frac{T}{\Delta C_v V} \frac{dV}{d\theta} \]

A.8. Equation 3.13

Energy balance for the exhaust stage:

\[ \frac{dU}{d\theta} = \dot{Q} - \dot{W} - \dot{H}_e \]

\[ \dot{m}_i = \dot{H}_i = 0 \quad \text{and} \quad \frac{dm}{d\theta} = -\dot{m}_e \]
• Total internal energy (U):

\[ u = C_{vb} \ast T + h_{fb} \]

and

\[ \frac{dU}{dt} = \frac{dm \ast u}{dt} = m \frac{du}{dt} + u \frac{dm}{dt} \]

• Power output to the piston (W):

\[ \delta W = P dV \quad \text{so} \quad \delta \dot{W} = P \frac{dV}{d \theta} \]

assuming ideal gas behavior,

\[ PV = mRT \quad \text{then,} \]

\[ P = \frac{mRT}{V} \]

where \( R = xR_b + (1 - x) R_u \)

As long as we only have burned gas comes,

\[ \delta \dot{W} = \frac{\dot{m} \ast R_b \ast T}{V} \frac{dV}{d \theta} \]

Energy balance equation comes,

\[ \dot{m} \frac{du}{d \theta} - u \dot{m}_b = \dot{Q} - \dot{W} - \dot{m}_b \ast (C_{pb} \ast T + h_{fb}) = \]

\[ \dot{m} \frac{du}{d \theta} - (C_{vb} \ast T + h_{fb}) \ast \dot{m}_b = \dot{Q} - \dot{W} - \dot{m}_b \ast (C_{pb} \ast T + h_{fb}) = \]

\[ \dot{m} \frac{du}{d \theta} = \dot{Q} - \dot{W} - \dot{m}_b \ast (C_{pb} - C_{vb}) \ast T = \]

Finally,

\[ \dot{m} \frac{du}{d \theta} = \dot{Q} - \dot{W} - \dot{m}_b \ast R_b \ast T \]

Finally,

\[ \dot{m} \frac{du}{d \theta} = -\dot{m}_b d \left( \frac{C_{vb} \ast T + h_{fb}}{d \theta} \right) = \dot{m} \ast C_{vb} \frac{dT}{d \theta} \]

so

\[ \frac{dT}{d \theta} = \frac{\dot{Q}}{\dot{m} \ast C_{vb}} - \frac{R_b \ast T}{V \ast C_{vb}} \frac{dV}{d \theta} - \frac{\dot{m}_b \ast R_b \ast T}{\dot{m} \ast C_{vb}} \]
A.9. Equation 3.19

Energy balance for the intake stage:

\[
\frac{dU}{d\theta} = \dot{Q} - \dot{W} + \dot{H}_i
\]

\[
\dot{m} = \dot{H}_e = 0 \quad \text{and} \quad \frac{dm}{d\theta} = \dot{m}.
\]

- **Total internal energy (U):**

\[
u = C_v \ast T + h_f
\]

and

\[
\frac{dU}{dt} = \frac{dm \ast u}{dt} = m \frac{du}{dt} + u \frac{dm}{dt}
\]

- **Power output to the piston (W):**

\[
\delta W = PdV \quad \text{so} \quad \delta \dot{W} = P \frac{dV}{d\theta}
\]

assuming ideal gas behavior,

\[
PV = mRT \quad \text{then,}
\]

\[
P = \frac{mRT}{V} \quad \text{where} \quad R = xR_h + (1 - x) R_u
\]

As long as we only have unburned gas comes,

\[
\delta \dot{W} = \frac{\dot{m} \ast R_u \ast T}{V} \frac{dV}{d\theta}
\]

Energy balance equation comes,

\[
\dot{m} \frac{du}{d\theta} + u \ast \dot{m}_u = \dot{Q} - \dot{W} + \dot{m}_u \ast (C_p \ast T \ast u + h_f)
\]

\[
\dot{m} \frac{du}{d\theta} - (C_v \ast T + h_f) \ast \dot{m}_u = \dot{Q} - \dot{W} + \dot{m}_u \ast (C_p \ast T \ast u + h_f)
\]
\[ \dot{m} \frac{du}{d \theta} = \dot{Q} - \dot{W} + \dot{m}_u (C_{p_u} T_u + h_{f_u} - C_{v_u} T - h_{f_u}) = \dot{m} \frac{du}{d \theta} = \dot{Q} - \dot{W} + \dot{m}_u (C_{p_u} T_u - C_{v_u} T) \]

Finally,

\[ \dot{m} \frac{du}{d \theta} = -\dot{m} \frac{d}{d \theta} \left( C_{v_u} T + h_{f_u} \right) = \dot{m} C_{v_u} \frac{d}{d \theta} \]

so

\[ \frac{dT}{d \theta} = \frac{\dot{Q}}{\dot{m} C_{v_u}} - \frac{R_{u} T}{V C_{v_u}} \frac{dV}{d \theta} + \frac{\dot{m}}{\dot{m} C_{v_u}} (C_{p_u} T - C_{v_u} T) \]
Appendix B

Definitions

B.1. Knock

“As the flame front travels across the combustion chamber the temperature and pressure of the gases ahead are rising, due to the continual release of heat. Above a minimum value of temperature and pressure, a mixture of fuel vapor and air with a particular concentration at a particular pressure and temperature has a delay in time after which it will spontaneously ignite, know as autoignition. That is, when the mixture reaches the particular temperature and pressure, a reaction begins, the end point of which is ignition.

This reaction does not take place all at once. If the unburned mixture in front of the advancing flame (known as the end-gas) in the combustion chamber were to reach its autoignition point simultaneously due to the temperature and pressure rise, then the entire remaining unburned mixture would ignite at once, not waiting for the arrival of the flame front. The combustion which previously had been an orderly progressive burning would now become an explosion.” [2] This phenomenon is called knock.
Appendix C

Computer simulations

C.1. CycleComQC

The “CycleComQC” can be divided in six parts:

1. Engine data
2. Auxiliary functions
3. Main functions
   a. Power cycle process
      i. Compression stage
      ii. Ignition
      iii. Combustion/Expansion stage
   b. Exhaust process
   c. Intake process
4. Outputs
   a. Numerical results
   b. Plots
(1) Engine data

```c
// The Complete Non-Adiabatic Engine

// Engine data
Rc=2; // Connecting rod/stroke length ratio
rc=1; // Compression ratio
Vm=0.00055; // Maximum cylinder volume (m^3)
ths=0.88*pi; // Ignition onset (rad)
thsb=0.33*pi; // Burn duration (rad)
thd=1.21*pi; // Burning end (rad)
rpm=6000; // Engine (rpm)
ws=2*pi*rpm/60; // Engine (rad/s)
Tw=400; // Cylinder wall temperature (K)

// Valve data, exhaust
thevo=2*pi-8*pi/9; // Exhaust valve opens (rad)
thevc=3*pi; // Exhaust valve closes (rad)
eportd=0.04; // Exhaust port diameter (m)
estmd=-0.015; // Exhaust valve stem diameter (m)
elm=0.035; // Exhaust valve max lift (m)

// Valve data, intake
thivo=3*pi; // Intake valve opens (rad)
thivc=4*pi; // Intake valve closes (rad)
iiportd=0.04; // Intake port diameter (m)
iiestmd=0.015; // Intake valve stem diameter (m)
iielm=0.035; // Intake valve max lift (m)

// Intake-exhaust state
P1=100; // Intake pressure (kPa)
Pe=150; // Exhaust pressure (kPa)
T1=320; // Intake temperature (K)

// Unburned fuel-air equation of state, CH4, phe-1
Ru=0.2968; // uf-air gas constant (kJ/kgK)
Cpuf=1.022; // Cv for uf-air (kJ/kgK)
ku=1.409; // Specific heat ratio for uf-air
hfuf=-692; // Zero degree enthalpy of uf-air (kJ/kg)
Cvuf-Cpuf-Ru; // Cp for uf-air (kJ/kgK)

// Burned fuel-air equation of state
Rb=0.2959; // bf-air gas constant (kJ/kgK)
Cpbf=1.096; // Cv for bf-air (kJ/kgK)
kb=1.37; // Specific heat ratio for bf-air
hfbf=-3471; // Zero degree enthalpy of bf-air (kJ/kg)
Cvbf=Cpbf-Rb; // Cv for bf-air (kJ/kgK)
```
// uf-air bf-air mixture data
49 dcv=Cvb-Cvu;
50 dhf=hfb-hfu;
51 dR=Rb-Ru;
52 //
53 // Volumetric efficiency calculation data
54 Vc=Vm/rc; // Clearence Volume (m^3)
55 Vd=Vm*(1-1/rc); // Displacement Volume (m^3)
56 Vef=Ru*Ti/(Pi*Vd);
57 //
58 // Bore and stroke
59 bo=(4*Vd/^pi)^(1/3); // Bore (m)
60 s=bo; // Stroke (m)
61 //
62 // Clearence Area
63 hc=4*Vc/(^pi*bo^2); // Clearence height (m)
64 Ac=^pi*bo*hc/^pi/2*bo^2; // Clearence area (m)
65 //
66 // Piston Speed
67 Upm=2*rpm*s/60; // Mean piston speed (m/s)
68 U=0.494*Upm; // Piston speed (m/s)
69 //
70 // Turbulence coefficients
71 fp=0.03;
72 fd=0.05;
73 cf=0.4;
74 vl=0.04; // Laminar speed (m/s)
(2) Auxiliary functions

```c
// Auxiliary functions

// Cylinder volume, its derivative and exposed cylinder area
function [v, dv, Aw] = volm(th, Rc, rc, Vm, bo, Ac, Vc)
    v = Vm * (1/rc + 0.5*(1-1/rc)*(1+cos(th)));
    dv = -Vm * 0.5*(1-1/rc)*sin(th);
    Aw = (v-Vc)/(bo/8)+Ac;
endfunction

// Turbulence
function dturb = turbu(Fp, Us, ws, Fd, K, th, Rc, rc, Vm, bo, Ac, Vc)
    [v, dv, Aw] = volm(th, Rc, rc, Vm, bo, Ac, Vc);
    dturb = [Fp*Aw*(abs(Us)^3)/(v*ws))-(2/3)*K*dv/(v)-Fd*K*sqrt(2*abs(K))/(v^(1/3))*ws];
endfunction

// Combustion Chamber
function [r, dr] = bradius(bo, ths, Vf, ws, th, thd)
    if th<ths then
        r = 0;
        dr = 0;
    else
        r = Vf/ws*(th-ths);
        dr = Vf/ws;
    end
endfunction

// Valve opening opening/closing
function A = valve(th, tho, thc, Dp, ds, lm)
    if th>thc then
        A = 0;
        return
    else
        A = A*Dp/2*ds^2;
    end
endfunction
```


// Mass flow equation
function mf=massf(Po,To,Pv,k,R,A,ws)
    if Pv>=Po
        mf=0;
    return
    end
    Ff=A*(Po/(R*To))^sqrt(1000*k*R*To)/ws;
    pc=(2/(k+1))^(k/(k-1));
    if Pv/Po>pc
        mf=Ff*((2/(k-1))*abs((Pv/Po)^(2/k)-(Pv/Po)^((k+1)/k)))^0.5;
    else
        mf=Ff*(2/(k+1))^((k+1)/(2*(k-1)));
    end
endfunction

// Heat transfer coefficient
function hg=coeff(P,U,bo,T)
    hg=(300*(P)^0.75*U^0.75*bo*(-0.25)*T^(-0.465))/1000;
endfunction

//
(3) Main functions

(a) Power cycle process

i. Compression stage

```c
// Initial Conditions
xr=0.05; // Residual mass fraction at intake
P1=Pi;
T1=Ti;
///~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~/
for i=1:4
th(1)=0; // Value of theta at beginning of compression
mb(1)=0;
ID(1)=0;
IT(1)=T1; // Temperature at beginning of compression
P(1)=P1; // Initial pressure
turb(1)=0.01;
m=P1*Vm/(((1-xr)*Ru-xr*Rb)*T1); // Initial fresh charge
V(1)=Vm; // Initial volume
W(1)=0; // Work at beginning of compression
mc(1)=m;
y(1)=0;
dy(1)=0;
Qj(1)=0;
qu=0;
[v, dv, Aw]=volm(th(1), Rc, rc, Vm, bo, Ac, Vc);
Aw1=Aw;
161
162
// Numerical Integration parameters
N=200; // Number of theta steps from 0 to 2pi
dth=thevo/N; // theta step increment
js=int(ths/dth);
rr(1)=0;
Vff(1)=0;
///~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~/
```
ii. Ignition

```c
199 // During the burning
200 ri=0.01*bo/2; 201 h=4*v/($pi*bo^2); 202 Vbi=($pi*h*ri^2); 203 mbi=m*Vbi/v; 204 mui=m-mbi; 205 Tb(j)=(Cpu*T(j)+(1-xr) *(hfu-hfb)-P(j)*Vbi/mbi)/Cvb; 206 //
```
iii. Combustion/Expansion stage

```c
// Temperatures after the spark plug goes off
for j=js:N=1
  th(j)=th(j-1)+dth;
  mc(j)=m;
  V(j)=v;
  [v,dv,Av]=voln(th(j),Rc,rc,Vm,bo,Ac,Vc);
  Awb(j)=Av;
  Us=i*dv/(bo^2*pi);
  turb(j)=turb(j-1)+dth*turbul(Fp,Us,ws,Fd,turb(j-1),th(j-1),Rc,rc,Vm,bo,Ac,Vc);
  // Flame speed
  Vt=sqrt(2*turb(j));
  Vf=ws*(Vl+Gs*Vt);
  [r,dr]=bradius(bo,th(j-1),Vf,ws,th(j),thd);
  // Burned and unburned volumes
  Vb=v*r^2/(bo/2)^2;
  Vu=v-Vb;
  dVb=4/bo^2*r^2*dv+ü*v*r/bo^2*dr;
  dVu=dv-dVb;
  // Mass Balance
  mb=m*Vb/v;
  dmb=m*(1/v*dVb-Vb/v^2*dv);
  mu=m-mb;
  dmu=-dmb;
  x=mb/m;
  Awb=2*pi*r^2;
  Awu=Aw-Awb;
  //
```
if r<0.95*bo/2

\[ h_g = \text{cosef}(P_{j-1}, U, bo, Tb_{j-1}) \];
\[ h = h_g; \]
\[ Q_w = h_g * A_{wb} * (T_b_{j-1} - T_w) / (C_{vu} + d_{cv} * rpm); \]
\[ h = \text{cosef}(P_{j-1}, U, bo, Tb_{j-1}) \];
\[ h_g (j) = (A_{wb} * h_g + A_{wa} * h_g) / A_w; \]
\[ Q_w = h_g * A_{wu} * (I_{j-1} - T_w) / (C_{wu} + x * d_{cv} * rpm); \]
\[ I (j) = I_{j-1} + ((Q_w - P_{j-1} + d_{vu} + d_{mb} * (C_{vu} - C_{psi}) * T_{j-1}) / (m * C_{vu})) * dth; \]
\[ T_b (j) = T_{b_{j-1}} + ((Q_w - P_{j-1} + d_{vb} + d_{mb} * (C_{vu} + T_{j-1} - C_{vb}) * (1 - x_r) * d_{hfu})) / (m * C_{vb}) * dth; \]
\[ P (j) = (m * R_u * I (j) + m_b * R_b * T_b (j)) / v; \]
\[ I_s (j) = (1 - x) * C_{vu} * I (j) + x * C_{vb} * T_b (j) / ((1 - x) * C_{vu} + x * C_{vb}); \]
\[ W (j) = W_{j-1} + P_{j-1} * d_v * dth; \]
\[ Q_t = Q_w + Q_{wu} * dth + Q; \]
\[ Q (j) = Q_w + Q_{wu}; \]
\[ r (j) = I; \]

else

\[ h_g = \text{cosef}(P_{j-1}, U, bo, Tb_{j-1}) \];
\[ Q_w = h_g * A_{wb} * (T_b_{j-1} - T_w) / (C_{vu} + d_{cv} * rpm); \]
\[ T_b (j) = T_{b_{j-1}} + ((Q_w - P_{j-1} + d_{vu} + d_{mb} * (C_{vu} - C_{psi}) * T_{j-1}) / (m * C_{vu})) * dth; \]
\[ I (j) = I_{j-1}; \]
\[ T (j) = 0; \]
\[ P (j) = m_b * R_b * T_b (j) / v; \]
\[ W (j) = W_{j-1} + P_{j-1} * d_v * dth; \]
\[ Q_t = Q_w; \]
\[ Q (j) = Q_w; \]
\[ h_g (j) = h_g; \]
\[ r (j) = bo / 2; \]
end

V_{ef} (j) = V_f; 
end
(b) Exhaust process

```plaintext
265 // Exhaust process
266 Kk=1014+N;
267 dth=\frac{(3*\pi-thevo)}{100};
268 for j=N+2:Kk
269 th(j)=th(j-1)+dth;
270 Ae=valve(th(j-1), thevo, thevc, eportd, estemd, elm);
271 Avalve(j)=Ae;
272 mf=massf(P(j-1), Tb(j-1), Pe, kb, Rb, Ae, ws);
273 [v, dv, Aw]=volm(th(j-1), Rc, rc, Vm, bo, Ac, Vc);
274 Aw(j)=Aw;
275 hg=coef(P(j-1), U, bo, Tb(j-1));
276 mc(j)=mc(j-1)-mf*dth;
277 Qw=-hg*Aw* (Tb(j-1)-Tw) / ((Cu+x*dcv)*rpm);
278 Tb(j)=Tb(j-1)+(Qw- (kb-1)*(dv/v+mf/mc(j-1))*Tb(j-1)) * dth;
279 W(j)=W(j-1)+P(j-1)*dv*dth;
280 [v, dv, Aw]=volm(th(j), Rc, rc, Vm, bo, Ac, Vc);
281 V(j)=v;
282 P(j)=mc(j)*Rb*Tb(j)/V(j);
283 Y=j;
284 Vef(j)=0;
285 hgg(j)=hg;
286 Qj(j)=Qw;
287 Ta(j)=Tb(j);
288 Qt=Qt+Qw*dth;
289 rr(j)=bo/2;
290 end
291 mr=mc(j);
292 //
```
(c) Intake process

```c
// Intake Process
L=Kk+101;
dth=pi/100;
for j=Kk:L
    \theta(j)=\theta(j-1)+dth;
    A=\text{valve}(\theta(j-1), \theta, \text{thivo}, \text{thivc}, \text{iportd}, \text{istemd}, \text{lim});
    A_valve(j)=A;
    mf=\text{massf}(P, Ti, P(j-1), ku, Ru, Ai, ws);
    [v, dv, Aw]=\text{voln}(\theta(j-1), \text{Ec}, \text{rc}, \text{Vm}, \text{bc}, \text{Ac}, \text{Vc});
    hg=\text{coef}(P(j-1), U, bo, Tb(j-1));
    x=mr/mc(j-1);
    a=Cv+xdcv;
    b=(Ru+x*dR)/a;
    Qw=hdg*Aw*(Tb(j-1)-Tw)/(Cv+x*dcv)*rpm;
    Tb(j)=Tb(j-1)+(Qw-b*dv*Tb(j-1)/v+mf*(Cpu-Ti-Cvu*Tb(j-1))/(mc(j-1)*a))*dth;
    mc(j)=mc(j-1)+mf*dth;
    W(j)=W(j-1)+P(j-1)*dv*dth;
    [v, dv, Aw]=\text{voln}(\theta(j), \text{Rc}, \text{rc}, \text{Vm}, \text{bo}, \text{Ac}, \text{Vc});
    Awv(j)=Aw;
    V(j)=v;
    x=mr/mc(j);
    P(j)=mc(j)*((x*Rb+(1-x)*Ru)*Tb(j)/v;
    Vff(j)=0;
    hgg(j)=hg;
    Qj(j)=Qw;
    Ta(j)=Tb(j);
    T(j)=0;
    Qt=Qt+Qw*dth;
    rr(j)=bo/2;
end
T(1)=T(j);
P(1)=P(j);
x=x;
```

(4) Outputs

(a) Numerical results

```c
// Output results
W(L)
Qt=Qt*rpm/120
Power=W(L)*rpm/120
eff=W(L)/(mc(L)-mr)*(hfu-hfb))
```
(b) Plots

```matlab
// Output plots
subplot(4,2,1)
plot(th,T,th,Tb)
xtitle ('Temperature vs Theta', 'theta (rad)', 'Temperature (K)');
subplot(4,2,2)
plot(th,Ta)
xtitle ('Temperature vs Theta', 'theta (rad)', 'Average Temperature (K)');
subplot(4,2,3)
plot(ch,rr)
xtitle ('Theta vs Burned Radius', 'theta', 'Burned Radius');
subplot(4,2,4)
plot(ch,Vff)
xtitle ('Theta vs Flame Speed running at 6000rpm', 'theta [degrees]', 'Flame Speed [m/s]');
subplot(4,2,5)
plot(V,P)
xtitle ('P-V Diagram', 'V (m^3)', 'P (kPa)');
subplot(4,2,6)
plot(V,W)
xtitle ('Work vs Volume', 'V (m^3)', 'W (kJ)');
subplot(4,2,7)
plot(ch,hqv)
xtitle ('hg vs Theta', 'theta (rad)', 'hg (kJ/m^2.K)');
subplot(4,2,8)
plot(ch,Qj)
xtitle ('Qw vs Theta', 'theta (rad)', 'Qw (kW)');
```
C.2. CycleCom

The main program developed by CVK can be divided in six parts:

1. Engine data
2. Auxiliary functions
3. Main functions
   a) Power cycle process
   b) Exhaust process
   c) Intake process
4. Outputs
   a) Numerical results
   b) Plots
(1) Engine data

```plaintext
2 // The Complete Adiabatic Engine
3 //
5 Rc=2; // Connecting rod/stroke length ratio
6 rc=11; // Compression ratio
7 Vm=0.00055; // Maximum cylinder volume, m^3
8 ths=0.88*pi; // Ignition onset
9 thb=0.33*pi; // Burn duration
10 rpm=10000; // Engine rpm
11 w=2*pi*rpm/60; // Engine radians/s
12 // Valve data, exhaust
13 thevo=2*pi; // Exhaust valve opens (radians)
14 thevc=3*pi; // Exhaust valve closes (radians)
15 sprot=0.04; // Exhaust port diameter in meters
16 estemd=0.015; // Exhaust valve stem diameter in meters
17 cowm=0.035; // Exhaust valve max lift in meters
18 // Valve data, intake
19 thivo=3*pi; // Intake valve opens (radians)
20 thivc=4*pi; // Intake valve closes (radians)
21 iprot=0.045; // Intake port diameter in meters
22 istemd=0.02; // Intake valve stem diameter in meters
23 iwm=0.035; // Intake valve max lift in meters
24 // Intake- exhaust state
25 Pi=100; // Intake pressure, kPa
26 Pe=150; // Exhaust pressure, kPa
27 Ti=320; // Intake temperature, Kelvin
28 //
29 // Unburned fuel-air equation of state, CH4, phi=1
30 Ru=0.2968; // uf-air gas constant, kJ/kgK
31 Cpu=1.022; // Cp for uf-air, kJ/kgK
32 ku=1.29; // Specific heat ratio for uf-air
33 hfu=692; // Zero degree enthalpy of uf-air, kJ/kg
34 Cv=1.022; // Cu for uf-air, kJ/kgK
35 //
36 // Burned fuel-air equation of state
37 Rb=0.2959; // bf-air gas constant, kJ/kgK
38 Cpb=1.096; // Cp for bf-air, kJ/kgK
39 kb=1.27; // Specific heat ratio for bf-air
40 hfb=3471; // Zero degree enthalpy of bf-air, kJ/kg
41 Cv=1.096; // Cv for bf-air, kJ/kgK
42 //
43 // uf-air bf-air mixture data
44 dcv=Cvb-Cvu;
45 dhf=hfb-hfu;
46 dR=Rb-Ru;
```
(2) Auxiliary functions

```c
48 // Auxiliary functions
49 //
50 // Cylinder volume and its derivative
51 function [r, dv]=volm(th, Rc, rc, Vm)
52 v=Vm*(1/rc+0.5*(1-1/rc)*(1+cos(th)));
53 dv=-Vm*0.5*(1-1/rc)*sin(th);
54 endfunction
55 //
56 // Combustion rate function
57 function [x, dx]=comb(th, ths, th, thb)
58 if th<ths
59   x=xr;
60   dx=0;
61 else
62   x=xr+(1-xr)*(1-exp(-5*((th-ths)/thb)^3));
63   dx=(1-xr)*(15/thb)*((th-ths)/thb)^2)*exp(-5*((th-ths)/thb)^3);
64 end
65 endfunction
66 //
67 // Valve opening/closing
68 function A=valve(th, thc, Dp, ds, ln)
69 if th>thc
70   A=0;
71 else
72   A=A0;
73 end
74 Ap=0.4*0.25*pi*(Dp^2-ds^2);
75 lift=0.5*ln*(1-cos(2*pi*(th-tho))/(thc-tho)));
76 Av=0.4*pi*dp*lift;
77 if Av<Ap then
78   A=Av;
79 else
80   A=A0;
81 end
82 endfunction
83 //
84 // Mass flow equation
85 function mf=massf(Po, To, PV, k, R, A, wa)
86 if Pv>=Po
87   mf=0;
88 else
89 end
90 if A<Po/(R*To)+sqrt((1000*R*To)/ws;
91 pc=(2/(k+1))^((k/(k-1)));
92 if Pv/Po>pc
93   mf=ff*((2/(k-1))*abs((Po/Po)^((2)/k)-(Po/Po)^((k+1)/k)))/0.5;
94 else
95   mf=ff*(2/(k+1))^((k+1)/(2*(k-1)))
96 end
97 endfunction
```
(3) Main functions

(a) Power cycle process

```matlab
99 // Initial Conditions
100 xr=0.1; // Residual mass fraction at intake
101 P1=50;
102 T1=600;
103 for i=1:3
104 th(1)=0; // Value of theta at beginning of compression
105 T(1)=T1; // Temperature at beginning of compression
106 P(1)=P1; // Initial pressure
107 m=P1*Vmn/((1-xr)*Ru+xr*Rb)*T1) // Initial fresh charge
108 V(1)=Vmn; // Initial volume
109 W(1)=0; // Work at beginning of compression
110 mc(1)=m;
111 y(1)=1;
112 dy(1)=0;
113 // Initial mass in the cylinder
114 // Numerical Integration parameters
115 N=200; // Number of theta steps from 0 to 2pi
116 dth=theta/N; // theta step increment
117 //%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
118 // Numerical Integration of the first law until exhaust valve opens
119 for j=2:N+1
120 th(j)=j*dth;
121 thm=th(j)-dth;
122 mc(j)=m;
123 [v, dv]=volm(thm, Rc, rc, Vmn);
124 [x, dx]=comb(th, xr, ths, chb);
125 q=(-dcv*T(j-1)+dth/((Cv+dx)*dcv));
126 s=-(1-x)*Ru+x*Rb)/((Cv+dx)*dcv);
127 T(j)=T(j-1)+(q*dx+p*T(j-1)*dv/v)*dth; // Temperature
128 W(j)=W(j-1)+P(j-1)*dv*dth; // Work
129 v, dv]=volm(th(j), Rc, rc, Vmn);
130 V(j)=v;
131 P(j)=m*((1-x)*Ru+x*Rb)*T(j)/v; // Pressure
132 end
133 PowercycleEff=W(j)/(m*(1-xr)*(hfu-hfb));
134 PowercycleEff
135 j=N+1;
136 a_valve(N+1)=0;
137 //
```
(b) Exhaust process

```plaintext
138 // Exhaust process
139 K=101+N;
140 dth=(3*pi-thevo)/100;
141 for j=N+2:K
142 th(j)=th(j-1)+dth;
143 Ae=valve(th(j-1),thevo,thvc,eportd,estend,eln);
144 A= Valve(j)=Ae;
145 nf=massf(P(j-1),T(j-1),Pe,kb,Rb,Ae,ws);
146 [v,dv]=voln(th(j-1),Rc,rc,Vm);
147 nc(j)=mc(j-1)-mf*dth;
148 T(j)=T(j-1)-(kb-1)*(dv/v+nf/mc(j-1))*T(j-1)*dth; // Temperature
149 W(j)=W(j-1)+P(j-1)*dv*dth; // Work
150 [v,dv]=voln(th(j),Rc,rc,Vn);
151 V(j)=v;
152 P(j)=nc(j)*Rb*T(j)/V(j); // Pressure
153 K=j;
154 end
155 thvo=th[K];
156 nr=mc[K]
157 //
```

(c) Intake process

```plaintext
158 // Intake Process
159 L=int((4*pi-th[K])/dth);
160 for j=K+1:K+L+1
161 th(j)=th(j-1)+dth;
162 Ai=Valve(th(j-1),thivo,thvc,iportd,istemd,ilm);
163 A= Valve(j)=Ai;
164 nf=massf(Ei,Ti,P(j-1),ku,Ru,Ai,ws);
165 [v,dv]=voln(th(j-1),Rc,rc,Vm);
166 x=mr/mc(j-1);
167 a=Cvu+x*dcv;
168 b=(Ru*x*Dr)/a;
169 T(j)=T(j-1)+(-b*dv*T(j-1)/v+mf*(Cpu*Ti-Cvu*T(j-1))/(mc(j-1)*a))*dth; // Temperature
170 nc(j)=mc(j-1)+mf*dth;
171 W(j)=W(j-1)+P(j-1)*dv*dth; // Work
172 [v,dv]=voln(th(j),Rc,rc,Vm);
173 V(j)=v;
174 x=mr/mc(j);
175 P(j)=nc(j)*(x*Rb+(1-x)*Ru)*T(j)/v; // Pressure
176 end
177 //
```
(4) Outputs

(a) Numerical results

```c
181 // Output Numerical Overall Results
182 xr=mr/mc(j);
183 T1=T(j);
184 T1
185 P1=P(j);
186 P1
187 Work=W(j);
188 Work
189 Eff=Work/((hfuf-hf)f*mc(j)-mr));
190 Eff
191 Power=rpm*Work/120;
192 Power
193 end
```

(b) Plots

```c
195 // Output Plots
196 subplot(2,2,1)
197 plot(V,P)
198 xtitle("P-V Diagram","V","P")
199 subplot(2,2,2)
200 plot(th,T)
201 xtitle("Temp vs theta","theta","T")
202 subplot(2,2,3)
203 plot(th,mc)
204 xtitle("Cylinder Mass vs Theta","Theta","m")
205 subplot(2,2,4)
206 plot(V,W)
207 xtitle("Work vs Volume","V","W")
```
C.3. Single zone heat transfer model

```
4 // Engine data
5 rpm=6000; // Engine rpm
6 ws=2*3.14159*rpm/60; // Engine radians/s
7 Rc=2; // Connecting rod/stroke length ratio
8 rc=11; // Compression ratio
9 Vm=0.00055; // Maximum cylinder volume, m^3
10 Vc=Vm/rc; // Clearance volume
11 Vd=Vm-Vc; // Displacement volume
12 bo=(4*Vd/(3.14159*(1/3))); // Bore assuming bore=stroke
13 s=bo; // Stroke
14 hc=4*Vc/(3.14159*bo^2); // Height of clearance volume
15 Ac=3.14159*bo*hc+(3.14159*(bo/2))*bo^2; // Clearance volume area
16 Upm=2*rpm*s/120; // Mean piston speed.
17 J=0.494*Upm; // Empirical piston speed.
18 /
19 chs=0.88*3.14159; // Ignition onset
20 chd=0.33*3.14159; // Burn duration
21 // // Valve data, exhaust
22 thevo=2*3.14159; // Exhaust valve opens (radians)
23 thevc=3*3.14159; // Exhaust valve closes (radians)
24 eportd=0.04; // Exhaust port diameter in meters
25 estemd=0.015; // Exhaust valve stem diameter in meters
26 elm=0.035; // Exhaust valve max lift in meters
27 // // Valve data, intake
28 ihvo=3*3.14159; // Intake valve opens (radians)
29 ihvc=4*3.14159; // Intake valve closes (radians)
30 iportd=0.04; // Intake port diameter in meters
31 istemd=0.015; // Intake valve stem diameter in meters
32 ilm=0.035; // Intake valve max lift in meters
33 // // Intake- exhaust state
34 Pi=100; // Intake pressure, kPa
35 Pe=150; // Exhaust pressure, kPa
36 Ti=320; // Intake temperature, Kelvin
37 Tw=400; // Cylinder wall temperature
38 // // Unburned fuel-air equation of state, CH4, phe=1
39 Ru=0.2968; // uf-air gas constant, kJ/kgK
40 Cpu=1.022; // Cp for uf-air, kJ/kgK
41 ku=1.409; // Specific heat ratio for uf-air
42 hfu=692; // Zero degree enthalpy of uf-air, kJ/kg
43 Cvu=Cpu-Ru; // Cu for uf-air, kJ/kgK
```
// Burned fuel-air equation of state
Rb=0.2959; // bf-air gas constant, kJ/kgK
Cpb=1.096;  // Cp for bf-air, kJ/kgK
kb=1.37;    // Specific heat ratio for bf-air
hfb=-3471;  // Zero degree enthalpy of bf-air, kJ/kg
Cvb=Cpb-Rb; // Cv for bf-air, kJ/kgK

// uf-air bf-air mixture data
dcv=Cvb-Cvu;
dhf=hfb-hfu;
dR=Rb-Ru;

// Auxiliary functions

// Cylinder volume and its derivative
function [v,dv,dAw]=volm(th,Rc,rc,Vm,bo,Ac,Vc)
v=Vm*(1/rc+0.5*(1-1/rc)*(1+cos(th)));
dv=-Vm*0.5*(1-1/rc)*sin(th);
dAw=4*(v-Vc)/bo+Ac;
endfunction

// Combustion rate function
function [x,dx]=comb(th,xr,ths,thd)
if th<ths
  x=xr;
else
  x=xr+(1-xr)*(1-exp(-5*((th-ths)/thd)^3));
end
endfunction
// Valve opening opening/closing

function A=valve(th,tho,thc,Dp,ds,lm)

if th>thc
    A=0;
else
    A=0.4*0.25*pi*(Dp^2-ds^2);
end

if lift>0.5*ln*(1-cos(2*pi*(th-tho)/(thc-tho)))
    Av=0.4*pi*Dp*lift;
if Av<A then
    A=Av;
else
    A=Ap;
end

endfunction

// Mass flow equation

function mf=massf(Po,To,Pv,k,R,A,ws)

if Pv>Po
    mf=0;
else
    pc=(2/(k+1))^(k/(k-1));
    mf=F*((2/(k-1))*abs((Pv/Po)^(2/k)-(Pv/Po)^((k+1)/k)))^0.5;
else
    mf=F*((2/(k-1))^((k+1)/(2*(k-1)));
end

endfunction

// Heat transfer coefficient

function hg=coef(P,U,bo,T)

c=300;

hg=c*((P*U)^0.75)*(bo^(-0.25))*(T^(-0.465))/1000;
endfunction
// Initial Conditions
xr=0.1; // Residual mass fraction at intake
P1=80;
T1=600;
for i=1:4
th(1)=0; // Value of theta at beginning of compression
T(1)=T1; // Temperature at beginning of compression
P(1)=P1; // Initial pressure
m=P1*Vm/(((1-xr)*Ru+xr*Rb)*T1); // Initial fresh charge
V(1)=Vm; // Initial volume
W(1)=0; // Work at beginning of compression
mc(1)=m;
y(1)=0;
dy(1)=0;
Qt=0;
// Initial mass in the cylinder
// Numerical Integration parameters
N=400; // Number of theta steps from 0 to 2pi
dth=th2vo/N; // theta step increment
// Numerical Integration of the first law until exhaust valve opens
for j=2:N+1
th(j)=j*dth;
thm=th(j)-dth;
mc(j)=m;
[th, dx] = coef(P(j-1), U, bo, T(j-1));
[V, dv, Aw] = voln(thm, Rc, rc, Vm, bo, Ac, Vc);
[x, dx] = comb(thm, xr, ths, thd);
Qw= -h*Aw*(T(j-1)-Tw)/((Cvu+x*dcv)*rpm);
g=-dcv*T(j-1)*dhf/(Cvu+x*dcv);
s= -((1-x)*Ru+x*Rb)/(Cvu+x*dcv);
T(j) = T(j-1) + (Qw/m+q*dx+s*T(j-1)*dv/v)*dth;
W(j) = W(j-1) + P(j-1)*dv*dth;
[V, dv, Aw] = voln(th(j), Rc, rc, Vm, bo, Ac, Vc);
V(j) = V;
P(j) = m*((1-x)*Ru+x*Rb)*T(j)/v;
end
PowercycleEff=W(j)/(m*(1-xr)*(hfu-hfb));
// PowercycleEff
j=N+1;
Avalve(N+1)=0;
//
158 // Exhaust process
159 while P(j)>Pe
160 j=j+1;
161 th(j)=th(j-1)+dth;
162 le=valve(th(j-1),thvo,thvc,eportd,estend,elm);
163 a=avel(j)=ae;
164 mf=massf(P(j-1),T(j-1),Pe,kb,Rb,Ae,ws);
165 hg=coef(P(j-1),U,bo,T(j-1));
166 [v,dv,Aw]=volm(th(j-1),Rc,rc,Vm,bo,Ac,Vc);
167 Qw=-hg*Aw*[(T(j-1)-Tw)/((Cvu+x*dcv)*rpm)];
168 mc(j)=mc(j-1)-mf*dth;
169 T(j)=T(j-1)+(Qw/mc(j-1)-(kb-1)*(dv/v+mf/mc(j-1))*T(j-1))*dth;
170 W(j)=W(j-1)+P(j-1)*dv*dth;
171 [v,dv,Aw]=volm(th(j),Rc,rc,Vm,bo,Ac,Vc);
172 V(j)=v;
173 P(j)=mc(j)*Rb*T(j)/V(j);
174 K=j;
175 end
176 thvo=th(K);
177 nr=mc(K);
178 //
179 // Intake Process
180 L=int((i*pi-th(K))/dth);
181 for j=K+1:K+L+1
182 th(j)=th(j-1)+dth;
183 ai=valve(th(j-1),thvo,thvc,iportd,istend,ilm);
184 a=avel(j)=ai;
185 mf=massf(Pi,Ti,P(j-1),ku,Ru,Ai,ws);
186 hg=coef(P(j-1),U,bo,T(j-1));
187 [v,dv,Aw]=volm(th(j-1),Rc,rc,Vm,bo,Ac,Vc);
188 x=mr/mc(j-1);
189 Qw=-hg*Aw*[(T(j-1)-Tw)/((Cvu+x*dcv)*rpm)];
190 a=Cvu+x*dcv;
191 b=(Ru+x*dR)/a;
192 T(j)=T(j-1)+(Qw/mc(j-1)-b*dv*T(j-1))/v+mf*(Cpu*Ti-Cvu*T(j-1))/(mc(j-1)*a)*dth;
193 mc(j)=mc(j-1)+mf*dth;
194 W(j)=W(j-1)+P(j-1)*dv*dth;
195 [v,dv,Aw]=volm(th(j),Rc,rc,Vm,bo,Ac,Vc);
196 V(j)=v;
197 x=mr/mc(j);
198 P(j)=mc(j)*(x*Rb+(1-x)*Ru)*T(j)/v;
199 end
C.4. Computer simulation of the turbulent model

```matlab
2 // Turbulence model
3 //
4 rpm=6000;
5 Rc=2;
6 rc=10;
7 Vm=0.00055;
8 Vd=Vm*(1-1/rc);
9 bo=(4*Vd/pi)^(1/3); // Bore
10 s=bo; // Stroke
11 Vc=Vm-Vd;
12 //
13 // Clearance Area
14 hc=4*Vc/(pi*bo^2); // Clearance height
15 Ac=pi*bo*hc+pi/2*bo^2; // Clearance area
16
17 function [v,dv,Ap]=volm(th,Rc,rc,Vm,bo,Ac,Vc)
18 v=Vm*(1/rc+0.5*(1-1/rc)*(1+cos(th)));
19 dv=Vm*0.5*(1-1/rc)*sin(th);
20 Ap=(v-Vc)/(bo/2)+Ac;
21 endfunction
22 //
23 //
24 Fp=0.03;
25 Fd=0.05;
26 Vl=0.3
27 Cf=1;
28 ws=2*pi*rpm*s/60;
29 //
30 // Turbulence
31 function durb=turbul(Fp,U,ws,Fd,K,th,Rc,rc,Vm,bo,Ac,Vc)
32 [v,dv,Ap]=volm(th,Rc,rc,Vm,bo,Ac,Vc);
33 durb=[Fp*Ap*(abs(U)^3)/(v*ws)-(2/3)*K*vdv/(v) -Fd*K*sqrt(2*abs(K))]/(v^(1/3)*ws);
34 endfunction
35
36 th=linspace(0.88*pi,1.21*pi,100);
37 dh=0.33*pi/100;
38 K(1)=0.01;
39 Vf(1)=ws*(Vl+Cf*sqrt(2*K(1)));
40 for j=2:100
41 [v,dv,Ap]=volm(th(j-1),Rc,rc,Vm,bo,Ac,Vc);
42 U=dv^4/(bo^2*pi);
43 durb=turbul(Fp,U,ws,Fd,K(j-1),th(j-1),Rc,rc,Vm,bo,Ac,Vc);
44 K(j)=K(j-1)+durb*dh;
45 Vf(j)=ws*(Vl+Cf*sqrt(2*K(j)));
46 end
47 subplot(2,1,1)
48 plot(th,K)
49 xtitle("Turbulence vs Theta","theta (rad)","K (m^2/s^3)"
50 subplot(2,1,2)
51 plot(th,Vf)
52 xtitle("Vf/ws vs Theta","theta (rad)","Vf/ws (m/rad)"
```