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Mathematical correlations for variation in heat release rate of a diesel engine fuelled with n-octanol blends

n-Oktanol karışımlarıyla çalışan bir dizel motorun ısı yayılımı oranının değişimi için matematiksel korelasyonlar

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Abstract

The current literature reports a few papers regarding the prediction of heat release rate of a diesel engine fuelled with n-octanol blends using numerical methods. To address this gap, the main objective of the presented study is to derive correlations for estimating the variation in heat release rate of a diesel engine fuelled with diesel fuel and diesel fuel-biodiesel-n-octanol blends. For this purpose, three different ternary blends were prepared by varying the n-octanol concentration to 6% (OCT6), 8% (OCT8), and 10% (OCT10) by volume. The estimation of heat release rate was accomplished using the least-squares regression (sine, piecewise, and rational equations) and the function approximation (Padé approximation) methods. The ignition delay and peak heat release rate increased by 3.8462%, 5.9501% for OCT6; 7.6923%, 3.7125% for OCT8; and 8.9744%, 3.0755% for OCT10, respectively, compared to diesel fuel. The peak cylinder pressure of OCT6 and OCT8 was observed to be higher by 2.4378% and 1.3982%, respectively, whereas that of OCT10 was found to be lower by 1.9458%, compared to diesel fuel. Compared to the others, the suggested rational equation qualitatively and quantitatively achieved the best correlation with all experimental heat release rate data measured by both the author and some other authors.

Keywords: n-Octanol, Heat release rate, Sine equation, Padé approximation, Piecewise equation

Öz

Mevcut literatür, n-oktanol karışımları ile çalışan bir dizel motorun ısı yayılımı oranının sayısal yöntemlerle tahmin edilmesiyle ilgili birkaç makale sunmaktadır. Bu boşluğu gidermek için, sunulan çalışmanın temel amacı, dizel yakıtı ve dizel yakıtı-biyodizel-n-oktanol karışımları ile çalışan bir dizel motorun ısı yayılımı oranındaki değişimi tahmin etmek için korelasyonlar elde etmektir. Bu amaçla n-oktanol miktarı hacimsel olarak %6 (OCT6), %8 (OCT8) ve %10 (OCT10) oranlarında değiştirilerek üç farklı üçlü karışım hazırlanmıştır. Isı yayılımı oranının tahmini, en küçük kareler regresyonu (sinüs, parçalı ve rasyonel denklemler) ve fonksiyon yaklaşımı yöntemleri (Padé yaklaşımı) kullanılarak gerçekleştirilmiştir. Tutuşma gecikmesi ve en yüksek ısı yayılımı oranı, dizel yakıtına kıyasla sırasıyla, OCT6 için %3.8462, %5.9501; OCT8 için %7.6923, %3.7125; ve OCT10 için %8.9744, %3.0755 oranlarında artmıştır. Dizel yakıtına kıyasla, OCT6 ve OCT8'in en yüksek silindir basınçlarının %2.4378 ve %1.3982 oranlarında daha yüksek olduğu, OCT10'un ise %1.9458 oranında daha düşük olduğu görülmüştür. Diğer denklemler ile karşılaştırıldığında, önerilen rasyonel denklem, nitelik ve nicelik olarak hem yazar hem de diğer bazı yazarlar tarafından ölçülen tüm deneysel ısı yayılımı oranı verileriyle en iyi korelasyonu sağlamıştır.

Anahtar kelimeler: n-Oktanol, Isı yayılımı oranı, Sinüs denklemi, Padé yaklaşımı, Parçalı denklem

1 Introduction

The ever-growing energy demand worldwide, the rise in environmental concerns (global warming), and the volatility of petroleum prices have led to a growing interest in alternative fuels [1, 2]. Among the alternative fuels for diesel engines, biodiesel and higher alcohols have been focused on in this study. Biodiesel is a type of fuel composed of mono-alkyl esters of long-chain fatty acids. Biodiesel is produced by the transesterification of animal fats or vegetable oils. Biodiesel has been gaining attention for decades because of its many advantages over diesel fuel (being renewable, biodegradable, non-toxic, and having a higher flash point) [3, 4]. Higher alcohols have been used as an additive to diesel fuel and biodiesel [5]. Among higher alcohols, n-octanol is a next-generation biofuel produced from renewable lignocellulosic biomass [6]. It has a higher cetane number and heating value (39 and 37.53 MJ/kg) than methanol, ethanol, n-butanol, and n-pentanol. Because of its superior hydrophobic nature, n-octanol is likely to cause less corrosion in fuel lines than n-butanol, n-pentanol, and n-hexanol [7]. The higher flash point temperature (81°C) and lower vapor pressure of n-octanol make it safer for storage and transport than diesel fuel [8]. Unlike ethanol and methanol, which are hydrophilic and tend to phase separate when mixed with diesel fuel, n-octanol exhibits high miscibility in diesel fuel. This property offers an encouraging opportunity to replace diesel fuel with a higher proportion of biofuel than methanol and ethanol [9]. Compared to biodiesels, n-octanol generally exhibits superior cold flow

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characteristics, as evidenced by its pour point of -13.5°C [10]. The use of n-octanol generally results in very low soot emissions owing to its high oxygen concentration (12.41%) [8]. Owing to the superior fuel properties of n-octanol, it has been the subject of extensive research in recent years as follows: Sidharth and Kumar [11] prepared three ternary blends (80% diesel fuel-10% waste cooking oil biodiesel-10% n-octanol, 70% diesel fuel-20% waste cooking oil biodiesel-10% n-octanol, and 70% diesel fuel-10% waste cooking oil biodiesel-20% n-octanol, v/v) and two binary blends (90% diesel fuel-10% waste cooking oil biodiesel, and 90% diesel fuel-10% n-octanol, v/v). They investigated the effects of ternary and binary blends on the performance, emission and combustion characteristics of a single-cylinder diesel engine under different brake mean effective pressures. The blend of 80% diesel fuel-10% waste cooking oil biodiesel-10% n-octanol exhibited improved brake thermal efficiency and brake specific energy consumption, compared to diesel fuel. Ashok et al. [12] researched the impacts of n-octanol-biodiesel blends. Five different blends were prepared by varying the n-octanol concentration from 10% to 50% on a volumetric basis. These blends were tested and compared with pure diesel fuel at different engine loads (0%, 25%, 50%, and 100%) and 1500 rpm. According to the results, increasing the amount of n-octanol led to a longer ignition delay, resulting in a higher cylinder peak pressure. The use of n-octanol increased carbon monoxide and smoke emissions and decreased nitrogen oxide emissions. Sekar et al. [13] investigated the effects of O10NBD90 (10% n-octanol-90% neem biodiesel, v/v) and O20NBD80 (20% n-octanol-80% neem biodiesel, v/v) on the performance, emissions, and combustion of a single-cylinder diesel engine under different brake powers (1.1, 2.2, 3.3, 4.4 and 5.5 kW). Increasing the volume percentage of n-octanol resulted in a higher heat release rate and in-cylinder pressure during premixed combustion. The fuel consumption was reduced by 2.4% with higher n-octanol content. Sharbuddin et al. [14] prepared three ternary blends including diesel fuel (80% v/v), waste cooking oil biodiesel (15% v/v), and oxygenates (5% v/v). Di-n-butyl ether, n-octanol, and 2-ethyl-hexanol were used as the oxygenates. Response surface methodology-based optimization was used to minimize nitrogen oxide and smoke opacity emissions while maximizing engine performance. It was determined that the blend (80% diesel fuel-15% waste cooking oil biodiesel-5% n-octanol) injected at a compression ratio of 19:1 with an EGR rate of 10% provided the best performance and emission characteristics. Konjevic et al. [15] investigated the effects of diesel fuel-n-pentanol and diesel fuel-n-octanol blends on engine performance and exhaust emissions in a diesel engine under different engine speeds and indicated mean effective pressures. The highest increment in specific fuel consumption (10.9%) was determined with the use of a diesel fuel-n-pentanol blend (including 10% n-pentanol v/v) at a low load and medium engine speed. The highest increment in nitrogen oxide emissions (11%) was determined for the use of a diesel fuel-n-pentanol blend (including 30% n-pentanol) under high load and high engine speed. Li et al. [16] performed a numerical analysis to investigate the effects of n-octanol and di-n-butyl-ether mixtures on the combustion characteristics and formation of emissions in a diesel engine using the KIVA4-CHEMKIN code. Various n-octanol-di-n-butyl-ether mixtures were prepared by changing the di-n-butyl-ether content from 10% to 90% (with an interval of 10%). The diesel engine was then simulated with pure n-octanol, pure di-n-butyl-ether, and their blends at engine speeds of 1500 rpm and 2280 rpm. Blending more di-n-butyl-ether into n-octanol decreased the ignition delay and the pressure rise rate, increased the peak pressure, and prolonged the combustion duration. Blending di-n-butyl-ether into n-octanol decreased carbon monoxide but increased nitrogen oxide emissions. The optimum di-n-butyl-ether blending ratio was determined to be 50%, resulting in carbon monoxide reductions of 69.91% and 65.98% at 1500 and 2280 rpm.

Considering the other relevant studies in the existing literature [17-19] as well as the literature review mentioned above, the effects of n-octanol blends on the performance, emissions, and combustion characteristics have been frequently investigated in recent decades. However, although accurate knowledge of the change in the heat release rate is essential in internal combustion engine studies to understand the ignition and combustion characteristics of the used fuel, few studies have focused on predicting the heat release rate of diesel engines. To overcome this limitation, this study aims to derive an equation and use the function approximation method (Padé approximation) to estimate the change in the heat release rate of a diesel engine fuelled with diesel fuel and n-octanol blends. In other words, the importance of this study is that it can offer an alternative approach for predicting the heat release rate, considering some technical and economic difficulties in experimentally determining the heat release rate.

2 Material and methods

2.1 Test fuels

The test fuels consist of diesel fuel (DF), biodiesel (vegetable oil methyl ester) [20], and n-octanol. Table 1 and Appendix Table 1 show the properties of n-octanol [7, 21-23] and diesel fuel (DF). Considering the European Directives [24, 25], a binary blend is prepared by combining DF and biodiesel in a volumetric ratio of 80:20 at room temperature. n-Octanol, as an oxygenated fuel additive, is added to the DF-biodiesel binary blend at 6% (OCT6), 8% (OCT8), and 10% (OCT10) by volume to obtain ternary blends at room temperature.

Table 1. Some fuel properties of n-octanol

Properties	n-octanol
Chemical formula	$C_8H_{17}OH$
Molecular weight (g/mol)	130.23
Carbon content (wt.%)	73.68
Hydrogen content (wt.%)	13.91
Oxygen content (wt.%)	12.41
Cetane number	39
Boiling point (ºC)	195
Lower heating value (MJ/kg)	37.53
Latent heat of evaporation (kJ/kg)	538
Flash point (ºC)	81
Self-ignition temperature (ºC)	270
Density at 15ºC (kg/m^3)	827
Viscosity at 40ºC (mm^2/s)	5.8

A magnetic stirrer is used to obtain all blends for nearly 30 min. All blends are prepared just before conducting the experiments. No phase separation is detected in any of the blends at room temperature. Owing to the high cost of n-octanol (analytical grade) in Turkey and its low cetane number, volume ratios exceeding 10% are not studied.

2.2 Experimental setup and procedure

To conduct the experiments, a single-cylinder diesel engine (Hatz) in the Internal Combustion Engines Laboratory at Karadeniz Technical University is used. The main technical specifications of the diesel engine are listed in Appendix Table 2. Appendix Figure 1 shows the test bed which includes the engine, an electric dynamometer (DC), a fuel tank, and monitoring systems. No modifications are made on the engine or the fuel supply/injection system. To measure the engine torque (± 0.1 Nm) and engine speed (± 1 rpm), a force sensor and an optical encoder are fixed to the electric dynamometer. The data acquisition system, consisting of an engine cycle analyzer, a cylinder head pressure piezoelectric transducer (made by Kistler, sensitivity: ~36 pC/bar, measuring range: 0-300 bar, and natural frequency: >70 kHz), and an optical crank angle encoder (with a resolution of 1 crank angle (degree)), collects data (cylinder pressure, cylinder volume, etc.). Cylinder pressure data are taken for every 1 crank angle (degree). The engine is allowed to run for a while at full throttle before measurements are taken to achieve a steady operating condition. All experiments are carried out under steady-state conditions at 1200 rpm, and before running the engine with a new fuel, any remaining fuel from the previous experiment is consumed. All measurements are conducted 20 times to minimize uncertainties. The cylinder pressure data from 50 consecutive engine cycles are averaged. The cylinder head pressure piezoelectric transducer exhibits a linearity of ≤ ±0.4. These factors contribute to the reliability and accuracy of the cylinder pressure data and the results related to the combustion parameters. After measurements are taken for each fuel, the engine is operated with pure diesel fuel to remove any remaining blends from the fuel line. No difficulties are encountered during the engine tests for each fuel [26].

2.3 Calculation of heat release rate

The apparent net heat release rate is the difference between the apparent gross heat release rate and the heat transfer rate to the walls. It is calculated using the following equation:

$$\frac{dQ_n}{d\theta} = \frac{k}{k-1} \cdot P \cdot \frac{dV}{d\theta} + \frac{1}{k-1} \cdot V \cdot \frac{dP}{d\theta} \tag{1}$$

where $dQ_n/d\theta$ is the apparent net heat release rate (J/degree), k is the ratio of specific heats, P is the instantaneous cylinder pressure (Pa), V is the instantaneous cylinder volume (m^3), θ is the crank angle (degree), $dV/d\theta$ is the derivative of cylinder volume over crank angle (m^3/degree), and $dP/d\theta$ is the derivative of cylinder pressure over crank angle (Pa/degree) [27].

2.4 Padé Approximation

The Padé approximation is not an interpolation approach, but a rational approximation (i.e., the quotient of two polynomials) [28, 29]. The Padé approximation seeks to approximate a function (f(x)) by finding a rational function that matches the function values and its derivatives at a specific point (x_0) [30]. The desired rational function (the numerator of degree m and the denominator of degree n) takes the following form [29, 30]:

$$r(x) = \frac{p_m(x)}{q_n(x)} = \frac{a_m \cdot x^m + \cdots + a_0}{b_n \cdot x^n + \cdots + b_0} \tag{2}$$

Assuming that the values of $f(x_0), \acute{f}(x_0), \ldots, f^{(k)}(x_0)$ are known for $k = m + n$, and x_0 is equal to zero for simplicity [30]. Let t(x) denote the Taylor polynomial of a given function (f(x)). The function (t(x)) can be written as:

$$t(x) = c_k \cdot x^k + \cdots + c_2 \cdot x^2 + c_1 \cdot x + c_0 \tag{3}$$

where c_k equals $f^{(k)}(0)/k!$ in terms of derivatives of f(x). We want r(x) to exactly match t(x) −to have the same value at x = 0 and the same derivatives of all orders up to, and including $k = m + n$ [30]. Therefore, the fundamental approach is to utilize the following equivalence of the expressions [30]:

$$t(x) = r(x) = \frac{p_m(x)}{q_n(x)} \tag{4}$$

and

$$q_n(x) \cdot t(x) = p_m(x) \tag{5}$$

Based on Eq. (5), the following relationship is established:

$$(b_n \cdot x^n + \cdots + b_0) \cdot (c_k \cdot x^k + \cdots + c_1 \cdot x + c_0) = a_m \cdot x^m + \cdots + a_0 \tag{6}$$

By considering the requirement that $q_n(0) \cdot t(0) = p_m(0)$, Eq. (6) gives us

$$b_0 \cdot c_0 = a_0 \tag{7}$$

The value of b_0 can be taken as unity [29]. With this convention, an equation is obtained to determine a_0 [30]. Similarly, with the use of derivatives of Eq. (6) at x = 0, all unknown coefficients can be determined for the desired rational function $(r(x))$ using the Naive Gauss Elimination method.

3 Results and discussions

Figures 1-5 show the variation in cylinder pressure and heat release rate (HRR) of DF, OCT6, OCT8, and OCT10 as a function of crank angle (degree). In the case of using OCT6, OCT8, and OCT10, the ignition delay is higher by

3.8462%, 7.6923%, and 8.9744% owing to the lower cetane number of n-octanol, compared to DF. The peak cylinder pressures of OCT6 (83.7289 bar) and OCT8 (82.8791 bar) are found to be 2.4378% and 1.3982% higher, respectively, whereas that of OCT10 (80.1459 bar) is found to be 1.9458% lower, compared to DF (81.7363 bar). The peak HRR increases by 5.9501%, 3.7125%, and 3.0755% for the use of OCT6 (28.9586 J/degree), OCT8 (28.3470 J/degree), and OCT10 (28.1729 J/degree), respectively, compared with DF (27.3323 J/degree). The increase in the peak cylinder pressure and peak HRR is linked to the oxygen concentration of n-octanol (enhances the combustion reaction) and the extended ignition delay (causes more fuel accumulation in the combustion chamber). However, the decrease in the peak cylinder pressure associated with OCT10 is due to the lower heating value of n-octanol. In other words, the lower heating value becomes more dominant over the change in cylinder pressure for the highest n-octanol content (10%). As shown in Figures 2-5, the experimental HRR data are correlated by the sine equation (Eq. (8)) and the piecewise equation (Eq. (9)) composed of quadratic and exponential terms using MATLAB and NCSS software [31, 32]:

$$y = a_1 \cdot sin(b_1 \cdot x + c_1) + a_2 \cdot sin(b_2 \cdot x + c_2) + a_3 \cdot sin(b_3 \cdot x + c_3) + a_4 \cdot sin(b_4 \cdot x + c_4) + a_5 \cdot sin(b_5 \cdot x + c_5) \quad (8)$$

$$y = \begin{cases} a_1 + b_1 \cdot x + c_1 \cdot x^2 + (x - d_1) \cdot sign(x - d_1) \cdot (e \cdot (x + d_1) + f), \; x < 0 \\ (a_2 + b_2 \cdot x) \cdot exp(-c_2 \cdot x) + d_2, \; x \geq 0 \end{cases} \quad (9)$$

where x is the crank angle (radian for Eq. (8), degree for Eq. (9)); y is the predicted HRR value; and $a_1, \dots, a_5, b_1, \dots, b_5, c_1, \dots, c_5, d_1, d_2, e$, and f are the regression constants. It can be noted that because HRR shows different characteristics in the negative and positive crank angle (degree) regions, the piecewise equation (Eq. (9)) is used to correlate the HRR data. In addition to the sine (Eq. (8)) and the piecewise (Eq. (9)) equations, their Padé approximations are also constructed to correlate the HRR data by using Mathematica software. Different numerator and denominator degrees are tried for their Padé approximations, and finally, rational functions with a numerator of degree 2 and a denominator of degree 6 are used in the Padé approximations of the sine (Eq. (8)) and the piecewise (Eq. (9)) equations for all HRR data. As shown in Figures 1-5, all fuels reveal almost similar characteristics of cylinder pressure and HRR variations depending on crank angle. It should be also noted that the predicted values of DF and OCT8 by Padé approximation of the sine equation slightly deviate from the related experimental data (i.e. the negative HRR values). Table 2 lists the regression constants of the sine (Eq. (8)) and piecewise (Eq. (9)) equations for the author's data. Table 3 lists the regression results of Eq. (8), Eq. (9), and their Padé approximations (r^2, relative errors (between measured peak HRR data and calculated peak HRR value), and mean absolute errors (between measured HRR data and calculated HRR values) for the author's data. The average (over the fuel type) r^2 values are calculated to be 0.9983 (the sine equation (Eq. (8)), 0.9852 (Padé approximation of the sine equation), 0.9976 (the piecewise equation (Eq. (9)), and 0.9974 (Padé approximation of the piecewise equation). The average (over the fuel type) relative errors are calculated as 0.9881%, 0.9882%, 0.7388%, and 0.7388% for the sine equation (Eq. (8)), Padé approximation of the sine equation, the piecewise equation (Eq. (9)), and Padé approximation of the piecewise equation, respectively. The average (over the fuel type) mean absolute errors are calculated as 0.3228, 0.8060, 0.2988, and 0.3180 for the sine equation (Eq. (8)), Padé approximation of the sine equation, the piecewise equation (Eq. (9)), and Padé approximation of the piecewise equation, respectively. Considering Figures 2-5, the sine equation (Eq. (8)), the piecewise equation (Eq. (9)), and Padé approximation of the piecewise equation (Eq. (9)) qualitatively agree very well with the experimental HRR data measured by the author. Moreover, the sine equation (Eq. (8)), the Padé approximation of the piecewise equation (Eq. (9)), and the piecewise equation (Eq. (9)) quantitatively outperform in terms of higher average r^2 (0.9983), lower average relative error (0.7388%), and lower average mean absolute error (0.2988) values, respectively. The predictive abilities of the sine equation (Eq. (8)), the piecewise equation (Eq. (9)), and their Padé approximations are evaluated against different experimental HRR data of n-octanol blends measured by Yeşilyurt and Çakmak [8] as well as Çakmak et al. [33]. Yeşilyurt and Çakmak [8] investigated the engine performance and combustion characteristics of a single-cylinder diesel engine fuelled with pure diesel and diesel-n-octanol blends (including 5%, 10%, 15%, and 20% n-octanol by volume) at a fixed engine speed of 1500 rpm and four different engine loads. The variation in HRR was investigated under the full load condition by Yeşilyurt and Çakmak [8]. Çakmak et al. [33] performed the exergy, exergoeconomic, and environmental analysis for a diesel engine fuelled with pure diesel and diesel-biodiesel-n-octanol blends at a constant engine speed (1500 rpm) and different engine loads. n-Octanol was added to the diesel-biodiesel blend at fractions of 5%, 10%, 15%, and 20% by volume [33]. They investigated the variation in heat release rate at the full engine load. Appendix Tables 3 and 4 list the regression constants of the sine (Eq. (8)) and the piecewise (Eq. (9)) equations for the experimental data measured by Yeşilyurt and Çakmak [8], and Çakmak et al. [33]. Appendix Tables 5 and 6 list the regression results of Eq. (8), Eq. (9), and their Padé approximations (r^2, relative errors (between measured peak HRR data and calculated peak HRR value), and mean absolute errors (between measured HRR and calculated HRR)) for the experimental data measured by Yeşilyurt and Çakmak [8] as well as Çakmak et al. [33]. As shown in Appendix Table 5 for the data measured by Yeşilyurt and Çakmak [8], the average (over the fuel type) r^2, relative error and mean absolute error values are calculated as 0.9357, 22.8316%, 1.2847; 0.3341, 22.7955%, 5.2281; 0.9512, 6.7514%, 0.9666; and 0.9503, 6.7515%, 0.9903 for the sine equation (Eq. (8)), Padé approximation of the sine equation, the piecewise equation (Eq. (9)), and

Padé approximation of the piecewise equation (Eq. (9)). As shown in Appendix Table 6 for the data measured by Çakmak et al. [33], the average (over the fuel type) r^2, relative error and mean absolute error values are calculated as 0.9522, 16.4322%, 1.0958; 0.0937, 16.4303%, 5.6557; 0.9793, 4.4275%, 0.7905; and 0.9792, 4.4274%, 0.7977 for the sine equation (Eq. (8)), Padé approximation of the sine equation, the piecewise equation (Eq. (9)), and Padé approximation of the piecewise equation (Eq. (9)). It is not necessary to investigate their qualitative predictive capabilities, because they have relatively high errors and low r^2 values (poor quantitative predictive capability). Considering Appendix Tables 5 and 6, since the sine equation (Eq. (8)), Padé approximation of the sine equation, the piecewise equation (Eq. (9)), and Padé approximation of the piecewise equation yield relatively high errors and low r^2 values (poor prediction accuracy), other piecewise equations (Eqs. (10)-(12)) are tested and fitted to the experimental HRR data measured by the author, Yeşilyurt and Çakmak [8] as well as Çakmak et al. [33]. Considering the regression results (given in Table 3, Appendix Table 5, and Appendix Table 6), to determine the best correlation for the data measured by both the author and other authors [8, 33], these piecewise equations (Eqs. (10)-(12)) are structured to include both sine, polynomial, and exponential terms (given in Eq. (8) and Eq. (9)).

$$y = \begin{cases} a_1 + b_1 \cdot x + c_1 \cdot x^2 + (x - d_1) \\ \cdot sign(x - d_1) \cdot (e_1 \cdot (x + d_1) + f_1),\ x < 0 \\ a_2 + b_2 \cdot x + c_2 \cdot (x - d_2) \cdot sign(x - d_2) \\ +e_2 \cdot (x - f_2) \cdot sign(x - f_2),\ x \geq 0 \end{cases} \quad (10)$$

$$y = \begin{cases} a_1 \cdot sin(b_1 \cdot x + c_1) + a_2 \cdot sin(b_2 \cdot x + c_2) \\ +a_3 \cdot sin(b_3 \cdot x + c_3) \\ +a_4 \cdot sin(b_4 \cdot x + c_4) \\ +a_5 \cdot sin(b_5 \cdot x + c_5), x < 0 \\ a_6 + b_6 \cdot x + c_6 \cdot (x - d) \cdot sign(x - d) \\ +e \cdot (x - f) \cdot sign(x - f), x \geq 0 \end{cases} \quad (11)$$

$$y = \begin{cases} a_1 \cdot sin(b_1 \cdot x + c_1) + a_2 \cdot sin(b_2 \cdot x + c_2) \\ +a_3 \cdot sin(b_3 \cdot x + c_3) \\ +a_4 \cdot sin(b_4 \cdot x + c_4) \\ +a_5 \cdot sin(b_5 \cdot x + c_5), x < 0 \\ (a_6 + b_6 \cdot x) \cdot exp(-c_6 \cdot x) \\ +d,\ x \geq 0 \end{cases} \quad (12)$$

Tables 4-6 and Appendix Tables 7-12 list the regression constants of Eqs. (10-12) for the experimental HRR data measured by the author, Yeşilyurt and Çakmak [8], and Çakmak et al. [33]. Table 7, Appendix Table 13, and Appendix Table 14 present the regression results of Eqs. (10)-(12) (r^2, relative errors (between measured peak HRR and calculated peak HRR), and mean absolute errors (between measured HRR data and calculated HRR values)) for the experimental HRR data measured by the author, Yeşilyurt and Çakmak [8], and Çakmak et al. [33]. In Table 7 for the author's data, the average values of r^2, relative error, and mean absolute error are listed as follows: 0.9916, 8.1590%, 0.4007 for Eq. (10); 0.9899, 8.1590%, 0.5276 for Eq. (11); and 0.9959, 0.7388%, 0.4257 for Eq. (12). In Appendix Table 13 for the data measured by Yeşilyurt and Çakmak [8], the average values of r^2, relative error, and mean absolute error are listed as follows: 0.9583, 6.7514%, 0.6970 for Eq. (10); 0.9900, 5.5069%, 0.4586 for Eq. (11); and 0.9829, 5.5069%, 0.7281 for Eq. (12). In Appendix Table 14 for the data measured by Çakmak et al. [33], the average values of r^2, relative error, and mean absolute error are listed as follows: 0.9853, 4.4275%, 0.5782 for Eq. (10); 0.9887, 2.7285%, 0.4792 for Eq. (11); and 0.9828, 2.7285%, 0.6916 for Eq. (12). According to these results, among Eqs. (10-12), a correlation with quantitatively sufficient accuracy (relative error of less than 5%, and r^2 of closer to 1.00) is not obtained for all experimental HRR data measured by the author, Yeşilyurt and Çakmak [8], and Çakmak et al. [33]. Finally, the experimental HRR data measured by the author, Yeşilyurt and Çakmak [8], and Çakmak et al. [33] are corrected by the following rational equation (x: crank angle (degree)) [31] (Eq. (13)):

$$y = \frac{(a_1 \cdot x^3 + a_2 \cdot x^2 + a_3 \cdot x + a_4)}{(x^4 + b_1 \cdot x^3 + b_2 \cdot x^2 + b_3 \cdot x + b_4)} \quad (13)$$

Table 8, Appendix Table 15, and Appendix Table 16 list the regression constants of Eq. (13) for the experimental HRR data measured by the author, Yeşilyurt and Çakmak [8], and Çakmak et al. [33]. The r^2, relative error, and mean absolute error (between measured HRR and calculated HRR) values from Eq. (13) for the HRR data measured by the author, Yeşilyurt and Çakmak [8], and Çakmak et al. [33] are listed in Table 9, Appendix Table 17, and Appendix Table 18. The average values of r^2, relative error, and mean absolute error arising from Eq. (13) are listed as follows: 0.9978, 0.6158%, 0.3178 for the author's data; 0.9939, 1.2185%, 0.4626 for Yeşilyurt and Çakmak's data [8]; and 0.9884, 1.5837%, 0.5991 for Çakmak et al.'s data [33]. Eq. (13) exhibits quantitatively more agreement with the experimental HRR data measured by both the author and other authors [8, 33], compared to other equations (Eq. (8)-(12)). As for qualitative predictive accuracy, Figure 6 and Appendix Figures 2-14 portray the comparison between the calculated HRR values using Eq. (13) and the experimental HRR data measured by the author, Yeşilyurt and Çakmak [8], and Çakmak et al. [33]. According to these figures, the calculated HRR values from Eq. (13) are also qualitatively well consistent with the experimental HRR data measured by the author, Yeşilyurt and Çakmak, and Çakmak et al. This result is likely due to the fact that the characteristic of Eq. (13) is similar to the variation characteristic of the HRR.

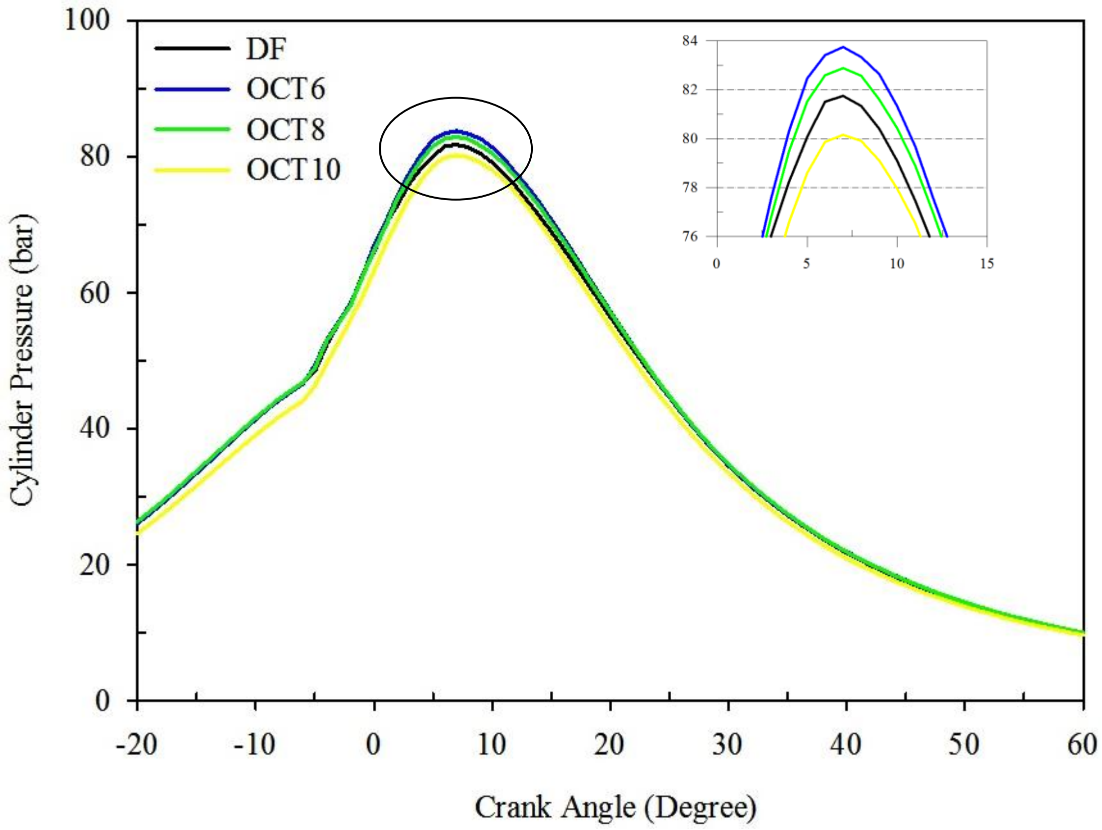

Figure 1. Variation of cylinder pressure depending on crank angle for all fuels

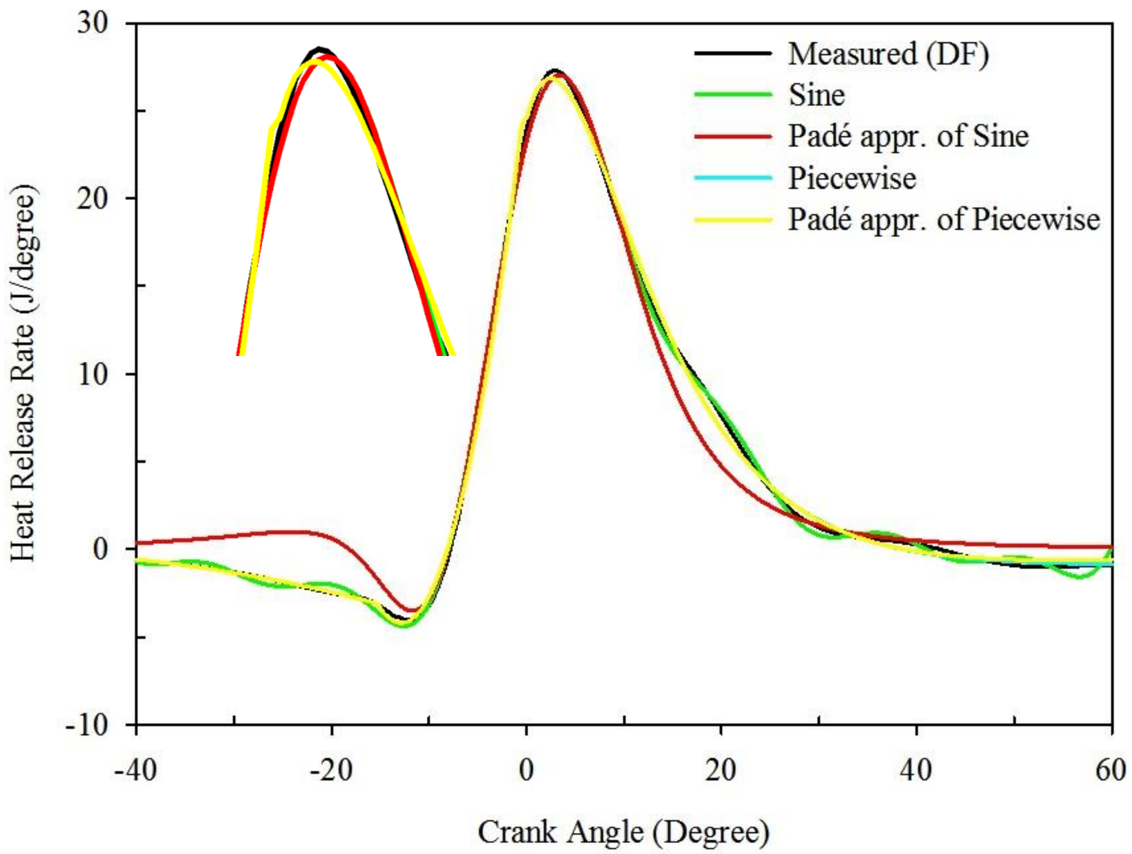

Figure 2. Comparison of measured HRR data of DF and calculated values from the sine (Eq. (8)) and the piecewise (Eq. (9)) equations and their Padé approximations

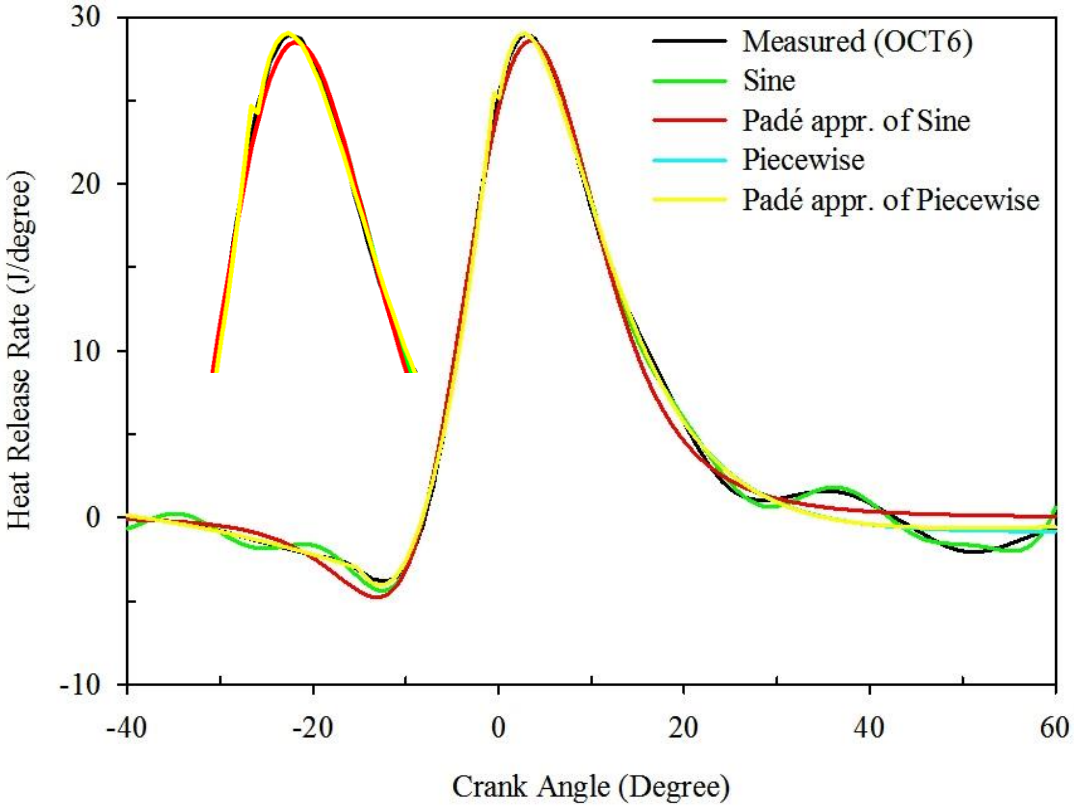

Figure 3. Comparison of measured HRR data of OCT6 and calculated values from the sine (Eq. (8)) and the piecewise (Eq. (9)) equations and their Padé approximations

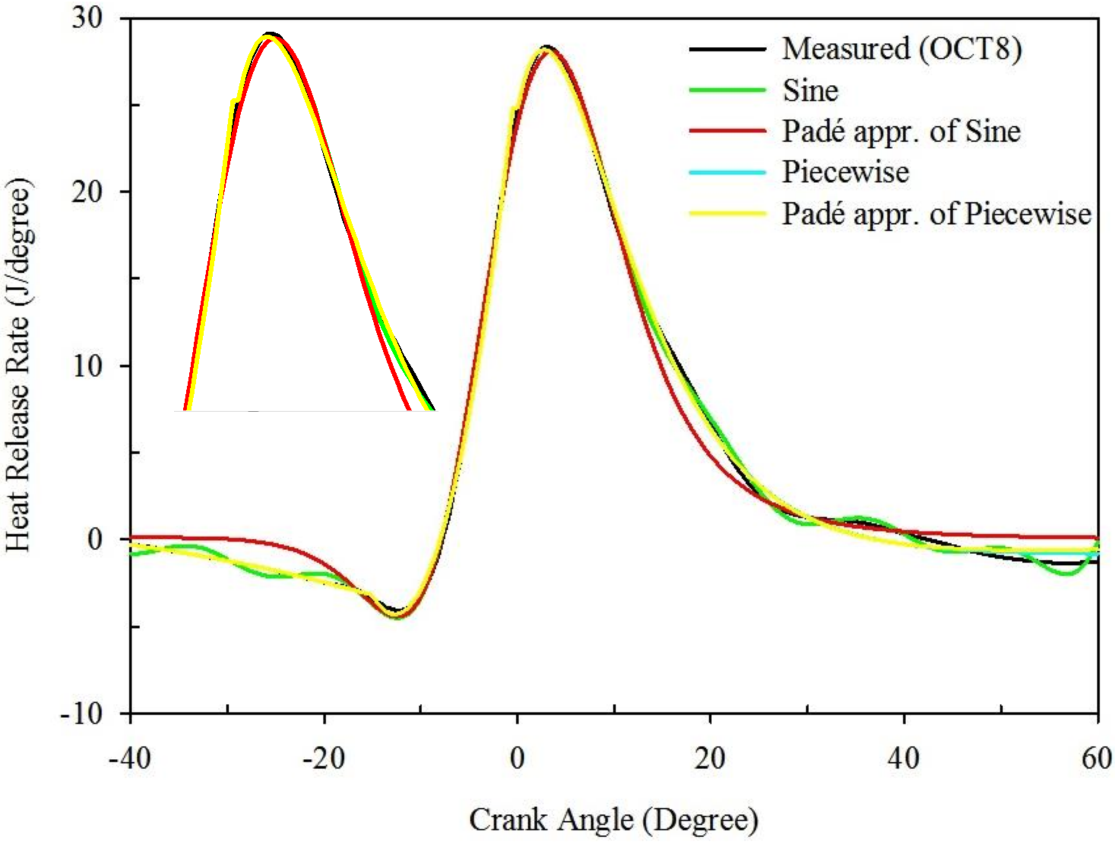

Figure 4. Comparison of measured HRR data of OCT8 and calculated values from the sine (Eq. (8)) and the piecewise (Eq. (9)) equations and their Padé approximations

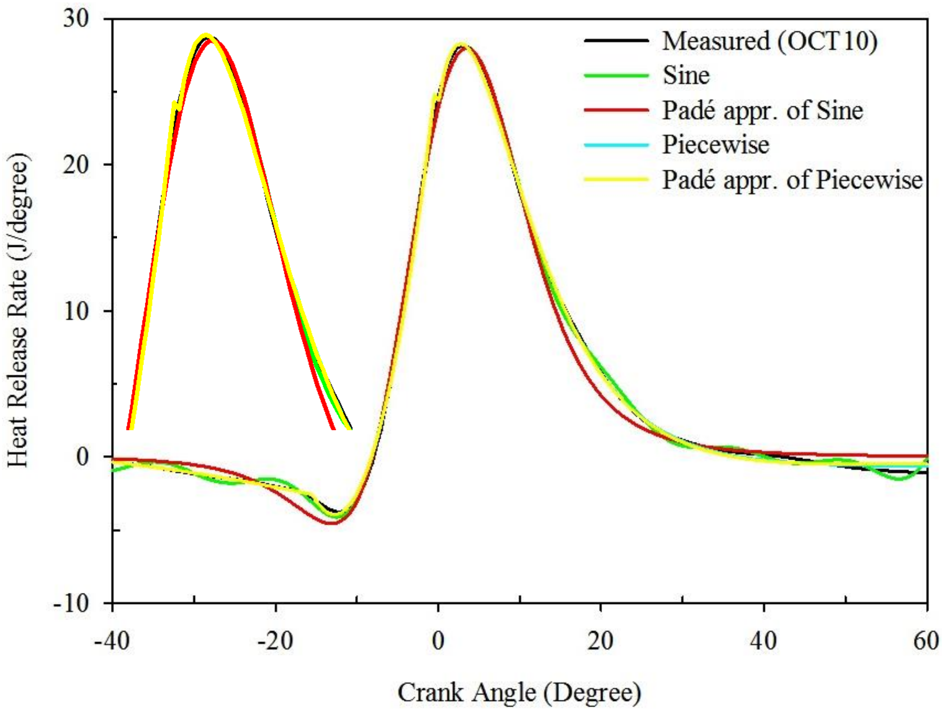

Figure 5. Comparison of measured HRR data of OCT10 and calculated values from the sine (Eq. (8)) and the piecewise (Eq. (9)) equations and their Padé approximations

Table 2. Regression constants of the sine (Eq. (8)) and the piecewise (Eq. (9)) equations for the author's data

Fuel	Equation	Regression constants						
		a_1	a_2	a_3	a_4	a_5	b_1	b_2
DF	Sine (Eq. (8))	11.67	37.93	5.978	2.897	1.568	5.213	0.03855
OCT6		11.92	960.9	7.077	2.707	1.561	5.211	0.001213
OCT8		10.98	7.885	6.379	2.879	1.534	5.499	1.246
OCT10		9.032	10.41	5.63	2.849	1.287	6.369	2.143
DF	Piecewise (Eq. (9))	10.45762	25.47713	-	-	-	2.29846	5.78886
OCT6		10.86057	25.84369	-	-	-	2.38726	7.73898
OCT8		10.67781	25.58212	-	-	-	2.38618	6.93811
OCT10		11.26198	24.87711	-	-	-	2.36364	7.58063

Table 2. (Continued)

Fuel	Equation	Regression constants						
		b_3	b_4	b_5	c_1	c_2	c_3	c_4
DF	Sine (Eq. (8))	10.39	15.44	20.52	0.8966	0.1672	0.7394	1.031
OCT6		10.47	15.56	20.32	0.9511	0.00672	0.7682	0.8721
OCT8		10.53	15.61	20.68	0.8905	1.245	0.7464	0.9233
OCT10		10.98	15.92	20.77	0.8569	1.23	0.7839	0.8928
DF	Piecewise (Eq. (9))	-	-	-	0.09231	0.14523	-	-
OCT6		-	-	-	0.09727	0.16550	-	-
OCT8		-	-	-	0.09726	0.15638	-	-
OCT10		-	-	-	0.09495	0.16650	-	-

Table 2. (Continued)

Fuel	Equation	Regression constants				
		c_5	d_1	d_2	e	f
DF	Sine (Eq. (8))	1.048	-	-	-	-
OCT6		1.134	-	-	-	-
OCT8		1.084	-	-	-	-
OCT10		1.068	-	-	-	-
DF	Piecewise (Eq. (9))	-	-15.33455	-0.92116	0.09400	2.49308
OCT6		-	-15.00712	-0.86288	0.09934	2.62792
OCT8		-	-15.07171	-0.85542	0.09884	2.58905
OCT10		-	-15.46649	-0.64289	0.09603	2.51447

Table 3. The r^2, relative error, and mean absolute error values coming from Eq. (8) and Eq. (9), and their Padé approximations for the author's data

Fuel	Equation	r^2	Relative error (%)	Mean absolute error
DF	Sine (Eq. (8))	0.9984	1.0772	0.2984
OCT6		0.9979	1.2612	0.3609
OCT8		0.9982	0.9343	0.3346
OCT10		0.9985	0.6797	0.2973
Average		0.9983	0.9881	0.3228
DF	Padé approximation of Sine (Eq. (8))	0.9699	1.0773	1.1710
OCT6		0.9898	1.2612	0.7088
OCT8		0.9883	0.9346	0.7614
OCT10		0.9929	0.6797	0.5828
Average		0.9852	0.9882	0.8060
DF	Piecewise (Eq. (9))	0.9982	1.7809	0.2651
OCT6		0.9950	0.2501	0.4401
OCT8		0.9981	0.5354	0.2962
OCT10		0.9990	0.3888	0.1938
Average		0.9976	0.7388	0.2988
DF	Padé approximation of Piecewise (Eq. (9))	0.9981	1.7807	0.2839
OCT6		0.9946	0.2502	0.4621
OCT8		0.9978	0.5353	0.3153
OCT10		0.9989	0.3888	0.2106
Average		0.9974	0.7388	0.3180

Table 4. Regression constants of the piecewise (Eq. (10)) equation for the author's data

Fuel	Equation	Regression constants					
		a_1	a_2	b_1	b_2	c_1	c_2
DF	Piecewise (Eq. (10))	10.45762	16.40062	2.29846	-0.60450	0.09231	0.19770
OCT6		10.86057	9.85106	2.38726	-0.55465	0.09727	0.57381
OCT8		10.67781	15.03272	2.38618	-0.60274	0.09726	0.53061
OCT10		11.26198	16.97065	2.36364	-0.67669	0.09495	0.39183

Table 4. (Continued)

Fuel	Equation	Regression constants					
		d_1	d_2	e_1	e_2	f_1	f_2
DF	Piecewise (Eq. (10))	-15.33455	18.61222	0.09400	0.32554	2.49308	28.49428
OCT6		-15.00712	22.24746	0.09934	0.16712	2.62792	53.35073
OCT8		-15.07171	23.63617	0.09884	0.05732	2.58905	51.65241
OCT10		-15.46649	19.94766	0.09603	0.21111	2.51447	28.61170

Table 5. Regression constants of the piecewise (Eq. (11)) equation for the author's data

Fuel	Equation	Regression constants					
		a_1	a_2	a_3	a_4	a_5	a_6
DF	Piecewise (Eq. (11))	38.22	40.15	12.47	9.189	-0.06939	16.40062
OCT6		26.71	1526	1503	1.212	-0.1556	9.85106
OCT8		20.28	371.8	354.8	1.185	-0.05414	15.03272
OCT10		18.77	525.7	509.4	0.7225	-0.1826	16.97065

Table 5. (Continued)

Fuel	Equation	Regression constants					
		b_1	b_2	b_3	b_4	b_5	b_6
DF	Piecewise (Eq. (11))	11.55	12.39	17	18.65	67.72	-0.60450
OCT6		13.23	16.52	16.57	25.5	47.97	-0.55465
OCT8		12.35	16.14	16.32	23.39	69.13	-0.60274
OCT10		12.56	16.43	16.54	26.55	48.15	-0.67669

Table 5. (Continued)

Fuel	Equation	Regression constants					
		c_1	c_2	c_3	c_4	c_5	c_6
DF	Piecewise (Eq. (11))	3.755	1.118	1.432	-6.87	5.113	0.19770
OCT6		3.92	2.292	-0.8264	-6.462	-1.422	0.57381
OCT8		3.608	2.221	-0.8382	-7.11	5.342	0.53061
OCT10		3.674	2.303	-0.7859	-6.048	-1.405	0.39183

Table 5. (Continued)

Fuel	Equation	Regression constants		
		d	e	f
DF	Piecewise (Eq. (11))	18.61222	0.32554	28.49428
OCT6		22.24746	0.16712	53.35073
OCT8		23.63617	0.05732	51.65241
OCT10		19.94766	0.21111	28.61170

Table 6. Regression constants of the piecewise (Eq. (12)) equation for the author's data

Fuel	Equation	Regression constants					
		a_1	a_2	a_3	a_4	a_5	a_6
DF	Piecewise (Eq. (12))	38.22	40.15	12.47	9.189	-0.06939	25.47713
OCT6		26.71	1526	1503	1.212	-0.1556	25.84369
OCT8		20.28	371.8	354.8	1.185	-0.05414	25.58212
OCT10		18.77	525.7	509.4	0.7225	-0.1826	24.87711

Table 6. (Continued)

Fuel	Equation	Regression constants					
		b_1	b_2	b_3	b_4	b_5	b_6
DF	Piecewise (Eq. (12))	11.55	12.39	17	18.65	67.72	5.78886
OCT6		13.23	16.52	16.57	25.5	47.97	7.73898
OCT8		12.35	16.14	16.32	23.39	69.13	6.93811
OCT10		12.56	16.43	16.54	26.55	48.15	7.58063

Table 6. (Continued)

Fuel	Equation	Regression constants				
		c_1	c_2	c_3	c_4	c_5
DF	Piecewise (Eq. (12))	3.755	1.118	1.432	-6.87	5.113
OCT6		3.92	2.292	-0.8264	-6.462	-1.422
OCT8		3.608	2.221	-0.8382	-7.11	5.342
OCT10		3.674	2.303	-0.7859	-6.048	-1.405

Table 6. (Continued)

Fuel	Equation	Regression constants	
		c_6	d
DF	Piecewise (Eq. (12))	0.14523	-0.92116
OCT6		0.16550	-0.86288
OCT8		0.15638	-0.85542
OCT10		0.16650	-0.64289

Table 7. The r^2, relative error, and mean absolute error values coming from Eqs. (10)-(12) for the author's data

Fuel	Equation	r^2	Relative error (%)	Mean absolute error
DF	Piecewise (Eq. (10))	0.9931	7.2153	0.3598
OCT6		0.9903	8.6836	0.5023
OCT8		0.9918	7.5255	0.3747
OCT10		0.9912	9.2117	0.3661
Average		0.9916	8.1590	0.4007
DF	Piecewise (Eq. (11))	0.9930	7.2153	0.4093
OCT6		0.9879	8.6836	0.6771
OCT8		0.9919	7.5255	0.3937
OCT10		0.9867	9.2117	0.6302
Average		0.9899	8.1590	0.5276
DF	Piecewise (Eq. (12))	0.9981	1.7809	0.3147
OCT6		0.9927	0.2501	0.6149
OCT8		0.9981	0.5354	0.3152
OCT10		0.9945	0.3888	0.4579
Average		0.9959	0.7388	0.4257

Table 8. Regression constants of Eq. (13) for the author's data

Fuel	Equation	Regression constants					
		a_1	a_2	a_3	a_4	b_1	b_2
DF	Eq. (13)	-70.64	-1399	1.318e5	1.09e6	-14.51	646.6
OCT6		-77.76	-694.3	1.057e5	8.519e5	-3.003	433.8
OCT8		-73.85	-1048	1.202e5	9.665e5	-8.067	536.2
OCT10		-51.73	-785	8.645e4	7.162e5	-6.25	381.4

Table 8. (Continued)

Fuel	Equation	Regression constants	
		b_3	b_4
DF	Eq. (13)	1456	4.472e4
OCT6		965.8	3.339e4
OCT8		1094	3.87e4
OCT10		785	2.879e4

Table 9. The r^2, relative error, and mean absolute error values coming from Eq. (13) for the author's data

Fuel	Equation	r^2	Relative error (%)	Mean absolute error
DF	Eq. (13)	0.9984	1.2667	0.2822
OCT6		0.9955	0.2562	0.4403
OCT8		0.9983	0.5027	0.3195
OCT10		0.9990	0.4377	0.2292
Average		0.9978	0.6158	0.3178

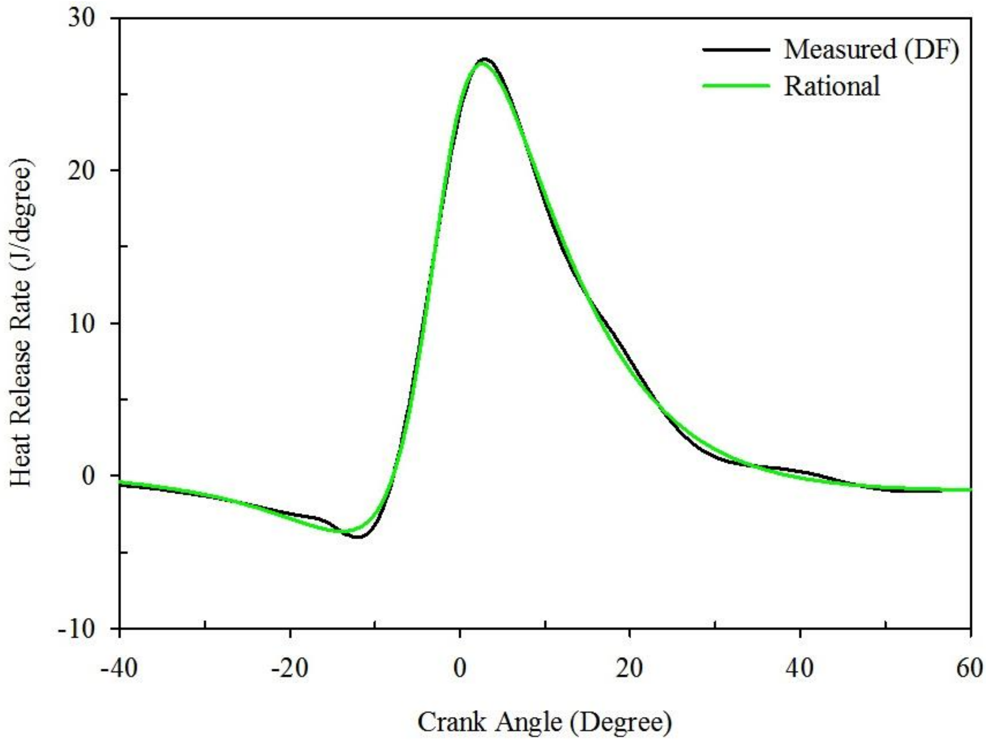

Figure 6. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of DF measured by the author

Table 10 summarizes the regression results of the investigated equations for all the experimental datasets. In Table 10, the "well" term indicates that the corresponding equation gives both an average relative error of less than 5% and an average r^2 of closer to 1.00 for the corresponding data set (i.e. well prediction accuracy), while the "poor" term indicates the opposite (i.e. poor prediction accuracy).

Table 10. Summary of regression results

Equation	Measured HRR data		
	The author	Yeşilyurt and Çakmak [8]	Çakmak et al. [33]
Eq. (8)	Well	Poor	Poor
Eq. (9)	Well	Poor	Well
Eq. (10)	Poor	Poor	Well
Eq. (11)	Poor	Poor	Well
Eq. (12)	Well	Poor	Well
Eq. (13)	Well	Well	Well

4 Conclusions

In recent years, n-octanol has emerged as a promising biofuel option, exhibiting considerable potential as an alternative to diesel fuel owing to its favourable fuel properties. Therefore, experimental studies have been performed to examine the effects of n-octanol blends on the performance, exhaust emissions, and combustion characteristics of diesel engines. On the other hand, there are a limited number of studies on the use of the function approximation methods for predicting combustion parameters. To eliminate this gap in the existing literature, this study focuses on the use of regression equations and their Padé approximations to predict the HRR of a single-cylinder diesel engine fuelled with DF and n-octanol blends (OCT6, OCT8, and OCT10). The predictive capabilities of suggested regression equations and their Padé approximations are also tested against the literature data measured by different authors. The main conclusions are as follows:

Compared with DF, the ignition delay and peak heat release rate show an increase of 3.8462% and 5.9501% for OCT6, 7.6923% and 3.7125% for OCT8, and 8.9744% and 3.0755% for OCT10, respectively.

Compared to DF, the peak cylinder pressure of OCT6 and OCT8 is observed to be higher by 2.4378% and 1.3982%, while that of OCT10 is found to be lower by 1.9458%.

The sine equation (Eq. (8)), the piecewise equation (Eq. (9)), and the Padé approximation of the piecewise equation (Eq. (9)) demonstrate superior quantitative performance in terms of higher average r^2 (0.9983, 0.9976, 0.9974), lower average relative error (0.9881%, 0.7388%, 0.7388%), and lower average mean absolute error values (0.3228, 0.2988, 0.3180), respectively, for the author's HRR data.

The sine equation (Eq. (8)), Padé approximation of the sine equation, the piecewise equation (Eq. (9)), and Padé approximation of the piecewise equation (Eq. (9)) yield relatively high average relative errors (22.8316%, 22.7955%, 6.7514%, 6.7515%; and 16.4322%, 16.4303%, 4.4275%, 4.4274%) and low average r^2 (0.9357, 0.3341, 0.9512, 0.9503; and 0.9522, 0.0937, 0.9793, 0.9792) values for the prediction of the HRR data measured by Yeşilyurt and Çakmak [8], and Çakmak et al. [33].

None of the other piecewise equations (Eqs. (10-12)) show a correlation with quantitatively sufficient accuracy for all experimental HRR data obtained by the author, Yeşilyurt and Çakmak [8], and Çakmak et al. [33]. Eq. (10), Eq. (11), and Eq. (12) exhibit relatively low average r^2 (0.9916, 0.9899, 0.9959 for the author's data; 0.9583, 0.9900, 0.9829 for Yeşilyurt and Çakmak's data; 0.9853, 0.9887, 0.9828 for Çakmak et al.'s data) and high average relative error (8.1590%, 8.1590%, 0.7388% for the author's data; 6.7514%, 5.5069%, 5.5069% for Yeşilyurt and Çakmak's data; 4.4275%, 2.7285%, 2.7285% for Çakmak et al.'s data) values when used for predicting HRR data.

Eq. (13) qualitatively and quantitatively exhibits better curve fitting with all experimental HRR data measured by the author and different authors compared to other equations.

This study can contribute to the literature by suggesting Eq. (13) as a useful tool to predict the heat release rate of a diesel engine fuelled with diesel fuel and n-octanol blends for internal combustion engine studies. In other words, given the technical and economic difficulties involved in determining the heat release rate, Eq. (13) appears to be one of the most favorable choices, particularly for numerical internal combustion engine studies.

For deriving general correlations depending on fuel properties, engine speed, engine load, injection timing, compression ratio, etc., more cylinder pressure data can be measured. Then, multiple regression models with independent variables can be used. Moreover, some machine learning methods can be used to generalize the regression constants. In addition, other function approximation methods can be investigated for predicting HRR.

As a future study, machine learning methods can be chosen for classification or prediction problems related to engine studies.

Conflict of interest

The author declares that there is no conflict of interest.

Similarity rate (iThenticate): 18%

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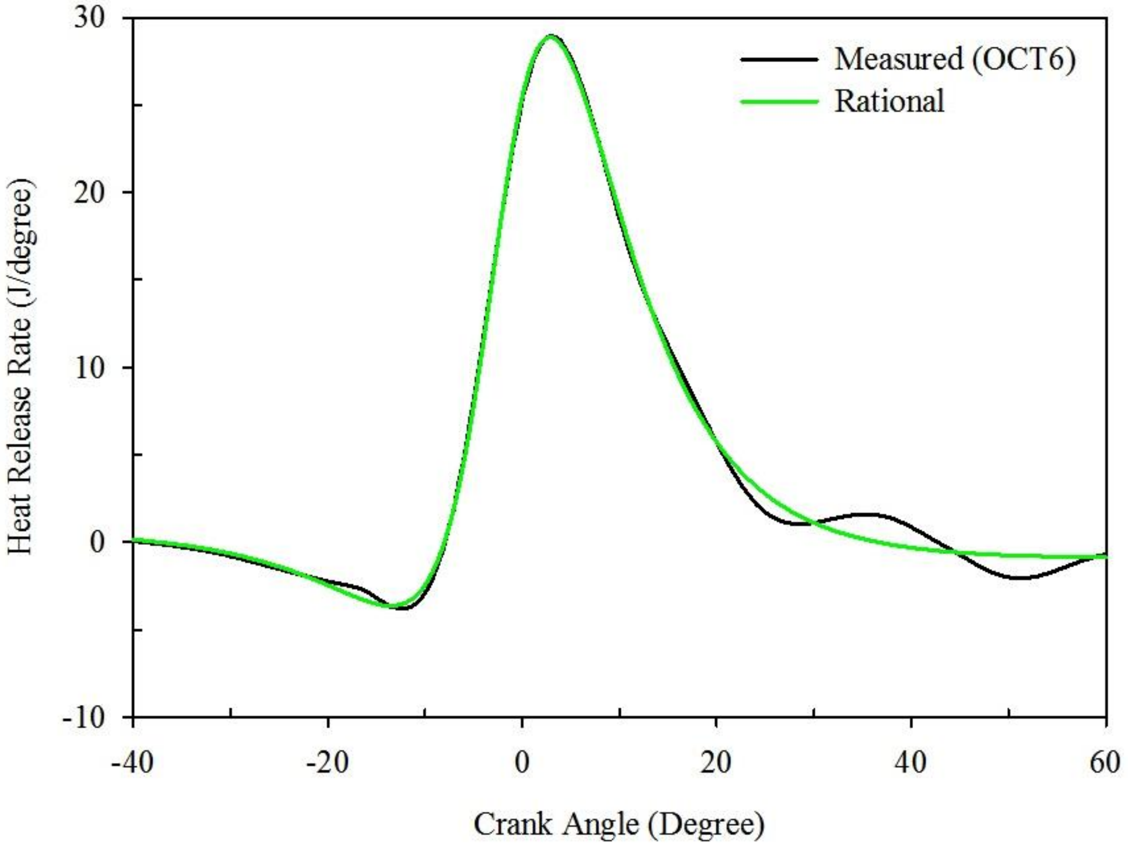
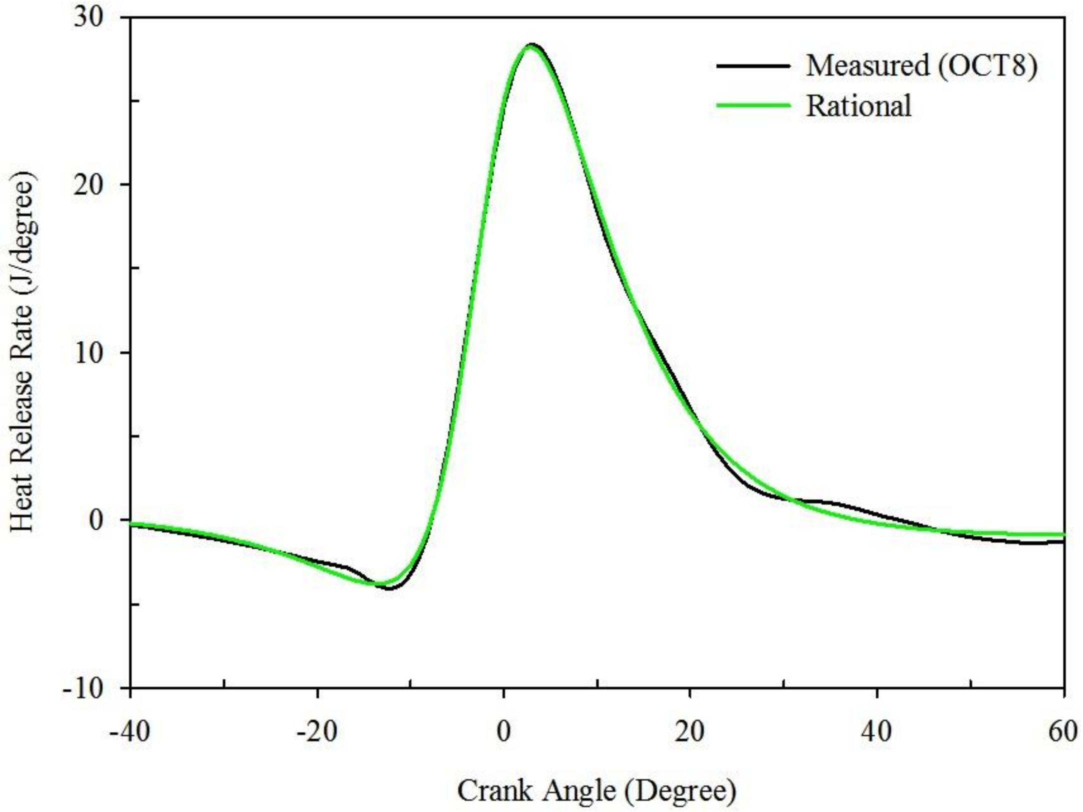
Appendix

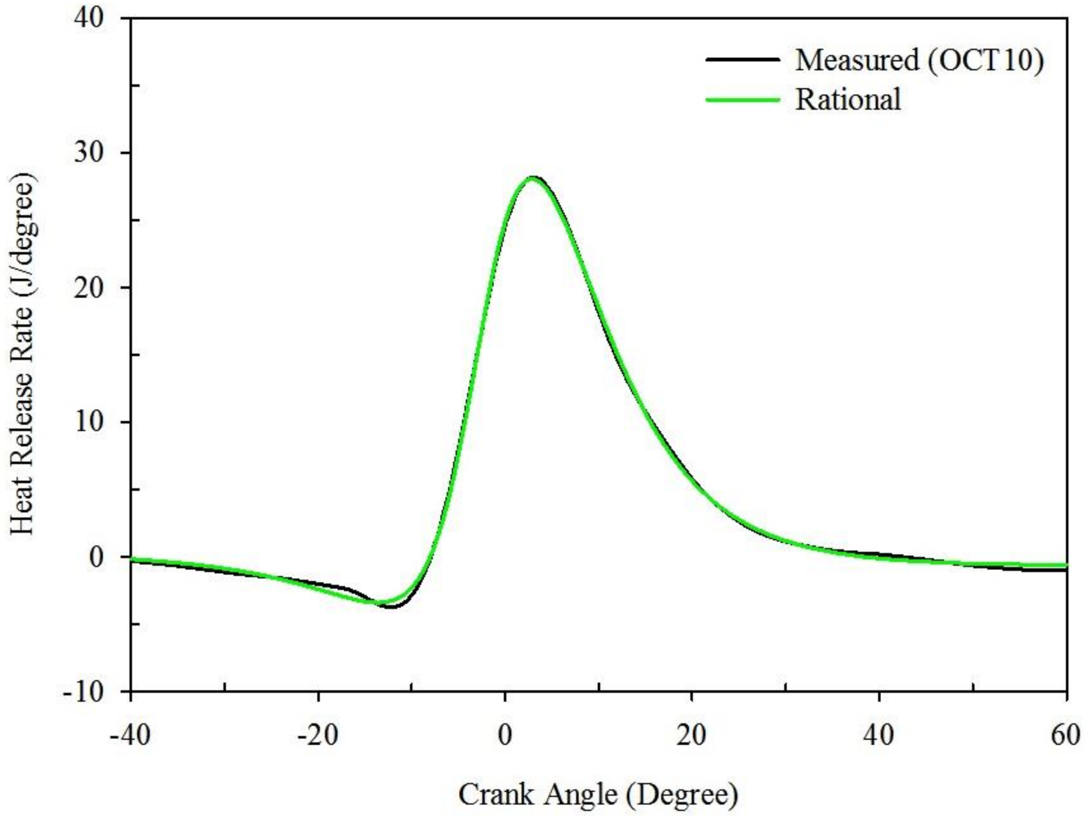
Appendix Figure 1. Schematic figure of the experimental setup



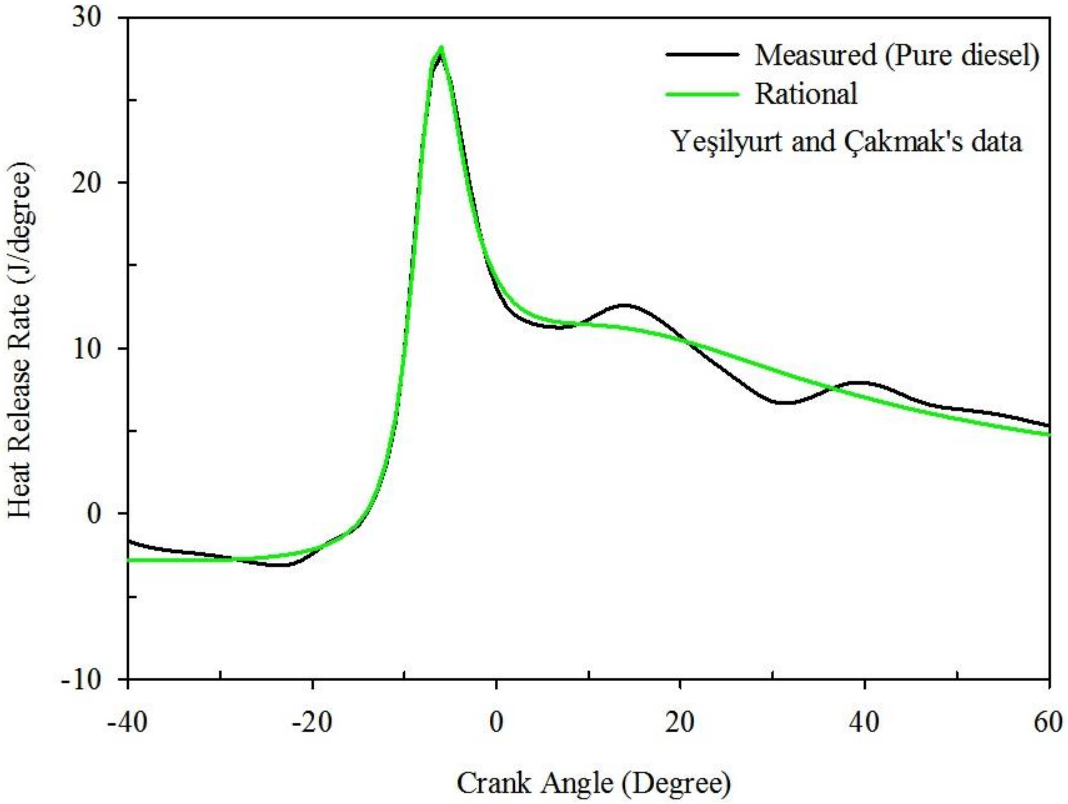
Appendix Figure 2. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of OCT6 measured by the author



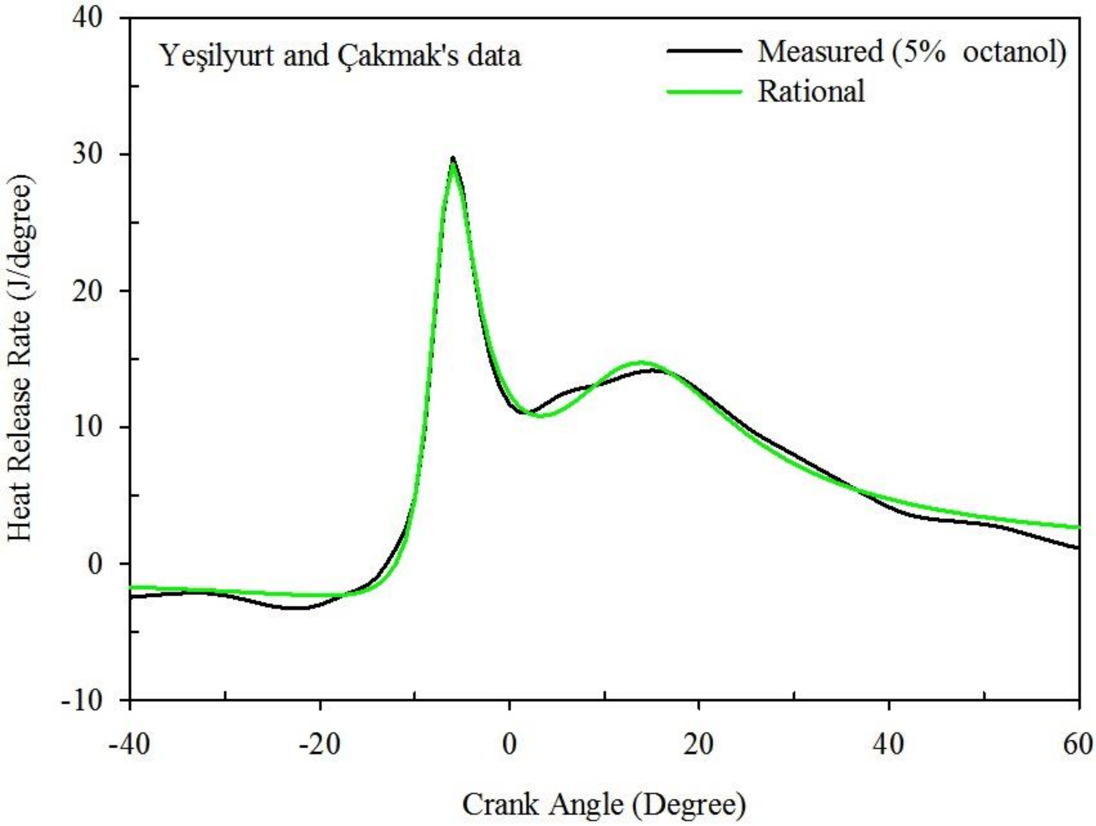
Appendix Figure 3. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of OCT8 measured by the author



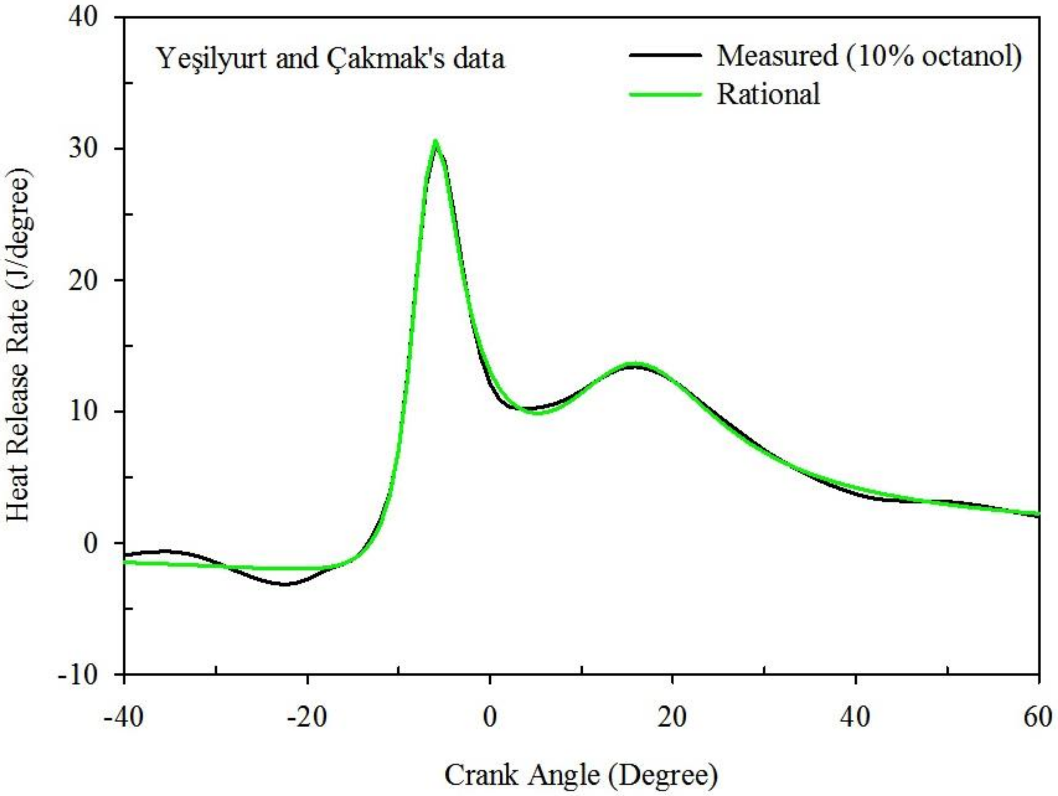
Appendix Figure 4. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of OCT10 measured by the author



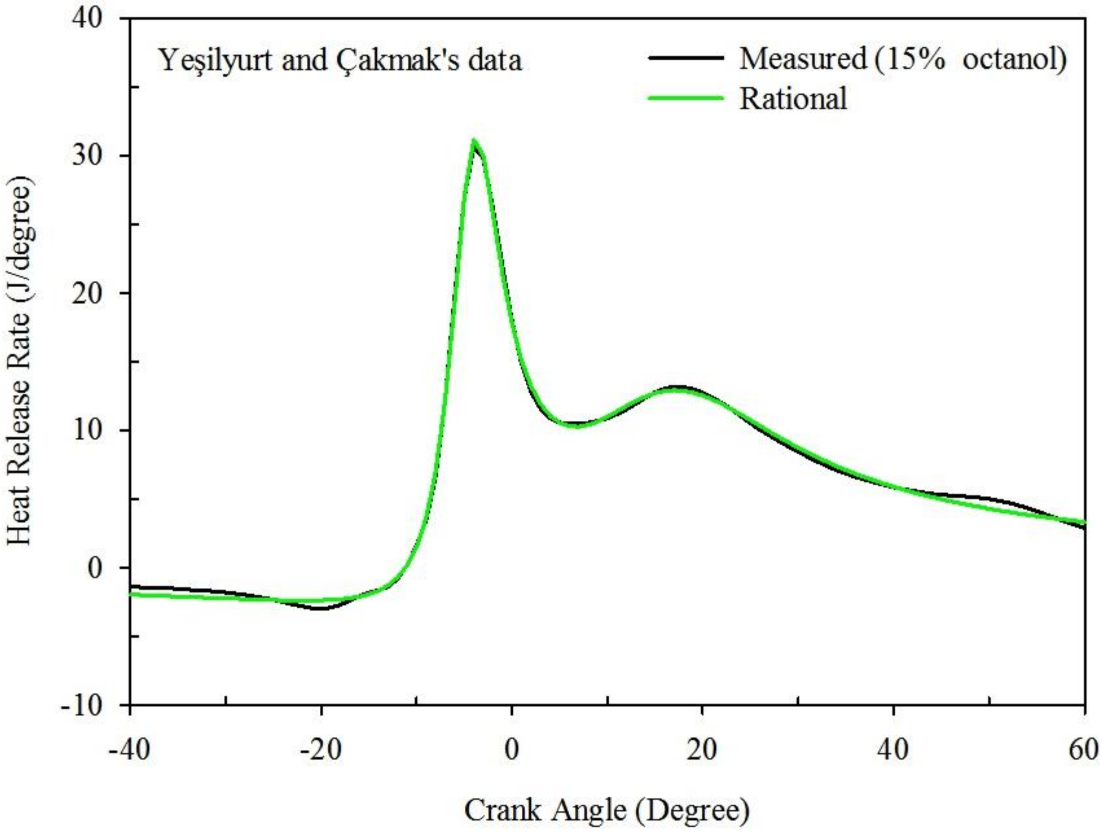
Appendix Figure 5. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of pure diesel measured by Yeşilyurt and Çakmak [8]



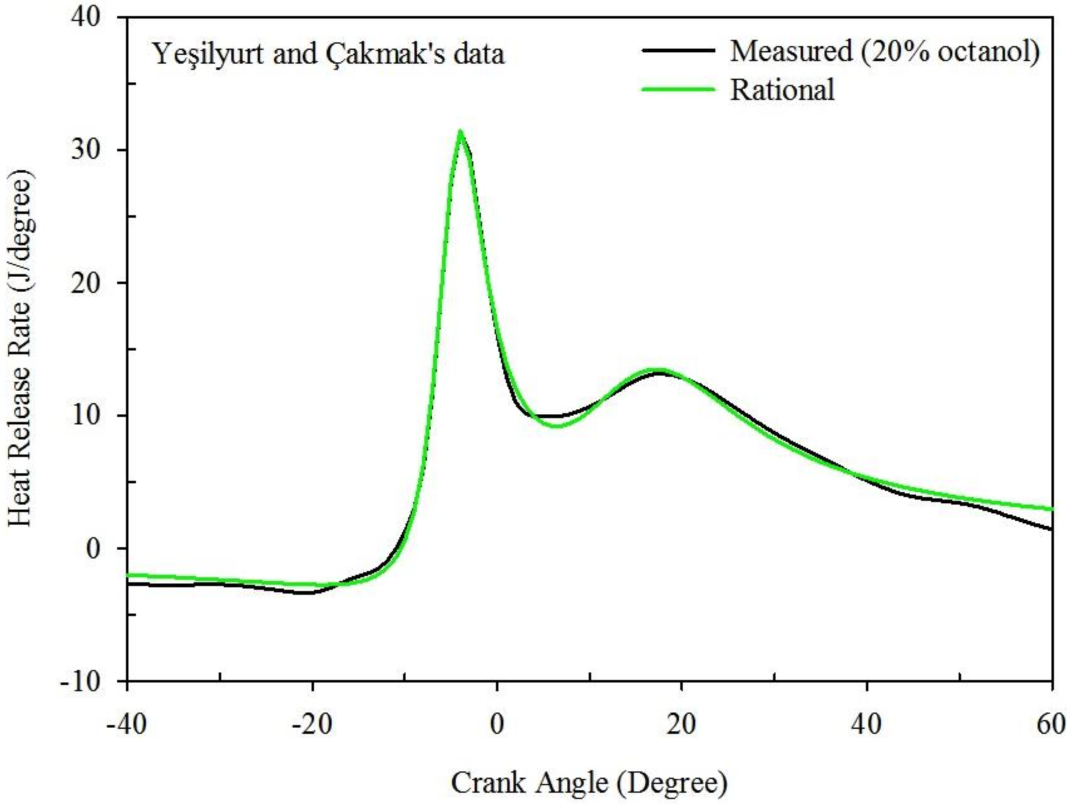
Appendix Figure 6. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of the blend (including 5% octanol) measured by Yeşilyurt and Çakmak [8]



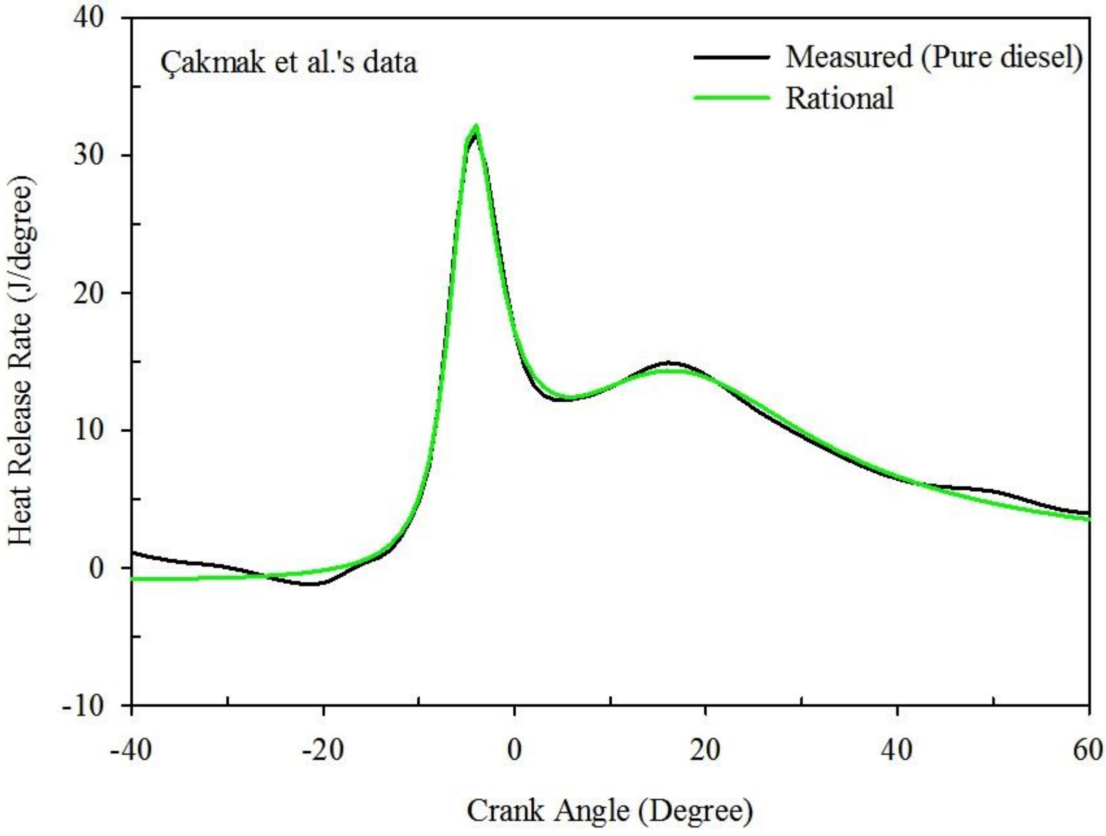
Appendix Figure 7. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of the blend (including 10% octanol) measured by Yeşilyurt and Çakmak [8]



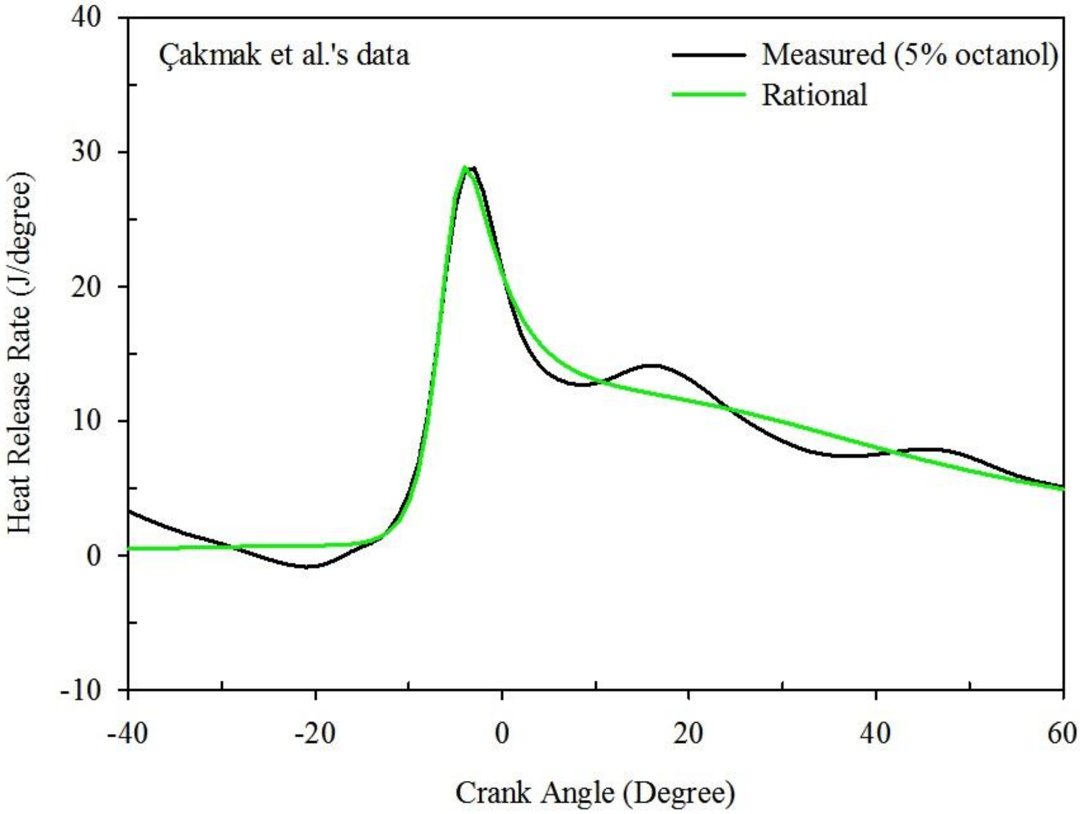
Appendix Figure 8. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of the blend (including 15% octanol) measured by Yeşilyurt and Çakmak [8]



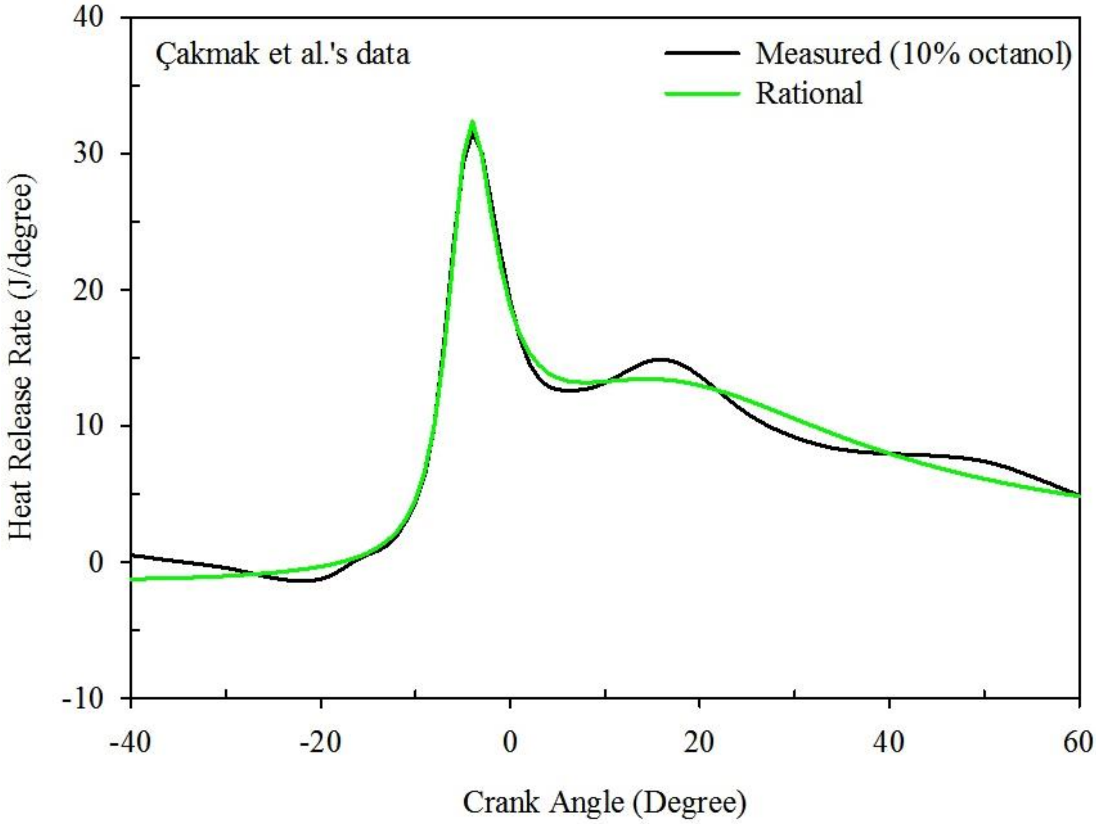
Appendix Figure 9. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of the blend (including 20% octanol) measured by Yeşilyurt and Çakmak [8]



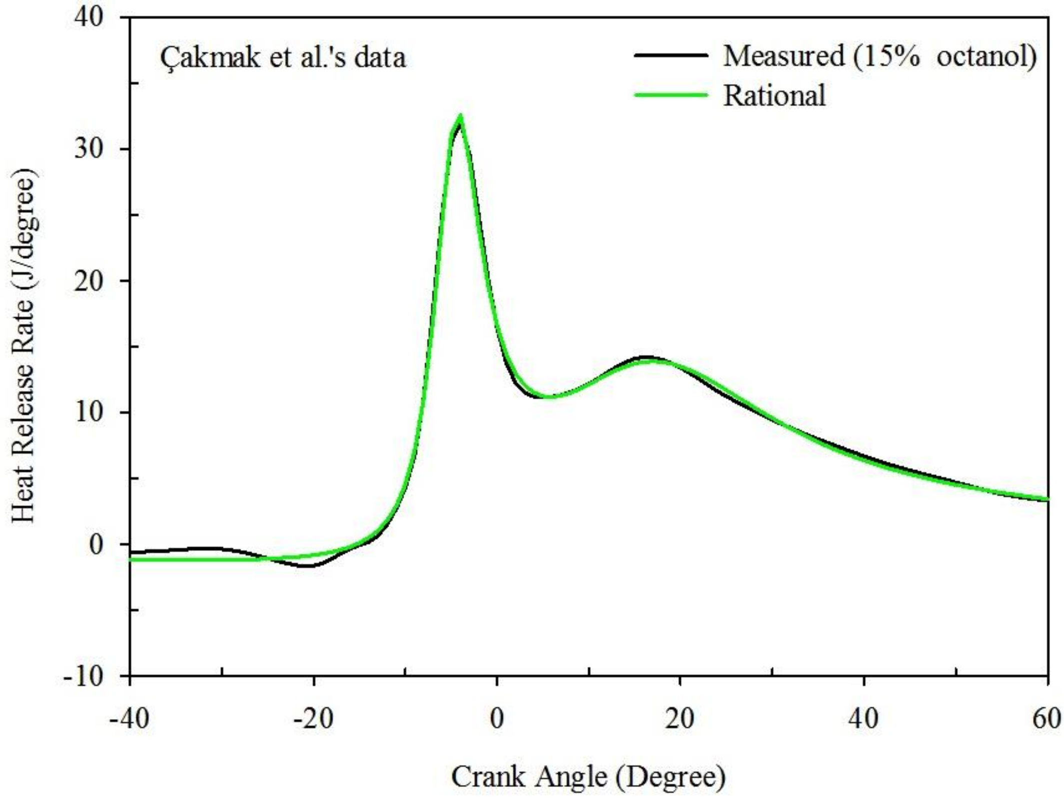
Appendix Figure 10. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of pure diesel measured by Çakmak et al. [33]



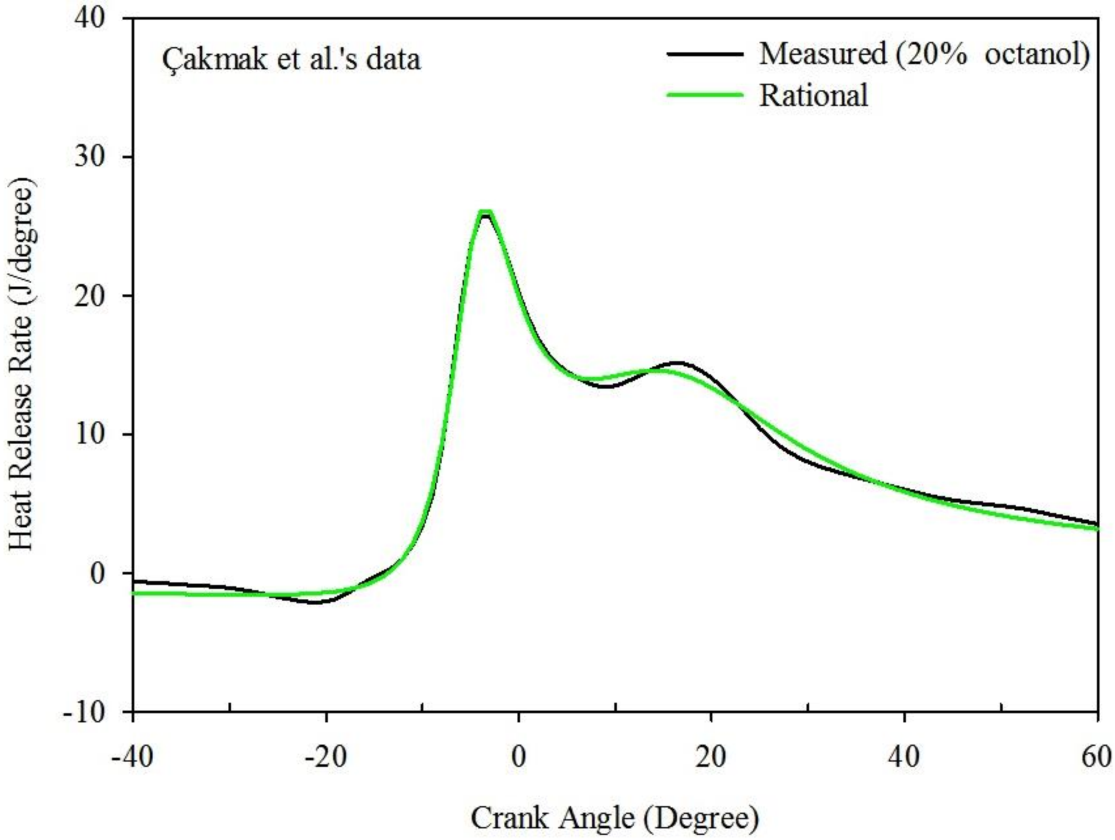
Appendix Figure 11. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of the blend (including 5% octanol) measured by Çakmak et al. [33]



Appendix Figure 12. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of the blend (including 10% octanol) measured by Çakmak et al. [33]



Appendix Figure 13. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of the blend (including 15% octanol) measured by Çakmak et al. [33]



Appendix Figure 14. Comparison of the predicted values (from Eq. (13)) with the experimental HRR data of the blend (including 20% octanol) measured by Çakmak et al. [33]

Appendix Table 1. The main fuel properties of DF

Property*		Test method	Limit		Value
			Min.	Max.	
Density at 15℃ (kg/m^3)		TS EN ISO 12185	820	845	834.8
Kinematic viscosity at 40℃ (mm^2/s)		TS EN ISO 3104	2	4.5	2.714
Flash point temperature (℃)		TS EN ISO 2719	>55	-	58.5
Higher heating value (MJ/kg)		DIN 51900-2	-	-	45.225
Total contaminat. (mg/kg)		TS EN 12662	-	24	16.5
Cold filter plugging point temperature (℃)		TS EN 116	-	+5 (Sum.) -15 (Win.)	-12
Copper strip corrosion at 3 h and 50℃		TS 2741 EN ISO 2160	1		1A
Lubrication property (µm)		TS EN ISO 12156-1	-	460	397
Sulfur (mg/kg)		TS EN ISO 20846	-	10	6.8
Distillation	250℃ (% v/v)	TS EN ISO 3405	-	<65	38.2
	350℃ (% v/v)		85	-	93.8
	95% (v/v)		-	360℃	356.1
Cetane index		TS EN ISO 4264	46	-	51.7
Cetane number**		EN ISO 5165 EN 15195	51	-	51

*: All properties except cetane number were measured at Prof. Dr. Saadettin GUNER Fuel Application and Research Center.
**: Cetane number is given by the supplier of DF used in this study.

Appendix Table 2. Technical specification of the test engine

Type of engine	Direct-injection and naturally aspirated
Valve	2 (One inlet and one exhaust)
Nozzle hole number/diameter	5/0.162 mm
Nozzle type	Standard
Injector opening pressure	220 bar
Injection pump type	Mechanical
Cooling system	Air
Bore x stroke (mm)	88 x 76
Connecting rod length (mm)	124
Engine capacity (cm^3)	462
Compression ratio	20.5:1
Start of fuel injection	13 crank angle (degree) before the top dead center

Appendix Table 3. Regression constants of the sine (Eq. (8)) and the piecewise (Eq. (9)) equations for Yeşilyurt and Çakmak's data [8]

Octanol Content	Equation	Regression constants						
		a_1	a_2	a_3	a_4	a_5	b_1	b_2
0 (Pure diesel)	Sine (Eq. (8))	4.94	13.17	3.614	2.048	3.243	7.453	2.176
5		3.515	13.94	3.789	2.955	-2.186	7.901	2.443
10		3.721	13.38	4.682	3.409	2.395	7.791	2.38
15		4.193	13.63	4.567	3.524	2.301	7.989	2.35
20		3.594	13.54	4.557	3.524	2.378	8.103	2.463
0 (Pure diesel)	Piecewise (Eq. (9))	8.22380	6.77598	-	-	-	-3.23415	0.75714
5		3.80474	11.42232	-	-	-	-4.62354	1.83147
10		5.90853	10.02813	-	-	-	-4.46131	1.55554
15		14.28259	19.42027	-	-	-	2.00227	0.59948
20		14.57193	22.04874	-	-	-	1.99629	1.02745

Appendix Table 3. (Continued)

Octanol Content	Equation	Regression constants						
		b_3	b_4	b_5	c_1	c_2	c_3	c_4
0 (Pure diesel)	Sine (Eq. (8))	12.06	22.02	16.85	1.620	1.089	2.825	-2.599
5		12.03	17.12	21.99	1.238	1.067	2.802	3.241
10		12.06	17.03	21.99	1.412	1.133	2.841	3.204
15		12.44	17.67	22.50	1.284	1.026	2.421	2.533
20		12.43	17.71	22.54	1.322	1.000	2.459	2.593
0 (Pure diesel)	Piecewise (Eq. (9))	-	-	-	-0.33508	0.07427	-	-
5		-	-	-	-0.47497	0.06283	-	-
10		-	-	-	-0.46152	0.06240	-	-
15		-	-	-	0.05609	0.02968	-	-
20		-	-	-	0.05407	0.03233	-	-

Appendix Table 3. (Continued)

Octanol Content	Equation	Regression constants				
		c_5	d_1	d_2	e	f
0 (Pure diesel)	Sine (Eq. (8))	3.236	-	-	-	-
5		6.733	-	-	-	-
10		3.538	-	-	-	-
15		2.841	-	-	-	-
20		2.908	-	-	-	-
0 (Pure diesel)	Piecewise (Eq. (9))	-	-11.37961	5.11708	-0.35157	-4.17335
5		-	-10.32028	-1.94341	-0.48798	-5.35529
10		-	-10.55624	-1.12643	-0.47895	-5.37384
15		-	-21.28344	-6.56398	0.06078	2.36784
20		-	-21.51955	-11.27791	0.05772	2.25004

Appendix Table 4. Regression constants of the sine (Eq. (8)) and the piecewise (Eq. (9)) equations for Çakmak et al.'s data [33]

Octanol Content	Equation	Regression constants						
		a_1	a_2	a_3	a_4	a_5	b_1	b_2
0 (Pure diesel)	Sine (Eq. (8))	4.042	15.1	3.328	4.389	-2.294	7.954	2.2
5		5.062	14.68	4.027	3.096	1.943	7.86	2.085
10		4.721	15.08	4.07	3.386	2.23	7.821	2.141
15		3.897	14.6	4.422	-2.422	3.563	8.022	2.245
20		14.94	3.555	4.68	2.901	1.522	2.287	12.07
0 (Pure diesel)	Piecewise (Eq. (9))	11.74727	14.24844	-	-	-	-3.55641	1.01905
5		15.77979	15.37784	-	-	-	-1.50551	0.00025
10		13.08163	13.47703	-	-	-	-3.75826	0.51029
15		10.38882	17.89887	-	-	-	-3.80176	0.96558
20		13.76048	16.92187	-	-	-	-1.40068	0.76323

Appendix Table 4. (Continued)

Octanol Content	Equation	Regression constants						
		b_3	b_4	b_5	c_1	c_2	c_3	c_4
0 (Pure diesel)	Sine (Eq. (8))	17.43	12.15	22.23	1.259	1.112	9.026	-3.688
5		12.19	17.38	22.17	1.211	1.132	2.454	2.458
10		12.34	17.54	22.45	1.309	1.087	2.52	2.638
15		12.26	22.36	17.41	1.366	1.093	2.565	-0.1094
20		7.776	17.37	22.2	1.073	2.404	1.062	2.454
0 (Pure diesel)	Piecewise (Eq. (9))	-	-	-	-0.48930	0.04633	-	-
5		-	-	-	-0.31175	0.02324	-	-
10		-	-	-	-0.56737	0.04064	-	-
15		-	-	-	-0.51000	0.03658	-	-
20		-	-	-	-0.28745	0.04968	-	-

Appendix Table 4. (Continued)

Octanol Content	Equation	Regression constants				
		c_5	d_1	d_2	e	f
0 (Pure diesel)	Sine (Eq. (8))	6.181	-	-	-	-
5		2.783	-	-	-	-
10		2.875	-	-	-	-
15		2.781	-	-	-	-
20		2.676	-	-	-	-
0 (Pure diesel)	Piecewise (Eq. (9))	-	-9.11591	-1.26027	-0.50455	-4.35598
5		-	-9.16442	1.76318	-0.32927	-2.34533
10		-	-8.41445	1.60137	-0.58481	-4.69576
15		-	-9.14452	-5.90583	-0.52145	-4.43124
20		-	-9.22525	-0.00061	-0.30054	-2.10746

Appendix Table 5. The r^2, relative error, and mean absolute error values coming from Eq. (8) and Eq. (9), and their Padé approximations for Yeşilyurt and Çakmak's data [8]

Octanol Content	Equation	r^2	Relative error (%)	Mean absolute error
0 (Pure diesel)	Sine (Eq. (8))	0.9545	16.6249	1.0632
5		0.9240	28.8298	1.3481
10		0.9335	22.3415	1.3172
15		0.9389	21.0810	1.2808
20		0.9276	25.2808	1.4141
Average		0.9357	22.8316	1.2847
0 (Pure diesel)	Padé approximation	0.3224	16.5582	5.3074

5	of Sine (Eq. (8))	0.3763	28.8159	5.0280
10		0.4200	22.2565	4.7129
15		0.2573	21.0725	5.5438
20		0.2944	25.2744	5.5484
Average		0.3341	22.7955	5.2281
0 (Pure diesel)	Piecewise (Eq. (9))	0.9852	5.7504	0.6740
5		0.9805	11.5225	0.7434
10		0.9762	6.7997	0.9321
15		0.9118	7.3347	1.2019
20		0.9025	2.3499	1.2815
Average		0.9512	6.7514	0.9666
0 (Pure diesel)	Padé approximation of Piecewise (Eq. (9))	0.9804	5.7504	0.7964
5		0.9805	11.5225	0.7409
10		0.9763	6.7997	0.9311
15		0.9118	7.3348	1.2019
20		0.9025	2.3500	1.2814
Average		0.9503	6.7515	0.9903

Appendix Table 6. The r^2, relative error, and mean absolute error values coming from Eq. (8) and Eq. (9), and their Padé approximations for Çakmak et al.'s data [33]

Octanol Content	Equation	r^2	Relative error (%)	Mean absolute error
0 (Pure diesel)	Sine (Eq. (8))	0.9383	20.2908	1.2574
5		0.9642	12.3517	0.9354
10		0.9463	18.8404	1.1893
15		0.9354	21.4228	1.3044
20		0.9768	9.2555	0.7927
Average		0.9522	16.4322	1.0958
0 (Pure diesel)	Padé approximation of Sine (Eq. (8))	0.0905	20.2883	5.6050
5		0.0862	12.3512	5.7791
10		0.0109	18.8363	6.0497
15		0.1733	21.4199	5.5042
20		0.1076	9.2559	5.3405
Average		0.0937	16.4303	5.6557
0 (Pure diesel)	Piecewise (Eq. (9))	0.9793	5.8774	0.7923
5		0.9764	3.6699	0.8142
10		0.9808	3.8426	0.7876
15		0.9794	6.4867	0.7814
20		0.9808	2.2611	0.7771
Average		0.9793	4.4275	0.7905
0 (Pure diesel)	Padé approximation of Piecewise (Eq. (9))	0.9793	5.8772	0.7920
5		0.9764	3.6698	0.8142
10		0.9799	3.8426	0.8232
15		0.9794	6.4866	0.7813
20		0.9808	2.2609	0.7778
Average		0.9792	4.4274	0.7977

Appendix Table 7. Regression constants of the piecewise equation (Eq. (10)) for Yeşilyurt and Çakmak's data [8]

Octanol Content	Equation	Regression constants					
		a_1	a_2	b_1	b_2	c_1	c_2
0 (Pure diesel)	Piecewise (Eq. (10))	8.22380	10.61204	-3.23415	-0.02448	-0.33508	-0.22091
5		3.80474	10.20356	-4.62354	0.04243	-0.47497	-0.32678
10		5.90853	8.41127	-4.46131	0.05494	-0.46152	-0.33204
15		14.28259	11.90488	2.00227	-0.07520	0.05609	-0.19699
20		14.57193	11.11728	1.99629	-0.04330	0.05407	-0.23786

Appendix Table 7. (Continued)

Octanol Content	Equation	Regression constants					
		d_1	d_2	e_1	e_2	f_1	f_2
0 (Pure diesel)	Piecewise (Eq. (10))	-11.37961	16.80460	-0.35157	0.18721	-4.17335	26.87172
5		-10.32028	15.43546	-0.48798	0.15014	-5.35529	39.14301
10		-10.55624	17.50194	-0.47895	0.20002	-5.37384	37.08696
15		-21.28344	21.32535	0.06078	0.13635	2.36784	34.12016
20		-21.51955	20.91682	0.05772	0.11891	2.25004	40.06140

Appendix Table 8. Regression constants of the piecewise equation (Eq. (10)) for Çakmak et al.'s data [33]

Octanol Content	Equation	Regression constants					
		a_1	a_2	b_1	b_2	c_1	c_2
0 (Pure diesel)	Piecewise (Eq. (10))	11.74727	12.49190	-3.55641	-0.03718	-0.48930	-0.23466
5		15.77979	13.52185	-1.50551	-0.13344	-0.31175	-0.14453
10		13.08163	13.50237	-3.75826	-0.07436	-0.56737	-0.23366
15		10.38882	12.91867	-3.80176	-0.05184	-0.51000	-0.21493
20		13.76048	13.94956	-1.40068	-0.13647	-0.28745	-0.24210

Appendix Table 8. (Continued)

Octanol Content	Equation	Regression constants					
		d_1	d_2	e_1	e_2	f_1	f_2
0 (Pure diesel)	Piecewise (Eq. (10))	-9.11591	18.91832	-0.50455	0.14173	-4.35598	36.29648
5		-9.16442	21.66059	-0.32927	0.19215	-2.34533	29.55688
10		-8.41445	19.50540	-0.58481	0.19374	-4.69576	28.37379
15		-9.14452	18.85122	-0.52145	0.08771	-4.43124	37.10636
20		-9.22525	20.38284	-0.30054	0.24352	-2.10746	30.11443

Appendix Table 9. Regression constants of the piecewise equation (Eq. (11)) for Yeşilyurt and Çakmak's data [8]

Octanol Content	Equation	Regression constants					
		a_1	a_2	a_3	a_4	a_5	a_6
0 (Pure diesel)	Piecewise (Eq. (11))	32.56	3.845	37.02	31.94	29.36	10.61204
5		24.44	3.657	27.54	46.88	45.24	10.20356
10		11.9	21.38	41.99	4.879	38.58	8.41127
15		8.56	7.47	67.83	153	62.01	11.90488
20		7.979	6.978	125.2	120	44.11	11.11728

Appendix Table 9. (Continued)

Octanol Content	Equation	Regression constants					
		b_1	b_2	b_3	b_4	b_5	b_6
0 (Pure diesel)	Piecewise (Eq. (11))	7.755	25.44	6.173	33.41	33.97	-0.02448
5		6.115	21.12	4.367	31.38	31.88	0.04243
10		7.695	2.767	30.95	23.89	31.59	0.05494
15		8.276	24.11	29.34	0.2841	29.8	-0.07520
20		8.387	23.61	29.53	29.78	0.9433	-0.04330

Appendix Table 9. (Continued)

Octanol Content	Equation	Regression constants					
		c_1	c_2	c_3	c_4	c_5	c_6
0 (Pure diesel)	Piecewise (Eq. (11))	0.4427	-0.691	2.769	-0.09667	-2.97	-0.22091
5		0.1658	-1.756	2.28	-0.2346	-3.146	-0.32678
10		0.7814	1.329	-0.5589	-0.7492	-3.394	-0.33204
15		0.7915	4.924	-2.087	0.1212	-5.012	-0.19699
20		0.9026	4.82	-1.898	-4.921	0.3896	-0.23786

Appendix Table 9. (Continued)

Octanol Content	Equation	Regression constants		
		d	e	f
0 (Pure diesel)	Piecewise (Eq. (11))	16.80460	0.18721	26.87172
5		15.43546	0.15014	39.14301
10		17.50194	0.20002	37.08696
15		21.32535	0.13635	34.12016
20		20.91682	0.11891	40.06140

Appendix Table 10. Regression constants of the piecewise equation (Eq. (11)) for Çakmak et al.'s data [33]

Octanol Content	Equation	Regression constants					
		a_1	a_2	a_3	a_4	a_5	a_6
0 (Pure diesel)	Piecewise (Eq. (11))	88.75	9.294	9.851	98.41	89.88	12.49190
5		52.7	10.89	4.375	32.49	29.27	13.52185
10		8.211	63.19	8.583	131.7	124.5	13.50237
15		7.788	105	7.118	85.92	80.36	12.91867
20		10.84	85.18	5.981	47.12	42.03	13.94956

Appendix Table 10. (Continued)

Octanol Content	Equation	Regression constants					
		b_1	b_2	b_3	b_4	b_5	b_6
0 (Pure diesel)	Piecewise (Eq. (11))	0.5271	7.802	25.48	29.68	30.06	-0.03718
5		0.9456	7.237	23.85	29.99	30.6	-0.13344
10		8.496	0.6916	25.18	29.84	30.08	-0.07436
15		9.061	0.3905	24.37	29.92	30.28	-0.05184
20		6.998	0.6569	25.44	29.95	30.44	-0.13647

Appendix Table 10. (Continued)

Octanol Content	Equation	Regression constants					
		c_1	c_2	c_3	c_4	c_5	c_6
0 (Pure diesel)	Piecewise (Eq. (11))	0.2555	0.6746	5.663	-1.81	-4.774	-0.23466
5		0.4749	0.405	4.784	-1.836	-4.692	-0.14453
10		0.936	0.3221	5.295	-1.977	-5.003	-0.23366
15		1.177	0.1786	5.137	-1.731	-4.705	-0.21493
20		0.2045	0.2982	5.414	-1.937	-4.848	-0.24210

Appendix Table 10. (Continued)

Octanol Content	Equation	Regression constants		
		d	e	f
0 (Pure diesel)	Piecewise (Eq. (11))	18.91832	0.14173	36.29648
5		21.66059	0.19215	29.55688
10		19.50540	0.19374	28.37379
15		18.85122	0.08771	37.10636
20		20.38284	0.24352	30.11443

Appendix Table 11. Regression constants of the piecewise equation (Eq. (12)) for Yeşilyurt and Çakmak's data [8]

Octanol Content	Equation	Regression constants					
		a_1	a_2	a_3	a_4	a_5	a_6
0 (Pure diesel)	Piecewise (Eq. (12))	32.56	3.845	37.02	31.94	29.36	6.77598
5		24.44	3.657	27.54	46.88	45.24	11.42232
10		11.9	21.38	41.99	4.879	38.58	10.02813
15		8.56	7.47	67.83	153	62.01	19.42027
20		7.979	6.978	125.2	120	44.11	22.04874

Appendix Table 11. (Continued)

Octanol Content	Equation	Regression constants					
		b_1	b_2	b_3	b_4	b_5	b_6
0 (Pure diesel)	Piecewise (Eq. (12))	7.755	25.44	6.173	33.41	33.97	0.75714
5		6.115	21.12	4.367	31.38	31.88	1.83147
10		7.695	2.767	30.95	23.89	31.59	1.55554
15		8.276	24.11	29.34	0.2841	29.8	0.59948
20		8.387	23.61	29.53	29.78	0.9433	1.02745

Appendix Table 11. (Continued)

Octanol Content	Equation	Regression constants				
		c_1	c_2	c_3	c_4	c_5
0 (Pure diesel)	Piecewise (Eq. (12))	0.4427	-0.691	2.769	-0.09667	-2.97
5		0.1658	-1.756	2.28	-0.2346	-3.146
10		0.7814	1.329	-0.5589	-0.7492	-3.394
15		0.7915	4.924	-2.087	0.1212	-5.012
20		0.9026	4.82	-1.898	-4.921	0.3896

Appendix Table 11. (Continued)

Octanol Content	Equation	Regression constants	
		c_6	d
0 (Pure diesel)	Piecewise (Eq. (12))	0.07427	5.11708
5		0.06283	-1.94341
10		0.06240	-1.12643
15		0.02968	-6.56398
20		0.03233	-11.27791

Appendix Table 12. Regression constants of the piecewise equation (Eq. (12)) for Çakmak et al.'s data [33]

Octanol Content	Equation	Regression constants					
		a_1	a_2	a_3	a_4	a_5	a_6
0 (Pure diesel)	Piecewise (Eq. (12))	88.75	9.294	9.851	98.41	89.88	14.24844
5		52.7	10.89	4.375	32.49	29.27	15.37784
10		8.211	63.19	8.583	131.7	124.5	13.47703
15		7.788	105	7.118	85.92	80.36	17.89887
20		10.84	85.18	5.981	47.12	42.03	16.92187

Appendix Table 12. (Continued)

Octanol Content	Equation	Regression constants					
		b_1	b_2	b_3	b_4	b_5	b_6
0 (Pure diesel)	Piecewise (Eq. (12))	0.5271	7.802	25.48	29.68	30.06	1.01905
5		0.9456	7.237	23.85	29.99	30.6	0.00025
10		8.496	0.6916	25.18	29.84	30.08	0.51029
15		9.061	0.3905	24.37	29.92	30.28	0.96558
20		6.998	0.6569	25.44	29.95	30.44	0.76323

Appendix Table 12. (Continued)

Octanol Content	Equation	Regression constants				
		c_1	c_2	c_3	c_4	c_5
0 (Pure diesel)	Piecewise (Eq. (12))	0.2555	0.6746	5.663	-1.81	-4.774
5		0.4749	0.405	4.784	-1.836	-4.692
10		0.936	0.3221	5.295	-1.977	-5.003
15		1.177	0.1786	5.137	-1.731	-4.705
20		0.2045	0.2982	5.414	-1.937	-4.848

Appendix Table 12. (Continued)

Octanol Content	Equation	Regression constants	
		c_6	d
0 (Pure diesel)	Piecewise (Eq. (12))	0.04633	-1.26027
5		0.02324	1.76318
10		0.04064	1.60137
15		0.03658	-5.90583
20		0.04968	-0.00061

Appendix Table 13. The r^2, relative error, and mean absolute error values coming from Eqs. (10)-(12) for Yeşilyurt and Çakmak's data [8]

Octanol Content	Equation	r^2	Relative error (%)	Mean absolute error
0 (Pure diesel)	Piecewise (Eq. (10))	0.9901	5.7504	0.4988
5		0.9849	11.5225	0.5046
10		0.9878	6.7997	0.5359
15		0.9180	7.3347	0.9713
20		0.9107	2.3499	0.9746
Average		0.9583	6.7514	0.6970
0 (Pure diesel)	Piecewise (Eq. (11))	0.9957	0.8526	0.3412
5		0.9900	10.0711	0.4485
10		0.9944	4.8528	0.3770
15		0.9842	4.4973	0.5640
20		0.9856	7.2607	0.5623
Average		0.9900	5.5069	0.4586
0 (Pure diesel)	Piecewise (Eq. (12))	0.9908	0.8526	0.5164
5		0.9856	10.0711	0.6873
10		0.9829	4.8528	0.7731
15		0.9780	4.4973	0.7946
20		0.9773	7.2607	0.8692
Average		0.9829	5.5069	0.7281

Appendix Table 14. The r^2, relative error, and mean absolute error values coming from Eqs. (10)-(12) for Çakmak et al.'s data [33]

Octanol Content	Equation	r^2	Relative error (%)	Mean absolute error
0 (Pure diesel)	Piecewise (Eq. (10))	0.9872	5.8774	0.5181
5		0.9796	3.6699	0.6766
10		0.9864	3.8426	0.5840
15		0.9850	6.4867	0.5792
20		0.9881	2.2611	0.5332
Average		0.9853	4.4275	0.5782
0 (Pure diesel)	Piecewise (Eq. (11))	0.9906	4.2514	0.4490
5		0.9838	0.8669	0.5555
10		0.9875	4.3333	0.5408
15		0.9903	4.0377	0.4519
20		0.9913	0.1534	0.3990
Average		0.9887	2.7285	0.4792
0 (Pure diesel)	Piecewise (Eq. (12))	0.9827	4.2514	0.7233
5		0.9805	0.8669	0.6931
10		0.9819	4.3333	0.7443
15		0.9847	4.0377	0.6542
20		0.9840	0.1534	0.6429
Average		0.9828	2.7285	0.6916

Appendix Table 15. Regression constants of Eq. (13) for Yeşilyurt and Çakmak's data [8]

Octanol Content	Equation	Regression constants					
		a_1	a_2	a_3	a_4	b_1	b_2
0 (Pure diesel)	Eq. (13)	234.5	5887	7.499e4	5.521e5	3.575	520.4
5		108.6	1163	1.403e4	1.877e5	-10.27	8.55
10		89.07	386.8	8821	2.474e5	-15.91	-11.18
15		134.5	565.6	8159	2.066e5	-19	159.1
20		123.7	8.992	3517	1.739e5	-19.53	94.49

Appendix Table 15. (Continued)

Octanol Content	Equation	Regression constants	
		b_3	b_4
0 (Pure diesel)	Eq. (13)	8140	3.893e4
5		2479	1.522e4
10		2867	1.905e4
15		2516	1.165e4
20		2189	1.058e4

Appendix Table 16. Regression constants of Eq. (13) for Çakmak et al.'s data [33]

Octanol Content	Equation	Regression constants					
		a_1	a_2	a_3	a_4	b_1	b_2
0 (Pure diesel)	Eq. (13)	107.7	2685	2.832e4	2.845e5	-19.25	251
5		86.38	8923	1.914e5	1.386e6	-25.13	1230
10		171.1	4721	5.152e4	3.82e5	-14.02	461.3
15		116.6	1848	1.693e4	2.415e5	-19.37	201.8
20		115.8	1377	2.191e4	3.305e5	-17.88	195.5

Appendix Table 16. (Continued)

Octanol Content	Equation	Regression constants	
		b_3	b_4
0 (Pure diesel)	Eq. (13)	3918	1.661e4
5		1.538e4	6.624e4
10		5377	2.041e4
15		3332	1.462e4
20		2827	1.666e4

Appendix Table 17. The r^2, relative error, and mean absolute error values coming from Eq. (13) for Yeşilyurt and Çakmak's data [8]

Octanol Content	Equation	r^2	Relative error (%)	Mean absolute error
0 (Pure diesel)	Eq. (13)	0.9883	1.6441	0.6273
5		0.9922	1.7033	0.5767
10		0.9960	1.1325	0.3557
15		0.9978	1.5626	0.2869
20		0.9950	0.0502	0.4663
Average		0.9939	1.2185	0.4626

Appendix Table 18. The r^2, relative error, and mean absolute error values coming from Eq. (13) for Çakmak et al.'s data [33]

Octanol Content	Equation	r^2	Relative error (%)	Mean absolute error
0 (Pure diesel)	Eq. (13)	0.9925	1.9242	0.5028
5		0.9721	0.2319	0.9537
10		0.9859	2.4487	0.7473
15		0.9966	1.8238	0.3499
20		0.9950	1.4900	0.4419
Average		0.9884	1.5837	0.5991