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Effect of Sauter Mean Diameter on the Combustion Related Parameters in Heavy-Duty Diesel Engines

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A mathematical model of combustion process in a diesel engine has been developed according to the theory of the chain reactions for the higher hydrocarbon compounds. The instantaneous rates of fuel vaporization and combustion are defined by the current values of temperature, pressure, concentration of fuel vapors, overall diffusion rate, fuel injection rate, and mean fuel droplet size in terms of the Sauter mean diameter (SMD). Numerical experiments have been carried out for investigating the interdependency between various combustion-related parameters. Specifically, the effect of fuel droplet size (in terms of SMD) on the subsequent combustion parameters, such as pressure, temperature, thermodynamic properties of air/gas mixture, heat transfer, fuel vaporization, combustion rate, current air/fuel ratio, and gas mixture composition have been investigated. In addition, the integral indicator parameters of the engine, such as mean indicated pressure, peak pressure, compression pressure, and specific fuel consumption have been analyzed. The results show very good agreement with the available data on heavy-duty diesel engines.

Nomenclature

A_0 = constant depending on the physical and chemical properties of the fuel applied to premixed combustion, 47–52
A_1 = constant depending on the physical and chemical properties of the fuel applied to diffusion combustion, 14–16
a = coefficient in the Redlich–Kwong's equation of state, $N \cdot m^4 \cdot kg^2$
b = coefficient in the Redlich–Kwong's equation of state, m^3/kg, volume per unit mass at $T = -273°C$
c_p = specific isobaric heat capacity, $J/kg \cdot K$
c_v = specific isochoric heat capacity, $J/kg \cdot K$
D_{SM} = Sauter mean diameter (SMD) of droplet, μm
D_t = overall coefficient of diffusion, m^2/s
f = branching coefficient of chain reactions
f_b = overall nondimensional fuel mass fraction burned up to the current moment of time, m_b/m_c ($= m_p/m_c$, that is, $f_b = f_p + f_d$, because $m_b = m_p + m_d$)
f_d = nondimensional fuel mass fraction burned up to the current moment of time under the conditions of diffusion flame, m_d/m_c
f_i = nondimensional fuel mass fraction injected up to the current moment of time, m_i/m_c
f_p = nondimensional fuel mass fraction burned up to the current moment of time under the conditions of premixed flame, m_p/m_c
f_v = nondimensional fuel mass fraction vaporized up to the current moment of time, m_v/m_c
f_{vi} = nondimensional fuel mass fraction vaporized during the self-ignition delay period
h = specific enthalpy of air/gas mixture, J/kg
k_t = coefficient of turbulence
M = current mass of air/gas mixture in the cylinder, kg
m_b = mass of fuel burned up to the current moment of time, kg
m_c = total fuel mass injected per cycle per cylinder, kg
m_d = fuel mass burned up to the current moment under the conditions of diffusion flame, kg
m_p = fuel mass burned up to the current moment of time under the conditions of premixed flame, kg
m_v = fuel mass vaporized up to the current moment, kg
p = pressure in the cylinder of the engine, N/m^2
Q = heat loss due to fuel vaporization, dissociation, heat transfer (see subscripts)
Q_f = calorific value of fuel, J/kg
R = gas constant, J/kg-K
r_i = mass fractions of pure air, pure gas, and fuel vapor ($i = 1, 2, 3$)
T = temperature of the air–gas mixture in the cylinder, K
T_d = surface temperature of the liquid fuel droplets, K
t = time, s
t_{sc} = time at the moment of the beginning of combustion
u = specific internal energy, J/kg
V = current volume of the cylinder, m^3
V_i = volume of the cylinder at the moment of ignition, m^3
v = specific volume of air/gas mixture, m^3/kg
λ = air/fuel (A/F) equivalence ratio, $(A/F)_{actual}/(A/F)_{stoichiometric}$
ρ = density of liquid fuel, kg/m^3
τ_{id} = ignition delay (time between the start of injection and detectable heat release)
φ_0 = total branching coefficient, $f - g$

Subscripts

b = fuel burned
c = cycle, cylinder
d = diffusion, droplet, dissociation
ev = evaporation
f = fuel
i = injection
liq = liquid fuel
p = premixed flame
SM = SMD
t = turbulence
v = fuel vaporized
w = cylinder wall
0 = initial, originating value
$\sum$ = overall, sum

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Introduction

COMBUSTION modeling provides a pivotal role for computer simulation of the actual behavior of diesel engine cycles. The combustion occurs in a three-dimensional time-dependent turbulent flow, with a fuel containing a blend of hydrocarbons, and with not well-understood combustion chemistry. Studies based on mathematical models can be very useful for the understanding of engine processes and for the design of engines with improved performance and reduced emissions. Presently existing mathematical models are not able to solve applied problems concerning the combustion process with respect to the controlling parameters such as instantaneous temperature and pressure in the cylinder, parameters of fuel injection, fuel atomization, and a large number of operating conditions, such as engine load and engine speed. The approaches used and techniques for modeling the diesel engine combustion process may be arranged into two categories: thermodynamics-based models and fluid dynamics-based models.

The thermodynamics-based models provide equations for describing the heat release curve in the cylinder of the engine by means of comparatively simple functions in conjunction with approximations of experimental data. In the 1960s, thermodynamics, combined with the advent of digital computers, gave rise to detailed cycle analysis, which is zero dimensional. Such an approach was introduced by Wiebe.[1] Later Shipinski et al.,[2] and Woschni and Anisits[3] composed new models based on one (single) or two (double) Wiebe's functions for simulating the rate of combustion in both direct injection and indirect injection engines. They found a correlation between the parameters and operating conditions. Ghojel[4] used a double Wiebe's function to describe the rate of combustion in a turbocharged direct injection engine over an engine speed of 1000–2500 rpm. He assumed the durations of premixed and diffusion combustion to be constants for a certain operating condition, but introduced corrections that took into account the influence of the ignition delay period, fuel injection rate, and equivalence ratio. Ghojel[4] expressed the Wiebe's function parameters with respect to the design factors and operating conditions. He assumed that the first maximum in the rate of combustion occurs at a constant crank angle interval after the ignition. Miyamoto et al.[5] developed an empirical model for describing the rate of combustion in the cylinder of an engine over a range of operating conditions, including speed, load, and fuel-injection timing. All of these models are zero dimensional, and the process lacks a direct means of coupling the engine fluid mechanics to the combustion. These models can be used to improve valve timing, study thermal loading, and investigate the effects of heat release, turbocharging, and other systems design parameters. Zero-dimensional analysis is, however, unable to probe very far into the combustion process itself.

The fluid dynamics-based models provide mathematical descriptions of airflow, fuel spray behavior, and physical and chemical modeling of spray combustion in closed systems. The most common practice has been to describe the combustion process by an Arrhenius form single-rate equation.[6] Later Butler et al.[7] introduced a multidimensional numerical simulation of reactive flow in internal combustion engines. Spatially resolved numerical methods and models developed in the 1970s began to appear in computer codes in the 1980s. By 1985 the generalized code KIVA, developed at Los Alamos National Laboratory, was available for public use. During the following 10 years the progress was remarkable, and several computational fluid dynamics (CFD) codes for simulating flow and combustion behavior in diesel design are now available commercially, for example, KIVA-II,[8,9] Fluent, CFDRC, and Answer. The KIVA-III code,[8] made available in 1993, further improves the grid resolution, and a more powerful KIVA code for computers using parallel processing is now available on an experimental basis. The University of Wisconsin version of KIVA-II includes also an ignition delay model, a spray model,[9] and emission models,[10] using a modified k–ε model (Re Normalized Group, RNG model), and multicomponent droplet vaporization models are now being introduced to KIVA. The problems accompanying the fluid dynamics-based models are provided in the review by Heywood.[11] The first problem is the presumption that the oxidation process of a complex hydrocarbon fuel can be adequately represented by a single or limited number of overall reaction(s). Second, thus far these models have worked with ensemble-averaged equations so that cyclic variability of the in-cylinder flows is not predicted. These models use average values of concentration and temperature to calculate the local reaction rate, whereas the instantaneous local values will actually determine the reaction rate. This problem is analyzed by Ozdor et al.[12] Third, the final phase of combustion occurs when the flame approaches the chamber surfaces. These phenomena are not well understood in the existing models. Fourth, the implied strong dependence of burning rate on chemical kinetics is at variance as evidenced by the experimental results from engine combustion. Engine designers have been forced to use greatly simplified reaction schemes. In addition, detailed reaction schemes are only available for the simpler hydrocarbon fuels. Accordingly, multidimensional engine calculations have used highly simplified chemical kinetic schemes to represent the combustion process. Fifth, the existing models do not take into account the effect of imperfections in the working medium on the combustion-related parameters under high-pressure conditions that prevail in the cylinders of the modern forced turbocharged engines. In summary, fluid dynamics-based modes of airflow, fuel spray behavior, and combustion are still under development. They have yet to substitute for good judgment and experience.

The following conclusions can be formulated about the existing models of diesel engine combustion process that are based on either the thermodynamic or fluid mechanic considerations.

1) No satisfactory models exist for simulating combustion process consisting of both premixed flame (for the combustion of fuel vaporized during the self-ignition delay period) and diffusion flame (for the combustion of fuel during the injection process).

2) The influence of fuel vaporization on the combustion process (as affected by, for example, the fuel preparation and precombustion processes effects) is not yet clearly understood.

3) There are no reliable mathematical models for the fuel vaporization process that take into account the fuel droplet sizes, fuel properties, and the instantaneous values of pressure, temperature, concentrations, and turbulence levels.

4) No reliable mathematical description exists for modeling the interdependencies between the fuel-injection rate and fuel-vaporization rate.

5) Multidimensional models of diesel engine combustion process use highly simplified chemical kinetic schemes, with one or at most a few reactions, to represent the combustion process. Although such schemes can be calibrated with experimental data to give acceptable results over a limited range of engine conditions, they lack an adequate fundamental basis.

6) Thermodynamic behavior of a working medium in the existing models is described by an equation of state for an ideal gas, and the internal energy u, enthalpy h, specific heat capacities c_v and c_p are defined depending on the temperature T and the gas-mixture composition only. There are no mathematical models that define the thermodynamic properties of working medium as a function of pressure (or density or specific volume). These idealizations appear as preconditions for errors that can be considerable for some modern forced diesel engines with high peak pressures.

Objectives

The overall objective of this study is to provide a numerical analysis of interdependencies between combustion-related parameters during the combustion process in the cylinder of a diesel engine via an improved mathematical model. Some specific objectives follow.

1) Provide an improved mathematical model for the fuel vaporization process, taking into account the fuel injection rate, droplet size in terms of the Sauter mean diameter (SMD), fuel properties, instantaneous values of temperature, pressure, diffusion coefficient, and concentrations of fuel vapors in the engine cylinder.

2) Develop an improved mathematical model both for the premixed and diffusion combustion process in the engine, based on the theory of the chain reactions for the higher hydrocarbon compounds and practical fuels that are blends of a large number of hydrocarbons.

3) Simulate the energy conversion processes during the combustion process in a diesel engine taking into account working medium imperfections via new mathematical descriptions for the caloric parameters (enthalpy, internal energy, and specific heat capacities c_v and c_p) that depend on the thermal parameters (temperature T and pressure P) and gas-mixture composition.

4) Create an algorithm and program to numerically solve the differential equations.

5) Calibrate the model and verify the model validation.

6) Investigate interdependencies between combustion-related parameters and engine performance via mathematical modeling with respect to the engine operating conditions and parameters of fuel injection and atomization in terms of the SMD.

The intent of this paper is to provide data and an explanation of engine operating characteristics with respect to the parameters influencing the combustion process and interdependencies between combustion-related parameters. The performance and efficiency of diesel engines and the effect of changes in major operating variables are related to the more fundamental material on engine combustion.

The approach used in this study for attaining the listed objectives involves parallel efforts between theoretical and experimental studies: The theoretical study is for the development of an improved mathematical model on the grounds of advanced thermodynamic property relations and the theory of the chain reactions for the higher hydrocarbon compounds. Practical fuels that are blends of a large number of hydrocarbons are emphasized. The experimental study is for model validation and model calibration.

Mathematical Model

The engine combustion process takes place under continuously changing volume, temperature, pressure, concentrations, mass (due to fuel injection and leakage through piston rings), heat transfer rate, diffusion, etc. Figure 1 is a schematic of the various interdependencies between the parameters during the combustion process in the engine cylinder.

The branching character of the links between the parameters reveal that there are great number of logical chains that can be specified to estimate the mutual influence between parameters. For example, the temperature influences pressure, diffusion, fuel vaporization rate, combustion rate, thermodynamic properties (c_v, c_p, h, and u) of the gas mixture, dissociation, heat transfer rate, etc. Simultaneously each one of these parameters influences the other parameters, which further affects the combustion process. From this point of view a great number of back loops can be counted. The best way for analysis of such extremely complicated interdependencies is via detailed mathematical modeling. The mathematical model must take into consideration all of these interactions and provide an opportunity both for qualitative and quantitative analysis.

In attempting to achieve these objectives, the authors have developed an improved mathematical model both for the premixed and diffusion combustion process in a diesel engine. The model is based on the theory of the chain reactions for the higher hydrocarbon compounds and practical fuels that are blends of a large number of hydrocarbons. The major equations of the mathematical model for describing the combustion process in a diesel engine are presented as follows:

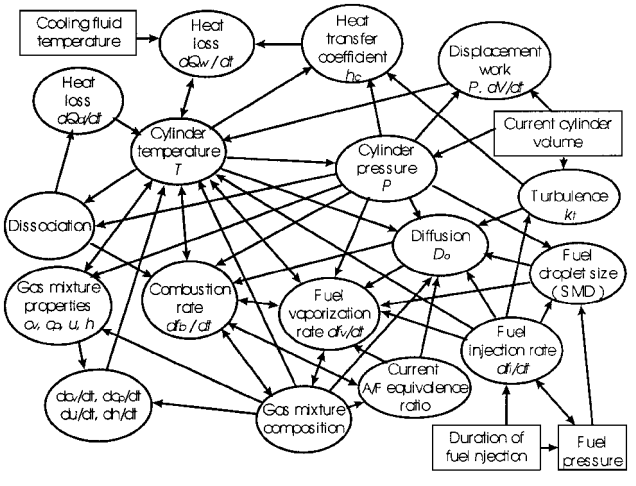

Fig. 1 Skeleton showing major interactions between various parameters during the combustion process in a diesel engine.

$$M\left[c_v(v,T)+T\sum_{i=1}^{3}\frac{\mathrm{d}c_{v_i}}{\mathrm{d}T}\right]\frac{\mathrm{d}T}{\mathrm{d}t}$$
$$=m_cQ_f\frac{\mathrm{d}f_b}{\mathrm{d}t}-M\left(\frac{\partial u}{\partial r_1}\frac{\partial r_1}{\partial f_b}+\frac{\partial u}{\partial r_2}\frac{\partial r_2}{\partial f_b}+\frac{\partial u}{\partial r_3}\frac{\partial r_3}{\partial f_b}\right)\frac{\mathrm{d}f_b}{\mathrm{d}t}$$
$$-M\left[\frac{\partial u}{\partial r_3}\frac{\partial r_3}{\partial f_v}\frac{\mathrm{d}f_v}{\mathrm{d}t}-\frac{\partial u}{\partial v}\left(\frac{1}{M}\frac{\mathrm{d}V}{\mathrm{d}t}-\frac{V}{M^2}\frac{\mathrm{d}M}{\mathrm{d}t}\right)\right]$$
$$+(h-u)\frac{\mathrm{d}M}{\mathrm{d}t}-\frac{\mathrm{d}Q_w}{\mathrm{d}t}-\frac{\mathrm{d}Q_{ev}}{\mathrm{d}t}-\frac{\mathrm{d}Q_d}{\mathrm{d}t}-p\frac{\mathrm{d}V}{\mathrm{d}t} \tag{1}$$

$$\frac{\mathrm{d}f_v}{\mathrm{d}t}=\frac{D_t}{p}\left(\frac{0.5T+0.5T_d}{273}\right)^2\frac{6}{\rho D_{\mathrm{SM}}}f_i^{\frac{1}{3}}(f_i-f_v)^{\frac{5}{3}}\frac{\lambda-f_v}{1.15f_v} \tag{2}$$

$$\frac{\mathrm{d}f_p}{\mathrm{d}t}=A_0\frac{m_c}{V_i}f_{vi}\{\exp[\varphi_0(t-t_{sc})]\}(f_{vi}-f_0)\Big|_{\text{from } f_0=0}^{\text{to } f_0=f_{vi}} \tag{3}$$

$$\frac{\mathrm{d}f_d}{\mathrm{d}t}=\psi\frac{\mathrm{d}f_v}{\mathrm{d}t}+A_1\frac{m_c}{V}(f_v-f_b)^2f_b \tag{4}$$

$$\frac{\mathrm{d}f_b}{\mathrm{d}t}=\frac{\mathrm{d}(m_b/m_c)}{\mathrm{d}t}=\frac{\mathrm{d}(m_p/m_c)}{\mathrm{d}t}+\frac{\mathrm{d}(m_d/m_c)}{\mathrm{d}t} \tag{5}$$

$$u(v,T)=u_0(T)+\frac{3}{2}\frac{a}{b}\frac{1}{\sqrt{T}}\ln\left(\frac{v}{v+b}\right) \tag{6}$$

$$h(v,T)=h_0(T)+\frac{3}{2}\frac{a}{b}\frac{1}{\sqrt{T}}\ln\left(\frac{v}{v+b}\right)+\frac{bRT}{v-b}-\frac{a}{(v+b)\sqrt{T}} \tag{7}$$

$$c_v(v,T)=c_{v_0}(T)-\frac{3}{4}\frac{a}{b}T^{-\frac{3}{2}}\ln\left(\frac{v}{v+b}\right) \tag{8}$$

$$c_p(v,T)=c_v(v,T)+T\left(\frac{R}{v-b}+\frac{a}{2v(v+b)T^{\frac{3}{2}}}\right)^2$$
$$\times\left(\frac{RT}{(v-b)^2}-\frac{a(2v+b)}{v^2(v+b)^2\sqrt{T}}\right)^{-1} \tag{9}$$

$$\left(p+\frac{a}{v(v+b)\sqrt{T}}\right)(v-b)=RT \tag{10}$$

where c_v and c_p are specific isochoric and isobaric heat capacities for the gas mixture in the cylinder; $\mathrm{d}f_b/\mathrm{d}t=\mathrm{d}(m_b/m_c)/\mathrm{d}t$ is the overall nondimensional combustion rate (OCR), 1/s; r_1, r_2, and r_3 are mass fractions of pure air, pure gases, and fuel vapors in the cylinder; $\mathrm{d}f_v/\mathrm{d}t=\mathrm{d}(m_v/m_c)/\mathrm{d}t$ is the fuel vaporization rate (FVR), 1/s; h is the specific enthalpy of the working medium in the cylinder; $\mathrm{d}M/\mathrm{d}t$ is the rate of mass change due to the fuel injection and leakage through the piston rings; $\mathrm{d}Q_w/\mathrm{d}t$, $\mathrm{d}Q_{ev}/\mathrm{d}t$, $\mathrm{d}Q_d/\mathrm{d}t$ (J/s) are rate of heat loses due to the heat transfer through the cylinder walls, fuel vaporization, and dissociation of fuel; T_d is the temperature of the fuel droplet, defined as $T_d=0.25T+380$ K; $\mathrm{d}f_p/\mathrm{d}t=\mathrm{d}(m_p/m_c)/\mathrm{d}t$ is the nondimensional premixed combustion rate (PCR), 1/s; $\varphi_0=5900$–6200; and ψ is the coefficient of proportionality ($\psi=0.84$–0.87).

Equations (1–10) have the following physical meaning.

Equation (1) represents energy balance in the engine cylinder according to the first law of thermodynamics.[13] This differential equation (1) describes the energy conversion process in a diesel engine cylinder from the beginning of the real compression process until the opening of exhaust valve/port. The equation is valid for a working medium, considered as a real gas, and takes into account the imperfections in the working media that appear in case of high pressures. This gives an opportunity to simulate the processes in the modern forced turbocharged engines with high peak pressure in the cylinder. During the indicator process (compression, combustion, and expansion) the intake and exhaust valves/ports are closed ($dM_{in}/dt = 0$; $dM_{ex}/dt = 0$), that is, there is no mass transfer and energy transfer through the inlet and exhaust valves/ports. The mass balance can be presented as follows:

$$\frac{dM}{dt} = m_c \frac{df_i}{dt} - \frac{dM_L}{dt} \tag{11}$$

that is, the change of mass at the cylinder is caused by the fuel injection df_i/dt and gas leakage through the piston rings, dM_L/dt.

Equation (2) represents the fuel vaporization rate.[14] This equation allows one to define the instantaneous rate of fuel vaporization and mixing with respect to the current values of pressure, temperature, air/fuel (A/F) equivalence ratio, SMD, and concentrations. Note that in spite of denoting df_v/dt as rate of vaporization, Eq. (2) has more global physical meaning. It represents the rate of preparing the fuel for combustion via atomization, vaporization, and mixing under the conditions of variable temperature, pressure, and concentrations and also accounts for diffusion via D_t and turbulence k_t. From this point of view df_v/dt is named vaporization rate only for simplicity, but its real meaning is rate of preparing the fuel for diffusion combustion. The overall diffusion coefficient D_t is defined by the equation of Popov,[15] giving an opportunity to take into account the diffusion process with respect to the temperature, pressure, and turbulence in the cylinder. Equation (2) plays very important role for defining the diffusion combustion rate.

Equation (3) gives the nondimensional combustion rate under the conditions of premixed flame.[14] Note that Eq. (3) for the premixed combustion rate is valid only in the interval $0 < f_0 < f_{vi}$, where f_0 is an integral sum of the right side of Eq. (3) from the beginning of combustion to the current moment of time:

$$f_0 = \int_{t=t_{sc}}^{t} A_0 \frac{m_c}{V_i} f_{vi} \{\exp[\varphi_0(t - t_{sc})]\}(f_{vi} - f_0)\, dt \tag{12}$$

where A_0 is constant depending on the physicochemical properties of the fuel. For diesel fuels Semenov[16] suggests $A_0 = 47$–52 and $\varphi_0 = 5900$–6200.

Equation (4) represents the nondimensional combustion rate under the conditions of diffusion flame.[14] It is obvious that the first term on the right side can work until the end of vaporization process ($df_v/dt = 0$), when the last fuel droplet is vaporized ($f_v = 1$), but there are some unburned fuel vapors. Their percentage is $1 - f_b$. The combustion of this amount of fuel can be presented only by the second term on the right side of Eq. (4). However, this amount of fuel burns under conditions that can not be considered as diffusion flame because there is no atomization and vaporization. During the same time this process can not be considered as a premixed flame. Whereas the premixed combustion in the engine cylinder is characterized with very high heat-release rate, the fuel fraction that has not yet burned after the end of vaporization burns with a comparatively low rate. Besides, because at this point of the process the premixed combustion does not exist ($df_p/dt = 0$), the combustion rate here is equal to the overall combustion rate (df_b/dt). To use Eq. (4), however, one needs data on the fuel injection rate and mean droplet size in terms of the SMD (discussed later).

Equation (5) gives overall combustion rate (premixed plus diffusion). On substituting Eq. (3) for the PCR and Eq. (4) for the diffusion combustion rate (DCR) ($df_d/dt = d(m_d/m_c/dt)$), 1/s, in Eq. (5), the final differential equation for the OCR can be written as follows:

$$\frac{df_b}{dt} = A_0 \frac{m_c}{V_i} f_{vi} \{\exp[\varphi_0(t - t_{sc})]\}(f_{vi} - f_0)\Big|_{\text{from } f_0 = 0}^{\text{to } f_0 = f_{vi}}$$

$$+ \psi \frac{C}{p} \left(\frac{0.5T + 0.5T_d}{273} \right)^2 \frac{6}{\rho D_{SM}} f_i^{\frac{1}{3}} (f_i - f_v)^{\frac{5}{3}} \frac{\lambda - f_v}{1.15 f_v}$$

$$+ A_1 \frac{m_c}{V} (f_v - f_b)^2) f_b \tag{13}$$

The first term on the right side describes the combustion rate of fuel vapors that are vaporized during the self-ignition delay period under the premixed flame conditions. The second term on the right side expresses the combustion of fuel in which the burning rate is controlled by the rate of vaporization. This is the main component of the DCR. The third term on the right side describes the rate of combustion of fuel vapors and products of incomplete combustion that have not burned up to the current moment of time, with the exception of the fuel vapors vaporized during the self-ignition period. From the beginning of combustion process up to the moment $f_b = f_{vi}$, all three terms on the right-hand side of the equation are involved in the modeling process. From the moment $f_b = f_{vi}$ to the moment $f_v = 1$, the second and third terms take part in the modeling process. Finally, after the end of vaporization process ($f_v = 1$) only the last (third) term on the right describes the combustion process that take place under the conditions of late combustion.

Equations (6–9) represent mathematical dependencies between the caloric parameters (internal energy u, enthalpy h, isochoric specific heat capacity c_v, and isobaric specific heat capacity c_p) and thermal parameters (P, T, and v). These equations have also been created in a previous study.[13] They were derived from generalized relations of thermodynamics in partial derivatives in conjunction with the Redlich–Kwong (see Ref. 17) equation of state for real gases. These equations have been applied to the various products encountered during the burning of fuel, such as nitrogen (N_2), oxygen (O_2), carbon dioxide (CO_2), carbon oxide (CO), hydrogen (H_2), and water or steam (H_2O). They have also been applied to the gas mixture as a whole, for describing the thermodynamic behavior of real gases in the engine cylinder under conditions of high pressures and temperatures, which occur during the combustion process. A comparison between the numerical and experimental data made by the authors is given Ref. 14.

Equation (10) is the Redlich–Kwong equation of state for real gases.[17] The coefficient a and b in this equation has been quantitatively evaluated in a previous study[13] on the grounds that all partial derivatives are equal to zero at the critical point, in conjunction with the equation of Planck–Gibbs for the critical point.[17]

In addition to these new equations, some known equations are also used for closing the system of differential equations. The mass flow rate of fuel injected through the nozzle dm_f/dt, and, hence, the nondimensional fuel-injection rate (FIR) $df_i/dt = d(m_i/m_c)/dt$ is modeled by the Hiroyasu and Kadota[18] equation. For defining the instantaneous heat transfer rate dQ_w/dt, we have used the equations for heat transfer coefficient of Woschni and Anisits[3] for the cylinder head and piston and of Dent (provided by Heywood[11]) for the cylinder walls. The rate of dissociation dQ_d/dt is modeled by the equation of Popov.[15] The mass leakage rate dM_L/dt through the piston rings is modeled by the equation of Danov.[13] To integrate Eq. (2), one needs the value for the SMD. For this purpose the empirical expression of Hiroyasu and Kadota[18] for the SMD is used. To define the nondimensional fuel mass fraction f_{vi} vaporized during the ignition delay period, the equation of Hardenberg and Hase (see Ref. 11) is used for predicting the duration of the ignition delay period. This equation has been shown to give very good agreement with experimental data over a wide range of engine operating conditions.

Computational Procedure

The fourth-order Runge–Kutta method (see Ref. 19) is applied for obtaining numerical solution of the proposed system of differential equations. The computing procedure is iterative. The numerical solution, that is, integration of the system of differential equations,

of the proposed mathematical model of diesel engine combustion process is carried out with respect to the crank angle (CA) rotation (degree). Because the proposed governing equations for modeling the diesel combustion process are presented with respect to the time, a change of the independent variable is carried out: $dP/dt = dP/d\varphi \times d\varphi/dt$, where P is any parameter, that is, the connection between these independent parameters (CA φ and time t) is the crankshaft angular velocity $\omega = d\varphi/t$. The step $\Delta\varphi$ of integration is variable. Its initial value is 0.2 CA deg, but the developed algorithm has capability to reduce the step automatically during the computation process. Its value depends on the current truncation error of the Runge–Kutta process. The current truncation error is estimated via the rule of Collatz (see Ref. 19). The algorithm is realized via a FORTRAN 90, using either a personal computer or UNIX workstation.

Model Validation

Figure 2 shows a comparison between the experimental data on the pressure history in the cylinder and calculated results for pressure using both ideal and real gas model for a two stroke slow-speed marine turbocharged diesel engine, Sulzer type 6RLB66.

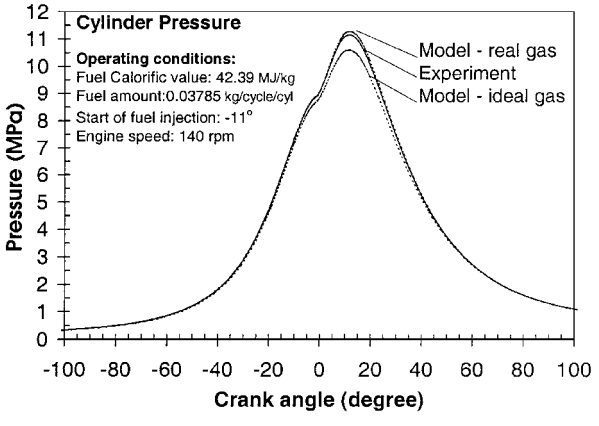

Fig. 2 Comparison between the experimental data on indicated pressure (for 6RLB-66 engine) and calculated results on pressure using real and ideal gas models.

The model used the same operating conditions as that in experiments, that is, engine speed $n = 140$ rpm, fuel calorific value = 42.39 MJ/kg (heavy diesel fuel), start of fuel injection = −11°BTDC, fuel amount = 0.03785 kg/cycle/cylinder, ambient pressure = 740 mm Hg column, and ambient temperature = 27°C. The experimental error in the measured experimental curve is filtered by means of a windowing method for filtration. In the case of ideal gas model, the influence of pressure, that is, density, on the caloric parameters (u, h, c_v and c_p) and, hence, the subsequent effects have been ignored. It can be seen that if the pressure at the engine cylinder is over 8–9 MPa, considerable differences exist between experimental and theoretical data from the ideal gas model. These differences exceed the errors of the experiment (see Table 1). The results clearly show that the ideal gas model is not adequate to represent the real energy conversion process in the engine cylinders.

Discussions about the magnitude of the errors and uncertainties in the experimental data used to validate the model have been provided in Ref. 13. The errors and uncertainties are caused by the stochastic nature of the cycle variability and are possibly due to some imperfections in the diagnostics. The relative errors of experiments for the parameters listed in Tables 1 and 2 are as follows: mean indicated pressure $\delta P_i = 3.03\%$, compression pressure $\delta P_c = 1.55$, peak pressure $\delta P_z = 3.42$, specific fuel consumption δSFC = 3.1, and engine power $\delta P = 3.05\%$.

The comparison between the experimental data and numerical results from the real gas model shows very good agreement. The relative differences between the experimental data and results from the real gas model for the integral indicator parameters (see Table 1) are commensurable with the experimental error. A comparison between the model predictions and experimental curves for the overall combustion rate for the nominal operating conditions (load and engine speed) is shown in Fig. 3. The experimental curve is obtained from the experimental curve of pressure (Fig. 2) and Eq. (1) of energy conservation, resolved with respect to the combustion rate $df_b/dt = d(m_b/m_c)/dt$, Table 2 shows a comparison between the major integral parameters of a 8DKRN74/160-3 marine diesel engine, for different rotational speeds and loads over a range of operational conditions. Good agreement between the experimental and predicted parameters allows one to use the mathematical model described here for solving applied problems and to predict or investigate the engine indicator parameters for various operational conditions.

Table 1 Calculated and experimental data for integral parameters of a Sulzer-6RLB-66 marine diesel engine

	Modeling		
Parameters	Ideal gas model	Real gas model	Experiment
Mean indicated pressure, MPa	1.451	1.572	1.554
Compression pressure, MPa	8.752	8.970	8.953
Peak pressure of cycle, MPa	10.609	11.284	11.150
Specific indicated fuel consumption, kg/kW · h	0.196	0.181	0.183
Heat losses in cooling fluid, %	13.88	14.97	14.50

Table 2 Theoretical and experimental parameters for a marine diesel engine, at different rotating speeds and loads on screw-propeller curve

	Condition 1[b]		Condition 2[c]		Condition 3[d]		Condition 4[e]	
Parameters[a]	Experiment	Model	Experiment	Model	Experiment	Model	Experiment	Model
P_C, MPa	3.589	3.391	4.325	4.312	5.246	5.248	5.639	5.682
P_Z, MPa	5.482	5.267	6.139	5.993	6.806	6.748	7.051	7.099
P_i, MPa	0.657	0.637	0.849	0.831	1,010	1.008	1.069	1.091
SFC, kg/kW · h	0.217	0.221	0.216	0.220	0.217	0.219	0.221	0.218
P, kW	5,040	4,945	7,570	7,430	10,075	9,980	11,080	11,220

[a] P_C = compression pressure, P_Z = peak pressure, P_i = mean indicated pressure, SFC = specific effective fuel consumption, and P = engine effective (break) power.
[b] Amount of fuel per cycle per cylinder, $m_C = 0.0237$ kg/cycle and engine rotational speed, $n = 96$ rpm.
[c] $m_C = 0.0312$ kg/cycle; $n = 109$ rpm. [d] $m_C = 0.0380$ kg/cycle; $n = 120$ rpm. [e] $m_C = 0.04116$ kg/cycle; $n = 124$ rpm.

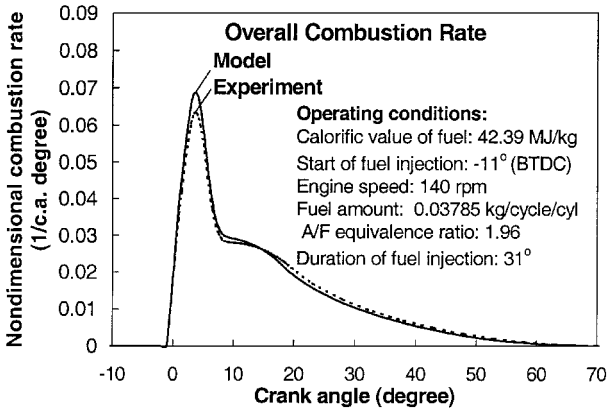

Fig. 3 Comparison of calculated results on overall combustion rate with the experimental data from a 6RLB-66 marine diesel engine.

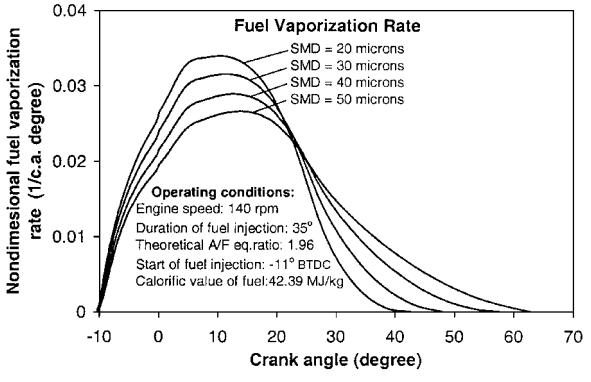

Fig. 4 Effect of SMD on the fuel vaporization rate in the cylinder during the combustion process for marine diesel engine 6RLB-66.

Results and Discussion

The atomization of a liquid fuel into a large number of small drops is necessary to create a large surface area across which liquid fuel can evaporate. Because the measurement of droplet characteristics in an operating diesel engine is extremely difficult, most results have come from studies of fuel injection into constant-volume chambers with high-pressure quiescent air at room temperature. These conditions, however, are totally different from the conditions in the cylinder of an operating engine. The mathematical model presented here allows one to quantify the rates of fuel vaporization and combustion under the conditions of variable pressure, volume, temperature, and concentration. Numerical experiments have been carried out for investigating the effect of SMD on the major parameters in the cylinder during the combustion process. The marine DI diesel engine (Sulzer 6RLB-66) used has a cylinder bore and stroke of 0.66 m and 1.4 m, respectively. For all numerical experiments, the operating conditions were as follows: amount of fuel = 0.03785 kg/cycle/cylinder, beginning of fuel injection = 11° BTDC, duration of fuel injection = 35 CA deg, ambient pressure = 740-mm Hg column, ambient temperature = 27°C, rotating speed = 140 rpm, and fuel = heavy diesel (mazut). The calorific value of the fuel was 42.39 MJ/kg. Figures 4–11 show shows the important results. The effect of SMD on the fuel vaporization rate is shown in Fig. 4. The overall combustion rate is shown in Fig. 5. The current mass fraction of the fuel vapors remaining, representing the unburned fuel as a difference between mass fraction vaporized and mass fraction burned, is shown in Fig. 6. The other figures show the current A/F equivalence ratio (Fig. 7), mass fractions of pure air and pure gases (Fig. 8), pressure in the cylinder (Fig. 9), temperature in the cylinder (Fig. 10), and overall heat transfer coefficient (Fig. 11). These parameters are evaluated quantitatively for a change of SMD from 20 to 50 μm.

Figure 4 shows the variation of fuel vaporization rate in the engine cylinder as affected by the SMD. The smaller size droplet contributes to enhance vaporization and to reduce the time duration for fuel vaporization. The droplet size strongly influences the overall combustion rate (Fig. 5). This influence is, however, rather indirect, mainly via the fuel vaporization rate. Accordingly, as the droplet size (SMD) is reduced, the maximum increases and the duration of the combustion process is reduced. An increase of SMD leads to lower combustion rates and a longer duration of combustion process. For smaller SMD, the fuel mass fraction burned under the conditions of premixed flame increases. For very small droplet sizes (SMD < 10 μm), usually the second maximum on the heat release curve does not appear for the investigated engine, 6RLB66. For larger SMD, the fuel mass fraction burnt under the conditions of diffusion flame increases, and for these cases the second maximum on the heat release curve appears (Fig. 5). The second maximum, however, is always lower than the first one. It can be seen that, for the specified operating conditions, there is a delay of 9–10° between

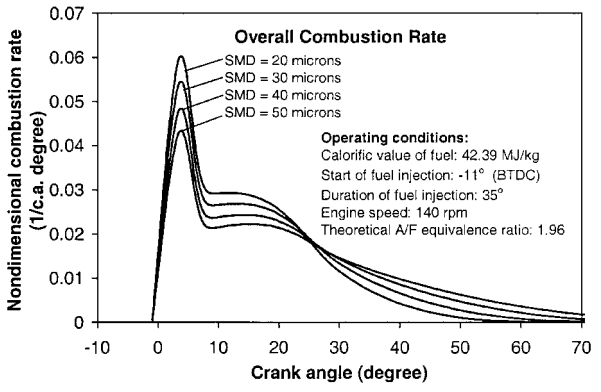

Fig. 5 Effect of SMD on the overall combustion rate in the cylinder for marine diesel engine 6RLB-66.

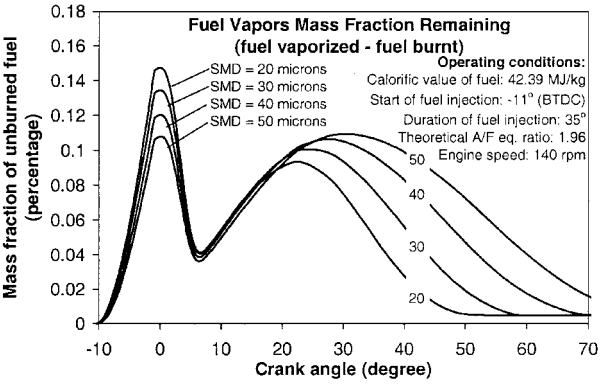

Fig. 6 Effect of SMD on the mass fraction of the unburned fuel in the cylinder during the combustion process for marine diesel engine 6RLB-66.

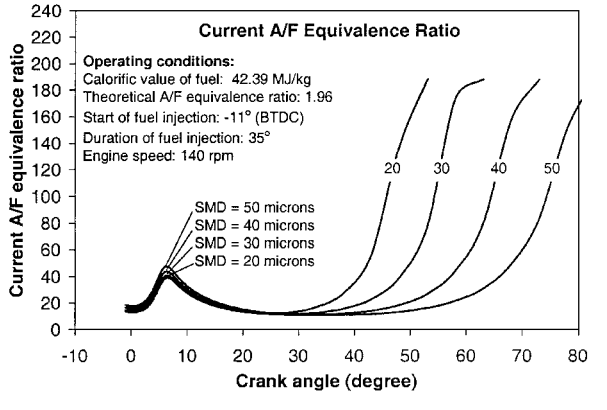

Fig. 7 Effect of SMD on the current A/F equivalence ratio in the cylinder during the combustion process for marine diesel engine 6RLB-66.

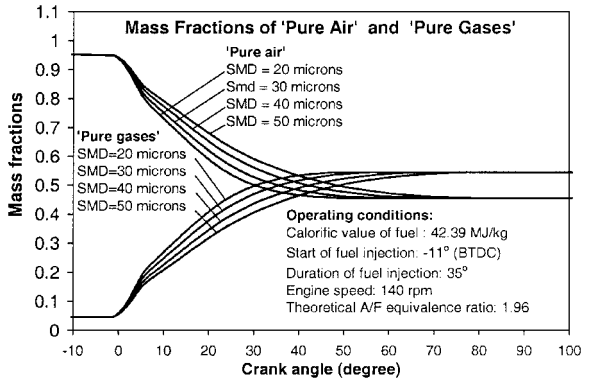

Fig. 8 Effect of SMD on the mass fraction of pure air and pure gas in the cylinder during the combustion process for marine diesel engine 6RLB-66.

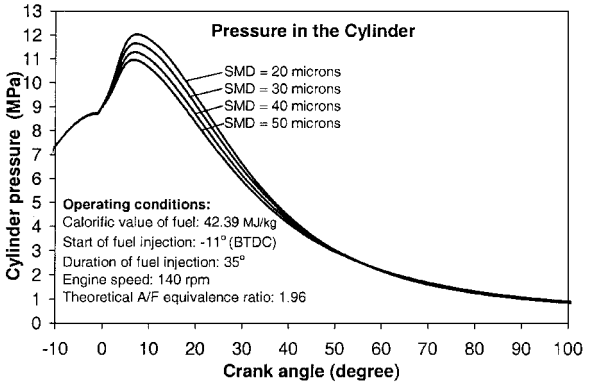

Fig. 9 Effect of SMD on the pressure in the cylinder during the combustion process for marine diesel engine 6RLB-66.

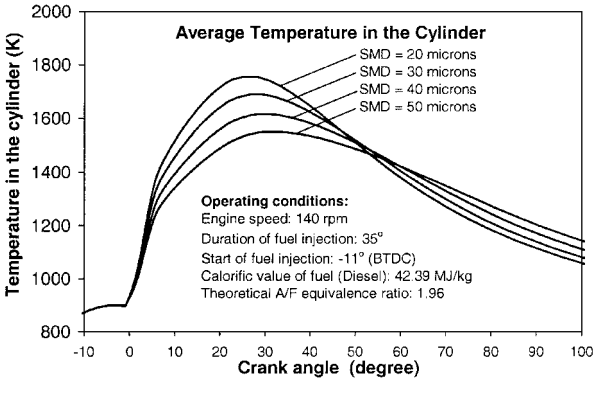

Fig. 10 Effect of SMD on the temperature in the cylinder during the combustion process for marine diesel engine 6RLB-66.

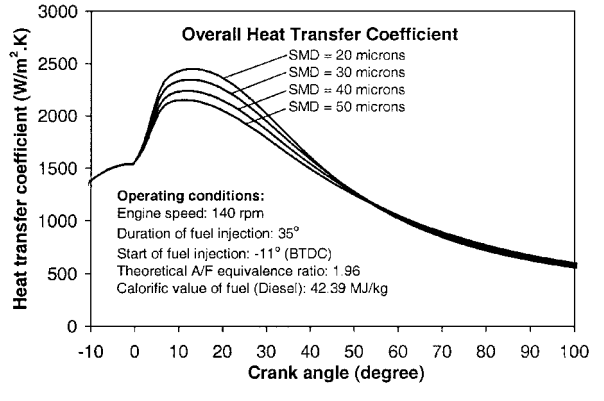

Fig. 11 Effect of SMD on the overall heat transfer coefficient in the cylinder during the combustion process for marine diesel engine 6RLB-66.

the start of fuel injection and combustion (Figs. 4 and 5). In spite of the droplet size, the overall combustion rate, that is, the heat release curve, is typical for the DI engine over its load and speed range. For all of the cases the combustion process proceeds in three distinguishable stages. In the first stage, the rate of burning is very high and it lasts only 8–9 CA deg (Fig. 5). This stage corresponds to the combustion of fuel vaporized during the ignition delay period, that is, combustion occurs under premixed flame condition. The second stage corresponds to the period of gradually decreasing heat-releaserate, though it initially may rise to a second, lower, peak. Figures 4 and 5 show that once the fuel and air, premixed during the ignition delay, have been consumed, the burning rate is controlled by the rate at which mixture becomes available for burning, that is, the burning rate here is controlled by the rates of fuel injection, vaporization, and mixing. The duration of vaporization process for these operating conditions is strongly influenced both by the SMD and the FIR. After the end of vaporization, the combustion process continues at a lower rate. This process is related to some 3–6% from the cycle amount of fuel (Fig. 6) that has not burned as yet at the end of vaporization process. The kinetics of the final burnout process become slower as the temperature and pressure of the cylinder gases fall during the expansion.

Figure 6 illustrates the variations of the current concentration of fuel vapors. This concentration is a difference between the fuel mass fraction vaporized and the overall fuel mass fraction burnt. The fuel vapor concentration strongly influences the combustion rate. In fact, it determines the current values of the fuel/air equivalence ratio (Fig. 7), the gas-mixture composition (Fig. 8) and the thermophysical properties of working medium in the cylinder. The instantaneousconcentrationsof the air and gases depend on the mass fraction of fuel burnt (the accumulated percentage as an integral curve) and the initial value of A/F equivalence ratio. Because the rates of fuel vaporization and burning are influenced by the current values of concentrations (Figs. 6–8), temperature (Fig. 9) and pressure (Fig. 10), the mutual consideration of these parameters give a clear understanding about the interactions between the combustion related parameters (Fig. 1). The values for the instantaneous heat transfer coefficient (Fig. 11) depend on the corresponding current values of the temperature and pressure. Besides, the gas mixture is considered as a mixture of real gases.[13] That is why the pressure also influences the specific heat capacities.

Conclusions

A mathematical model of combustion process in a diesel engine has been developed and is based on the theory of branched chain reactions for higher hydrocarbon compounds. The combustion process is considered as one consisting of both premixed and diffusion flame:

1) The combustion of fuel vaporized during the self-ignition delay period is modeled according to the conditions of premixed flame. A kinetic differential equation has been created for modeling this kind of combustion.

2) The combustion of fuel during the injection and fuel vaporization processes is modeled as diffusion flame. This process is described by means of a newly developed differential equation.

A mathematical model for the instantaneous fuel vaporization rate has been developed. The vaporization rate is defined by the current values of temperature, pressure, concentration of fuel vapors, FIR, and the mean fuel droplet size in terms of the SMD.

The proposed mathematical model has a clear physical meaning and is simple to use for providing the numerical solution of the nonlinear simultaneous differential equations.

Mathematical dependencies between the caloric parameters and thermal parameters have been provided for describing the thermodynamic behavior of real gases under high-pressure and high-temperature conditions during the combustion process. As a result, an improved mathematical model for the energy conversion processes, taking account of working media imperfections in the diesel engine cylinder, has been provided.

The model gives an opportunity to investigate the interactions between combustion-related parameters and combustion process and

engine performance with respect to the engine operating conditions and the parameters for fuel injection and atomization.

The model assists in better understanding of various ongoing physical and chemical processes that occur during the combustion in the cylinder of a diesel engine. The processes of fuel vaporization and combustion are simulated and quantified with respect to the following controlling parameters: FIR, current temperature, current pressure, current concentrations, A/F equivalence ratio, and droplet size in terms of the SMD.

The mutual influence between the vaporization and combustion processes is investigated and estimated quantitatively. The influence of the quality of fuel atomization process, estimated via the SMD, on the FVP and OCR has been estimated. The results show very strong influence of SMD on the vaporization and combustion processes, both with respect to the maximum rates and the duration of these processes. The results show that the ratio of amount of fuel burnt under the premixed flame conditions to amount of fuel burnt under diffusion flame conditions for one cycle is strongly influenced by the SMD.

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