CFD Simulation for Predicting Combustion and Pollutant Formation in a Homogeneous-Charge Spark-Ignition Engine

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ABSTRACT

A Flame Area Evolution (FAE) model was integrated into a CFD simulation program so as to predict combustion and pollutant formation in homogeneous-charge spark-ignition engines. Gas flows and combustion in a natural-gas engine was simulated by a fully three-dimensional numerical calculation with FAE model and $k$-$\varepsilon$ turbulence model. Pressure changes were successfully reproduced with those measured in the corresponding experiments for a variety of conditions. Based on the spatial profiles of velocity, local heat-release rate, temperature and the local production rate of NO, effects of gas flows and turbulence on flame propagation and pollutant formation were investigated with special attention to the mixing of heat and mass. In addition, the wall-quenching effect was also investigated to elucidate the mechanism of formation of unburned hydrocarbon in the combustion processes.

INTRODUCTION

In recent years, many computational fluid dynamic (CFD) approaches for predicting the combustion process in spark-ignition engines have been proposed to clarify the combustion phenomena and to predict the pollutant formation. Since it is difficult to describe the turbulent combustion directly, most CFD simulations include the turbulence and combustion models. A $k$-$\varepsilon$ two-equation model and a large-eddy simulation have been developed for turbulence and an eddy break-up model [1] and a finite rate Arrhenius kinetics [2] for combustion. In particular, the eddy break-up model has been usually employed in combination with a $k$-$\varepsilon$ two-equation turbulence model. In this combustion model, however, the combustion rate is governed only by the mixing rate represented by the ratio of turbulent kinetic energy to dissipation rate. Weller et al. [3] pointed out that the burning rate in the near-wall region becomes unnaturally high because of a smaller length scale there. It results in a poor prediction of flame evolution in the top clearance of the engine cylinder. Also, because the characteristic time scale of chemical reaction is not included, the appropriate selection of empirical constants is required for the individual calculation in different conditions.

In the present study, a fully three-dimensional numerical calculation with flame area evolution (FAE) model [3] and $k$-$\varepsilon$ turbulence model is established. In this combustion model, it is assumed that flames having a wrinkled structure expand at laminar burning velocity and turbulence effects are empirically assessed, thereby reflecting the development of turbulent premixed-combustion. In particular, the local flame temperature in each computational cell is also estimated, which enables us to reasonably predict the pollutant formation. This model is applied to simulate gas flows and combustion in a natural-gas engine having a deep-bowl combustion chamber with swirl motion. The results will show that in-cylinder pressure changes are successfully reproduced with measured ones in the corresponding experiments for different equivalence ratios and swirl ratios.

THEORETICAL MODEL

Method of Solution

The computer code is based on that developed in a previous study [4]. Necessary revisions are made to enable a fully three-dimensional calculation. The conservation equation of mass, momentum, enthalpy, turbulent kinetic energy $k$, dissipation rate $\varepsilon$ and mass fraction of fuel $m_f$ are calculated in a fully implicit manner. Also, equations of the concentration of nitrogen oxide NO and mass fraction of unburned fuel $G_f$ are considered to investigate the pollutant formation.
The unburned fuel, which is a factor in HC emission, is considered based on a wall-quenching effect. Flame-quenching processes are analyzed by relating the heat release within the flame to the heat loss to the walls under conditions where quenching just occurred. Figure 2 shows a schematic of interaction between wall and flame. Assuming laminar flow near the wall, heat release rate per unit area of flame front \( q_f \) is expressed by the following equation:

\[
q_f = \rho_s S_t m_{fu} h_q
\]

where \( m_{fu} \) is mass fraction of fuel before combustion and \( h_q \) is the lower calorific value of fuel. The heat flux to the wall \( q_w \) is given by the equation in a laminar boundary-layer using the distance between flame front and wall, \( d \).

\[
q_w = \frac{\mu_b C_{pb} (T_b - T_w)}{Pr d}
\]

where \( \mu_b \) is the viscosity, \( C_{pb} \) the specific heat at constant pressure, \( T_b \) and \( T_w \) the temperature of flame and wall, \( Pr \) the Prandtl number, respectively. The local Peclet number defined as the ratio of \( q_f \) to \( q_w \) where the wall quench occurs, \( Pe \), is obtained by Lavoie: \( Pe = C p^{0.26} \) where \( C \) is equal to 3 from experimental data of single wall quenching. Thus the quenching distance \( d_q \) is given by

\[
d_q = \frac{Pe \mu_b C_{pb} (T_b - T_w)}{Pr \rho_s S_t m_{fu} h_q}
\]

Using this equation, the production rate of unburned fuel in the cell neighboring wall, \( dG_f/ dt \), is estimated by \( d_q \) and \( R_f \) as the following equation.

\[
\frac{dG_f}{dt}_{\text{est}} = R_f d_q \frac{d}{\Delta x}
\]

where \( \Delta x \) is the cell size. The unburned fuel that once occurs due to the above mechanism is oxidized slowly in a hot region. The rate of oxidation is evaluated from the following expression, which was taken for propane:

\[
\frac{dG_f}{dt}_{\text{ox}} = -6.7 \times 10^{14} \exp \left( -\frac{37230}{RT} \right) f_f f_o \left( \frac{P}{RT} \right)^2
\]

where \( f_f \) and \( f_o \) are the mole fractions of fuel and oxygen, respectively.

**Engine Condition for Computation**

The present simulation for a homogeneous-charge spark-ignition engine deals with a four-cycle natural-gas engine with deep-bowl chamber (bore 102 mm, stroke 106 mm, compression ratio 11.5:1, cavity diameter and depth 50 mm and 23 mm respectively) [7]. Figure 3 shows the configuration of the engine and grid systems. Ignition is simulated by instant burning-up of 0.1% of the whole mixture around the ignition plug at the assigned timing. All calculations were made under the

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**Combustion Modeling**

FAE concept proposed by Weller is used to model the progress in combustion; the thin flame sheet having a wrinkled structure represents an effective discontinuity separating burned and unburned regions, and local burning velocity is equal to that of laminar flame \( S_l \), as shown in Fig. 1. The ensemble-averaged burning rate \( R_f \) at each cell is related with the turbulent burning velocity \( S_t \) and the gradient of \( m_{fu} \), then

\[
R_f = \rho_s S_t |\nabla m_{fu}|
\]

where \( \rho_s \) is the density of mixture. \( S_t \) is estimated from the empirical equation of turbulence intensity \( u' \) and \( S_0 \) [5].

\[
S_t / S_0 = 1 + 1.25 \left( \frac{u'}{S_0} \right)^{0.5}
\]

\( S_t \) is assumed as a function of temperature and determined based on the experimental data [6].

\[
S_t = S_0 \left( \frac{T}{298} \right)^2
\]

where \( S_0 \) is 0.43 m/s at \( \phi = 1.0 \) and 0.21 m/s at \( \phi = 0.68 \) for natural-gas mixture.

**NO Formation and Unburned Fuel**

The FAE model can reasonably estimate local flame temperature in each computational cell, which enables us to predict the NO formation and wall-quenching effect. NO concentration during combustion is calculated from the extended Zeldovich mechanism, where the chemical equilibrium in the burned-gas temperature is assumed to obtain the chemical species included.
conditions in the corresponding experiments of the ignition timing at maximum brake torque (MBT) and the engine-revolution speed of 1200 rpm. The initial temperature, pressure and flow at the inlet valve closure at 120°BTDC were assumed to be 350 K, 0.1 MPa and forced vortex motion according to the swirl ratio $r_s$. The boundary conditions of the wall are given by the logarithmic wall law on the quasi-steady assumption with temperature of 400K.

RESULTS AND DISCUSSIONS

Combustion Process

To ascertain the accuracy of this calculation, we first compared the pressure changes with those measured for a variety of conditions. Figure 4 demonstrates the predicted courses of in-cylinder pressure $p$ against crank angle $\theta$ for different equivalence ratios $\phi = 1.0$ and 0.68 at swirl ratio $r_s = 2.2$, where the initial value of $k$ and $e$ are 15.4 m$^3$/s$^2$ and 1350 m$^3$/s$^3$, respectively, based on laser homodyne measurements [8]. In the case of $\phi = 1.0$, $p$ is successfully reproduced with that measured. Also for $\phi = 0.68$, a degree of consistency is simulated except for a larger pressure-rise in the initial stage of combustion. In Fig. 5, the result for different swirl ratios $r_s = 0$ and 4.5 is shown at $\phi = 1.0$. The initial values of $k$ and $e$ are 3.84 m$^3$/s$^2$ and 339 m$^3$/s$^3$ at $r_s = 0$ and 35.6 m$^3$/s$^2$ and 3140 m$^3$/s$^3$ at $r_s = 4.5$, respectively. Although such different swirl conditions cause a big change in gas flows and turbulent characteristics, the predicted courses of in-cylinder pressure coincide well with the measured ones. In summary, a reasonable degree of reproduction for a wide range of operating conditions is achieved in describing the turbulent combustion in a spark-ignition engine.

In Fig. 6 the histories of average temperature $T$, concentrations of HC and NO are shown for $\phi = 1.0$ and 0.68. NO concentration rapidly increases with an increase in temperature during combustion and approaches a constant level.
which may be compared with the measured exhaust value indicated in the figure. Although the calculated NO level is lower for $\phi = 1.0$ and higher for $\phi = 0.68$, the change of the level with equivalence ratio is consistent with the measured one, suggesting the availability of this simulation for analyzing NO formation processes. Hydrocarbon fuel is consumed with the progress in combustion. The rate of a decrease in HC concentration due to combustion for $\phi = 1.0$ is higher than that for $\phi = 0.68$, whereas a larger amount of fuel remains as an unburned HC in the later crankangle.

**Spatial Profiles of Gas Flows and Temperature**

Now, the combustion process and pollutant formation will be discussed based on the profiles of gas flows and temperature on the specific cross-section indicated in Fig. 7. Figure 8 shows the profiles of local heat release rate $\dot{q}$, temperature $T$, the rate of NO formation, together with the resultant radial and axial velocities relative to the piston motion $\dot{u}_{z}$, calculated at $\theta = $ TDC and $5^\circ$ATDC of $\phi = 1.0$. The flame front is displayed in the figure as a maximum of dispersive profile of ensemble-averaged $\dot{q}$. The semi-spherical flame kernel initially develops, then expands from the ignition point associated with swirl and squish flows at $\theta = $ TDC. At $\theta = 5^\circ$ATDC, about 15% mass of the mixture burns and the flame front reaches the cylinder axis. A higher-temperature region distributes near the spark plug, where the flame kernel initially occurs and is adiabatically compressed due to combustion that follows. Although NO formation mainly depends on a high
temperature, the rate of NO production is higher around the flame front rather than in the higher-temperature regions. Next, in Fig. 9 the profiles are shown under the lean condition of $\phi = 0.68$ at $\theta = TDC$ when 15% of mixture is burned. A flame propagation is slower, so that the region with high temperature exists at a position downstream of swirling flow. Unlike the stoichiometric case, the rate of NO production exhibits a maximum at the high temperature region. Such difference in the region for NO formation is caused by the concentration of oxygen. NO formation is dominated by temperature under the condition that there is sufficient oxygen. This suggests that an effective suppression of NO formation can be achieved by disturbing the of high temperature region especially.

**Formation of NO and Unburned Fuel**

To investigate the NO formation with an attention paid to the mixing of heat and mass, time-changes of flame temperature and NO concentration are traced at eleven selected cells as shown in Fig. 10. Figure 11 shows their courses at two ignition positions of bowl edge (E) and bowl center (C) for lean combustion $\phi = 0.68$. In the case of (E), temperature and NO concentration at the opposite side from spark plug represented at the cells '6', '7' and '8' become much higher during combustion, rather than those at the spark plug as the cell '0'. The value of $T_a$ and NO at each fixed position fluctuate with crankangle, which reflects heat and mass exchange with other elements by mixing. However in the case of ignition (C), the element that burns initially '0' is adiabatically compressed from time to time, reaching a higher level of temperature and NO, due to combustion of the element that follows. Thus, NO concentration at 60°ATDC in the case of bowl-center ignition is more than double the NO concentration in the case of bowl-edge ignition.

Lastly, the interaction between the heat release and wall quenching is investigated to clarify unburned HC for the two conditions of Fig. 8 (b) and 9. Figure 12 shows the changes of mean reaction rate $R_f$ and the wall-quenching distance $d_q$ against the positions on the wall a-b-c-d-e'-d'-c'-b'-a as shown in Fig. 10. From the equation (6), $d_q$ is inversely proportional to fuel mass-fraction of mixture, so that $d_q$ at $\phi = 0.68$ is longer than that at $\phi = 1.0$. Especially for the lean combustion, $d_q$ in squish region is much greater than that in the other region. This suggests that the unburned fuel is produced in greater quantities in this end-gas region without arrival of flame.

**CONCLUSIONS**

A three-dimensional numerical calculation was established to simulate gas flows and combustion in a natural-gas spark-ignition engine. The flame area evolution concept was employed for modeling the progress in combustion, which features to estimate a local flame temperature related with NO formation and flame quenching on the wall. From the calculated results, it is shown that a reasonable degree of reproduction in the pressure changes is achieved for a wide range of operating conditions without changing empirical constants. Furthermore, based on the distributions of velocity vectors, temperature, turbulent characteristics and the rate of NO production, the process of formation of NO and unburned fuel during
Fig. 10 Positions of eleven elements selected in the combustion chamber.

Fig. 11 Changes of $T_s$ and NO against $\theta$ at eleven selected elements.

Fig. 12 Distribution of fuel-consumption rate $R_f$ and wall quenching distance $d_q$.

Combustion is revealed.

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