Study on NOx and Soot Emissions in Diesel Engines with Multi-Stage Injection Based on a Stochastic Combustion Model

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ABSTRACT: In this study, a phenomenological combustion model, which had been developed based on a stochastic combustion model for simulating combustion with multi-stage injection in diesel engines, was improved to estimate the NOx and soot emissions with modifications in the model for the interaction of sprays from sequent injection stages. Model validation was performed by comparison with experimental data from a single-cylinder diesel engine. To understand the variation of NOx and soot production with injection conditions, analysis of combustion process was conducted based on the calculation results from different injection parameters including injection timing and quantity.

KEY WORDS: heat engine, compression ignition engine, numerical calculation, Diesel engine, Multi-stage injection, Stochastic combustion model, Swirl flow, NOx, Soot [A1]

1. INTRODUCTION

Recently, in order to satisfy the increasingly stringent emission regulations for diesel engines, the multi-stage injection strategies utilizing the common-rail injection system are paid more attentions due to the potential for reducing NOx and soot emissions. However because of the complicated mechanisms of the combustion with multi-stage injection, the NOx and soot production processes have not been fully comprehended when varying the injection parameters such as injection pressure, timing and quantity, which results in difficult selection of proper injection strategy from numerous combinations of parameters.

To better understand the combustion processes with multi-stage injection, the phenomenological combustion model(1) with stochastic approach(2) was developed in the previous study. In the present study, to predict exhaust emissions, NOx and soot models were embedded into the model and the effects of swirl flow on the interaction between sprays from sequent injection stages was considered. The calculated results were compared with experimental data from a single cylinder test engine for pilot/main two-stage injection. The results show the well prediction of heat release rates and NOx emissions except soot emissions. Thus the analysis of soot production process was performed to improve the prediction of soot emission.

2. MODEL DESCRIPTION

In the previous model, a combustion chamber was divided into three zones: the first spray, the second spray and the surrounding air. The injected fuel and surrounding air were treated as many fluid elements with same mass. The spray zone was composed of the fuel elements and entrained surrounding air elements whose amount was determined by a zero-dimensional (0D) spray propagation model. Meanwhile, the fuel-air mixing was considered as a stochastic process in which the fluid elements in a combustion chamber meet and exchange their properties each other to approach the homogeneous state. And fuel vaporization, chemical reaction, and heat loss were calculated for each fluid element. Whence, the temporal variation of probability density functions (PDF) of fluid thermodynamic states, pressure, temperature, and heat release rate can be obtained by the statistics of all fluid elements.

As the primary solutions for realizing the combustion calculation with multi-stage injection the following treatments were employed. The 0D spray propagation model was developed based on Musculus’ model(3), which is able to calculate the spray tip penetration, spray tail penetration, and overall entrainment rate after the end of injection (EOI) besides the spray tip penetration and overall entrainment rate during injection. Thereby the interaction between the sequentially injected sprays could be judged by arrival of the second spray tip at the first spray tail. And the interaction was modeled as the entrainment of the second spray from the first spray. In addition, the lower fuel-air mixing rate caused by the spray flowed in squish region, enhancement of spray entrainment by wall impingement, and entrainment suppression by the interaction between adjacent sprays were
modeled and employed to improve the prediction on the heat release rate.

According to the work above, fairly well prediction was obtained for the heat release rates with various pilot injection conditions. However, some discrepancies remained between the calculated and measured heat release rates, which are needed to improve for reasonable emission calculation results.

The entrainment rates from the pilot spray (gray solid lines) of the main spray (black solid lines), air entrainment rates (black broken lines), and from the pilot spray. The heat release rate of the main spray is lower than that of the pilot spray due to the entrainment rate is proportional to the spray surface area (marked with a circle). This discrepancy is mainly caused by the controlled combustion phase than those of experimental data release rates from the previous study show lower peaks of mixing.

2.1. Modeling of interaction between the sprays from sequent injection stages with swirl flow effect

2.1.1 Problem in the previous model

As shown in Fig.1, for the larger pilot injection quantity cases in the pilot/main two-stage injection, the calculated heat release rates from the previous study show lower peaks of mixing-controlled combustion phase than those of experimental data. This discrepancy is mainly caused by the low air entrainment rate of the main spray due to the entrainment from the pilot spray. The heat release rate of the main spray decreases due to the lower oxygen concentration in the burned gas from the pilot spray. Figure 2 shows the total entrainment rates (black solid lines), air entrainment rates (black broken lines), and the entrainment rates from the pilot spray (gray solid lines) of the main spray in the case of a pilot injection quantity of 6 mm³. This figure indicates that the air entrainment rates of main spray shows a low level due to the high entrainment rates from the pilot spray.

2.1.2 Swirl flow effects on interaction between sequentially injected sprays

To improve the calculation, the effects of swirl flow on the spray behavior are considered. The swirl flow does not only decrease the spray penetration, but also deviates the spray path. These effects make the second spray (main spray) tip overtake the first spray (pilot spray) tail and tip earlier than the case without swirl flow effects, and reduce the overlap region between the first and second sprays as shown in Fig.3. Consequently the intensity of interaction between the two sprays is attenuated, which results in the reduction of the entrainment rate of the second spray from the first spray, and thereby the air entrainment is enhanced. Thus, based on the assumption that the entrainment rate is proportional to the spray surface area, for the second spray, the ratio \( R_e \) of the entrainment rate from the ambient gas and that from the first spray can be expressed as

\[
R_e = \frac{A_{\text{spr}} + (1 - R_{3a}) A_{\text{blt}}}{R_{3a} A_{\text{blt}}},
\]

where the numerator expresses the area in air zone, and the denominator expresses the area in the first spray zone. \( A_{\text{spr}} \) is the surface area of the second spray up to the first spray tail, \( A_{\text{blt}} \) the surface area below the first spray tail, and \( R_{3a} \) the ratio of the second spray surface area included in the first spray zone to \( A_{\text{blt}} \), which can be treated as the interaction intensity.

![Diagram of sprays interaction](image)

(a) without swirl effects  (b) with swirl effects

Fig. 3 Diagram of sprays interaction

After the interaction starts, the surface area of the second spray up and below the first spray tail can be determined by the first spray tail position. Therefore the interaction start timing is required. Because of the swirl flow effects, the reduction of spray penetration in injection direction should be considered to calculate the timing at which the second spray tip touches the first spray tail. In this study, the ratio (\( R_{\text{ID}} \)) between the momentum from injected fuel (\( M_j \)) and total momentum in the spray, which includes the momentum from the injected fuel (\( M_j \)) and the entrained gas (\( M_e \)), is introduced as a factor for the spray penetration. The specific expressions are as follows,

\[
R_{\text{ID}} = \frac{M_j}{\sqrt{M_j^2 + M_e^2}},
\]
The soot model is based on the model proposed by Patterson et al.\(^{(3)}\). In the soot model, the net soot production rate is determined by the difference between soot formation rate and soot oxidation rate as expressed by equation (7),

\[
\frac{dm_s}{dt} = \frac{dn_{so}}{dt} - \frac{dn_{sof}}{dt},
\]

where \(m_s\) is the soot mass, \(dn_{so}/dt\) the mass rate of soot formation, and \(dn_{sof}/dt\) the mass rate of soot oxidation. The soot formation rate is same as in Hiroyasu’s soot formation equation\(^{(9)}\),

\[
\frac{dn_{so}}{dt} = A_t m_f P^{0.3} e^{-\frac{E}{RT}},
\]

where \(A_t\) is the model constant, \(m_f\) the fuel mass fraction, \(P\) the pressure, \(E\) the activation energy, and \(T\) the temperature. The oxidation rate adopts the Nagle and Strickland-Constable (NSC) model. In addition, to predict the soot oxidation accurately in fuel-rich regions, the effect of hydroxyl radical (OH) on soot oxidation rate (\(R_{SOH}\)) is considered by referring Neoh’s equation\(^{(9)}\) as follows,

\[
R_{SOH} = 1.29 \times 10^7 a_{OH} T^{-1/2}
\]

where \(a_{OH}\) is the partial pressure of OH, \(T\) the temperature, and \(a\) represents the collisions efficiency of OH with the soot particle surface and it is selected as 0.13 that was suggested by Neoh and often introduced into soot models for diesel engines. As a result, the final soot oxidation rate is rewritten as follows,

\[
\frac{dn_{sof}}{dt} = r C_{SO} \frac{6m_s}{\rho D_s} R_{SOH} + C_{SOH} \frac{6m_s}{\rho D_s} R_{SOH},
\]

where \(C_{SO}\) and \(C_{SOH}\) are the constants of oxidation rate by \(O_2\) and \(OH\) respectively, \(\rho\) the soot particles density, \(D_s\) the average diameter of soot particles, and \(R_{SOH}\) the soot oxidation rate calculated by NSC model.

In this combustion model, the chemical reaction process is realized by a quasi-global chemical kinetics model (Schreiber’s model) and a chemical equilibrium reactions model. At first, the ignition process of fluid elements is mimicked using the Schreiber’s model. Once the mole fraction of the final products exceeds the threshold, the chemical reaction calculation is switched to the equilibrium reactions. Considering that \(NO_x\) and soot are produced in high-temperature mixtures, the \(NO_x\) and soot calculations are conducted in each fluid element which reached the equilibrium state. Temperature of the fluid element is used for \(T\) in the equations (8) and (9), \(m_f, P_{O_2}\), and \(P_{OH}\) are obtained based on the species amount in fluid elements.

\section*{3. RESULTS AND DISCUSSION}

Based on the modifications above, simulations were carried out for a single-cylinder diesel test engine with pilot/main two-
stage injection. The specifications of test engine are listed in Table 1, and the calculation conditions are listed in Table 2.

Table 1 Standard specifications of test engine

| Engine type            | Single-cylinder, DI-Diesel engine |
|------------------------|----------------------------------|
| Bore × Stroke          | 85×96.9 mm                      |
| Compression ratio      | 16.3                            |
| Combustion chamber     | Reentrant type (Φ51.6 cavity)   |
| Injection system       | Common-rail system              |
|                       | 0.125 mm × 7 holes nozzle       |

Table 2 Calculation conditions

| Injection pressure     | 125MPa                          |
| Total injection quantity | 32 mm$^3$                      |
| Pilot injection quantity ($q_{pilot}$) | 2, 4, 6, 8 mm$^3$               |
| Pilot injection timing ($\theta_{pilot}$) | $-9$, $-19$, $-24$ ATDC         |
| Main injection timing  | 1 ATDC                          |
| EGR rate               | 20%                             |
| Swirl ratio            | 2.0                             |

3.1. Entrainment rate

After the modification, the comparison of the entrainment rates of main spray in the case with pilot injection quantity of 6 mm$^3$ is shown in Fig.5. In this figure, the cases without and with swirl flow effects are displayed in the left and right graphs, respectively. It can be observed that the starts of entrainment from the pilot spray are advanced by swirl flow effects. The lower entrainment rate from the pilot spray in the cases with swirl flow effects, due to the reduction of interaction intensity, causes the higher air entrainment rate.

In addition, the entrainment rate from the pilot spray sharply decreases to zero at the early timings (around 10 and 12°ATDC for $\theta_{pilot}$ of $-9$ and $-24$°ATDC) in the cases without swirl flow effects. This indicates that all of the pilot spray has been entrained into the main spray, however, this phenomenon is postponed in the cases with swirl flow effects. It can be found that the depletion of surrounding air occurs prior to that of pilot spray at around 22 and 27°ATDC for pilot injection timings of $-9$ and $-24$°ATDC. And the earlier depletion of surrounding air is observed in the case of the later pilot injection timing. This is because the larger heat release of the pilot spray in the case of later pilot injection timing leads to higher surrounding air density in the cylinder before main injection, so that the main spray entrainment rate is higher and the surrounding air is consumed at the earlier timing compared to the case of earlier pilot injection timing.

3.2. Pressure and heat release rate

Calculated heat release rates without and with swirl flow effects are shown in Fig.6 with those from experiments for a pilot injection quantity of 6 mm$^3$. This figure shows that the heat release rates peaks of mixing-controlled combustion phase have been improved after considering swirl effects, and the similar shapes of heat release rates to those of experimental data are obtained.

Fig.7 shows the in-cylinder pressures and heat release rates for different pilot injection timings and quantities after considering swirl flow effects. The simulation results obtain the similar levels of pressures and heat release rates to those of experiments. It is also observed that the model is able to capture the tendencies of the pressure and heat release rate when varying the pilot injection timing and injection quantity.
Fig. 7 Effects of pilot injection quantity on the in-cylinder pressure and the heat release rate ($\theta_{\text{pilot}}=-9, -24$ ATDC).

### 3.3. Emissions calculation

Based on the good agreement in the pressures and the heat release rates, the NOx and soot emissions were calculated. The soot model constants $A_f$, $C_{SO}$, and $C_{SOH}$ were set at 200, 2 and 2 respectively to fit the soot emissions level. Fig. 8 shows the NOx (left) and soot (right) emissions against the pilot injection timing. In this figure, the NOx emissions from the simulation are represented as the in-cylinder NOx mole fraction at exhaust valve open (EVO), and the calculated soot emissions are represented as the in-cylinder soot concentration at EVO, which are converted to the condition of standard temperature and pressure (25°C and 1.0 bar). The results reveal that the NOx calculation obtains the emission level and variation with the change in pilot injection conditions similar to the measured data. Regarding the soot emission, the calculated soot emissions also attain the comparable level with the measured data, and the increase with retarding pilot injection timing coincides with that of experiment in the case of smaller pilot injection quantity. However, the calculated soot emissions decrease when the pilot injection quantity is increased, which is an inverse trend to the measured data.

As shown in Fig. 7, the shorter ignition delay of the main spray and the increased in-cylinder pressure in the case of the larger pilot injection quantity are well reproduced by the calculation, which should cause higher soot emission as in the measured data. From the Fig. 9, which shows the histories of total soot mass for different pilot injection quantities at pilot injection timings of -9 and -24 ATDC, the soot mass tends to increase with increasing pilot injection quantity during the initial period in which soot formation is a primary factor. This indicates a reasonable tendency: the high in-cylinder pressure and short ignition delay cause soot formation increase. Nevertheless, after the soot mass starts to decrease due to the predominance of soot oxidation, the rate of the decrease presents faster in the larger pilot injection quantity case, eventually, the variation of final soot level along with the change in pilot injection quantity is reversed to that in the initial period, which is also opposite to the measured data. This is caused by excessive mixing rate and/or excessive soot oxidation rate in larger pilot injection quantity case.

Therefore it can be deduced that the microscopic mixing process and/or soot model are not accurate enough and need to be improved. In this study, as a first step of improvement, adjustment of model constants was performed and then another soot model was tested.

#### 3.3.1 Decrease of soot oxidation constants

Since the fast soot oxidation rate is one of the reasons for underestimation of the soot emissions when increasing the pilot injection quantity, the values of soot oxidation constants are decreased in Patterson's model. The calculations are performed with $C_{SO}$ and $C_{SOH}$ of 0.5, and $A_f$ is reduced to 8.0 to fit the soot emissions level. Figure 10 shows the comparison of soot histories before and after changing soot oxidation constants. Although the observed decrease rate of soot mass in the later period is attenuated using the smaller soot oxidation constants, the soot mass of 6 mm$^3$ case is still smaller than that of 2 mm$^3$ case. The measured tendency of soot emission could not be reproduced.
solely by changing the constants when the soot emissions are kept in the same level.

\[ \frac{d}{dt} \left( \frac{n}{N_A} \right) = \alpha - \beta \left( \frac{n}{N_A} \right)^2, \]  
\[ \frac{d}{dt} \left( \rho \gamma f_s \right) = \rho n + \delta \left( \frac{36\pi}{\rho^2} \right) n^2 (\rho f_s)^3 (C_{SOH} + C_{SOH}^2), \]

where \( n \) is the soot particles number density, \( f_s \) the soot volume fraction, \( N_A \) Avogadro’s number. \( \alpha, \beta, \gamma \) and \( \delta \) are the source terms for the number density and the volume fraction, they are expressed by equations (13) through (16).

\[ \alpha = C_a T^\gamma X_t \exp\left(-\frac{T}{T_a}\right), \]  
\[ \beta = C_B T^\gamma, \]  
\[ \gamma = C_c T^\gamma X_t \exp\left(-\frac{T}{T}\right), \]  
\[ \delta = C_D T^\gamma, \]

where \( C_a, \beta, \gamma, \delta \) are the model constants, \( T_a \) and \( T \) the activation temperatures, \( \rho \) the local mixture density, \( T \) the local mixture temperature, and \( X_t \) the fuel mole fraction. The calculation of soot is conducted for each fluid element, therefore, \( \rho, T, \) and \( X_t \) are represented by those of fluid elements. In order to fit the soot emissions level, \( C_a \) and \( C_B \) are modified to \( 3.0 \times 10^{-2} \) and \( 1.25 \times 10^{10} \), and both the constants of soot oxidation rate (\( C_{SO} \) and \( C_{SOH} \)) are set at 0.5.

**3.3.3 Analysis of soot calculations based on different soot models**

As shown in Fig.11, the calculated soot emissions based on Moss’s model are able to reproduce the increase with the increase in pilot injection quantity at fixed pilot injection timings, which is observed in the experimental data. The histories of total soot mass are shown in Fig.12 for the cases with pilot injection timings of \(-9\) and \(-24\) ATDC and pilot injection quantities of 2 and 6 mm\(^3\). This figure shows that the peak soot mass of 6 mm\(^3\) case is much larger than that of 2 mm\(^3\) case and the soot mass in the later period is still larger although the oxidation rate is slightly higher for the case of a pilot injection timing of \(-24\) ATDC. On the other hand, in the case of \(-9\) ATDC, the peak of 6 mm\(^3\) case is slightly larger and appears earlier compared with the 2 mm\(^3\) case and the decrease rates of soot mass are almost the same, as a result, the later soot level is close to each other. Thus, the calculation with selecting parameters in Moss’s model partly reproduces the measured soot emission tendency; however, there remains a problem from a microscopic viewpoint.
However, when the pilot injection quantity is large enough ($q_{pilot} = 8 \text{ mm}^3$), the increased tendency of soot emissions with advancing pilot injection timing is consistent with the measured data.

From the aspect of fuel-air mixing, this means that a part of mixture undergoes slow mixing. There is possibility that the submodels of sprays interaction and/or mixing in the squish area partly attribute to this phenomenon. Further study is required for the soot oxidation rate relative to fuel-air mixing rate to improve the soot calculation.

![Fig. 13 Soot mass distribution against equivalence ratio at 35° ATDC of Patterson's and Moss's models.](image)

4. CONCLUSION

In this paper, the swirl flow effects on the spray penetration and spray deflection were considered to model the interaction between the sprays, and NO$_x$ and soot model were introduced into combustion model for emissions calculation. Based on the results comparison with experiment data and analyses of the emissions production process, especially the production process of soot, the conclusion are derived as follows.

(1) The model of interaction between sprays considering the spray deflection by swirl flow enables the combustion model to accurately predict in-cylinder pressures and heat release rates with pilot/main two-stage injection.

(2) Combining with the extended Zeldovich mechanism, the combustion model reasonably predicts the NO$_x$ emissions level and captures the tendencies with increased pilot injection quantity and retarded pilot injection timing.

(3) The combustion model with Moss's soot model is able to reproduce the measured increase of soot emission with increasing pilot injection quantity at fixed pilot injection timings. However, larger soot emissions are predicted in the cases of earlier pilot injection timing, which is remarkable in the larger pilot injection quantity case.

(4) Based the comparison of results from Patterson's and Moss's model, the lower soot oxidation rate relative to fuel-air mixing rate causes unreasonable distribution of soot mass against mixture equivalence ratio. Thus the soot oxidation rate relative to fuel-air mixing rate should be paid attention to improve the soot calculation.

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