SIMULATING COMBUSTION AND EXHAUST GAS EMISSIONS IN A DI DIESEL ENGINE BY USING A CFD CODE COMBINED WITH DETAILED CHEMISTRY

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1. Introduction

Complicated, fast and unsteady phenomena including the temporal changes of the concentration of chemical species and temperature have been observed during diesel combustion process. Thus, it is beneficial during the process of the engine development that the diesel combustion will be reproduced or even predicted by means of CFD (Computed Fluid Dynamics) codes such as KIVA-3[1] developed by Los Alamos national laboratory in the U.S. With the extensively advanced sub-models used in these CFD codes concerned with atomization and evaporation of fuel spray, current sub-models [i.e. Ref. 2] have consistency with the results of visualization experiments to some extent. Nevertheless, chemical reactions relative to ignition and combustion processes in the calculation codes are usually expressed by those with one or several stages, and unfortunately these simplified reactions can’t properly describe the low temperature oxidation process and the high temperature oxidation process that play important roles in auto-ignition of fuel. Therefore, if the more detailed chemical reactions are considered, we will be able to analyze ignition and combustion processes or NOx and PM formation processes in detail in diesel combustion. Then beneficial information will be given in the engine’s R&D. Of course, the current chemical kinetic scheme cannot describe the close phenomena occurs in the cylinder of engines. Moreover, LES (Large Eddy Simulation) in which the variables are filtered not in time scale but in physical space may be introduced in future. However, it is assumed very productive in the current situation to simulate and observe the phenomena inside a cylinder by combining the detailed chemistry with the current CFD code which utilizes the k- \( \varepsilon \) type turbulence model.

From a point of view described above, in this study, we tried to conduct a calculation analysis of diesel combustion by using the CFD code combined with the detailed elementary reaction processes, and considered the calculation results about ignition and combustion and NOx and soot formation processes calculation procedure

2. Calculation procedure

2.1 Test Engine

The calculation was conducted to simulate the turbo-charged DI diesel engine with common-rail fuel injection system that has 7.79 l of total swept volume, inline 6 cylinders and 4 stroke-cycle, manufactured for the medium-duty trucks. The engine specification is shown in Table
1. PM was measured by using AVL SPC472 while exhaust gas emissions were measured by using HORIBA MEXA9100DEGR.

2.2 Calculation Model
This calculation code based on KIVA-3 [1], which was developed in Los Alamos national laboratory in the U.S, is directly linked with the originally modified subroutines in CHEMICIN-II [3], which was developed in Sandia national laboratory. As a model of a spray, modified Wave Model proposed by Wakisaka et al [4] was employed. In the stratified combustion field such as diesel combustion, its rate of fuel/air mixing is very slow compared to that of chemical reactions. As a result, because the fuel oxidation is mainly governed by the mixing rate, it was necessary to introduce a mixing process into calculation. In the conventional CFD code, sub-models based on Magnussen model [5] are used. Magnussen model, in which a single-step oxidation reaction resides, is usually used for the oxidation reaction rate that is controlled by the mixing before fuel/air mixing reaches molecular level. However, when hundreds of elementary reactions are considered, because of the existence of many reactions, Magnussen model can’t be applied. From this point of view, as a model for the interaction between turbulent mixing processes and gas phase chemical kinetics, the model based on PaSR (Partially stirred Reactor) [6] concept by Valeri Golovichev et al was introduced into the calculation code.

2.3 Chemical Reaction Scheme
Chemical reaction scheme for hydrocarbon fuel of which carbon number corresponds to that of light gas oil has not been found yet. Thereupon, in the calculation, we assumed that the hypothetical fuel had surface tension and vapor pressure equal to those of light gas oil, and its kinetics adopted those of n-heptane that has the cetane index almost equal to that of light gas oil. Thus the calculation results on penetration and evaporation characteristics were to become highly close to those of diesel oil, in the mean time, for the thermal decomposition, oxidation reactions were considered under control of the rates of reactions of n-heptane. The chemical reactions were based on the reduced scheme for n-heptane [7], and incorporated N series reactions by Sano et al [8]. N series reactions includes extended Zeldovich mechanism, Fenimore NO and NO formed via N$_2$O. Currently, several calculation models for each PAHs, soot formation reactions [i.e. Ref. 9] have been proposed. However, these models included too many elementary reactions to finish the calculation in an allowable CPU time. Considering CPU time, the simple soot model, in which olefin hydrocarbons grow into benzene before they finally produce solid soot, was employed as shown in Fig.1. The total number of elementary reactions was 336, and that of chemical species was 68.

2.4 Calculation Conditions
Calculation conditions are shown in Table 1. Calculations were conducted on the tenth measuring point (revolution 60%, load 80%) in Japanese D-13 mode test.

<table>
<thead>
<tr>
<th>Table 1 Engine specifications</th>
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<tbody>
<tr>
<td>Engine type</td>
</tr>
<tr>
<td>Number of cylinders</td>
</tr>
<tr>
<td>Chamber shape</td>
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<tr>
<td>Bore × stroke mm</td>
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<td>Swept volume L</td>
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3. Results and Discussion

3.1 Pressure Diagram, Rate of Heat Release (RHR)

In this interaction model between turbulence and chemical kinetics, the turbulent characteristics time-scale, $\tau_{\text{mix}}$, is defined as follows:

$$\tau_{\text{mix}} = A \frac{V}{k} \quad (1)$$

Here, $V$ and $k$ represent kinetic viscosity and turbulent energy, respectively. The notation ‘A’ is a model constant as well as a function for the crank angle. ‘A’ was adjusted in order to agree the predicted pressure diagram and RHR with the actual measurement. Fig. 2 shows the comparisons of pressure diagram and RHR between actual measurement and prediction. Since the calculation result reproduced the similar tendency of actual measurement, we will analyze this calculation result in the next section.

3.2 Ignition and Combustion Process

Iso-contours of fuel vapor and HCHO concentrations are shown in Fig. 3. Iso-contours of CO (carbon monoxide) and CO$_2$ (carbon dioxide) concentration, OH concentration and isotherms are also shown in Fig. 4. To simplify the explanation of the calculation results, the discussion is firstly focused on the mixture that evaporates. As shown in Fig. 3, fuel evaporated to form rich mixture at the crank angle $\theta \approx 4$ deg. ATDC. This mixture was decomposed to HCHO during the low-temperature reaction. Thus, HCHO was formed in the same region where the high concentration fuel vapor was observed at the same crank angle. After that, this mixture penetrated...
the surroundings accompanied by its progressing chemical kinetics. Since CO was also formed during low temperature reactions after the HCHO formation, which was observed at $\theta = 4$ deg ATDC in Fig.3, a little CO was also observed at the same crank angle in Fig.4. Finally, CO$_2$, which was formed after being converted from CO observed at $\theta = 4$ deg ATDC, appeared at $\theta = 8$ deg ATDC. It is suggested from Fig.4 that the slight temperature increase was also observed in the place where CO$_2$ started being formed during high temperature reaction. At this time, OH was also formed. This sequential phenomena of the fuel vapor and the HCHO and CO formation at $\theta = 4$ deg ATDC followed by the CO$_2$ and OH formation and temperature increase at $\theta = 12$ deg ATDC continued to occur one after another. For example, the result in vapor and HCHO and CO formation at 8 deg ATDC and CO$_2$, OH formation and high temperature region at 12 deg ATDC was in the same sequence as the above.

3.3 Formation Processes of NO and NO$_2$

Results of concentrations of NO and NO$_2$ are shown in Fig. 5. When the initial stage of combustion was observed at crank angles like $\theta = 12$, 16, deg. ATDC, NO was formed around the same area as where high OH concentration was observed in Fig.4. At $\theta = 20$ deg. ATDC, its band shaped formation area with high concentration more than 1000 ppm of NO appeared, and the area of NO formation diffused in the cylinder. On the other hand, NO$_2$ appeared around the NO formation area. NO$_2$ was initially formed after being converted from NO. Thus, formed NO was diffused in the lean area and it was converted to NO$_2$ there. However, the concentration of NO$_2$ itself was less compared to that of NO.

3.4 Evaluation of NO(Nitric Mono Oxide) Formation Paths

As described above, in diesel combustion, it has the wide window of excess air ratios ranging from rich to lean exists, and variation becomes transitional at higher speed. Moreover, temperature and amount of the chemical species also change. Therefore various NO formation paths should be considered. In truth, 41 elementary reactions concerned with NO$_2$ formation and destruction were taken into account in our model. Thus, the simple technique as described below was used accordingly to estimate the amount of NO formed through three different paths. Here, NO formation path was classified into following three paths, thermal NO, Fenimore NO and NO
via NO$_2$. In the analysis, it was assumed that these were independent of one another. Needless to say, though each path isn’t actually independent, the rough dependence on each formation path became known through this simple method. Calculations were conducted individually using the reaction relative to NO formation only in each scheme, and the results for amount of NO were compared to that of full scheme including all reactions relative to NO formation. The history of NO formation and the frozen NO values for each path are shown in Figs.6 and 7 respectively. It is clear from these figures that NO formation in diesel combustion is mainly governed by thermal NO described by the extended Zeldovich mechanism. The NO that was generated through thermal NO accounted for 88% of total NO. Fenimore NO and NO via N$_2$O accounted for 7% and 1.5%, respectively.

3.5 Formation Process of Soot

As shown in Fig.1, there are mainly three paths for soot (Solid Carbon; C(S)) formation in the
present chemical reaction scheme. Distributions of the concentration for olefin hydrocarbon \( \text{C}_2\text{H}_2 \) (acetylene), \( \text{C}_6\text{H}_6 \) (benzene), soot, and \( \text{O}_2 \) in the cylinder are shown in Fig. 8. At crank angles 8 deg. ATDC, \( \text{C}_2\text{H}_2 \) was observed in the core region of fuel spray where the oxygen concentration became lower. After that, the acetylene started to disappear after \( \theta =12 \) deg. ATDC. At crank angles from 8 to 16 deg. ATDC, aromatic hydrocarbon benzene and soot were apparently observed in the core region of fuel spray, which existed at the \( \text{C}_2\text{H}_2 \) formation region observed at 4 deg. ATDC. This can be explained by the fact that \( \text{C}_2\text{H}_2 \) was polymerized to be converted to soot. After \( \theta =16 \) deg. ATDC, soot was decomposed, and the mass concentration became low due to the increased cylinder volume. The histories of formations of soot and \( \text{C}_2\text{H}_2 \) as the olefin hydrocarbon are shown in Fig. 9. Amount of soot increased rapidly during the initial combustion stage, and at 20 deg. ATDC the formation decreased, then it increased again. Around 60 deg. ATDC, the reactions in soot formation froze. However, the further extensive study to find more accurate oxidation reactions in soot formation and decomposition are necessary to predict
soot formation since calculation result was ten times more than the actual measurement, which was obtained by using the micro dilution PM sampling system.

4. Conclusions

Simulation of the ignition and combustion processes of a DI diesel engine with a supercharger and a common rail fuel injection system were tested under 60% of engine speed and 80% of load condition using the multi-dimensional model combined with detailed chemistry. The conclusions were drawn as follows
(1) The fuel directly injected into the cylinder is decomposed to HCHO and CO as it penetrates inside the cylinder during the low temperature reaction. After that, the high temperature reaction occurs when OH and CO$_2$ are observed.

(2) NO is formed immediately around the fuel rich area after 16 deg. ATDC, and diffused in the combustion chamber. This NO is partially converted into NO$_2$ in the outer area of NO formation region.

(3) 88% of NO formed in diesel combustion is governed by the expanded Zeldovich mechanism. 7% and 1.5% NOs are formed through Fenimore NO and NO via N$_2$O, respectively.

(4) In the mechanism applied in this study, the quantitative soot prediction was hardly achieved since the calculation result was ten times more than the actual result. More detailed oxidation reactions of soot are necessary. However, there is a possibility to predict where and when soot is formed, by considering a simplified soot formation kinetic model.

References


