Engine combustion modeling – An Introduction

Modeling, in science and engineering, may be generally regarded as the process of describing the physical phenomena in a particular system with the help of mathematical equations (subject to “reasonable” assumptions) and solving the same to understand more about the nature of such phenomena. Usually, engineering models help in designing better devices by understanding more about the fundamental physical processes occurring therein. Engine modeling activities, at least in recent decades, have largely been concentrated in the direction of designing better performing engines with lower emissions. In this regard, modeling of engine combustion processes assumes importance.

The various engine combustion models that have been developed to date may be grouped into three categories:

1. Zero dimensional models
2. Quasi-dimensional models
3. Multi-dimensional models

In the above classification, although the level of detail and proximity to physical reality increases as one proceeds downward, so does the complexity of creating and using those models.

Zero dimensional models are the simplest and most suitable to observe the effects of empirical variations in the engine operating parameters on overall heat release rates.\footnote{The phrase “heat release rate” is a misnomer, since heat is essentially a form of energy in transit and cannot be “released” from a substance, say a fuel. The correct phrase could be either “rate of conversion of chemical energy to thermal energy” or simply “energy release rate.” However, since “heat release” is widely used in engine literature and is semantically compact, it will be retained here.}
cylinder pressure schedules. These models are zero dimensional in the sense that they do not involve any consideration of the flow field dimensions.

Zero dimensional models are further sub-divided into:

1. Single zone models
2. Two zone models
3. Multi-zone models

In single zone models, the working fluid in the engine is assumed to be a thermodynamic system, which undergoes energy and/or mass exchange with the surroundings and the energy released during the combustion process is obtained by applying the first law of thermodynamics to the system.

In two zone models, the working fluid is imagined to consist of two zones, an unburned zone and a burned zone. These zones are actually two distinct thermodynamic systems with energy and mass interactions between themselves and their common surroundings, the cylinder walls. The mass-burning rate (or the cylinder pressure), as a function of crank angle, is then numerically computed by solving the simplified equations resulting from applying the first law to the two zones.

A brief note is in order when referring to the nature of single zone and two zone models. These models have been traditionally used in two different directions (shown in Figure 1):

1. In one way, both these models have been used to predict the in-cylinder pressure as a function of crank angle from an assumed energy release or mass burned profile (as a function of crank angle).
2. Another use of these models lies in determining the energy release/mass burning rate as a function of crank angle from experimentally obtained in-cylinder pressure data.

Multi-zone models take this form of analysis one step further by considering energy and mass balances over several zones, thus obtaining results that are closer to reality.

**Assumptions for a typical two zone model**

1. The burned and unburned zones are ideal gases of different properties.
2. The unburned zone is assumed to consist of a premixed fuel-air mixture. Though this may not be exact for diesel combustion, it is more realistic for SI engine combustion.
3. The characteristic gas constants of the burned and unburned zones do not vary much with temperature and pressure; or if any such variations exist, they can be suitably modeled using explicit relationships between gas constants and properties (T, P, etc.)
4. No heat transfer occurs from the burned to the unburned zone and vice versa.
5. Enthalpy associated with injected fuel is usually not significant and hence ignored.
6. Crevice losses may be significant but are not included.
7. Spatially averaged instantaneous heat transfer rates are adequate to estimate heat transfer to the cylinder walls.
8. Instantaneous pressure in both the zones is the same since the flame is a deflagration combustion wave.
9. The work required to transfer fluid from the unburned zone to the burned zone is negligible.
Figure 1. The directions followed by different variations of the single and two zone models for different purposes.
Figure 2. Schematics of the single zone (a) and two zone (b) combustion models depicting the associated energy and mass transfers
**Single zone Model (to find heat release rates from measured pressure)**

Applying the First Law of Thermodynamics to the system (single zone):

\[
\frac{\delta Q_{ch}}{d\theta} - \frac{\delta Q_{ht}}{d\theta} = \frac{\delta W}{d\theta} + \frac{dm}{d\theta} h_f = \frac{dU}{d\theta}
\]

where:

\[
\frac{\delta Q_{ch}}{d\theta} : \text{Apparent rate of chemical energy (or heat) release}
\]

\[
\frac{\delta Q_{ht}}{d\theta} : \text{Rate of heat transfer out of the system}
\]

\[
\frac{\delta W}{d\theta} : \text{Rate of work transfer out of the system}
\]

\[
\frac{dm}{d\theta} h_f : \text{Rate of enthalpy inflow with the fuel}
\]

\[
\frac{dU}{d\theta} : \text{Rate of change of internal energy of the system}
\]

All the energy rates are expressed with respect to the crank angle \(\theta\).

The sum of the work transfer term and the internal energy change of the working fluid term may be expressed in terms of \(P\) and \(V\) alone as follows:

\[
\frac{\delta W}{d\theta} + \frac{dU}{d\theta} = P \frac{dV}{d\theta} + \frac{d}{d\theta} (mc_c T)
\]

where

\[
m : \text{Total mass of in-cylinder gases (the system) in kg}
\]

\[
c_c : \text{Specific heat of the working fluid at constant volume in kJ/kg.K}
\]
From the ideal gas equation,
\[ PV = mRT \] \tag{3}

where

\[ R : \text{ Characteristic gas constant of the cylinder gases in kJ/kg. K} \]

Upon logarithmic differentiation, the above equation becomes
\[
\frac{dP}{P} + \frac{dV}{V} = \frac{dm}{m} + \frac{dR}{R} + \frac{dT}{T}
\]

However, considering the fact that the mass in the control volume remains constant (neglecting crevice losses and quantity of fuel injected) and also assuming that the gas constant remains constant throughout the combustion process, we get
\[
\frac{dP}{P} + \frac{dV}{V} = \frac{dT}{T} \tag{4}
\]

Substituting for \( m \) (from Equation 3) and \( \frac{dT}{T} \) (from Equation 4) in Equation 2, we get
\[
\frac{dW}{d\theta} + \frac{dU}{d\theta} = P \frac{dV}{d\theta} + \left( \frac{PV}{R} \right) c_v \left( \frac{dP}{P} + \frac{dV}{V} \right)
\]

Rearranging and simplifying,
\[
\frac{dW}{d\theta} + \frac{dU}{d\theta} = \left( 1 + \frac{c_v}{R} \right) P \frac{dV}{d\theta} + \left( \frac{c_v}{R} \right) V \frac{dP}{d\theta} \tag{5}
\]

Now for an ideal gas,
\[
c_p - c_v = R \tag{6}
\]
\[
\frac{c_p}{c_v} = \gamma \tag{7}
\]
where

\( c_p \): Specific heat of the working fluid at constant pressure in kJ/kg.K

\( \gamma \): Ratio of specific heats at constant pressure and constant volume

Using Equations (6) and (7) and simplifying, Equation (5) becomes

\[
\frac{dW}{d\theta} + \frac{dU}{d\theta} = \left( \frac{\gamma}{\gamma - 1} \right) P \frac{dV}{d\theta} + \left( \frac{1}{\gamma - 1} \right) V \frac{dP}{d\theta}
\]  

(8)

Substituting Equation (8) in Equation (1), neglecting the fuel enthalpy term, and rearranging,

\[
\frac{dQ_n}{d\theta} = \frac{dQ_{ch}}{d\theta} - \frac{dQ_{ht}}{d\theta} = \left( \frac{\gamma}{\gamma - 1} \right) P \frac{dV}{d\theta} + \left( \frac{1}{\gamma - 1} \right) V \frac{dP}{d\theta}
\]  

(9)

where

\[ \frac{dQ_n}{d\theta} \]: Net apparent rate of heat release

**Two zone Model (to find heat release rates from measured pressure)**

In order to perform parametric simulation studies on engine combustion, a simple thermodynamic model, which incorporates two zones, viz. an unburned zone and a burned zone is desirable. Naturally, it is important to understand the suitability (or lack thereof) of the two zone model to predict heat release rates in diesel and spark-ignited engine combustion. Whereas in spark-ignited engines relatively well-defined (continuous) flame propagation might occur, diesel engine combustion might consist of several distinct burned and unburned regions scattered throughout the cylinder, as shown in Figure 2. Despite the differences in the nature of combustion, the two zone model
would still be applicable for both diesel and spark-ignited engine combustion since it is basically a zero dimensional model that considers only unburned and burned zones without any consideration of the spatial location of such zones. The basic idea behind the two-zone model is to utilize the conservation of mass and energy (First Law of Thermodynamics) and also the ideal gas equations in obtaining an “apparent” rate of heat release curve or “apparent” mass burned fraction curve. The adjective “apparent” should be stressed in order to realize the fact that whatever be the heat release or mass burned fraction obtained indirectly from measuring in-cylinder pressure, its accuracy is limited by both the assumptions of the model as well as the accuracy of the pressure data.

The conservation of mass inside the cylinder is

\[ m = m_u + m_b, \]  

(10)

where

\[ m : \] Total mass of charge inside the cylinder \((= m_{\text{fuel}} + m_{\text{air}})\)

\[ m_u: \] Mass of unburned charge

\[ m_v: \] Mass of burned charge

Also, since the mass inside the cylinder is assumed to be constant in any given engine cycle,

\[ \dot{m}_b = -\dot{m}_u \]  

(11)

Since the unburned and burned zones together constitute the total cylinder charge volume at any instant, we have

\[ V = V_u + V_b \]  

(12)

where
\[ V : \text{Total volume of charge inside the cylinder} \]

\[ V_u : \text{Volume of unburned charge} \]

\[ V_b : \text{Volume of burned charge} \]

The ideal gas equations for the unburned and burned zones are

\[ PV_u = m_u R_u T_u \quad (13) \]
\[ PV_b = m_b R_b T_b \quad (14) \]

The generic form of the first law of thermodynamics applied to a control volume is

\[ \frac{\delta Q}{dt} - \frac{\delta W}{dt} + \sum_{\text{in}} m h_i - \sum_{\text{out}} m h_o = \frac{dE_{cv}}{dt} \quad (15) \]

Now, considering the above expression for the unburned zone in terms of the respective rates of the energy terms with crankangle,

\[ -Q_{br,u} - PV_u + m_u h_u = m_u u_u \quad (16) \]

Similarly, applying the first law (Equation 14) for the burned zone and remembering that the total energy input into the burned zone is due to the chemical energy (released by the fuel when it burns), we get

\[ Q_{ch} - Q_{hr,b} - PV_b - m_u h_u = m_b u_b \quad (17) \]

The governing equations for the two zone model are Equations (10-14) and (16-17). These equations are solved simultaneously each time (or crank angle) step to determine the unknown quantities \( T_u, \ T_b, \ V_u, \ V_b, \ m_u, \ m_b, \) and heat release rate from the known cylinder pressure \( P \) and total volume \( V \).
In-cylinder pressure measurement – general procedure

The schematic of a typical in-cylinder pressure measurement system is given in Figure 3. The pressure transducer used to measure in-cylinder pressure is of the piezoelectric type. When there is time-varying pressure acting on the diaphragm of the transducer, which consists of a piezoelectric crystal, an electric charge, proportional to the magnitude of the applied pressure is induced on the opposite edges of the crystal (“transverse cut crystal”) or on the same sides of the crystal (“longitudinal cut crystal”, as shown in Figure 4). This charge is converted and scaled into DC voltage by the dual mode charge amplifier. A high-speed data acquisition board (that has an Analog/Digital Converter) reads the analog output of the amplifier and digitizes the data. The digitized data are then converted into the corresponding pressure values. An optical encoder coupled to the engine crankshaft, controls acquisition of the pressure data at the required crank angles. An important fact concerning the pressure values thus obtained is that these are actually relative (with respect to the pressure sensed by the transducer when the amplifier is initially “reset”) pressures at different crank angles. Therefore, they need to be “scaled” with a known absolute pressure during the engine cycle. Typically, the pressure at BDC during the intake stroke is assumed to equal the measured absolute intake manifold pressure and the relative pressures at other crank angles in the cycle are scaled with respect to the pressure at BDC.
Figure 3. Typical in-cylinder pressure measurement system

Figure 4. Schematic illustrating the piezoelectric principle