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Thermodynamic modeling of direct injection methanol fueled engines

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ABSTRACT

In-cylinder pressure is an important parameter that is used to investigate the combustion process in internal combustion (IC) engines. In this paper, a thermodynamic model of IC engine combustion is presented and examined. A heat release function and an empirical conversion efficiency factor are introduced to solve the model. The pressure traces obtained by solving the thermodynamic model are compared with measured pressure data for a fully instrumented laboratory IC spark ignition (SI) engine. Derived scaling parameters for time to peak pressure, peak pressure, and maximum rate of pressure rise (among others) are developed and compared with the numerical simulations. The models examined here may serve as pedagogic tools and, when suitably refined, as preliminary design tools.

1. Introduction

In an IC engine the cylinder pressure is an important parameter for analyzing the progress and intensity of the combustion process. Even without combustion (as in idealized engine cycles such as the Otto and combined cycles [1,2]) the pressure trace is required in order to calculate the work output. In fact, given the engine turnover rate (RPM) the pressure trace forms the basis of the engine cycle power computation. Examples of these calculations are provided in thermodynamics textbooks [1,2] and in classical "engines" textbooks [3–5]. Although the models examined in these books are simple, they yield order-of-magnitude estimates of satisfactory accuracy. Various sophisticated models with empirically determined parameters and heat release (i.e., combustion rate) profiles have been developed using these methods.

There are many pressure-based combustion studies in the literature. Rassweiler and Withrow [6] investigated the pressure change in an engine cylinder finding that mass burned and the pressure change were proportional. Daw and Kahl [7] used peak SI engine cylinder pressure as the primary parameter to study cycle-to-cycle variations during engine operation. Brunt et al. [8] analyzed knock in a gasoline engine. Shen et al. [9] analyzed combustion in a direct injection methanol engine using cylinder pressure data. Ludwig et al. [10] introduced a method to describe in-cylinder diesel combustion by monitoring the pressure trace. These works all ascribed primary importance to the engine cylinder pressure trace in determining the rates and magnitudes of other affiliated processes.

In this article, we present an analysis of the in-cylinder pressure variations and examine scaling relationships that correlate well with the experimental data for an IC test engine. A heat-release model is examined, producing mathematical parameters for scaling pressure traces between (and during) important IC engine combustion signposts, such as the instants of ignition, Top Dead Center (TDC), location of peak pressure and burnout. This article is a lengthier version of Ref. [11].

2. Thermodynamic analysis

A thermodynamic analysis is applied to a control volume in the engine cylinder. The analysis employs the following four assumptions: (1) The mixture inside the cylinder is an ideal gas, thus the relationship among the pressure (p), volume (V), and temperature (T) is given by the equation of state, $\ln p + \ln V = \ln m + \ln R + \ln T$. (2) Conditions in the engine cylinder are homogeneous and characterized by unique values of the pressure (p), temperature (T), volume (V) and heat release (Q). (3) The intake and exhaust valves are both closed during combustion so the mixture mass (m) is constant. (4) The ideal gas constant R is assumed constant throughout the engine cycle. Then, the above equation of state may be written as

$$dp/p + dV/V = dT/T. \tag{1}$$

According to the first law of thermodynamics, the differential form of the energy conservation equation in the engine cylinder is $dU = dQ - dW$. Using $dU = mc_v dT$ and $dW = pdV$ gives $mc_v dT = dQ - pdV$. Dividing this equation by $pV = mRT = m(c_p - c_v)T = mc_v(\gamma - 1)T$,

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Nomenclature

a, b, c	dimensionless parameters used in Section 4
c_v, c_p	specific heats at constant volume, pressure ($e/m-T$)
$f(\theta)$, $g(\theta)$	coefficient functions in Eq. (2)
K	nondimensional heat transfer to charge, $K = (\gamma-1)Q_{in}/p_1V_1$ (–)
m	mass of gas in piston cylinder (m)
p	pressure (F/L^2)
$\bar{p}$	dimensionless pressure, $\bar{p} = p/p_1$ (–)
$Q(\theta)$	heat release during combustion of fuel (e)
Q_{in}	total heat energy added during cycle (e)
r	compression ratio, $r = V_{BDC}/V_{TDC}$ (–)
R	gas constant ($e/m-T$)
s	dummy variable of integration (–)
T	temperature (T)
U	internal energy (e)
V	volume (L^3)
$\bar{V}$	dimensionless volume, $\bar{V} = V/V_1$ (–)
W	work (e)
$x(\theta)$	heat release progress variable (–)
z	dummy variable of integration (–)

Greek symbols

α	positive dimensionless parameter in Eq. (5) (–)
γ	specific heat ratio, $\gamma = c_p/c_v$ (–)
Δ	angular coordinate centered at TDC, $\Delta = \theta - 2\pi$ (–)
ζ	mathematically defined dimensionless function in Section 3.1, $\zeta = ln[(\xi + x)/\xi]$ (–)
θ	angular coordinate (–)
ξ	positive dimensionless parameter in Eq. (5) (–)
τ	normalized angular coordinate used in Section 3.1, $\tau = (\theta - \theta_i)/(\theta_f - \theta_i)$ (–)
ϕ	dummy variable of integration in Eq. (5) (–)
χ	positive dimensionless parameter in Eq. (5) (–)

Subscripts

f	burnout value ("final")
i	ignition value
m	value at maximum pressure
1	inlet (BDC) value ("initial")

Acronyms

BDC	Bottom Dead Center
CAD	crank angle degrees (same as θ)
IC	internal combustion
RPM	revolutions per minute
TDC	Top Dead Center

then writing the differentials with respect to the crank angle degree θ (CAD) and using Eq. (1) for the term containing the factor $T^{-1}\ dT/d\theta$ yields [Ref. [5], p. 388] the differential equation for the engine cylinder pressure trace $p(\theta)$,

$$dp/d\theta + (\gamma/V)(dV/d\theta)p = ((\gamma-1)/V)dQ/d\theta. \tag{2}$$

The engine geometry dictates the cylinder volume. Thus, $V(\theta)$ and $dV(\theta)/d\theta$ are known, given functions of θ. Eq. (2) then becomes $dp/d\theta + f(\theta)p = g(\theta)$, where $f(\theta) = (\gamma/V)(dV/d\theta)$ is a known coefficient function and $g(\theta) = ((\gamma-1)/V)dQ/d\theta$ is the forcing function, which is known when the heat release trace $Q(\theta)$ is known.

The function $Q(\theta)$, however, is known only once the in-cylinder combustion problem is solved, a difficult (and so far impossible) task. Consequently, in our analysis we specify this function, either *a priori* or *a posteriori*, in order to proceed with our analysis.

We develop two models in this paper. In the first model, Model (i), the heat release $Q(\theta)$ is deduced by comparing the predictions of Eq. (2) with the experimental $p(\theta)$ profiles, producing an accurate and reasonably sophisticated $Q(\theta)$ expression. Model (i) produces a version of Eq. (2) that must be solved numerically. Model (ii) produces a version of Eq. (2) that can be solved analytically. This analytical solution is used to derive mathematical scaling parameters for use in engine analysis. Without such a simplification, the mathematical analysis is too difficult and scaling parameters cannot be analytically derived. This is true for Model (i).

For both Models (i) and (ii), we write $Q(\theta) = Q_{in}x(\theta)$ where $x(\theta)$ is a heat release progress variable defined such that $x(\theta_i) = 0$ at the start of combustion and $x(\theta_f) = 1$ at its completion. Here, θ_i is the 'ignition' crank angle while θ_f is the burnout or 'final' crank angle. All of the heat Q_{in} has been released when $x(\theta_f) = 1$. In terms of $x(\theta)$ Eq. (2) becomes

$$dp/d\theta + (\gamma/V)(dV/d\theta)p = ((\gamma-1)/V)Q_{in}dx/d\theta. \tag{3}$$

Subject to the assumptions (1)–(4) Eq. (3) is exact. Eq. (3) is nondimensionalized using $\overline{p} = p/p_1$, $\overline{V} = V/V_1$, where p_1, V_1 are inlet or Bottom Dead Center (BDC) values. For future reference p_2 and V_2 are TDC values. The mathematical solution of the nondimensional Eq. (3) uses the nondimensionalizations for $\bar{p}$ and $\bar{V}$ given above in Eq. (3) and then employs Euler's solution for linear first-order ordinary differential equations $d\bar{p}/d\theta + \bar{f}(\theta)\bar{p} = \bar{g}(\theta)$ in the form

$$\bar{p}(\theta) = \left\{const. + \int^{\theta} \bar{g}(s)\exp\left(\int^{s}\bar{f}(z)dz\right)ds\right\}\exp\left[-\int^{\theta}\bar{f}(z)dz\right],$$

where s and z are dummy variables of integration. A brief calculation including the application of the initial condition $\bar{p}(\theta_i) = \bar{p}_i$ yields

$$\bar{p}(\theta) = \frac{\overline{p_i}}{(\overline{V}/\overline{V_i})^{\gamma}} + \frac{K}{\overline{V}^{\gamma}}\int_{\theta_i}^{\theta}\frac{dx}{d\phi}\overline{V}(\phi)^{\gamma-1}d\phi, \tag{4}$$

where ϕ is the dummy variable of integration and $K = (\gamma-1)Q_{in}/p_1V_1$ is the dimensionless heat release. Various possible heating functions are illustrated in Fig. 1, showing the rise from zero heat release at ignition to full heat release at burnout, approximately $\theta \approx 385$ CAD in Fig. 1.

3. Empirical heat release function

3.1. Theoretical model

In order to deduce an empirically accurate $Q(\theta)$ profile, six physically justified restrictions on the heat release function are presented below in the form of bullet points (1)–(3) [9]:

(1) At $\theta = \theta_i$: $x = 0$ and $(dx/d\theta)_i > 0$. These conditions denote ignition or start of combustion.
(2) When $\theta_i < \theta < \theta_f$: $0 < x < 1$ and $(dx/d\theta) > 0$. These conditions are commensurate with flame propagation and the continuation of combustion.
(3) At $\theta = \theta_f$: $x = 1$ and $(dx/d\theta)_f = 0$. These conditions identify the termination of combustion.

By normalizing θ to values ranging between zero at ignition and unity at burnout according to the mathematical definition $\tau = (\theta - \theta_i)/(\theta_f - \theta_i)$ it has been shown [9,12] that conditions (1)–(3) can be satisfied by the following equation: