Numerical Simulation of Premixed Lean Diesel Combustion in a DI Engine

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ABSTRACT

Relationship among fuel injection, fuel-air mixture formation, combustion and emissions for a PREmixed lean Diesel Combustion (PREDIC) engine has been studied numerically by the KIVA II modeling package. The software was modified with an improved autoignition and combustion submodel, which describes the formation of combustible or ignitable fuel-air mixtures by turbulent mixing, and describes four chemical reactions, including low-temperature oxidation. Definitions of a weighted mean mixture ratio and a fuel-air mixture length scale have been introduced and used to obtain overall fuel-air mixture characteristics. The results show that two stage ignition is successfully predicted by the present model, and that the advantage of extremely early fuel injection for lean mixture formation consists of not only a longer mixture formation period, but also the possibility of grater mixture penetration.

INTRODUCTION

It is known that premixed lean diesel combustion engines are able to achieve smokeless and low NOx operation by extremely early direct fuel injection [1-3]. Takeda et al. call this type of combustion PREDIC(PREmixed lean Diesel Combustion) [1]. Their report indicates that the PREDIC fuel-air mixture formation process should be controlled for development of practical PREDIC engines. To control the fuel-air mixture formation process, the relationship among fuel injection, fuel-air mixture formation, combustion and emissions, should be known. However, the relationship has not been clarified yet. To this end, numerical simulation of injection and combustion in a PREDIC engine has been conducted using a modified version of the KIVA II [4] modeling code. This version of KIVA was updated with an improved autoignition and combustion submodel, which describes the formation of combustible or ignitable fuel-air mixtures by turbulent mixing and four chemical reactions, including low temperature oxidation. A method of fuel-air mixture characterization has been introduced and used to analyze the numerical results. This method provides the average value of physical quantities in the fuel-air mixture, and the size of fuel-air mixture region. The computations were applied to reproduction and interpretation of some experimental results.

COMPUTATIONAL MODELS

KIVA II Submodels

The conservation equations of species, mass, momentum, and energy for the gas and droplets, and the k-ε turbulence model considering droplet motion used in this study are the same as in the KIVA II computer program. The spray-wall interaction model developed by Naber and Reitz [5] is used along with the original KIVA II models. Furthermore, three kinetic reaction equations describing the extended Zeldovich mechanism, and six chemical equilibrium equations are used to predict the mass of NO emissions. Since the chemical reactions are considered without microscopic or instantaneous inhomogeneities, the emission mass can only be predicted in a qualitative fashion. The following model has been incorporated into the KIVA II code to predict the rate of heat release due to auto-ignition and combustion.

Autoignition and Combustion Model

The autoignition and combustion model used here describes the formation of combustible or ignitable fuel-air mixtures by turbulent microscopic mixing [6], and also describes a four-step chemical reaction mechanism, which includes the low temperature oxidation reactions [7].

The mass conservation equations of vaporized fuel before and after turbulent mixing can be written in the form:

\[
\frac{\partial \rho_n}{\partial t} + \nabla \cdot (\rho_n \mathbf{U}) = \nabla \cdot \left( \frac{\mu_e}{\text{Sc}} \nabla \left( \frac{\rho_{EVAP}}{\rho} \right) \right) + \Gamma_{EVAP} - \Gamma_{FMIX}
\]

\[ (1) \]

\[
\frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v \mathbf{U}) = \nabla \cdot \left( \frac{\mu_e}{\text{Sc}} \nabla \left( \frac{\rho_{FMIKX}}{\rho} \right) \right) + \Gamma_{FMIX} - \Gamma_{FCHEM}
\]

\[ (2) \]

where \( \rho_n \) indicates the density of vaporized fuel before turbulent microscopic mixing, \( \rho_v \) indicates the density of microscopically mixed fuel(vapor) with oxygen, which is ignitable or combustible. \( \mathbf{U} \) denotes the fluid velocity vector, while \( \rho \), \( \mu_e \), and \( \text{Sc} \) are the density, effective viscosity, and effective Schmidt number of the gas, respectively. \( \Gamma_{FMIX} \) and \( \Gamma_{FCHEM} \) are the rate of mass exchange by turbulent mixing, droplet evaporation, and chemical reaction, respectively. \( \Gamma_{EVAP} \) is obtained by the evaporation model used in KIVA II. The equation to evaluate \( \Gamma_{FMIX} \) is given by [6,8]:

...
where B is a model constant, τ (kg/kg) is the stoichiometric oxygen required to burn 1 kg of fuel, k and ε are the local turbulence kinetic energy and dissipation rate, respectively, which are obtained from their own conservation equations employed in the original KIVA II code.

\[ \Gamma_{\text{CHEM}} = \text{B} \cdot (\varepsilon / k) \min \left( \rho_{\text{fb}} \cdot \rho_{\text{ot}} / \tau \right) \]  

(3)

Equations (R1)-(R3) describe a reduced low temperature kinetic oxidation mechanism, based on the reduced scheme introduced by Schreiber et al. [7]. It is assumed here that their low temperature oxidation mechanism can be applied to auto-ignition of diesel fuel, even though their model was based on experimental data of iso-octane and n-heptane. F denotes vaporized diesel fuel, represented by n-dodecane, which is microscopically mixed with O₂ by turbulence. Species I represents an oxygenated product radical, and Y represents a chain-propagating species. Reaction (R4) represents the simplest description of high temperature oxidation. This four-step scheme needs only two species and three chemical reaction equations, in addition to the commonly used single step scheme described by reaction (R4). The rate of reaction for (R1)-(R3) is given by [7]:

\[ R_{\text{f}} = k_{\text{f}}[F][O_2][M](p/p_0)^{2.2}C_{\text{ir}} \]  

(4)

\[ R_{\text{i}} = k_{\text{i}}[I](p/p_0)^{3.5} \]  

(5)

\[ R_2 = k_2[I]C_2 \]  

(6)

\[ R_3 = k_3[I][O_2][Y] \]  

(7)

where \( R_f \) and \( R_i \) are the rates of reactions (R1)-(R3), and subscripts f and i indicate forward and backward rates, respectively. \( k_f \) and \( k_i \) are the rate constants for the Arrhenius-type reactions (R1)-(R3), and \([M]\) is the total concentration of all species. The empirical coefficients \( C_{\text{ir}} \) in Eq. (4) and \( C_2 \) in Eq. (6) are regarded as functions of the fuel octane number. The reference pressure \( p_0 \) corresponds to 1MPa. To calculate the rate of reaction (R4), the following equation is used:

\[ R_4 = k_4[F]^{2.5}[O_2]^{1.5} \]  

(8)

The numerical solutions of Eqs. (R1)-(R3) and (4)-(7), may not be stable at high temperatures because of the explicit solution method employed in KIVA II. Therefore, the following equations for \( R_{\text{inc}} \) and \( R_{\text{inc}} \) are used instead of \( R_f \) and \( R_i \) to avoid this problem.

\[ R_{\text{inc}} = k_{\text{inc}}[F][O_2][M](p/p_0)^{2.2}C_{\text{ir}} \]  

(if \( R_{\text{f}} > 0 \) )  

(9)

\[ R_{\text{inc}} = 0 \]  

(if \( R_{\text{f}} \leq 0 \) )  

(10)

\[ R_{\text{i}} = R_{\text{f}} \cdot 1 - \varepsilon \Delta t \cdot k_{\text{f}}(p/p_0)^{3.5} \]  

(11)

\[ k_{\text{inc}} = k_4[1-1/[1+C_2(p/p_0)^{1.5}(k_2k_{\text{inc}})])] \]  

(12)

where \( \Delta t \) is the computational time step. In the present computations, the coefficient \( c \) in the Eq. (12) was set to 0.1. Eq. (13) is obtained by applying a quasi-steady state assumption for the concentration of the intermediate I. For reaction equation (R1), Eqs. (10) - (12) imply that if the backward reaction returns fuel consumed by the forward reaction in a very short time (compared to \( \Delta t \)), then reaction (R1) is regarded as being in equilibrium.

The Arrhenius parameters for the rate constants in Eqs. (4)-(8) and the model constant in Eq. (3), which are shown in Table 1, were determined by limited data from a single cylinder PREDIC engine for the present calculations. While these parameters and constants involve some uncertainty, they were fixed in the present calculations in order to predict the relative effects of varying other parameters.

A METHOD OF FUEL-AIR MIXTURE CHARACTERIZATION

The "In-Mixture" Average

To globally characterize fuel-air mixtures, let us employ the concept of a weighted mean, defined by:

\[ \rho_{\text{fb}} = \sum_c \rho_{\text{fb}} \cdot dV \]  

(14)

where \( \rho_{\text{fb}} \) is the fuel-air mass fraction at each control volume. The coefficients \( \rho_{\text{fb}} \) are determined by a user-specified mixing time. The mixing time selected in the present calculations can be used to characterize the fuel-air mixture at each control volume.

Table 1 Arrhenius parameters for reactions (R1)-(R4), heat of formation of I and Y, and model constant B

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( A_i ) (mol·cc·sec)</th>
<th>( E_i / R ) [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(R1)</td>
<td>( 1.0 \times 10^{22} )</td>
<td></td>
</tr>
<tr>
<td>(R1b)</td>
<td>( 6.0 \times 10^{22} )</td>
<td></td>
</tr>
<tr>
<td>(R2)</td>
<td>( 1.5875 \times 10^{8} )</td>
<td></td>
</tr>
<tr>
<td>(R3)</td>
<td>( 5.0 \times 10^{14} )</td>
<td></td>
</tr>
<tr>
<td>(R4)</td>
<td>( 1.2 \times 10^{14} )</td>
<td></td>
</tr>
</tbody>
</table>

Heat of formation at absolute zero [kJ/mol]

| I    | 1 | \(-2.7468 \times 10^{2} \) |
| Y    | 1 | \(-1.6779 \times 10^{2} \) |

Model constant [-] B in Eq. (3)

| B    | 0.4 |

(If \( i=1f \) or 2, the data for \( A_i \) includes \( C_{\text{ir}} \))
where $g_Y$ is the fuel mass weighted mean of an arbitrary physical quantity $g$, $\rho_{F,FB}$ is the local density of vaporized fuel, which consists of vaporized fuel before and after mixing, denoted by subscripts F and FB, respectively. The integral over $dV$ is the volume integral over the in-cylinder region. We call the weighted mean defined by Eq. (14) the "in-mixture average," as opposed to the in-cylinder average.

**Evaluation of the Fuel-Air Mixture Volume**

Using the in-mixture ($Y_F$) and in-cylinder ($Y_C$) averages of the mass fraction of vaporized fuel, an overall volume fraction of fuel-air mixture $X_F$ can be defined as follows:

$$X_F = \frac{V_C}{V_Y}$$  \hspace{1cm} (15)

The limits for $X_F$ are $X_F = 0.0$ to $1.0$. $X_F$ can be regarded as an efficiency or a degree of relative spatial occupation of fuel-air mixture. For example, if the fuel-air mixture has spread over the entire chamber, $X_F$ will be $1.0$.

A fuel-air mixture length scale $L_Y$, can be also defined by:

$$L_Y = \left( X_F \cdot \text{Vol} \right)^{1/3}$$  \hspace{1cm} (16)

where Vol is the volume of the in-cylinder region. The time histories of $L_Y$ can be observed in contrast to a length scale of the in-cylinder region $L_C$. $L_C$ is described by:

$$L_C = \text{Vol}^{1/3}$$  \hspace{1cm} (17)

**COMPUTATIONAL CONDITIONS**

**Fuel Injection Input Parameters**

The directional input parameters for fuel injection, i.e. "cone" or "dcone," the injection velocity $V_{inj}$ (see Fig. 1), and input Sauter mean diameter SMD$_I$, were determined so that the computational spray shapes and the fuel spray photographs were matched in a visualization chamber under certain test conditions. These parameters were assumed to be constant, except for the input Sauter mean diameter SMD$_I$. Since the fuel and injection pressure were not changed in the present study, SMD$_I$ was assumed to be expressed by a simple function of only the ambient gas density given by:

$$\text{SMD}_I = \text{SMD}_I(\rho_o / \rho)^0$$  \hspace{1cm} (18)

where the subscript 0 indicates atmospheric conditions. Three fuel injection nozzles were used to compare the computations and experiments using the assumed input parameters for the fuel injection nozzles shown in Table 2. Fig. 2 shows drawings of the fuel injection nozzle geometry for the three nozzles compared. Below are shown photographs of fuel sprays in a visualization chamber and corresponding calculated spray cross sections obtained using the parameters shown in Table 2.

**Other Conditions for PREDIC Simulations**

A single cylinder engine was used to compare the computations and experiments. Fig. 3 shows the schematic of the combustion chamber and basic engine parameters. Eight different combinations of engine operating conditions used in this study are shown in Table 3. The present (axisymmetric two-dimensional) calculations have been evaluated in terms of how well we could model the effects of injection timing, piston cavity shape, and nozzle configuration. The initial crank angle, at which compression began in the computations, was assumed to be BDC (-180 deg. ATDC). The initial temperatures were determined using the experimental data before ignition. For details of the PREDIC engine experiments, the reader can be referred to Ref. [9].

**RESULTS AND DISCUSSION**

**Comparison Between Computations and Experiments**

Figure 4 shows the effect of injection timing on the calculated and measured emissions. The data for the other parameters were averaged to generalize the effects of the difference in injection timing. Next, Fig. 5 shows the effect of piston cavity...
Table 3 Combinations of engine operating condition to compare the computation with experiment

<table>
<thead>
<tr>
<th>RUN NO.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOZZLE TYPE</td>
<td>A</td>
<td>B</td>
<td>C</td>
<td>C</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PISTON CAVITY</td>
<td>SHALLOW</td>
<td>DEEP</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: Number of computational mesh = 45(r) x 95(z, maximum) for the shallow dish, 44(r) x 100(z, maximum) for the deep dish

shape for nozzle C, in which the data for the injection timing difference were averaged. In these figures, the model yields NO and unburned fuel emissions, while for comparison, the experimental results consist of NO and HC emissions. Both Figs. 4 and 5 show good qualitative agreement between the computational and experimental NO and unburned fuel emissions results.

Figure 6 shows the effects of fuel injector nozzle configuration on the calculated and measured emissions. The results are for the shallow dish chamber, and the data for the injection timing difference were averaged to generalize the effects of the nozzle configuration. These results show good qualitative agreement between the computational and experimental results, except for nozzle A. This discrepancy will be discussed later, with reference to the modeled heat release rate and spray evaporation process.

Figures 7-9 show the heat release rate results. Examination of these plots reveals that the autoignition and combustion model can successfully predict two-stage ignition, and the basic influence of the variation in injection timing, piston cavity shape, and nozzle configuration. The results also indicate that the combustion submodel has a tendency to over-estimate the heat release rate in high-temperature oxidation. The model should be modified by considering the temperature heterogeneities after ignition.

Underestimating the heat release rate for the nozzle A, however, seems to cause the predicted NO emissions to be too low, compared to the other nozzles. Prediction of the in-cylinder overall burning rate depends not only on the predicted results of turbulent mixing rate and the temperature, but also on the fuel evaporation rate and the vaporized fuel concentration distribu-
Fig. 8 Effect of piston cavity shape on heat release rate
(Injection start: -80 deg. ATDC, nozzle type: C)

Fuel Sprays and Fuel-Air Mixtures

Figures 10 and 11 show computational results for the fuel spray particle location and local equivalence ratio just before ignition. The model results show that nozzle B may be the best in terms of evaporation, and also that a large fraction of fuel droplets remain in the squish region for the other two cases. The PREDIC fuel injection should not result in excessive fuel droplets in the squish region, since the fuel-air mixture resulting from these droplets is too rich to be burned completely. Figure 11 also shows that there seems to be too little vaporized fuel with nozzle A, which may be caused by an excessively large input SMD. Therefore, the underestimation of NO emissions for nozzle A might be caused by a failure to input an accurate SMD. This implies that the fuel injection input parameters must be determined more carefully to obtain more realistic model results.

Effect of Injection Timing

Figure 12 shows the predicted effects of injection timing on the mixture size, and NO and unburned fuel emissions. In these calculations, although the input conditions were fixed (ex-
except for the injection timing), the predicted relationship between NO emissions and injection timing shows a similar tendency as that obtained in previous experiments using various fuel injection nozzles [1, 2, 9]. The results confirm that advancing the start of fuel injection results in lower NO emissions because of a lower in-mixture average equivalence ratio. This means the mixture extent is very important to form a lean mixture.

The fuel-air mixture length scale ($L_v$), and the length scale of the chamber ($L_c$) for reference, are shown in Fig. 13, as a function of crank angle. Figure 14 shows the overall volume fraction of fuel-air mixture ($X_v$) as a function of crank angle relative to injection start. These figures indicate that the advantage of extremely early fuel injection for lean mixture formation consists of not only a long mixture formation period, but also an adequate mixture penetration. When the fuel is injected at extremely early stage, the in-cylinder gas density is low, and this allows the fuel-air mixture to penetrate easily.

CONCLUSIONS

The experimentally observed trends in NO and unburned fuel emissions could be reproduced by the present computational model. The sub-model describing autoignition and combustion could predict typical two-stage ignition, but further modification is needed. The concept of an "in-mixture average" was shown to be a useful technique to obtain overall fuel-air mixture characteristics from the results of multidimensional CFD modeling.

The advantage of extremely early fuel injection for lean mixture formation consists of not only a long period of mixture formation but also the level of mixture penetration. The fuel injection process in PREDIC engines should not result in an excessive amount of fuel droplets in the squish region, to maintain low unburned fuel emissions.

REFERENCES