Heat Release Model Based on Combustion Phenomena

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ABSTRACT

The authors have carried out the systematic and fundamental investigation on the combustion processes and characteristics of diesel spray injected into a quiescent atmosphere, using model chambers. The simple combustion model has been developed for calculating the rate of heat release of diesel spray based on the experimental results. The model is then implemented into a cycle simulation of a diesel engine to estimate the performances and the rate of heat release in a quiescent DI medium-speed diesel engine. The paper presents the combustion model and the comparison of the results obtained from simulation and from experiments.

INTRODUCTION

It is important to describe the relation between the rate of heat release (ROHR) and combustion phenomena of diesel spray in order to simulate the performance of diesel engines. Numerous methods have been presented to predict the ROHR, for example by Lyn (1), Shipinski (2), Hiroysu (3), Ikenami (4) and Aoyagi (5). Although each model has some features and agrees with the ROHR in practical engines, they do not always describe the relation between combustion phenomena and ROHR properly. In these models, furthermore, the calculation methods are too complicated to apply to the design of an engine.

The authors have carried out the systematic and fundamental works on the diesel combustion processes through the no-combustion and combustion experiments at a high pressure with a high temperature using model chambers (6,7,8). The range of experimental condition covers completely the practical diesel engine operating condition. The characteristics of diesel spray, that is, the shape and structure of spray and the air movement around it, were obtained from no-combustion experiments. The characteristics of flames were made clear by combustion experiments.

From these systematic experiments, a simple combustion model has been developed to predict the ROHR in a quiescent direct injection combustion system (9).

The model is installed into an engine simulation code which predicts cylinder pressure, fuel consumption and so on. The ROHR calculated from the model is compared with the experimental re-}

ults using a 250 mm bored single cylinder engine, which was operated with various compression ratio, boost pressure and injection timing. From the comparisons, the model has been confirmed to be capable of predicting the engine performance satisfactorily.

ENGINE SIMULATION

The engine simulation model is based on the well established step by step emptying and filling technique. The effects arising from interference between cylinders, inertia of gases or any form of pressure waves in the intake and exhaust manifolds are not catered for.

The structure diagram of the simulation program is shown in Fig. 1. Starting with an estimated cylinder pressure and temperature at exhaust valve opening moment, the program works in a step-by-step manner in crank angle increments until inlet valve closure. Increments of exhaust and intake flows are calculated. The cylinder pressure, temperature and gas composition are re-estimated after each step. Empirical values are employed in this step on the exhaust and intake port characteristics, which are given by a blowing rig test (10).

In-cylinder pressure and temperature are calculated using the combustion model, which will be described in the latter section, during compression and expansion strokes. Heat transfer between the in-cylinder medium and the combustion chamber wall is calculated with Annand’s equation (11). After the convergence of iteration, the indicated engine performances are calculated from the work done in the cylinder over the latest 720 degree cycle.

COMBUSTION MODEL

Phenomena of Combustion
Formulation of the layer of premixed mixture and first break-out a visible flame. Figure 2 shows the macroscopic structure of a fully developed diesel spray proposed by the authors (12). The spray, which is injected into a hot and pressured atmosphere, evaporates at first and then the ignition occurs in this evaporated part, as indicated in Fig. 2. The evaporation process is not a spatially or temporally uniform in diesel spray. Authors have found that the evaporation proceeds mainly in the mixing flow region of spray (13).
The spray tip penetration of different spray has the same length when each spray is injected into two types of atmosphere whose densities are equal, even if each pressure and/or each temperature are different. The visible spray angle, in the other hand, decreases as the initial temperature increases or the initial pressure decreases (7).

The reason for phenomena above is explained as following (12). The majority of injected fuel flies through the main jet region along spray axis and reaches the spray tip. The fuel evaporates scarcely until it reaches the tip, because the temperature is relatively low in the main jet region. The temperature affects therefore slightly on the penetration length of the visible spray, in other words, nonevaporated spray.

After reaching tip, fuel is driven outward radially by the radial pressure difference, i.e., pressure is higher near the axis in the stagnation part than that of the atmosphere. The driven fuel reduces its velocity and arrives at the mixing flow region of the mixing part, as spray grows down stream. In the mixing flow region, the vaporization process of droplets at mixing flow region is enhanced by eddy mixing (14) and by heat exchange between spray envelope and surrounding air. Visible spray angle thus decreases as temperature increases, although penetration length doesn't.

The evaporated part of spray injected into heated and compressed atmosphere can be taken by schlieren photography, although it can not be caught by direct photography (15,16). Ruber and coworkers, for example, indicates through their schlieren study that the evaporated spray, which is injected into atmosphere with a high temperature at a high pressure, has almost the same volume as spray which is injected into atmosphere with a room temperature at a high pressure, if both atmosphere has the same density (15). As a consequence, the volume of the premixed mixture formed at spray envelope can be given as a remainder of the evaporated and nonevaporated sprays, each of which is injected into atmosphere of the same density and of high or room temperature.

Figure 3 shows the example of sketches of flame growing process. Figure 4 indicates relation among growth of spray, growth of flame and ROHR corresponding to the case of Fig. 3. The first visible flame appears at the mixing part of the layer of premixed mixture as a luminous white spot (6). The distance \( h \) [m] between position of the first visible flame and nozzle tip is mainly
influenced by the initial pressure $p_0$ (MPa). The following relation is drawn from experiments (6):

\[ h = 10.0 \times 0.04 \times 10^{0.25} - 0.1 \]  

(1)

**Period of premixed flame burning.** After the first break-out of visible flame, the flame grows both in the direction of spray tip and in that of nozzle tip, along the layer of premixed mixture. The tone of flame is tinged with blue. This means that the flame is premixed one.

The flame growing velocity $V_n$ towards spray tip is approximately constant in the range from $55$ m/s to $60$ m/s, which is independent on the initial pressure and initial temperature. The same order of velocity was reported in a practical high-speed DI engine by Lyn et al. (1). It is remarkable that the velocity $V_n$ [m/s] is only linear to the oxygen concentration $\phi$ (ratio of oxygen partial pressure of charged gas to that of air in normal state). The following relation can be drawn:

\[ V_n = 56 \phi - 1 \]  

(2)

The flame growing velocity $V_n$ [m/s] towards nozzle tip is also only proportional to the oxygen concentration $\phi$ and is expressed as follows:

\[ V_n = 56 \phi - 34 \]  

(3)

It is notable that the flame never enters into initial part as far as the fuel is being injected. The heat quantity by burning of fuel in the layer of premixed mixture is nearly equal to the cumulative heat release from the first break-out of a visible flame to the time when the the ROHR has the first maximum, if fuel concentration in the layer is assumed as a stoichiometric value. Consequently, the fuel in the layer of premixed mixture can be considered to burn with stoichiometric ratio as a premixed flame.

**Period of diffusion flame burning.** The tone of the flame turns into white and the brightness of flame increases after the period of premixed flame burning (6). The phenomena is a diffusion flame. In the portion of the mixing region, where the premixed flame burning is completed, diffusion burning takes place between entraining fresh hot air and fuel, among which are the unburned vaporized one, the vapor and droplet diffusing from the main jet region. Then in Fig. 3, premixed flame burning and diffusion flame burning are going on simultaneously until the premixed flame reaches the spray tip, and all the premixed mixture is burnt out. The burnt out time is $5.8$ ms in the case of the conditions shown in Fig. 3.

Thereafter, only the phenomena of diffusion flame progresses and the ROHR indicates the gentle slope as shown in Fig. 4. The ROHR reaches the second peak nearly at the end of the injection. During injection period, the mass of entrained air

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**Fig. 3** Sketches of growth of flame in diffusion burning

**Fig. 4** Relations among growth of spray, growth of flame and ROHR.
in the burning diesel spray is almost the same as that in the unburning spray, if both of them are injected into the surroundings of the same density (17). So the mass of surrounding air in flame during period of injection is calculated from the volume of spray injected into the same condition as that of the flame. Nevertheless, the small quantity of surrounding air can enter into main jet region and the mean air/fuel ratio in the region is not so large that the combustion is progressing, because the mass flux of fuel is very great. Then diffusion flame burning is provided by diffusion among the vapor of fuel remained at mixing flow region after end of premixed flame burning, the droplets and vapor entering into mixing flow region from main jet region, and the surrounding charge entrained into spray during period of injection.

**Burning after end of injection.** The envelope of flame is broken out and the lump of flame is falling down after end of injection, as shown in Fig. 5. The flame proceeds into initial part as well. The fairly dark luminous dots appear there and are also falling down. ROHR decreases with gentle slope until the burning finishes.

**CALCULATION MODEL**

**Calculation of ROHR during Period of Injection**

As mentioned before, the burning of stoichiometric premixed mixture at mixing flow region controls the heat release during premixed flame burning. The burning of fuel remained at mixing flow region after premixed flame burning and the fuel entered the region from main jet region controls the heat release during diffusion flame burning. The air used in this period is entrained into spray after premixed flame burning.

Then the rate of heat release \(\frac{dQ_d}{dt}\) [J/s] during period of premixed flame burning and diffusion flame burning are expressed by following forms:

\[
\frac{dQ_d}{dt} = \frac{dV_b}{dt} \tag{4}
\]

where

\(V_b\) : volume of premixed mixture consumed during premixed flame burning [m³]

\(V_{ba}\) : volume of surrounding air entrained into mixing flow region where premixed flame burning already finished [m³]

The premixed mixture in the layer of premixed mixture burns at stoichiometric ratio during the period of premixed flame burning. The fuel burns also at stoichiometric ratio entraining surrounding air during period of diffusion flame burning. Then above two equations are rearranged as following forms.

\[
\frac{dQ_d}{dt} = \frac{Hi}{(O_2/F)_{at}} \frac{n_{nr}}{dV_b} \tag{6}
\]

where

\(n_{nr}\) : number of nozzle holes
\(Hi\) : low calorific value of fuel [J/kg]
\(F\) : mass fraction of oxygen in surrounding charge [-]
\((O_2/F)_{at}\) : stoichiometric ratio of mass of oxygen to that of air [-]

\[
\frac{dQ_d}{dt} = \frac{Hi}{(O_2/F)_{at}} \frac{n_{nr}}{dV_{ba}} \tag{7}
\]

The volume of the layer of premixed mixture and that of surrounding charge, which is entrained into flame, are presumed by the volume of spray, which is injected into atmosphere with a high pressure at a room temperature of the same density as one when the burning is progressing. So volumes \(V_b\) and \(V_{ba}\) are calculated from the model of spray injected into atmosphere with a high pressure at a room temperature shown in Fig. 6. The shape of solid line expresses a spray. The spray is formed by the cone with vertical angle \(\beta\),
that is, equivalent spray angle shown in Fig. 2, and sphere. The shape is made by the cone with vertical angle \( \theta \), that is, spray cone angle shown in Fig. 2, and ellipsoidal solid of revolution. Spray tip penetration \( l \) [mm], equivalence spray angle \( \Omega \) [sr] and spray cone angle \( \Omega_k \) [sr] are calculated from following experimental equations (7):

\[
1 = 27.1 \ t_{so}^{0.65} \ t_{so}^{0.35} \ \rho \ t_{so}^{0.29} \ \log \ t_{so} = 0.41 \ \rho \ t_{so}^{0.35}
\]

where

- \( u_{so} \) : mean discharge velocity of fuel at outlet of nozzle tip [m/s]
- \( t \) : time from start of injection [m/s]
- \( \rho_v \) : density of charge [kg/m³]
- \( \Omega \) : diameter of nozzle hole [mm]

\[
\Omega = 0.17 \ \rho_v^{0.30}
\]

\[
\Omega_k = 0.35 \ \rho_v^{0.16}
\]

Figure 7 displays the model of process of premixed flame burning and diffusion flame burning during period of injection, obtained from Eq. 3 and Eq. 6. Then volume \( V_t \) of premixed mixture consumed during premixed flame burning in equation (4) corresponds to that of part drawn by oblique line. Then volume \( V_t \) [m³] is expressed by following expressions:

\[
V_t = \ln \frac{dV_{t+}}{dz} dt\]

where

\( V_t \) : distance between flame front growing in the direction of spray tip and nozzle tip [m]

\( \ln \) : distance between position of the first visible flame and nozzle tip (See Eq. (1)) [m]

\( t \) : time from start of injection [s]

\( \tau \) : illumination delay (6) [s]

\[
\tau = 1.17 \times 10^{-3} \ \rho_v^{-0.30} \ \varphi^{-1.09} \ \exp(5130/T_s)
\]

\[
p_0 < 3.92 \ \text{[MPa]}
\]

\[
p_0 > 3.92 \ \text{[MPa]}
\]

where

- \( p_0 \) : initial pressure [MPa]
- \( \varphi \) : oxygen concentration [-]
- \( T_s \) : initial temperature [K]

\( V_f \) : velocity of flame growth in the direction of spray tip (See Eq. (2)) [m/s]

\( \ln \) : distance between flame front growing in the direction of spray tip and nozzle tip [m]

\[
\ln = \frac{1 - \int_{t_1}^{t} V_f dt}{\tau_1}
\]

where

- \( V_f \) : velocity of flame growth in the direction of nozzle tip (See Eq. (3)) [m/s]

\( V_{st} \) : volume of mixing flow region [m³]

\[
V_{st} = V_0 - V_{st}
\]

where

- \( V_0 \) : equivalent spray volume [m³]

\( V_{st} \) : volume of main jet region [m³]

\( z \) : axial distance from outlet of nozzle tip [m]

The velocity of surrounding charge entrained into spray is nearly reciprocal to the distance from nozzle tip along the spray axis (18). This tendency is as same as in the case of steady flow jet (19). So the quantity of surrounding charge entrained into spray in a unit width and a unit time is nearly constant regardless of the distance \( z \). And the surrounding charge entrained into mixing flow region after premixed flame burning only relates to diffusion flame burning. Considering these facts, \( dV_{st}/dt \) in Eq.(7) is rearranged in following form:

\[
\frac{dV_{st}}{dt} = \ln \frac{V_{st}}{V_{st1}}
\]

\[
\frac{dV_{st}}{dt} = \frac{\ln V_{st} - \ln V_{st1}}{\ln dt}
\]

The growth of flame in the direction of nozzle tip is terminated near the initial part as shown in Fig. 3. The length \( L \) is defined as the

AT FIRST
BREAK-OUT OF
A VISIBLE FLAME

FLAME FRONT

AT END OF INJECTION

PRE-MIXED FLAME BURNING AND
DIFFUSION FLAME BURNING

\[
t = \frac{T_s}{T_s - t_{11}}
\]

where

\( l_1 \) : spray tip penetration

\( l_2 \) : distance between position of visible flame and nozzle tip

\( l_3 \) : distance between flame front growing in the direction of spray tip and nozzle tip

\( l_4 \) : distance between flame front growing in the direction of nozzle tip and nozzle tip

\( l_5 \) : distance between limit position of flame front growing in the direction of nozzle tip and nozzle tip

\( V_f \) : velocity of flame growth in the direction of spray tip

\( V_n \) : velocity of flame growth in the direction of nozzle tip

Fig. 7 Model of process of premixed flame burning and diffusion flame burning during period of injection
The premixed mixture with stoichiometric ratio is burnt out when the flame reaches the spray tip. Then following conditions are obtained:

\[ \ln \frac{dQ_e}{dt} = 1 \quad \text{and} \quad \frac{dQ_e}{dt} = 0, \]

if \[ \ln \frac{dQ_e}{dt} < 1 \]

(17)

As a consequence, from the first break-out of a visible flame to the end of injection, the rate of heat release \( dQ_e/dt \) by premixed flame burning and the rate of heat release \( dQ_e/dt \) by diffusion flame burning are obtained by solving simultaneous equations (1) through (16) with the conditions (17) and (18). The total rate of heat release \( dQ_e/dt \) can be given as the summation of \( dQ_e/dt \) and \( dQ_e/dt \).

Calculation of ROHR after End of Injection

The volume \( V_{nj} \) [m³] of main jet region and the concentration \( C_{nj} \) [kg/m³] of fuel in main jet region, that is, the mass of fuel in a unit volume of main jet region, are expressed as following forms, by applying the experimental results on temporal concentration profile in non-steady hydrogen jet (14):

\[ V_{nj} = V_{nj}(t) \exp\left(\frac{-t}{\tau_1}\right) \]

if \( t > \tau_0 \)

(19)

\[ C_{nj} = C_{nj}(t) \exp\left(\frac{-t}{\tau_2}\right) \]

if \( t > \tau_0 \)

(20)

where

- \( \tau_0 \): time at end of injection [s]
- \( V_{nj}(t) \): volume of main jet region at end of injection [m³]
- \( t \): time from start of injection [s]
- \( \tau_1 \): time constant as for the rate of decrease in volume of main jet region after end of injection [s]
- \( C_{nj}(t) \): concentration of fuel in main jet region at end of injection [kg/m³]
- \( \tau_2 \): time constant as for the rate of decrease in concentration of fuel in main jet region after end of injection [s]

Furthermore, it is assumed that the fuel diffused from main jet region is burnt out and the unburnt fuel lies only in main jet region. Then the spray after the end of injection is devided into burnt region and unburnt region, as shown in Fig. 8. Cumulative heat release \( Q \) [J] after the end of injection is expressed by

\[ Q = H_i \left( M_{ro} - V_{nj} \cdot C_{nj} \right), \]

if \( t > \tau_0 \)

(21)

where

- \( H_i \): low calorific value of fuel [J/kg]
- \( M_{ro} \): total injected quantity of fuel in mass [kg]

The mass \( M_{nj}(t) \) of unburnt fuel in main jet region at the end of injection is written by
following form:

\[ M_{a1}(t_{ro}) = V_{a1}(t_{ro}) C_{a1}(t_{ro}) \]  \hspace{1cm} (22)

Substituting equations (19) and (20) into Eq. (21), and rearranging with Eq. (22) the following relation is obtained:

\[ Q = H_t \left( M_{ro} - M_{a1}(t_{ro}) \right) \exp\left( - \frac{t - t_{ro}}{\tau} \right) \]

if \( t > t_{ro} \)  \hspace{1cm} (23)

Hence the time constant \( \tau \) [s] as for the rate of decease in mass of unburnt fuel in main jet region after the end of injection is written by following relation:

\[ \frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2} \]  \hspace{1cm} (24)

Differentiating both sides of Eq. (23) with respect to the time \( t \), the rate of heat release \( \frac{dQ}{dt} \) [J/s] after the end of injection is expressed as follows:

\[ \frac{dQ}{dt} = \frac{H_t M_{a1}(t_{ro})}{\tau} \exp\left( - \frac{t - t_{ro}}{\tau} \right) \]

if \( t > t_{ro} \)  \hspace{1cm} (25)

At the time when the injection is ended, the continuity of the ROHR and cumulative heat release should be satisfied between the injection period and after the injection. The unknown factor can be obtained by solving this condition.

Figure 9 displays the schematic model of ROHR obtained from above-mentioned method. ROHR starts at first break-out of visible flame. The region A shows premixed flame burning controlled by the consumption of stoichiometric mixture at the layer of premixed mixture. At the first peak, the pre-mixed flame passes through the thickest part of the layer of premixed mixture.

The region B expresses diffusion flame burning controlled by the quantity of surrounding charge entrained into mixing flow region after passage of premixed flame. The region C shows also diffusion flame burning controlled by the break-out of main jet region.

COMPARISON OF ROHR FROM MEASURED DATA WITH ROHR FROM CALCULATION

The rate of heat release calculated from this model were compared with that obtained from a single cylinder research engine operations at changing compression ratio, boost pressure and injection timing.

Fig. 10 An example of ROHRs obtained from prediction and from experiment

Fig. 11 Effect of injection start timing on predicted and measured ROHRs
Fig. 12 Effect of compression ratio on predicted and measured ROHRs

Fig. 13 Effect of boost pressure on predicted and measured ROHRs

TEST ENGINE

The rate of heat release were measured with the medium-speed single-cylinder direct injection diesel engine. The details of the engine specification is shown in Table 1.

Table 1. Specification of experimental engine

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>250 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>320 mm</td>
</tr>
<tr>
<td>Rated Output</td>
<td>177 kW</td>
</tr>
<tr>
<td>Rated Speed</td>
<td>750 rpm</td>
</tr>
<tr>
<td>Rated B.M.E.P.</td>
<td>1.79 MPa</td>
</tr>
</tbody>
</table>

RESULTS AND DISCUSSION

Figure 10 shows an example of predicted and experimentally obtained ROHRs. The predicted ROHR reflects the typical diesel combustion phenomena, those are, the premixed and diffusion burnings. The model further expresses the phenomenon after the injection well, which have not been able to be described properly by most of previously published models. Present model intends to predict three different combustion periods with suitable description of each phenomena, while most of previous models have employed one mechanism to predict through the combustion periods.

Present model however tends to estimate the premixed burning effects higher and the diffusion
Fig. 14 Typical examples of Pressure-Crank angle diagrams as a function of injection start timing obtained from prediction and from experiments

(b) Measured data

Fig. 15 The relation between specific fuel consumption and injection timing

177 kW/750 rpm
Compression ratio 12.6
Boost pressure 0.160 MPa
Injection start timing
11.0 degCA BTDC
15.3
16.7

occurred at several points in the actual engine (20). The multi point ignition would shorten the premixed flame burning.

Present model indicates the effect of engine parameters well. Figure 11 shows, for example, the effect of injection start timing on predicted and measured ROHRs. The predicted results indicate the effects of injection start timing qualitatively well, i.e., the first peak of ROHR due to premixed burning increases and the second one due to diffusion burning decreases as the injection start timing is advanced.

Figure 12 shows the effects of compression ratio. In both experiments and prediction, combustion starts and finishes at early crank angle as compression ratio increases. Figure 13 shows the effects of boost pressure.

Engine performances are predicted sufficiently, although there lie some quantitative differences between predicted and experimentally obtained ROHRs.

Figure 14 shows typical examples of pressure-crank angle diagrams as a function of injection start timing obtained from prediction and from experiments. Prediction gives similar pressure diagram to experimental one.

Figure 15 shows the relation between specific fuel consumption and injection start timing under the same conditions represented as a form of difference against at injection timing of 11.0 deg BTDC. Specific fuel consumption decreases as injection start timing advances. The predicted specific fuel consumption gains agree with experimentally measured one within the tolerance of measurement.

From the comparisons above, the availability of the model has been confirmed to predict engine performance. And also this combustion model will be the base for predicting NOx, Soot and so on in the future, because the model is faithful to the combustion phenomena. The results could suggest that the simulation by the simple model intended to estimate the tendency of engine performance is very useful for a strategic decision of engine development.
CONCLUSIONS

The relations among ROHR, characteristics of diesel spray and combustion processes of diesel spray, which is injected into a quiescent atmosphere with a high pressure at a high temperature, have been discussed with detailed experiments. Using these relations the model of combustion processes of diesel spray is proposed. And the comparison with ROHR calculated by this model and that obtained from single cylinder engine data is presented in this paper.

The following conclusions can be drawn:
(1) The present model of combustion processes of diesel spray expresses fully the tendency of ROHR obtained from experimental data.
(2) The period of premixed flame burning is controlled by the consumption of stoichiometric mixture in length of premixed mixture formed at spray envelope.
(3) The heat release by diffusion flame until end of injection is controlled by the quantity of surrounding charge entrained into burnt region of length of premixed mixture.
(4) The heat release by diffusion flame after end of injection is controlled by the break-out of main jet region.

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