Modeling Ignition and Combustion in Direct Injection Compression Ignition Engines Employing Very Early Injection Timing*

Takeshi MIYAMOTO**, Tadashi TSURUSHIMA***, Naoki SHIMAZAKI***, Akira HARADA****, Satoru SASAKI*****; Koichi HAYASHI******, Yasuo ASAUMI******* and Yuzo AOYAGI****

An ignition and combustion model has been developed to predict the heat release rate in direct injection compression ignition engines employing very early injection timing. The model describes the chemical reactions, including low-temperature oxidation. The KIVA II computer code was modified with the present ignition and combustion model. The numerical results indicate that the model developed in this work reproduces major features of two-stage autoignition, as well as experimentally observed trends in NOx and unburned fuel emissions. The computational results show that fuel injection timing significantly influences NOx emissions. Results also indicate that fuel droplets that enter the squish region possibly become unburned fuel emissions. Some graphical results demonstrate the relationships among the in-cylinder fuel spray distributions, fuel-air equivalence ratio, temperature, and mass fractions of NO and unburned fuel.

** Key Words: **Ignition, Combustion, Diesel Engine, Compression Ignition Engine, Computational Fluid Dynamics

1. Introduction

An engine combustion method, where fuel lean mixtures formed by directly injecting fuel in the compression stroke are automatically ignited, is a promising combustion method that allows NOx and smoke emissions to be very low. Takeda et al.(1) experimentally studied an extremely early direct injection compression ignition engine using diesel fuel, and achieved combustion with little emissions of both of NOx and smoke. They call this combustion concept PREDIC (PREmixed lean Diesel Combustion), since they have aimed to make premixed lean combustion in diesel engines. Afterwards, multi-dimensional numerical simulation with the Magnussen combustion model(2) was tried in order to examine the possibility of computational prediction(3). That simulation qualitatively reproduced experimental tendency of spray shapes, timing of heat release, in-cylinder pressure, NOx emissions. However, the heat release rates versus crank angle were insufficiently predicted. The calculation results have only one peak in each curve of heat release rate versus crank angle, although the engine combustion actually shows two peaks in the heat release rate curve in the case of very early fuel injection. The cause of inaccurate predictions is that the calculation model did not include any low oxida-
tion chemical reactions.

The objective of this study is to sufficiently predict the heat release rate of direct injection compression ignition engines employing very early injection timing. The authors developed a new ignition and combustion model by considering both turbulent mixing and reduced chemical kinetics including low temperature oxidation. The new model was examined by simulating engine combustion, using the KIVA II computer code.

2. Nomenclature

\( A \): preexponential factor

\( CN \): cetane number

\( F \): vaporized fuel that was mixed with oxygen at a temperature not greater than \( T^* \)

\( F^* \): vaporized fuel that was mixed with oxygen at a temperature greater than \( T^* \)

\( I \): intermediate products in a low temperature oxidation model

\( K \): turbulent kinetic energy

\( M \): all chemical species

\( P \): pressure

\( R \): chemical reaction rate

\( Sc \): turbulent Schmidt number

\( SMR \): Sauter mean radius

\( T \): temperature

\( T^* \): threshold temperature

\( U \): flow velocity vector

\( Y \): intermediate products in a low temperature oxidation model

\( k \): reaction rate coefficient

\( r \): stoichiometric oxygen mass required to burn unit mass of fuel

\( t \): time

Greek

\( \Gamma \): mass exchange rate per unit volume

\( \varepsilon \): dispersion rate of turbulent kinetic energy

\( \mu_\text{e} \): effective viscosity

\( \rho \): density

Subscripts

\( AC \): activation (temperature)

\( EVAP \): evaporation

\( FB \): vaporized fuel before mixing with oxygen

\( F\text{CHEM} \): fuel oxidation

\( FMIX \): turbulent mixing between vaporized fuel and oxygen

\( H \): turbulent mixing between vaporized fuel and high temperature oxygen

\( L \): turbulent mixing between vaporized fuel and low temperature oxygen

\( U \): unburned fuel

0: a standard condition

3. Ignition and Combustion Model

The following are the assumptions for modeling ignition and combustion.

1. The gaseous flow can be expressed by ensemble-averaged (Reynolds-averaged) equations.

2. The states of vaporized fuel are represented by only two ones, although the number of the possible states is very large. The first state is assigned to fuel mixed with oxygen not sufficient to react and the second state is assigned to fuel mixed with oxygen sufficient to react. Additionally, the oxygen concentration in the second state is regarded as same as the local oxygen concentration obtained by solving the ensemble-averaged equations of fluid dynamics.

3. When turbulence mixed vaporized fuel with oxygen is sufficient and the local temperature at that mixing area is not higher than \( T^* \), it is assumed that the vaporized fuel mixed with oxygen is treated as chemically reactive fuel species \( F \). On the other hand, if the local temperature is higher than \( T^* \) at that time, the vaporized fuel mixed with oxygen is assumed to be treated as \( F^* \) instead of \( F \). \( F^* \) is chemically reactive fuel that includes propulsive chemical species.

4. For all of chemical species except fuel species (FB, F, F*), the effects of microscopic inhomogeneity of concentration and temperature on chemical reactions are negligible.

5. When a temperature rise by fuel oxidation is not significantly greater than that by compression in a local area, the temperature dominating chemical reaction rates is represented by the ensemble-averaged temperature in the local area.

6. The oxidation process of vaporized fuel \( F \) is categorized into low and high temperature oxidation processes, while that of \( F^* \) is categorized into the high temperature oxidation process only.

7. \( F^* \) is oxidized in the high temperature process as the same chemical species as \( F \).

8. When the concentration of \( F^* \) is greater than a certain value, \( F^* \) is distinguished from \( F \) and is oxidized with a higher reaction rate than that of the high temperature oxidation of \( F \).

9. When an increase in local temperature in a computational control volume caused by fuel oxidation is much greater than that caused by compression, the rate control factor of combustion in that control volume is regarded as chemical reaction or turbulent mixing.

Figure 1 shows a schematic process of fuel consumption in cylinders of direct injection compression ignition engines. The hatched part in the figure is modeled in this study. Based on the above stated
Fig. 1  Block diagram of modeled fuel consumption process

assumptions, the fuel mass conservation equations can be written in the form:

\[ \frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f U) = 0 \]

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where \( \rho_{\text{mix}} \) is turbulent mixing rate. Referring to literature reported by Ikegami et al.\(^9\), \( \rho_{\text{mix}} \) can be obtained by the Magnussen's form\(^9\) Eq. (4) including a model constant \( B \).

Chemical reaction equations (R1) - (R5) in Fig. 1 are described concretely in the following. The fuel is represented by \( n \) - dodecane. A reduced kinetic reaction scheme presented by Schreiber et al.\(^8\) is applied to describe the low temperature oxidation mechanism. In this scheme, intermediate products, which appear in the low temperature oxidation process, are represented by means of I and Y. Species I represents oxygenated intermediate products. Y represents intermediate chain-propagating species including OH radical.

\[ \begin{align*}
F + 2O_2 & \rightarrow I \quad \text{(R1)} \\
I & \rightarrow 2Y \quad \text{(R2)} \\
2Y + 5O_2 + F & \rightarrow 24CO_2 + 26H_2O \quad \text{(R3)} \\
2F + 37O_2 & \rightarrow 24CO_2 + 26H_2O \quad \text{(R4)} \\
2F^* + 37O_2 & \rightarrow 24CO_2 + 26H_2O \quad \text{(R5)}
\end{align*} \]

In the above chemical reaction equations, Eqs. (R1) - (R3) correspond to the low temperature oxidation mechanism. At first, the chemical reaction (R1) produces I, peroxyde of fuel F, secondly, the reaction (R2) produces Y, and at last, Y is consumed to release heat. But this heat release or compression caused by a piston rise increases the temperature to intensify the backward reaction in Eq. (R1). When the temperature is sufficiently increased, that backward reaction stops producing species I. This causes to end the heat release by the reaction (R3). More increase in the temperature leads principal heat release by the reaction (R4). The reaction (R4) mainly corresponds to the high temperature oxidation process, while it is regarded that the reaction (R4) includes a part of the low temperature oxidation.

When the vaporized fuel is mixed with oxygen where the temperature \( T \) is higher than \( T^* \), fuel oxidation process is modeled using the assumptions (6)\(^-\) (8). First, \( F^* \) is accumulated by Eqs. (3) and (6). When the molecular fraction of \( F^* \) becomes equal to or greater than a certain value \( S_{\text{mix}} \), \( F^* \) is oxidized by the reaction (R5) whose reaction rate is faster than that of the reaction (R4). When the molecular fraction of \( F^* \) is lower than \( S_{\text{mix}} \), \( F^* \) is treated as the same species as F, regarding that \( F^* \) can be reacted by (R4).

The rate Eqs. (7)\(^-\) (10)\(^6\), (11) and (12)\(^5\) for the reaction (R1) - (R5) are expressed by the following equations:

\[ R_{i,j} = k_{j,i}[F][O_2][M][\text{Products}]^{\nu} \quad \text{(7)} \]

\[ R_{i,j} = k_{i,j} \quad \text{(8)} \]

\[ R_{i,j} = k_{i,j} \quad \text{(9)} \]

\[ R_{i,j} = k_{i,j}[O_2][Y] \quad \text{(10)} \]

\[ R_{i,j} = k_{i,j} \quad \text{(11)} \]

where \( k_{i,j} \) is rate constant described by:

\[ k_i = A_i \exp(-T_{ac}/T^*) \quad \text{(13)} \]

The subscript \( i \) denotes chemical reaction numbers added to "R"s in Eqs. (R1) - (R5). The subscripts \( f \) and \( b \) correspond to forward and backward reactions, respectively. \( T_{ac} \) denotes activation temperature, which equals activity energy divided by universal gas constant. \( C_{\text{fr}} \) and \( C_b \) are constants to express the difference in ability of ignition, which are written in the following forms\(^6\) using an octane number \( N_o \).

\[ C_{\text{fr}} = (110 - N_o)/10 \quad \text{(14)} \]

\[ C_b = C_{\text{fr}} \quad \text{(15)} \]

In Fig. 2, a modeled combustion process through reactions (R4) and (R5). Instead of \( R_i \) and \( R_b \), we use \( R^f \) and \( R^b \), respectively, to calculate the reaction rates of (R4) or (R5) considering the microscopic heterogeneity of temperature and turbulent mixing.

\[ R^f = \min(R_i, R_{i,j} + R_{\text{mix}}) \quad \text{(16)} \]

\[ R_{\text{mix}} = D(E/K)[F]/a[(\text{Products})/M] \quad \text{(17)} \]

\[ R^b = \min(R_i, R_{i,j} + R_{\text{mix}}) \quad \text{(18)} \]
The governing equations of spray droplets and gas phase are coupled with the same equations, which describe droplet evaporation, droplet aerodynamic drag, heat exchange between droplets and their surrounding gas, and so on. To improve the original KIVA II code, we adopt a spray/wall collision submodel and as well as previous paper and the present autoignition and combustion model.

The autoignition and combustion model is incorporated here to KIVA II, mainly by adding some chemical reaction rate equations to the source code of CHEM, one of the subroutine programs of KIVA II. Those additional rate equations include the chemical reaction rates of Eqs. (7) and (8), which describe the rates of the first reaction (R1) in the low temperature reaction mechanism. If the forms of those rate equations were directly used, the numerical solution could not converge under high temperature conditions, because of an explicit solution procedure employed in CHEM. To avoid this problem, \( R_{REC} \) and \( R_{LOC} \), which are calculated by the following equations (20) – (24), are used for \( R_{17} \) and \( R_{18} \), the rate of chemical reaction (R1).

\[
R_{17} = k_{17}[F][O_2][M][P/P_0]^{2/3}C_{17} \quad (R_{17}^* > 0)
\]
\[
R_{REC} = 0 \quad (R_{17}^* \leq 0)
\]
\[
R_{LOC} = 0
\]

The \( R_{17}^* \) and \( k_{17} \) are expressed by the equations:

\[
R_{17}^* = R_{17}/(1 - c_d k_{17}[P/P_0]^{2/3})
\]
\[
k_{17} = k_{17}/[1 - 1/(1 + c_d[P/P_0]^{2/3}(k_0/k_{17})]]
\]

where \( \Delta t \) is the computational time step. In the present computations, the coefficient \( c \) in Eq. (23) was set to 0.1. Equations (20), (22) and (24) are obtained by applying a quasi steady state assumption to the concentration of intermediate species I. The Eqs. (21) and (23) imply that if the backward reaction returns I, which is produced in \( \Delta t \), it is \( P \) in \( c_d \Delta t \) (a very short time compared to \( \Delta t \)), then reaction (R1) is regarded as being in equilibrium.

5. Computational Conditions

Table 1 shows the constants of the present model. Figure 3 shows the specifications of the engine and the operating conditions. Assuming that the flow and sprays were three dimensional and axisymmetric, 45 grids were used in the radial direction and up to 90 grids in the axial direction in the engine cylinder. Some values of the model constants in Table 1 were assumed using the results of parametric pre-calculations. Each of them has a supplementary comment "Present" instead of a reference number in parentheses in Table 1. The pre-calculations were performed under the basic conditions shown in Fig. 3, with
Table 1 Model constants

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$A_i$ [mol·cm⁻³·sec⁻¹]</th>
<th>$T_{cal}$ [1000K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(R1)</td>
<td>$3.5 \times 10^{10}$ (Ref. (6))</td>
<td>19.5 (Ref. (6))</td>
</tr>
<tr>
<td>(R1b)</td>
<td>$6.0 \times 10^{10}$ (Ref. (6))</td>
<td>37.5 (Ref. (6))</td>
</tr>
<tr>
<td>(R2)</td>
<td>$6.0 \times 10^{11}$ (Ref. (6))</td>
<td>59 (Ref. (6))</td>
</tr>
<tr>
<td>(R3)</td>
<td>$1.5 \times 10^{10}$ (Present)</td>
<td>16.5 (Ref. (6))</td>
</tr>
<tr>
<td>(R4)</td>
<td>$1.1 \times 10^{10}$ (Present)</td>
<td>15.1 (Ref. (7))</td>
</tr>
<tr>
<td>(R5)</td>
<td>$3.0 \times 10^{11}$ (Present)</td>
<td>15.1 (Ref. (7))</td>
</tr>
</tbody>
</table>

Other model constants assumed in the present study

<table>
<thead>
<tr>
<th>B</th>
<th>CTH</th>
<th>D</th>
<th>T* [K]</th>
<th>SMDC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>2.2</td>
<td>240.0</td>
<td>750.0</td>
<td>0.0028</td>
</tr>
</tbody>
</table>

Fig. 3 Combustion chamber schematic and basic engine parameters

Injection timings at 120 degree of crank angle before top dead center TDC (−120 deg. ATDC) and TDC (0 deg. ATDC). The model constants $B$, $D$ for turbulent mixing, $C_{TH}$, $A_3$, and $A_4$ for reaction rates were adjusted so that the calculated heat release rate could agree with the measured one in the case of that injection timing of −120 deg. ATDC. The injection timing of TDC was selected as a representative condition where fuel spray is injected in high temperature air. Assuming a threshold temperature $T^*$ and a constant for reaction rate $A_3$ as shown in Table 1, the pre-calculations for TDC injection were performed to adjust a molecular concentration threshold $S_{MIN}$ in order that the calculated heat release rate might agree with the measured one. The standard enthalpy of formation of chemical species I as well as $Y$ was assumed to be equal to that of fuel $F$ ($n$-dodecane), whose enthalpy datum is automatically quoted from a fuel library in KIVA II.

In addition to the reaction equations (R1) - (R5), we used three kinetic reaction equations describing the extended Zeldovich mechanism and six chemical equilibrium equations in order to predict the amount of NO emissions. The attached input data of KIVA II software package for these nine chemical reactions were used for the rate and equilibrium constants, without any consideration of the process of microscopic turbulent mixing. We consider that the qualitative tendency of NO emissions can be predicted without consideration of the turbulent mixing process, since it is expected that microscopic heterogeneity of the mixture concentration is relaxed well and that the rate of NO production kinetics is relatively slow compared to that of combustion mechanism.

A pintle swirl nozzle (Fig. 4) with 100 MPa fuel injection pressure was used in an engine experiment to be compared with the present computations. The injection speed of fuel at the nozzle exit was assumed to be 200 m/s based on the nozzle geometry and injection pressure. “cone” and “dcone” in Fig. 4 denote injection direction and its scatter respectively, which are defined as input data of KIVA II. We assumed “cone” and “dcone” are 70 and 20 degrees respectively, expecting from the nozzle geometry. We assumed $\chi^2$ distribution for initial fuel droplet diameter, and didn’t use any models describing droplet breakup or coalescence. The initial Sauter mean radius of fuel droplets $SMR_i$ was assumed to be written in the form:

$$SMR_i=SMR_0\left(\frac{\rho_\infty}{\rho_0}\right)^p$$

The empirical coefficients $G$ and $SMR_0$ were determined so that KIVA II computational plots of droplet parcels would agree with spray photographs obtained by laser light sheet in a visualization chamber as shown in Fig. 5. $\rho_\infty$ denotes air density under a
standard condition, $\rho_A$, density of ambient air. $\rho_A$ was assumed to equal 1.15 kg/m$^3$. Using this assumption, $G$ and $SMR_0$ were determined to be 0.25 and 7.5 micrometers, respectively. To make computations for engine combustion, the input data of initial Sauter mean radius of fuel droplets were calculated using Eq.(25) with $\rho_A$ of in-cylinder air at injection start.

In this study, it was assumed that the compression started from the bottom dead center. The temperature of in-cylinder gas at the compression bottom dead center as the initial temperature was set at 355 K, which was predicted from the experimental data of in-cylinder pressure before combustion. The piston and cylinder were assumed to be always at a temperature of 400 K.

6. Results and Discussion

6.1 Comparison with experimental results

Fixing the computational conditions described in the former section, we made computations with varied injection timing. The results were compared with the experimental results reported by Harada et al.\(^{(9)}\) to examine the validity of the present model. The results are shown in Fig. 6. The measurement data show that every heat release rate curve vs. crank angle has two peaks in earlier fuel injection timing cases. We consider that the heat release of the low temperature oxidation leading the one of the high temperature oxidation causes this two-peaked heat release curve, since the fuel–air mixture is formed at a low temperature. Moreover, each curve of the measured heat release rates with later injection timing shows only one peak. These experimental tendencies are reproduced by the computations with the present model. The effects of injection timing on the timing and period of heat release are also reproduced by the computations. The experimental data of heat release rate were obtained by the pressure data, while the pressure results from not only chemical heat release but also release of latent heat and heat exchange between in-cylinder gas and solid walls. Therefore, individual comparison for those items between computations and experiments is desired to make more detail examinations.

Figure 7 shows the effect of injection timing on measured and calculated emissions. In this figure, the model yields NO$_x$ and unburned fuel emissions on the left side, which are NO$_x$ and unburned fuel mass...
emissions normalized by injected fuel mass. As experimental results to be compared with computational results of unburned fuel emissions, smoke and total hydrocarbon emissions (THC) are shown on the lower right side in Fig. 7 since both of them indicate incompleteness of combustion. The figure shows qualitatively good agreement between computational and experimental results of the emissions. The comparisons can be concluded that the present model is proper, at least under the conditions in this study. Using visualized results of the computations, the relation among the injection timing, the heat release start region in the engine cylinder and the emissions will be demonstrated in the following.

6.2 Relation between fuel injection timing and heat release start region

The region, where heat release starts at the earliest time in the cylinder, is greatly related to fuel injection timing. Retarding the injection timing, the spray-dispersed area is restricted within a smaller region because of higher air density and smaller distance between the injection nozzle exit and the piston head (Fig. 8). This leads to a fuel rich mixture, which consists of vaporized fuel and air (Fig. 9). Before the reaction with heat release, the richer the mixture is, the lower the temperature (Fig. 9). The region where chemical reaction progresses earlier compared to the other region is determined by suitable combination of the concentration and temperature, because the concentration and temperature dominate the chemical reaction rate. Figures 10 and 11 show the distributions of mass of combustion products when the heat release rate begins to rise (See Fig. 6). In these figures, the region where the mass fraction of combustion products corresponds to the heat release region. The results show that relatively uniform mixture distribution (Injection timing = −120 deg. ATDC) causes a wider region of heat release, while the mixture in the other case starts heat release in a narrower region near the boundary of the mixture and pure air regions. Note that we make no distinction between, FB, F and F* in Figs. 9, 11 and 12.

6.3 Effects of injection timing on emissions

In this engine, fuel droplets in the earlier injection case where the injection timing is 120 deg. BTDC are dispersed over a wider range (Fig. 8(a)). This causes an entirely leaner mixture (Fig. 9(a)) result-
ing in a relatively uniform and lower increase in temperature compared to the other cases (Fig. 12(a)). Then it is hard for that early injection case to produce a high temperature. This means, it is hard for such early injection to produce NO\textsubscript{x} emissions except too high in-cylinder average temperature that could be caused by excessive fuel quantity, excessive compression ratio or excessive advanced ignition timing. On the other hand, the fuel droplets impinged on the piston wall during injection become unburned fuel emissions in squish region (Fig. 12(c)). If the injection timing is later than 100 deg. BTDC, spray dispersion is restricted to make fuel-air mixture region narrow (Fig. 8(b)). This causes a higher temperature region after combustion (Fig. 12(a)). NO is produced in that higher temperature region (Fig. 12(b)). As shown by experimental and computational results in Fig. 7, if the fuel is injected after the timing that obtains maximum NO\textsubscript{x} emissions, unburned fuel emissions are increased while retarding the injection timing toward top dead center. Figure 11(b) indicates that impingement of fuel spray droplets on the piston wall makes a mixture too rich, which can be the main cause of unburned fuel emissions.

7. Conclusions

An autoignition and combustion submodel has been developed by considering reduced chemical reaction mechanisms including a low temperature oxida-
tion process, which are combined with turbulent mixing processes. The present submodel has been incorporated into the KIVA II multidimensional computer simulation program to conduct numerical simulations of combustion in a compression ignition engine employing extremely early injection timing.

The computational results show the typical time history of heat release rate, which is produced by this kind of engine. The results also show good agreement with the experimentally observed trends in the effects of fuel injection timing on heat release rate and NOx and unburned fuel emissions.

Furthermore, the following are shown by the computational results. The fuel injection timing influences the region of heat release start, through the spatial distribution of the fuel spray droplets, which affects the spatial distribution of temperature and equivalence ratio before combustion. This means that the fuel injection timing affects the temperature distribution before and after combustion, which dominates the region of NOx production and its total amount. Extremely early fuel injection makes the fuel droplet distribution in the cylinder very wide to cause an overall lean fuel mixture, which restrains the increase in the in-cylinder temperature to realize low NOx combustion. Regardless of the injection timing, fuel spray impinging on the piston wall makes a rich mixture. Therefore, the spray wall impingement can be a cause of unburned fuel and smoke emissions.

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