Fuel 117 (2014) 1096–1110

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Emissions–calibrated equilibrium heat release model for direct injection compression ignition engines

Jonathan M.S. Mattson *, Christopher Depcik

Department of Mechanical Engineering, University of Kansas, 1530 W. 15th Street, 3138 Learned Hall, Lawrence, KS 66045, United States

HIGHLIGHTS

- An equilibrium heat release model for diesel engine combustion is developed.
- Combustion is expressed by Arrhenius expression, and calibrated using emissions data.
- Model accounts for alternative fuels (biodiesels) and testing modes (EGR).
- Model has been validated with existing data acquisition, with time-efficient results.
- Effects on combustion of variable fuels and fuel properties are highlighted.

ARTICLE INFO

Article history:
Received 6 August 2013
Received in revised form 9 October 2013
Accepted 14 October 2013
Available online 1 November 2013

Keywords:
Heat release
Compression ignition
Emissions
Arrhenius
Biodiesel

ABSTRACT

The heat release analysis of an internal combustion engine is essential for understanding the process of combustion, with models commonly used as tools during engine testing. This effort describes a zero-dimensional (0-D), three-zone model (burned, unburned, and fuel mass zones) for computing the rate of heat release using in-cylinder pressure–time history. Each zone is thermodynamically independent except for the shared use of the pressure trace. By utilizing fundamental mass and energy balances, the model balances numerical accuracy with time-efficient computation. Improvements to the literature in this area include the incorporation of an Arrhenius-based function for the rate of combustion, freeing the user from having to diagnose the duration of the combustion event. Additionally, this methodology allows the rate of heat release to be calculated from a thermodynamic analysis of the change in the bulk gas as indicated by the pressure trace. The model is calibrated to a combustion efficiency found through a separate emissions analysis, providing a stable numerical platform. Model results demonstrate the rate of heat release of various fuel chemistries (mineral diesels, oxygenates, and other fuels) and testing modes (Exhaust Gas Recirculation), utilizing pressure data acquired from the testing of a single-cylinder compression ignition engine.

1. Introduction

Analysis of the combustion process within an internal combustion (IC) engine is essential to engine research. Two distinct techniques exist in order to characterize combustion. The first is a measurement of emissions species, whereby quantifying exhaust gases allows for calculation of the degree of combustion within the cylinder. The second is a combustion model, used to calculate various thermodynamic characteristics throughout the engine's thermodynamic cycle. One of the primary tools used by researchers for this analysis is a heat release (HR) model [1]. The diagnostic HR model functions by calculating the total energy released by the combustion of fuel based on the measurement of in-cylinder pressure [1,2]. In regards to the specifics of the HR model, there is a wide divergence in available models.

Of importance to the creation of an HR model is the number of dimensions used to model the flow characteristics within the control volume. For example, a three-dimensional model treats the change in cylinder characteristics as a function of time and three spatial dimensions. Conversely, a zero-dimensional (0-D) model ignores spatial dimensions, and evolution of the cylinder contents is treated as a function of time only. Of importance, higher dimensional models (often computational fluid dynamics based) see greatly increased accuracy when quantifying the energy output of fuels [3,4]. However, these added dependencies introduce a significant number of equations that must be solved at the cost of greatly increased computational time. In contrast, 0-D models do not account for these changes, and only evaluate the evolution of the "bulk" gas. As a result, 0-D models are favored when computational speed is a concern. These 0-D HR models have been widely

* Corresponding author. Tel.: +1 4027301120.
E-mail address: jmattson@ku.edu (J.M.S. Mattson).

0016-2361/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.fuel.2013.10.026

Nomenclature

A	area (m^2), first Arrhenius coefficient (ms)
A_n	injector nozzle area (m^2)
A_s	surface area within cylinder (m^2)
a	coefficient for gas emissivity correlation (unitless, Pa^{-1} - m^{-1}, Pa^{-2} m^{-2}, Pa^{-3} m^{-3})
C_d	coefficient of discharge
c_f	liquid fuel specific heat (J kg^{-1})
c_p	constant pressure specific heat (J kg^{-1})
E_a	activation energy (kJ $mole^{-1}$)
g	global reaction equation coefficients, dependant variable in the Newton–Raphson method
h_c	conductive heat transfer coefficient (W m^{-2} K^{-1})
K	fuel combustion rate coefficient (m^3 kg^{-1} s^{-1})
l	local combustion formula coefficient
m	mass (kg)
$m_{f,rem}$	mass of fuel remaining after combustion (kg)
n	moles of material (mol)
n_a	second Arrhenius coefficient
n_h	number of holes on a single fuel injector
n_{inj}	number of fuel injectors within a cylinder
p	pressure (Pa)
Q_{hr}	heat release (J)
Q_{ht}	heat transfer (J)
Q_{LHV}	lower heating value (J kg^{-1})
R	gas constant (J kg^{-1} K^{-1})
R_{univ}	universal gas constant (J mol^{-1} K^{-1})
T	temperature (K)
T_{vap}	fuel vaporization temperature (K)
T_w	cylinder wall temperature (K)
t	time (s)
U	internal energy (J)
V	volume (m^3)
W	work (J), molecular weight (kg $mole^{-1}$)
x	dependant variable in Newton–Raphson method
Y_{mb}	fraction of mass burned
y	mass fraction

Greek symbols

α_w	wall absorptivity
δ	molar amount of intake air (moles)
ε_1, ε_2	molar amount of gases recycled by residual fraction or EGR, respectively (moles)
ε_g	emissivity of the bulk gas
ζ	molar amount of unburned products of combustion (moles)
θ	crank angle (degree)
λ	molar amount of burned products of combustion (moles)
ξ	molar amount of injected fuel (moles)
ρ	density (kg m^{-3})
τ	ignition delay (s)

Subscripts

b	burned zone, burned
cv	control volume, bulk gas
e	entrained
f	fuel zone, fuel
fa	fuel added
fb	fuel burned
i	index for zones
inj	injected
j	index for species
k	index for data points
p	produced
u	unburned zone

used by researchers in the past because of this reduced computational load. However, they are often dependent on a correct diagnosis for the start and end of combustion; particularly, if they make use of the expressions pioneered by Wiebe or Matekunas [5–7]. While the correct methods for finding the onset of combustion are controversial, the approximate timing can be found using a wide variety of techniques, such as Arrhenius-based ignition delay functions or indications from the derivatives of the pressure trace. However, the appropriate end of combustion within the cylinder is less well understood, and so may lead to significant errors if the diagnosis is incorrect [7–10]. In addition, while the Wiebe and Matekunas expressions have proven particularly useful, they are ultimately approximations based on prior experimentation. As a result, 0-D models are often called Apparent Heat Release (AHR) or Net Heat Release (NHR) models, as the true RHR within the system cannot be known explicitly within the framework of a 0-D model [11,12]. This is (primarily) because the correlations of mass fraction burned used to control the rate of combustion are not governed by the rate of change of pressure within the cylinder. As a result, any fluctuations in the pressure trace away from the case "expected" by the mass fraction burned approximation will lead to error in RHR calculation. It is important to note that within this work, 0-D, NHR, and AHR models are treated as being synonymous.

For 0-D HR models, the bulk gas is often subdivided into a number of "zones," which are used to separate the control volume into distinct areas depending on the different species or processes within the cylinder [1]. Each zone is treated as being somewhat independent of the others, with some properties being shared, and some being distinct to a zone. This aids in the modeling of certain in-cylinder phenomenon, particularly blow-by effects or fuel stratification (in Direct Injected or DI engines). The addition of zones will lead to a larger system of equations that must be solved [13,14]. This has led many authors to make assumptions as to which thermodynamic variables are shared between zones. The most commonly shared variable is pressure, due to the impracticality of splitting a measured pressure trace into unique components for each zone [15,16]. Other models allow for a shared temperature between zones [14].

In this effort, the authors present an improved methodology for calculating the gross rate of heat release (RHR) with the full details presented in the first author's thesis [17]. The basis of the model is a three zone 0-D model, similar to previously constructed models, and is split into fuel, unburned, and burned mass zones [13,14]. The supplied pressure trace is the only thermodynamic variable shared between zones in order to preserve the rate of change of the fuel zone temperature for the calculation of ignition delay. However, the rate of fuel consumption by combustion within the cylinder is calculated through an Arrhenius-based equation as given by Hiroyasu et al. [18–20]. This expression only requires the user to diagnose the onset of combustion, as the use of an Arrhenius function becomes self-limiting since it is largely dependent on the amount of fuel remaining in the cylinder, as well as the temperature of the bulk gas. More importantly, this functional dependence on cylinder temperature leads to an implied dependence on pressure, meaning the RHR is not completely divorced