Numerical Modeling of Combustion Processes and Pollutant Formations in Direct-Injection Diesel Engines

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The Representative Interactive Flamelet(RIF) concept has been applied to numerically simulate the combustion processes and pollutant formation in the direct injection diesel engine. Due to the ability for interactively describing the transient behaviors of local flame structures with CFD solver, the RIF concept has the capabilities to predict the auto-ignition and subsequent flame propagation in the diesel engine combustion chamber as well as to effectively account for the detailed mechanisms of soot formation, NOx formation including thermal NO path, prompt and nitrous NOx formation, and reburning process. Special emphasis is given to the turbulent combustion model which properly accounts for vaporization effects on the mixture fraction fluctuations and the pdf model. The results of numerical modeling using the RIF concept are compared with experimental data and with numerical results of the commonly applied procedure which the low-temperature and high-temperature oxidation processes are represented by the Shell ignition model and the eddy dissipation model, respectively. Numerical results indicate that the RIF approach including the vaporization effect on turbulent spray combustion process successfully predicts the ignition delay time and location as well as the pollutant formation.

Key Words : Flamelet Model, Autoignition, Detailed Chemistry, Pollutant Formation, Vaporization Effects on Turbulent Spray Combustion Process

1. Introduction

In comprehensively modeling the spray combustion processes in DI diesel engines, numerical modeling of auto-ignition process is quite important to correctly predict the combustion and pollutant formation characteristics. The Shell ignition model (Halstead et al., 1975 ; Kong at al., 1995 ; Sazhina et al., 2000) is generally used to simulate the spray ignition process. However, the Shell ignition model is unable to include the turbulent effects on the ignition process and it has the basic shortcoming that the parameters must be tuned according to the combustion conditions. In order to overcome this defect, Pitsch et al. (1996) suggested the Representative Interactive Flamelet (RIF) Model. This model does not require the tuning of parameters and it can account for the turbulence-chemistry interaction based on the detailed chemistry. Hence, auto-ignition, partially premixed burning, diffusive combustion and pollutants (NOx, soot) formation need not to be modeled individually. This transient flamelet model has the basic advantage to efficiently simulate the three-dimensional combustion processes of the internal combustion engines with the widely varying chemical and fluid dynamic time

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scales. Wan et al. (1997) predicted auto-ignition delay time and location using RIF model. Pitsch and Peters (1988) reduced the detailed kinetic reaction mechanism to 14-step mechanism and then studied auto-ignition process and relationship between auto-ignition delay time and scalar dissipation rate in detail. To account for the spatial inhomogeneity of the scalar dissipation rate in the spray flame field, Barths et al. (1998) devised the multiple flamelets procedure. On the other hand, most of the previous works for simulation of spray combustion have neglected the effects of spray vaporization except the source term due to vaporization for mean mixture fraction. However, the recent DNS results by Reveillon and Vervisch (2000) revealed that the impact of vaporization sources on the small scales of the turbulent fuel distribution modifies significantly the fluctuations of mixture fraction and subsequently the scalar dissipation rate. Demoulin and Borghi (2000) also proposed the new model to include these major effects of spray vaporization on the mixture fraction fluctuations and the pdf model.

Our ongoing reseach is ultimately aiming at developing the reliable, stable and efficient combusion model which can realistically simulate the spray dynamics, vaporization, auto-ignition, combustion and pollutant formation process in DI diesel engine. In order to include the spray vaporization effects on the mixture fraction fluctuations and the pdf model, the present study employs the model proposed by Demoulin and Borghi (2000). The coupling between complex chemistry and turbulence are treated by employing the Representative Interactive Flamelet (RIF) Model.

This study has been mainly motivated to critically evaluate the predicative capability of two combustion models including the Shell ignition/ eddy dissipation model and the RIF model as well as to numerically investigate the vaporization effects on the turbulent spray combustion processes in the DI engines. Since the cetane numbers of Diesel fuel(CN-50) and n-heptane (CN-56) that control the ignition delay times are quite close, numerical simulations for combustion processes of an n-heptane fueled DI Diesel engine have been carried out. The detailed chemical mechanism used in this study comprises 114 elementary reactions with 43 species for n-heptane and 101 irreversible reactions with 13 additional species to predict NOx formation. The reaction scheme includes fuel oxidation, low temperature degenerate chain branching to describe auto ignition, and a reaction mechanism for NOx formation, including thermal(Zel'dovich), prompt, nitrous NOx and reburn by hydrocarbon radicals. All relevant physical submodels are implemented in the modified KIVA-3V code (Amsden, 1997). Computations are performed for four injection timings by using the Shell ignition/ eddy dissipation model and the RIF model with and without the vaporization effects on the turbulent combustion. In terms of ignition delay, cylinder pressure histories and pollutant emission, numerical results are compared with measurements of Venkatesan and Abraham (2000).

2. Numerical and Physical Models

All the gas-phase and liquid-phase processes are modeled by a system of unsteady, multi-dimensional equations. The gas-phase equation is written in an Eulerian coordinate whereas the liquid-phase is presented in Lagrangian coordinates. The two-way coupling between the two phases is described by the interaction source terms that represent the rates of momentum, mass and heat transfer. To realistically represent the physical processes involved in the spray dynamics, the present approach employs the hybrid breakup model (Beatrice et al., 1995), the stochastic droplet tracking model (Kim et al., 1994) and collision model (O'Rourke, 1994). In this study, two combustion models including the shell ignition/ eddy-dissipation model and the RIF model are implemented in the KIVA-3V code. In the present RIF approach, the modified formulations have been employed to account for the spray vaporization effects on the mixture fraction fluctuations and the pdf model. The main features of two combustion models are briefly described below.

2.1 Shell ignition/Eddy-dissipation model

The Shell ignition model (Halstead et al., 1975 ; Kong at al., 1995 ; Sazhina et al., 2000) is generally used to simulate the spray ignition process. However, the Shell ignition model is unable to include the turbulent effects on the ignition process and it has the basic shortcoming that the parameters must be tuned according to the combustion conditions. This model also requires the solution of some species transport equations including semi-empirical chemical source terms in CFD calculation. Moreover, for simulating the high-temperature combustion processes after auto-ignition, the eddy-dissipation model (Magnussen, and Hjertager, 1977) need to be turned on.

In terms of the pollutant model, soot formation and oxidation have been modeled by using the Hiroyasu soot formation and Nale and Strickland-Constable oxidation models, respectively (Patterson et al., 1994). For NO, the extended Zeldovich mechanism (Heywood, 1988) has been used to estimate the thermal NOx. This model is incapable of predicting the prompt and fuel NOx contribution. The ad-hoc correction factor is usally used to convert NO predictions to NOx estimation.

2.2 RIF-based combustion model

In the Representative Interactive Flamelet (RIF) model, the turbulent flow field can be calculated with a Computational Fluid Dynamics (CFD) code and the laminar flamelet equations can be solved with a flamelet code. However the flamelet equations are solved in a separate code, interactively coupled with a main code. Flamelet parameters obtained from the main code are used for calculating flamelet equations, and then species mass fractions gained from flamelet code are passed to the main code.

Introducing a conserved scalar Z, which is the mixture fraction, the one-dimensional flamelet equations (Peters, 1984) solved in the flamelet code can be written as:

$$\rho\frac{\partial Y_i}{\partial t}-\frac{\rho\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2}-\dot{m}_1=0 \tag{1}$$

$$\rho\frac{\partial T}{\partial t}-\frac{\rho\chi}{2}\frac{\partial^2 T}{\partial Z^2}-\frac{\rho\chi}{2}\frac{1}{c_p}\frac{c_p}{\partial Z}\frac{\partial T}{\partial Z}+\frac{\rho\chi}{2}\frac{\partial T}{\partial Z}\sum_{k=1}^{N}\left(1-\frac{c_{pk}}{c_p}\right)\frac{\partial Y_k}{\partial Z}+\frac{1}{c_p}\left(\sum_{k=1}^{N}h_k\dot{m}_k-\frac{\partial p}{\partial t}\right)=0 \tag{2}$$

where, N denotes the number of chemical species, p the pressure, c_{pk}, $\dot{m}_k$, h_k, Y_k, are the heat capacities at constant pressure, the chemical production rates, the enthalpies, and the mass fractions of the chemical species k, respectively. Instantaneous scalar dissipation rate χ which represents strain effects of the flow field on the transport of the scalars in mixture fraction space can be expressed as:

$$\chi(Z)=\chi_{st}f(Z)=\chi_{st}\frac{Z^2\ln Z}{Z_{st}^2\ln Z_{st}} \tag{3}$$

In addition two transport equations for the local mean mixture fraction $\tilde{Z}$ and its variance $\tilde{Z}''^2$ have to be solved in the CFD code to define the local mean species composition. So far, most of the turbulent combustion models originally developed for gaseous flames have been applied to simulate the spray combustion processes without considering the vaporization effects on the small-scale turbulent mixing and the turbulent combustion. In order to account for the vaporization effects on the turbulent spray combustion, the present study adopts the model proposed by Demoulin and Borghi (2000). The transport equation of mixture fraction variance is derived by using the pdf transport equation for mixture fraction. The equations for the mean mixture fraction $\tilde{Z}$ and its variance $\tilde{Z}''^2$ coupled with the vaporization effects can be written as follows;

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Z})+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{Z})=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_Z}\frac{\partial\tilde{Z}}{\partial x_j}\right)+\bar{\rho}\tilde{\omega}_v \tag{4}$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Z}''^2)+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{Z}''^2)=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_{Z''^2}}\frac{\partial\tilde{Z}''^2}{\partial x_j}\right)+\frac{2\mu_t}{\sigma_{Z''^2}}\frac{\partial^2\tilde{Z}}{\partial x_j^2}-\bar{\rho}\tilde{\chi}+2(\bar{\rho}\tilde{Z}\omega_v-\bar{\rho}\tilde{Z}\tilde{\omega}_v)+\bar{\rho}\tilde{Z}^2\tilde{\omega}_v-\bar{\rho}\tilde{Z}^2\omega_v \tag{5}$$

The last four additional source terms appeared in Eq. (5) account for the vaporization effects on mixture fraction variance. These new correlations taking into account the fluctuation of equivalence

ratio due to vaporization are in an unclosed form. By assuming that the spray vaporization takes places only at the liquid surface, Demoulin and Borghi (2000) have proposed the model for these correlations:

$$\bar{\rho}\widetilde{Z}\omega_v \approx \bar{\rho}\widetilde{Z}_s\omega_v = \sum_p Z_s^p \frac{\dot{m}_p}{V} \tag{6}$$

and

$$\bar{\rho}\widetilde{Z}^2\omega_v \approx \bar{\rho}\widetilde{Z}_s^2\omega_v = \sum_b (Z_s^p)^2 \frac{\dot{m}_p}{V} \tag{7}$$

where the subscript s denotes the value at the liquid surface. These additional source terms are mainly contributed to the production of mixture fraction fluctuations. In spray combustion processes, these terms are contributed to increase the scalar dissipation rate and the ignition delay time as well as to modify the small-scale mixing processes and the spray structure.

Another important effect due to vaporization is related to the fact that the upper limit of mixture fraction is not unity in spray combustion processes. Therefore, the upper limit (Z_{ini}) of mixture has to be determined. By utilizing the conditional pdf of Z_{ini} and mixture fraction equation, Demoulin and Borghi (2000) derived the following balance equation.

$$\begin{aligned}&\frac{\partial}{\partial t}(\bar{\rho}\widetilde{Z}\overline{Z}_{ini}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\widetilde{Z}\overline{Z}_{ini}) \\ &= \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_z}\frac{\partial \widetilde{Z}\overline{Z}_{ini}}{\partial x_j}\right) + \bar{\rho}\int_0^1 Z_{ini}\tilde{\omega}_{v|Z_{ini}}dZ_{ini}\end{aligned} \tag{8}$$

For a given position, therefore, the allowable space for mixture fraction Z has to be automatically adjusted from 0 to $\overline{Z}_{ini}$. In the present study, the β-pdf $\tilde{P}(Z;\vec{x}, t)$ is employed and its shape has been renormalized from the three constraints:

$$\begin{aligned}1 &= \int_0^{\overline{Z}_{ini}} \tilde{P}(Z)\,dZ, \\ \widetilde{Z} &= \int_0^{\overline{Z}_{ini}} Z\tilde{P}(Z)\,dZ, \\ \widetilde{Z}''^2 &= \int_0^{\overline{Z}_{ini}} (Z-\widetilde{Z})^2\tilde{P}(Z)\,dZ\end{aligned} \tag{9}$$

This modified upper limit of mixture fraction also influences the ignition delay and the spray combustion processes. Decease in the upper limit mixture fraction is contributed to increase the probability of combustion in a given mixture fraction.

Unlike the shell ignition/eddy dissipation model, the RIF concept has the capabilities to realistically predict the detailed soot formation process, NOx formation including thermal NO path, prompt and nitrous NOx formation, and reburning process by hydrocarbon radical without any ad-hoc procedure as well as the main turbulent combustion processes. In order to estimate the soot emission, this study employs the soot formation model proposed by Moss et al. (1995). This model is required to solve the following two transport equations for the volume fraction and number density of soot.

$$\frac{d(\rho_s f_v)}{dt} = \gamma n + \delta - \left(\frac{36\pi}{\rho_s^2}\right)^{1/3} n^{1/3}(\rho_s f_v)^{2/3}\omega_{NSC} \tag{10}$$

$$\frac{d(n/N_0)}{dt} = \alpha - \beta(n/N_0)^2 \tag{11}$$

where, f_v, ρ_s, n, N_0, ρ, T, α, δ, γ, β are the soot volume fraction, soot particulate density, particle number density, Avogadro number, local mixture density, temperature, soot nucleation terms, surface growth, and coagulation, respectively. The dependence of these terms on the mole fraction of the fuel, density and temperature is modeled by the following expressions.

$$\alpha = C_\alpha \rho^2 T^{1/2} X_f \exp(-T_\alpha/T) \tag{12}$$

$$\beta = C_\beta T^{1/2} \tag{13}$$

$$\gamma = C_\gamma \rho T^{1/2} X_f \exp(-T_\gamma/T) \tag{14}$$

$$\delta = C_\delta \alpha \tag{15}$$

where, T_α, T_β are activation temperatures, X_f is the mole fraction of a representative fuel species, and C_α, C_β, C_γ, C_δ are model constants obtained by calibrating against detailed measurements in laminar diffusion flames for several fuels (Moss et al., 1995). In the flamelet approach , the laminar diffusion data from OPPDIF is employed to express the source terms in equations (10) and (11) as a function of the mixture fraction Z. By convoluting these source terms with PDF, the mixture fraction averaged source terms are obtained. These source terms can be utilized to obtain the solution of the above two transport equations.

3. Results and Discussion

The RIF-based turbulent combustion models and the Shell ignition/eddy dissipation model have been applied to simulate the spray dynamics, vaporization, auto-ignition, combustion process and pollutant(NOx, soot) formation in the DI diesel engine.

The validation case was chosen as the experimental results (Venkatesan and Abraham, 2000) for Cummins N-14 engine. The engine specification and computational conditions are given in Tables 1 and 2. Computation starts at bottom dead center (BDC) and continues until the exhaust valve opens at 130°CA. In experiments, a diesel fuel is used. Since the detailed chemical kinetics of diesel fuel are still uncertain, n-heptane is used as a fuel in numerical simulation. The detailed chemical mechanism used in this study comprises 114 elementary reactions with 43 species for n-heptane and 101 irreversible reactions with 13 additional species related to NOx formation. The orifice diameter is 200 microns and a spray angle is 14°. Computations are performed for 45° sector of combustion chamber. Numerical results are compared with the experimental data of Venkatesan and Abraham (2000).

For simplicity of presentation, Model 1, Model 2 and Model 3 will be used to refer to the the Shell ignition/eddy dissipation model, the RIF model, and the RIF model with accounting for vaporization effects on turbulent combustion. In Fig. 1, the simulated cylinder pressure histories obtained by the Shell ignition/eddy dissipation model are compared with the measured data for 4 injection timings. For the injection timing near TDC, computed results agree well with experimental data. By continuously retarding the injection timing, the agreement between prediction and measurement becomes much worse. The largest deviations in ignition delay time and pressure histories are corresponding to the latest injection timing (9.5 CA). For the relatively late injection timings (7 and 9.5 CA) where the nonequlibrium chemistry effects are dominant due to the relatively low chamber temperature and intense turbulence associated with the high-speed injection, the Shell ignition/eddy dissipation model substantially underestimates the ignition delay time and predicts the quantitatively and qualitatively wrong pressure histories. These discrephancies could be related to the defect of the Shell ignition/eddy dissipation model which is unable to properly account for the turbulence-chemistry interaction. These numerical results suggest that

Table 1 Engine specification of Cummins N-14 DI diesel engine

Engine type	Cummins N-14
Bore (cm)	13.97
Stroke (cm)	15.24
Squish (cm)	0.378
Compression Ratio	16.5
Diplacement Volume (cm3)	2340
Connecting Rod Length (cm)	30.48
Injection Nozzles	8
Injector Hole Diameter (cm)	0.02
Spray Inclination Angle (deg)	76

Table 2 Computational conditions

Case	Computation Sector (°)	RPM	Initial Air Pressure (MPa)	Initial Air Temp. (K)	Mass of Air (g)	Mass of Fuel (g)	Wall Temp. (K)	SOI (°CA)	EOI (°CA)
A	45	1200	0.1244	408	2.627	0.0657	400	−2.5	4.5
B	45	1200	0.1244	408	2.627	0.0657	400	2	10
C	45	1200	0.1244	408	2.627	0.0657	400	7	15
D	45	1200	0.1244	408	2.627	0.0657	400	9.5	17.5

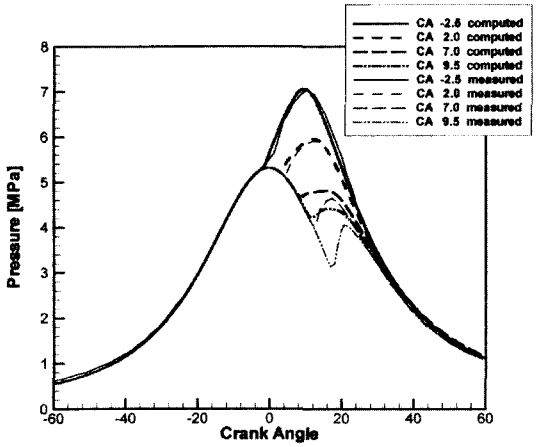


Fig. 1 Cylinder pressure histories for 4 injection timings (Model 1)

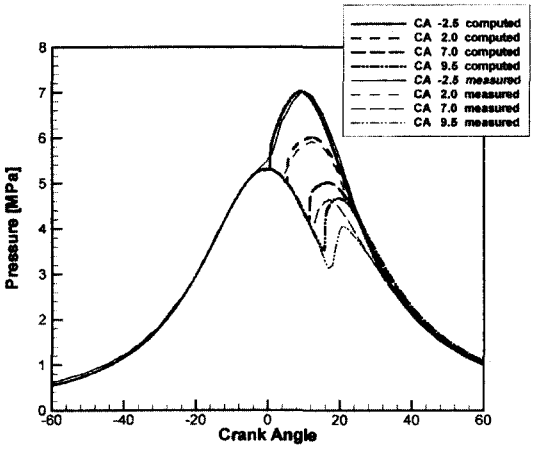


Fig. 2 Cylinder pressure histories for 4 injection timings (Model 2)

the Shell ignition/eddy dissipation model can not be applicable to simulate the combustion processes of DI diesel engine with the far retarded injection.

Figure 2 presents the simulated cylinder pressure histories obtained by the RIF model and the measured data for 4 injection timings. The computed and measured pressure histories and ignition delay times have the reasonably good agreement for all cases. Even if the agreement in the relatively late injection timings (7 and 9.5 CA) has been considerably improved in comparison with the Shell ignition/eddy dissipation

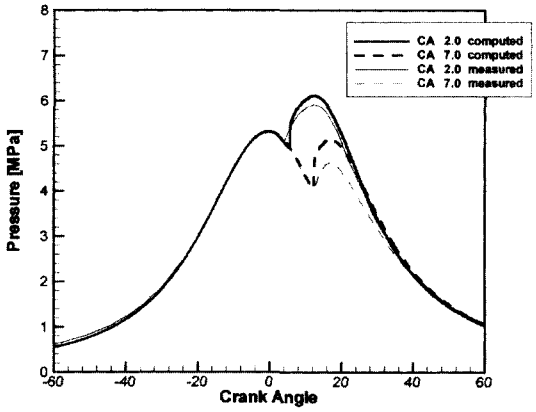


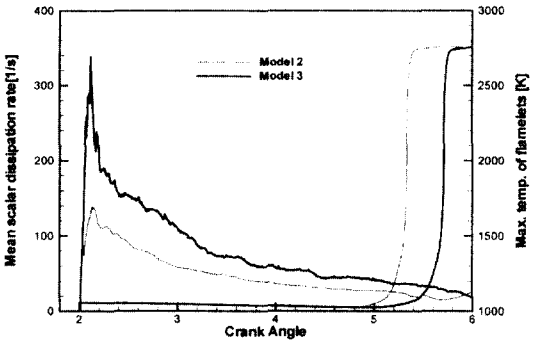
Fig. 3 Cylinder pressure histories for 4 injection timings (Model 3)

model, there are still a noticeable underestimation of ignition delay time for the relatively late injection timings (7 and 9.5 CA). These discrepancies could be attributed to the neglect of the radiative cooling and the vaporization effects on the turbulent combustion process, neglect of the spatial inhomogeneity of scalar dissipation rate, uncertainties in the spray dynamics models, the spray combustion processes of the multi-component diesel fuel, and the defects of the RANS-based turbulence model for treating the fast transient turbulent flows with the large-scale motion.

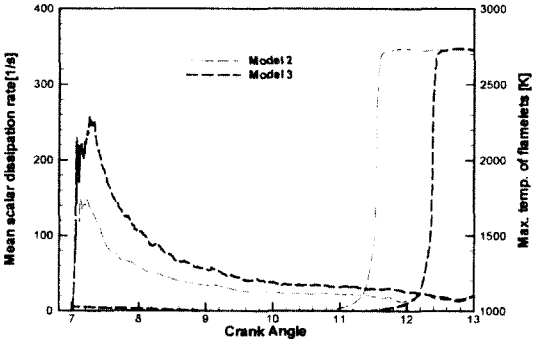
In order to improve the predicted ignition delay time, the RIF model including vaporization effects on turbulent combustion process is used to simulate the spray combustion processes for two injection timings (2 CA and 7 CA). Figure 3 displays the simulated cylinder pressure histories obtained by the RIF model with vaporization effect and the measured data for 2 injection timings. When the vaporization effects on turbulent combustion model are taken into account, it can be clearly seen that the agreement in the predicted and measured ignition delay times has been significantly improved especially for the relatively late injection timing (9.5 CA). These numerical results indicate that the vaporization effects on turbulent combustion process play a crucial role in the relatively late injection timing with the much lower cylinder temperature and

pressure. However, in terms of the cylinder pressure histories, the present model noticeably overestimate the cylinder pressure after auto-ignition at the relatively late injection timing (7 CA). These deviations might be related to the defects of the present turbulent combustion model described above.

Figure 4 shows the temporal evolutions of the mean scalar dissipation rate and mean temperature for two injection timings (2 CA and 7 CA). At the initial stage of liquid fuel injection, the scalar dissipation rate rapidly increases and reaches to a peak value due to the high vaporization rate and the intense tur-bulence generated by the high-velocity injection process. The high injection velocity enhances the liquid jet disintegration, droplet breakup, interphase convective heat transfer, droplet vaporization and gas-phase turbulence. Particularly, the droplet vaporization rate is greatly increased by reducing the vaporization characteristic time in the strong droplet breakup process as well as by increasing the interphase convective heat transfer. As a result, this high injection velocity abruptly increases the scalar dissipation rate by elevating these nonequilibrium effects such as the enhanced turbulence, the high spray evaporation rate and the large gradient of mixture fraction. Shortly after this initial injection period, the scalar dissipation rate gradually decreases to the slow-varying low value since the fuel vapor spreads out the ambient flow field and the turbulence is continuously dissipated. At the small scalar dissipation rates, the diffusive losses become so small that heat and radicals produced by the chemical reaction are continuously increased and the mixture field can be finally ignited. Compared to the RIF model(Model 2), the RIF model with vaporization effect(Model 3) predicts the relatively high level of the averaged conditional scalar dissipation rate. This trend directly reflects the spray vaporization characteristics predicted by these models. When the vaporization effects are coupled with the RIF turbulent combustion model, the averaged scalar dissipation rate considerably increases due to the increased production of mixture fraction fluctuations. These numerical results suggests that the vaporization effects coupled with the turbulent combustion models could be progressively influencing to the auto-ignition process and the spray combustion processes in the relatively retarded injection operation of DI diesel engines.



(a) 2°CA



(b) 7°CA

Fig. 4 Temporal evolution of the sclalar dissipation rates and the maximum temperature for 2 ignition timings

Figure 5 illustrates the instantaneous contours of mean temperature, OH radical mass fraction, NO concentration and soot volume fraction at CR 20 in the retarded injection timing (7 CA). Compared to two RIF models (Model 2 and Model 3), the Shell ignition/eddy dissipation model (Model 1) predicts the distinctly different flame structure and pollutant (NOx, soot) formation characteristics. These trends result from the defects of the the Shell ignition/eddy dissipation model (Model 1) which is unable to account for the effects of turbulence-chemistry interaction on auto-ignition and spray combustion processes in the DI diesel engines.

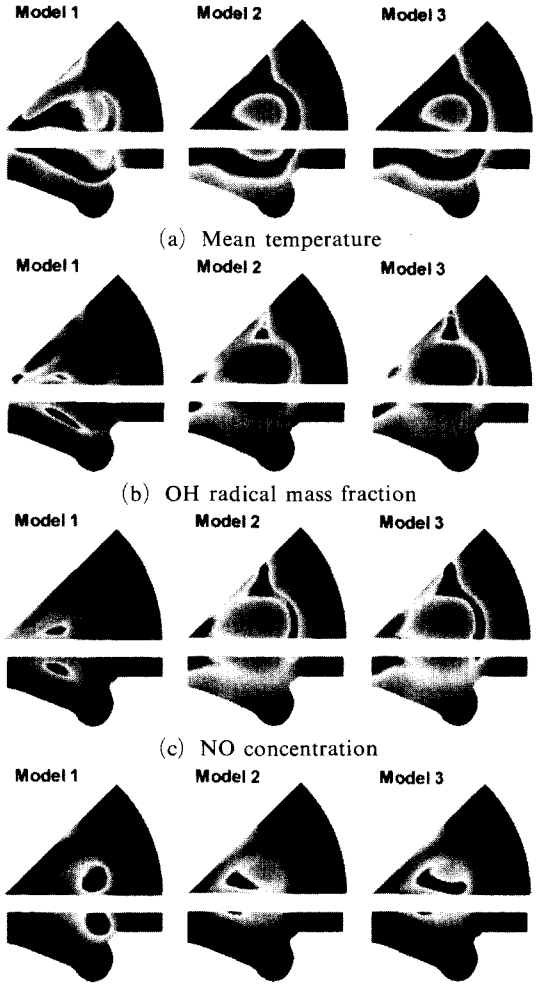


Fig. 5 Instantaneous contours of mean temperature, OH radical mass fraction, NO concentration, and soot volume fraction at 20 CR (injection timing 7 CA)

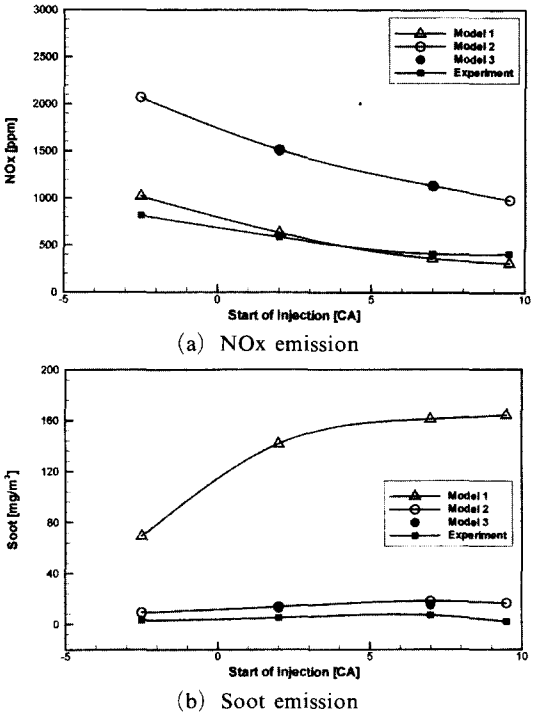


Fig. 6 NOx and soot emission for 4 injection timings

Figure 6 presents the measure and predicted NOx and soot emission charteristics for 4 injection timings of DI diesel engines. The measured and predicted results indicate that the NOx emission level decreases by retarding the injection timings. In terms of NOx emission, the Shell ignition/eddy dissipation model (Model 1) predicts the surprisingly good conformity with the measure emission characteristics while two RIF models (Models 2 and 3) considerably overestimate the NO emission level for 4 injection timings. However, it is necessary to note that all these models neglect the radiative cooling arising from soot and gaseous species (CO_2, H_2O). The recent numerical results (Kim et al., 2001) of the hydrogen jet flames indicates that the inclusion of radiative cooling effect results in the substantial decrease of NOx emission level. Therefore, it is expected that two RIF models with the radiative cooling effect could provide the much better agreement with the measured NOx emission level. In this aspect, the good conformity predicted by the Shell ignition/eddy dissipation model (Model 1) does not imply the physically correct representation and it might be related to the ad-hoc adjustment of correction factor used in the NOx emission model of Model 1.

In terms of soot emission, two RIF models (Model 2 and 3) predict the favorably good agreement with the measured soot emission level while the Shell ignition/eddy dissipation model (Model 1) predicts the completely wrong soot emission characteristics. Compared to the RIF model (Model 2), the RIF model with vaporization effect (Model 3) predicts the much better

conformity with the measured soot emission levels. These numerical results suggest that the RIF model including vaporization effect together with the Moss soot model (1995) has the great potential to correctly predict the soot emission for the wide range of injection timings.

4. Conclusion

The RIF-based turbulent combustion models and the Shell ignition/ eddy dissipation model have been applied to simulate the spray dynamics, vaporization, auto-ignition and combustion process in the DI diesel engine. Based on numerical results, the following conclusion can be drawn.

(1) Numerical results indicate that the RIF model including the vaporization effects on turbulent combustion process is capable of predicting auto-ignition and spray combustion processes in the wide range of injection timings in the DI diesel engines.

(2) For the relatively late injection timings (7 and 9.5 CA) where the nonequlibrium chemistry effects are dominant due to the relatively low chamber temperature and intense turbulence associated with the high-speed injection, the Shell ignition/eddy dissipation model substantially underestimate the ignition delay time and predict the quantitatively and qualitatively wrong pressure histories.

(3) In terms of NOx emission, the Shell ignition/eddy dissipation model (Model 1) predicts the surprisingly good conformity with the measure emission characteristics while two RIF models (Model 2 and 3) considerably overestimate the NO emission level for 4 injection timings. However, it is expected that two RIF models with the radiative cooling effect could provide the much better agreement with the measured NOx emission level. In this aspect, the good conformity predicted by the Shell ignition/ eddy dissipation model (Model 1) does not imply the physically correct representation and it might be related to the ad-hoc adjustment of correction factor used in the NOx emission model.

(4) In terms of soot emission, two RIF models (Models 2 and 3) predict the favorably good agreement with the measured soot emission level while the Shell ignition/eddy dissipation model (Model 1) predicts the completely wrong soot emission characteristics. Compared to the RIF model (Model 2), the RIF model with vaporization effect (Model 3) predicts much better conformity with the measured soot emission levels.

(5) The future works include the coupling of the RIF model with LES turbulence model, the development of the improved model to account for the vaporization effects on pdf and the scalar dissipation rate, the multiple RIF model to account for the spatial inhomogeneity of the scalar dissipation rate, the inclusion of radiative cooling, the implementation of comutationally efficient high-pressure vaporization model, and the development of multi-component fuel combustion model.

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