

First and Second Law Heat Release Analysis in a Single Cylinder Engine

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ABSTRACT

In-cylinder engine modeling is a necessary aspect of combustion research. In particular, simulating heat release connects variable combustion behavior to fuel properties through the 1st Law of Thermodynamics. One extension of such models is to evaluate changes to in-cylinder behavior using the Second Law of Thermodynamics in order to identify the peak period of availability for work extraction. Thus, Second Law models are a useful tool to augment research into alternative fuel usage and optimization. These models also help identify internal irreversibilities that are separate from heat transfer and exhaust gas losses.

This study utilizes a multi-zone 1st and 2nd Law Heat Release model to characterize the changes in combustion behavior of a number of neat fuels used in a single-cylinder compression ignition (CI) engine. This includes standard Ultra Low Sulfur Diesel (ULSD), biodiesels derived from jatropha and tallow feedstocks, Jet A aviation fuel, and a synthetic aviation fuel derived from renewable sources. In all cases, fuel injection timing was adjusted to align the peak pressure timing of each fuel with that of ULSD.

Overall, variations in fuel properties were found to bring about considerable changes in engine operation when investigating the 2nd Law. Most prominently, fuel density, energy content, cetane number, and viscosity serve as the primary fuel characteristics that drive combustion timing, duration, and intensity. In particular, it is shown that large viscosities (a characteristic of biodiesels) lead to delayed and prolonged combustion, which serves to add availability to the working fluid later in the expansion stroke, subsequently making it more difficult to extract that availability as useful work. In addition, the strengths of incorporating the 2nd Law analysis are expressed, both alone and in tandem with the traditional 1st Law analysis.

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INTRODUCTION

The thermodynamic modeling of in-cylinder combustion processes helps to characterize fuel behavior. The standard in-cylinder model uses the calculation of the engine-out rate of heat release (RHR) [1, 2]. Through RHR modeling, the changes in combustion rates between fuels and engine loads can be effectively categorized, and the premixed- and diffusion- dominated portions of the combustion cycle (and their mutual effects on engine performance and efficiency) can be identified and further separated from one another. This is particularly important within CI engine combustion, where changes in fuel properties can lead to variation in fuel breakup, ignition delay, and combustion duration. Hence, this type of modeling provides a window into in-cylinder combustion allowing injection parameters and engine operation to be optimized for a given fuel. The overall governing equation for RHR is given as [1]:

$$\frac{dQ_{hr}}{d\theta} = \frac{dU_{cv}}{d\theta} + \frac{dW_{cv}}{d\theta} + \frac{dQ_{ht}}{d\theta} + \sum h \frac{dm_{cv}}{d\theta} \quad (1)$$

where the RHR at a given crank angle (Q_{hr}) is a function of the rate of change of the bulk gas internal energy (U_{cv}), the rate of work being done (W_{cv}), the rate of heat transfer through the cylinder walls (Q_{ht}), and the rate of mass transfer into or out of the cylinder through various processes ($dm_{cv}/d\theta$).

An alternative (or expansion) to traditional RHR modeling is to incorporate the 2nd Law of Thermodynamics. A 2nd Law analysis, also known as an availability or exergy analysis, is similar to the 1st Law examination, but instead focuses on the generation and exchange of entropy within the bulk gas, and also through the cylinder walls. Whereas 1st Law models can calculate the peak thermal efficiency of an engine cycle, 2nd Law models calculate the periods of peak availability, and also analyze the means by which availability is utilized as work, or lost as entropy. The 2nd Law analysis utilizes an equation similar in nature to that used for 1st Law models [3]:

$$\frac{dA_g}{d\theta} = \frac{dA_c}{d\theta} - \left(\frac{dA_w}{d\theta} + \frac{dA_{ht}}{d\theta} + \frac{dA_{ir}}{d\theta} \right) \quad (2)$$

where the change in total availability of the bulk gas at a given crank angle (A_g) is given as the difference between the amount of availability added by the combustion of fuel (A_c) and the sum availability either leaving the cylinder through work (A_w) or heat transfer (A_{ht}), or being lost to irreversibilities and entropy generation (A_{ir}). The model then seeks to evaluate the component terms of Eqn. (2) individually in order to calculate the net change in availability within the cylinder.

The evaluation of availability transferred as work is well-established as the following [3, 4]:

$$\frac{dA_w}{d\theta} = \frac{dW_{cv}}{d\theta} - p_0 \frac{dV}{d\theta} \quad (3)$$

where p_0 is the ambient (reference) pressure, and V is the cylinder volume. As such, the rate of availability transferred is related to the work done by the engine, as well as the work done by the ambient atmosphere against the engine's motion.

The rate of availability loss through heat transfer is calculated as [3, 4]:

$$\frac{dA_{ht}}{d\theta} = \frac{dQ_{ht}}{d\theta} \left(1 - \frac{T_0}{T_w} \right) \quad (4)$$

where T_0 and T_w are the temperatures of the ambient and the cylinder walls, respectively. Similar to the work availability equation, the heat transfer availability losses compare the heat transfer out of the cylinder to the temperature of the ambient, as well as the medium (the cylinder walls) through which heat transfer occurs.

The rate of availability loss due to irreversibilities is defined as follows [3, 5, 6]:

$$\frac{dA_{ir}}{d\theta} = T_0 \frac{dS}{d\theta} - \frac{T_0}{T_w} \frac{dQ_{ht}}{d\theta} \geq 0 \quad (5)$$

where S is the entropy generated. Of note, Eqn. (5) only accounts for internal irreversibilities, while external irreversibilities (i.e., heat transfer) are given in Eqn. (4). In some situations, Eqns. (4) and (5) are unified into a single expression, representing all irreversibilities encountered by the system.

Next, the rate of availability addition (similar to the RHR) is given by [3]:

$$\frac{dA_c}{d\theta} = e_c \frac{dm_c}{d\theta} \quad (6)$$

where m_c is the mass of fuel consumed at a given crank angle, and e_c is the chemical availability of a given fuel. The value for e_c is analogous to the lower heating value of the fuel, and as such the lower heating value is typically used to approximate e_c [7, 8]:

$$\begin{aligned} \frac{e_c}{Q_{lhw}} = r = & 1.0401 + 0.1728 \frac{y_H}{y_C} + 0.0432 \frac{y_O}{y_C} \\ & + 0.2169 \frac{y_S}{y_C} \left(1 - 2.0628 \frac{y_H}{y_C} \right) \end{aligned} \quad (7)$$

where the ratio (r) between the chemical availability and the energy content (Q_{lhw}) of the fuel is expressed as a function of the mass fraction (y) of hydrogen (H), oxygen (O), carbon (C), and sulfur (S) in the fuel molecule. Alternatively, the value of r for ULSD has been found to be approximately 1.065 [9, 10].

By utilizing Eqns. (3)-(7), the various components of Eqn. (2) may be evaluated for a given crank angle, leaving only the availability retained by the bulk gas (A_g) to be solved for directly. Once the entire engine cycle has been solved in this manner, the 2nd Law Efficiency (or the exergetic efficiency, η_e) may be determined [10]:

$$\eta_e = \frac{A_w}{A_c} = 1 - \frac{(A_g + A_{ht} + A_{ir})}{A_c} \quad (8)$$

In essence, the exergetic efficiency is the 2nd Law analogue to the thermal efficiency used in 1st Law models. As a result, where the thermal efficiency calculates the ratio of work energy recovered by the system to heat energy input, Eqn. (8) expresses the ratio of recovered work to chemical availability added.

For this study, a previously constructed heat release model incorporating both 1st and 2nd Law modeling was utilized [11, 12]. The chosen model functions as a zero-dimensional, equilibrium-basis model, which calculates RHR from a measured pressure trace, and utilizes an Arrhenius reaction rate equation to control the rate of combustion (and thus the rate of availability addition into the cylinder by Eqn. (6)) [13]. Thermodynamic variables are calculated at each degree of crank angle using CHEMKIN-III [14]. Finally, the model is calibrated to the cycle combustion efficiency, calculated from the measured exhaust gases of the engine during operation.

EFFECT OF FUEL PROPERTIES

The 1st and 2nd Law models provide the basics needed to model engine combustion, particularly in the investigation of fuel physical and chemical properties. Combustion in CI engines is typically broken into two distinct phases; a premixed combustion phase, with rapid combustion and higher heat release, and a diffusion-dominated phase, with diffusion and mixing properties controlling the rate at which energy or availability is added to the cylinder [1]. Both phases of combustion are highly responsive to changes in fuel properties (as well as engine speed and load). The RHR analysis provides the means to link fuel properties to behavior within these two combustion phases, and it has the ability to identify both the benefits and shortcomings of a given fuel.

The link in combustion variability and fuel properties is particularly true in the case of biodiesel fuels, which generally suffer from lower energy content by mass and higher viscosity, but also offer high

density and significant oxygen content, in comparison to ULSD [15]. When switching between two fuels (either directly, or through blending of fuels), it becomes important to isolate the effects of each fuel property, either to optimize combustion for a given fuel, or to find the amount of deviation from the behavior of ULSD that is acceptable before engine operating parameters must be changed [16, 17]. The primary means by which fuel parameters come into play is through the injection and ignition delay process [18]. Before ignition can occur and combustion can proceed in a CI engine, fuel must first be injected into the cylinder at high pressure, atomize, vaporize, and chemically prepare [1]. Various factors affect the length of this ignition delay period, and are vital to consider.

One of the primary properties defining CI engine combustion behavior is fuel viscosity [18]. Viscosity is closely linked to the physical aspects of ignition delay, through spray breakup and atomization [19-21]. As a result, when fuel viscosity is raised (as is typically the case with biodiesel fuels), fuel breakup becomes more prolonged, increasing the ignition delay period by physically inhibiting the ignition process, and has been found to decrease thermal efficiency [18]. When viscosity is lowered, however, fuel breakup is much faster, leading to shortened ignition delays and advanced combustion, leading to the potential for increased temperatures and nitrogen oxide (NO_x) emissions without retarding the injection event, or decreasing injector pressure.

Fuel density is an important variable in the injection discharge rate, and so is one of the variables central to engine fuel flow rate that is not within a researcher's direct control. As fuel flow rate is inherently volumetric for high-pressure common rail systems, the density of the fuel is deterministic of the mass flow rate of fuel that may enter the cylinder at a given time [1]. Therefore, fuel density becomes a limiting factor in the ability of the injector to deliver fuel energy into the cylinder, alongside the fuel's energy content. In addition, lower fuel densities have been linked to shorter fuel ignition delay periods [18].

Cetane number is a parameter utilized to generalize the likelihood of fuels to autoignite, and so is used as a predictive measure of ignition delay in CI engines. In particular, cetane number is often used as a stand-in for chemical ignition delay parameters despite the fact that it does account for some physical properties as well [18]. Higher cetane numbers are indicative of shorter ignition delay periods, leading to a fuel igniting more promptly, but potentially leading to premature combustion before enough fuel may be prepared.

In order to further demonstrate the effects of variation in fuel properties, this study explores the usage of a number of different fuels in a high compression ratio CI engine. In particular, the variations in fuel density, viscosity, cetane number, and energy content serve as the primary focus, and their effects on engine operation are demonstrated through their effects on the RHR and the 2nd Law efficiency.

EXPERIMENTAL SETUP

The selected fuels were utilized with a Yanmar L100V single-cylinder engine, paired with a DyneSystems Dymond Series alternating current dynamometer [22]. Engine and dynamometer information can

be found in Table 1 and Table 2, respectively. The Yanmar engine was operated with a high-pressure single-rail electronic fuel injection system, in place of its original mechanical fuel injection system. In addition, the standard EGR port was blocked.

Table 1. Engine Specifications [22].

Manufacturer/Model	Yanmar L100V
Type	Vertical Direct-Injected
Intake	Naturally Aspirated
Colling	Air-Cooled
Cycle	4-Stroke
Displacement [cc]	435
Number of Cylinders	1
Number of Valves	2 (1 intake, 1 exhaust)
Bore [mm]	86
Stroke [mm]	75
Connecting Rod Length [mm]	118
Crank Radius [mm]	38
Clearance Volume [cm^3]	21.611
Piston Area [cm^2]	58.088
Compression Ratio	21.2
Injection Timing	Variable
Injection Pressure	Variable, Limited below 200 MPa
Continuous Rate Output [hp (SAE)]	8.3
Rated Speed [RPM]	3600
Engine Oil Used	Shell 15W-40

Table 2. Dynamometer Specifications [22].

Manufacturer/Model	DyneSystems, Inc. Dymod Series 12
Continuous Rated Torque [N-m]	28.61
Continuous Power [hp (SAE)]	12
Maximum Speed [RPM]	7500
Voltage [VAC]	480
Phase	Three Phase
Frequency [Hz]	60
Controller	DyneSystems, In. Linter-Loc V OCS

The fuels utilized during experimentation were Jet A, an aviation fuel derived from renewable through hydroprocessing (R-8), and two biodiesel fuels derived from beef tallow and jatropa oils. The characteristics for these fuels can be found in Table 3 [12, 23]. In addition, standard ULSD was utilized as a control. The engine was operated without added turbocharging, and without multiple injection events per cycle, in order to simplify the comparisons in engine operation between each fuel.

Table 3. Properties of Tested Fuels [12, 23].

Property	ULSD	Jet A	R-8	Tallow Biodiesel	Jatropa Biodiesel
Density (kg/m^3)	837.58	801.02	758.54	870.98	876.81
Kinematic Viscosity (cSt)	2.578	1.431	1.542	4.70	4.44
Dynamic Viscosity (cP)	2.159	1.146	1.170	4.094	3.893
Cetane Number	40.0	43.4	68.8	61.0	52.0
Energy Content (kJ/kg)	41530	42700	43101	39933	39809
Volumetric Energy Content (MJ/m^3)	34785	34204	32694	34781	34905

Engine operation and performance was monitored through a system created through LabVIEW, recording at a rate of 10 Hz for 120 seconds of engine operation. A second LabVIEW system was used in order to capture the in-cylinder pressure trace, recording 120 consecutive engine revolutions (amounting to 60 engine cycles) at a