Flamelet Modeling with LES for Diesel Spray Combustion by using KIVA-LES with CIP Scheme

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ABSTRACT

LES of Diesel spray flame has been conducted using KIVA-LES code where flamelet model is incorporated to improve the modeling of the diesel spray flame. To reduce the computational cost, the ignition reaction is simulated with Shell model, while the combustion is modeled using FTS model with one-step reaction. The results show that the unsteady process of diesel spray flame was predicted with flamelet approach, although the 333 hour is needed to simulate 5.0 ms after start of injection. Furthermore the mixture fraction and temperature map shows that the combustion phase is complicated significantly compared to the jet flame, because the droplet evaporation is affected on the fuel vapor supply and cooling locally in the diesel spray flame.

INTRODUCTION

The LES (Large Eddy Simulation) technique has been very popular as the turbulent analysis method for engineering problems, such as burner, turbine and engines, developing the computational devices over the pasted ten years. In LES approach, the resolved part of turbulent velocity which is larger than the grid size is simulated without models like direct numerical simulation (DNS), while only the unresolved part of turbulent velocity is modeled using sub grid scale (SGS) model. Compared to Raynolds Averaged Navier Stokes (RANS) which is widely used for the engineering problems, the LES technique can predict the unsteady turbulent motions based on the large scale instability accurately. Hence The LES technique for the engine was conducted to improve the prediction of unsteady engine characteristics and to estimate the cycle to cycle validation [1]-[11]. However LES technique for the diesel spray hardly is performed [12][13].

We have been developed the diesel spray simulation with the LES technique [14]-[17] to predict the unsteady process of the diesel spray like experimental images, using KIVA-LES code where LES is incorporated into KIVA 3V res.2 according to Sone's method [10]-[12]. In order to reduce the numerical diffusion, CIP(Cubic-Interpolated Pseudo-Particle) scheme [18] for the convective scheme of the momentum equation was incorporated into KIVA-LES. CIP scheme is also used in GTT (General Tank Tube) code which is developed by Wakisaka [19]. As the results, the unsteady behavior was able to be predicted and temporal images were obtained like experimental images under non-evaporative, evaporative spray and diesel spray flame conditions. On the other hand, in early studies one-step reaction is used for the oxidation mechanism of fuel the combustion mechanism, and the combustion model used in our code is mixing control model base on the filtered value on the computational grid. This model is low computational cost, but the accuracy is not enough to predict the diesel spray flame in the LES approach.

Flamelet model which is assumed that the flame is composed of many laminar flamelet has been very popular as the combustion model for LES approach [20]-[26]. In this model, many chemical species are considered using only two transport equation in respect to the mixture fraction and its variance. Moreover the chemical reaction calculation is not necessarily performed interactively with detailed chemical mechanism using Aurora in CHEMKIN code [27][28], since the chemical composition after combustion is able to be estimated using the flamelet library which is contracted before the LES spray simulation from the one dimensional opposed flame simulation.

In this study, flamelet model is incorporated into KIVA-LES code to improve the modeling of the diesel spray flame for the LES approach. To account for the unsteady effect of premixed flame propagation flamelet time scale (FTS) model is used for the flamelet model which is developed by Rutland et. al [4][26]. Furthermore the mixture fraction and temperature map is examined to confirm the computational results with flamelet approach.

LES ANALYSIS OF DIESEL SPRAY FLAME WITH FLAMELET MODEL

In this study, the low temperature oxidation is simulated using Shell model, while the high temperature oxidation mechanism is modeled using FTS model. The ignition model was used wherever the temperature was lower than 1000 K. If the temperature was higher than 1000 K, the FTS model was activated for the high temperature chemistry. Shell model constant is used in ref. [29]

LES GOVERNING EQUATION

The governing equations used in KIVA-LES are continuous, momentum, internal energy equation and chemical species equations. In addition to the above equations, the mixture fraction $\tilde{Z}$ and its variance $\tilde{Z}''^2$ transportation equations are solved in FTS model.

$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_i\tilde{Z}}{\partial x_i}=\frac{\partial}{\partial x_i}\left[\frac{\mu+\mu_t}{Sc}\frac{\partial \tilde{Z}}{\partial x_i}\right]+\dot{\rho}^s \quad (1)$$

$$\frac{\partial\left(\bar{\rho}\widetilde{Z''^2}\right)}{\partial t}+\frac{\partial\left(\bar{\rho}\tilde{u}_i\widetilde{Z''^2}\right)}{\partial x_i}$$
$$=\frac{\partial}{\partial x_i}\left[\frac{\mu+\mu_t}{Sc}\frac{\partial \widetilde{Z''^2}}{\partial x_i}\right]+\frac{2\left(\mu+\mu_t\right)}{Sc}\left(\frac{\partial \tilde{Z}}{\partial x_i}\right)^2-2\bar{\rho}\tilde{\chi} \quad (2)$$

where ρ and u are the density and velocity, respectively. μ and μ_t denote the viscosity and turbulent viscosity, respectively. μ_t is modeled using k-Δ model. Sc is the schmit number, and Sc = 0.9 is used in this study. $\dot{\rho}^s$ at right hand side in Eq. (1) is the source term representing the effect of fuel droplet evaporation. χ denotes scalar dissipation rate. This is given as following formulas,

$$\tilde{\chi}=\frac{\left(v+v_t\right)}{ScC_l\bar{\Delta}^2}\widetilde{Z''^2}, \quad (3)$$

where v and v_t are kinematic viscosity and turbulent kinematic viscosity, which is model using k-Δ model. Δ and C_l are the grid size and model constant, respectively. C_l is 0.07 used in this study.

DEFINITION OF MIXTURE FRACTION

Mixture fraction Z is defined using the following equation,

$$Z=\frac{v_{st}Y_F-Y_{O_2}+Y_{O_2,o}}{v_{st}Y_F+Y_{O_2,o}}, \quad (4)$$

where v_{st} represents the stoichiometric oxygen-to fuel mass ratio. Y_F and Y_{O2} are the mass fraction of fuel and oxygen, respectively. $Y_{O2,o}$ denotes Y_{O2} at the initial condition.

REACTION MECHANISM AND REACTION RATE

In this study, dodecane is used for the fuel. To reduce computational time global reaction equation of dodecane is used,

$$2C_{12}H_{26}+37O_2 \rightarrow 24CO_2+26H_2O. \quad (5)$$

In FTS model, the reaction rate of fuel is described using the characteristic timescale τ_c,

$$\frac{\partial Y_F}{\partial t}=-\frac{Y_F-Y_F^*}{\tau_c}, \quad (6)$$

where Y^*_F is the equilibrium mass fraction of fuel estimated using the flamelet library.

Characteristic time scale is given [29], .

$$\tau_c=\tau_l+f\tau_t \quad (7)$$

where τ_l is laminar time scale, τ_t is turbulent time scale and f is the factor corresponding to the progress variable. For dodecane used as fuel in this study, the laminar time scale τ_l is given as

$$\tau_l=\alpha_l\tau_{l,o}=\alpha_l A^{-1}\left(Y_f\right)^{0.75}\left(Y_{O_2}\right)^{-1.5}\exp\left(E_A/RT\right), \quad (8)$$

where α_l is the model constant and $\tau_{l,o}$ is the laminar time scale based on the global mechanism. The pre-exponential constant and activation energy are A =3.1x10^{12} and E_A=30.0 kJ/mol, respectively. The factor f is defined as a function of the local composition,

$$f=\frac{1-e^{-r}}{0.632}, \quad (9)$$

where the progress variable r is the ratio of the amount of products to that of total reactive species,

$$r=\frac{Y_{CO}+Y_{CO_2}+Y_{H_2O}}{1-Y_{N_2}}. \quad (10)$$

In FTS model, the predicted heat release rate depends on the characteristic time scale significantly. In particularly, the laminar time scale have influenced on the heat release rate in the premixed burn. In this study the laminar time scale is changed using the model constant α_l, and α_l,=0.01 and τ_t =10.0μs are used.

FLAMELET LIBRARY

To estimate the Y^*_F in Eq. (7), the flamelet library is constructed using the one-dimensional counter flow diffusion flames with OPPDIF code. Figure 1 shows that the mass fraction of fuel is plotted as a function of mixture fraction at different scalar dissipation rates. The scalar dissipation is changed by the boundary condition of velocity. The mass fraction of fuel increased with increasing the scalar dissipation. In referring to the dissipation in the spray flame simulation, the computational cell over χ = 50 s^{-1} is regard as the one of χ = 50 s^{-1}, and the flame extinction is not considered.

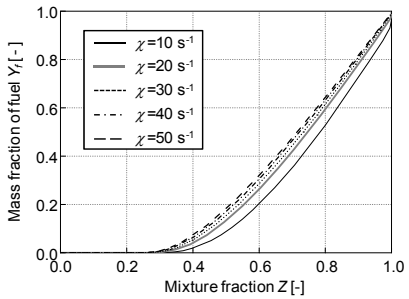

Fig. 1 Flamelet library

THE PRESUMED SHAPE PDF

To combine the flamelet library into the LES spray simulation field, the mixture fraction of fuel at equilibrium sate are estimated using proper probability density function (PDF) described by mixture fraction, variance of mixture fraction and scalar dissipation,

$$\tilde{Y}_f^* = \int_0^1 Y_f(\tilde{\chi}, Z) P(Z) dZ, \tag{11}$$

where $P(Z)$ is the beta function and $Y_f(\tilde{\chi}, Z)$ is the fuel mass fraction in the flamelet library. The beta function pdf has the form

$$P(Z) = \frac{Z^{\alpha-1}(1-Z)^{\beta-1}}{\Gamma(\alpha)\Gamma(\beta)}\Gamma(\alpha+\beta). \tag{12}$$

Here Γ is the gamma function. The two parameters and are related to mean and variance by

$$\alpha = \tilde{Z}\gamma\,, \quad \beta = \left(1-\tilde{Z}\right)\gamma\,, \tag{13}$$

where

$$\gamma = \frac{\tilde{Z}\left(1-\tilde{Z}\right)}{\widetilde{Z''^2}} \tag{14}$$

SPRAY MODELS

Blobs model where the injected droplet diameter in parcels equals to the nozzle diameter is used for the injection model. The injection velocity profile is constant in the injection duration. The effects of the internal nozzle flow, such as the cavitation and velocity fluctuation, are not considered. The droplet breakup is modeled using KHRT (Kelvin Helmholtz Rayleigh Taylor) model where model constant B_1 of 10 is adapted. The droplet evaporation model is KIVA original model where it is assumed that the droplet temperature distribution is uniform and the rate of droplet diameter change is given using the Frossling correlation. The collision and coalescence of droplets is not considered, because with collision and coalescence model the liquid length is overpredicted compared to the experimental results.

COMPUTATIONAL SCHEME

The LES governing equations are calculated based on Arbirorary Lagrangian Eulerian (ALE) as well as KIVA code[30]. The temporal differencing is divided into three part; phase A, phase B and phase C. Phase A calculates the spray dynamics and the source terms in governing equations. In phase B, diffusion terms are simulated inexplicitly using the SIMPLE (Semi-Implicit Mehtod for Pressure-Linked Equation) scheme. Phase C is the calculation of convective terms using the QSOU (Quasi Second Order Upwind) scheme [30].

However QSOU is the high stability, but the high numerical diffusion. The LES spray simulation with QSOU is unable to capture the unsteady process in diesel sprays and similar to the RANS spray simulation, since the numerical diffusion suppresses the unsteady motion related to large scale instability in the turbulence. Hence we incorporated CIP (Cubic-Interpolated Pseudo-Particle) scheme which are high numerical stability and low numerical diffusion into KIVA-LES. It is noted that the CIP scheme is not conservative and monotone scheme strictly. Hence, the convective term in the momentum equation which is related to the vortex motion and the unsteady characteristic is calculated using CIP sheme while the other convective schemes are simulated using QSOU.

COMPUTATIONAL CONDITIONS AND DOMAIN

Table 1 is the computational conditions. The spray predicted in the LES simulation is the diesel spray flame in the constant volume vessel with the injection pressure of 70MPa and the nozzle diameter of 0.20mm. The ambient gas is composed of the oxygen of 21 vol.% and nitrogen of 79 vol. %.

The computational domain is the cylindrical shape where the diameter and the height are 30mm and 100mm, respectively. The numbers of computational cells in radial, azimuthal and axial directions are 60, 60 and 200, respectively. The total number of computational cells is 780,000 cells. This corresponds to the grid resolution of 0.05mm in radial, 6degree in azimuthal and 0.5 mm in axis direction respectively. The number of parcels to be injected is 40,000. The time step is 1.0 μs and is changed using auto time step control with lowest time step of 0.1 μs [30]. The workstation with CPU of Xeon woodcrest is used as the computational device. The simulation consumed 333 CPU hour (4.8 million cycle) to simulate from injection start to 5.0 ms after start of injection with one-node and one CPU.

Table 1 Computational conditions

Hole diameter	[mm]	0.20
Injection pressure	[MPa]	70
Injection duration	[ms]	2.2
Fuel	[-]	C12H26
Fuel amount	[mg]	20.0
Fuel temperature	[K]	300
Ambient gas oxygen concentration	[-]	21 vol.%
Ambient pressure	[MPa]	4.1
Ambient temperature	[K]	900

RESULT AND DISCUSSION

HEAT RELEASE RATE

The heat release rate of LES simulation and experiment are shown in Fig.2. The ignition in the experiment is occurred at approximate 0.25ms. The good agreement is obtained between LES and experimental results in terms of the ignition time. The shape of the premixed and diffusion burn carve are predicted well, although the magnitude is not matched perfectly and the fluctuation is recognized at the computational heat release shape. The overprediction of the premixed burn is due to the prediction accuracy of FTS model. In the FTS model, the characteristic time scale used depends on the heat release rate significantly. Furthermore the pressure wave is generated from the massive heat release in the premixed burn phase, so that to improve the prediction the combustion model to treat the premixed flame front should be combined into the flamelet model due to the control of the computational premixed burn, such as coherent flamelet model and G-equation model.

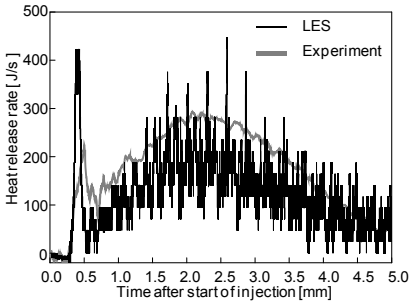

Fig. 2 Comparison of temporal change in heat release rate between LES and experimental result.

INSTANTANEOUS SPRAY IMAGES

Figure 3 shows the predicted 3D spray shape and sectional image at 2.2 ms in addition to the shadowgraph image. The section temperature distribution as shown in Fig. 3(b) the high temperature region is located at the spray periphery. In the internal of high temperature zone, the mixture fraction is significant high. This zone is mainly composed of the unburned fuel. The soot precursor and soot would be generated in this zone. On the other hand, the high temperature zone is existed near the nozzle and the flame lift-off length is unable to be predicted. In the case of this conditions flame lift-off length would be 15mm at least [31].

Figure 3 (c) is the 3D spray shape using the volume rendering technique to represent diesel spray flame with the in-situ effect like shadowgraphy method. The diesel spray flame defines the region over mixture fraction of 0.001. This region is visualized using the volume rendering whereas the fuel parcels is visualized as spheres of the constant size. If the temporal sequence images of the LES diesel spray flame are generated using these visualization techniques, the unsteady formation process of fuel vapor and the combustion gas expansion due to ignition and premixed burn are visualized like experimental shadowgraph images.

Figure 3 (d) is the coherent vortex generated in the gas phase. This vortex is identified using iso-surface of the second invariant of the velocity gradient tensor. The vortex structure composed of many hearpin-like structures is confirmed in the diesel spray flame, but the many turbulent tubes are generated besides the spray flame region. This is due to the pressure wave generated in the premixed burn.

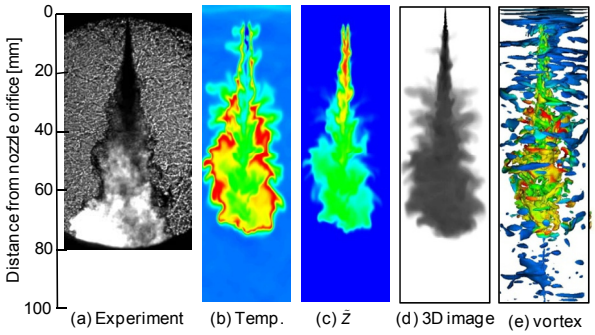

Fig.3 Comparison of instantaneous spray image between LES and Experimental results at 2.2ms .

DIESEL SPRAY FLAME STRUCTURE USING MIXTURE FRACTION AND TEMPERATURE MAP

The diesel spray structure is complicated compared to jet flame which fuel and oxygen is supplied separately from the boundary. This is because in spray flames fuel vapor is supplied locally from the droplet evaporation in the spray flame directly and cooling effect is occurred due to latent heat the droplet evaporation.

Figure 4 shows that the mixture fraction and temperature map to examine the detailed structure of diesel spray flame. Mixture fraction is not changed before and after chemical reaction. This is increased for the droplet evaporation and decreased for the turbulent diffusion. The computational cells where mixture fraction is over 0.001 are plotted in this figure.

Ignition delay time (*t*= 0.0-0.25ms)

In this period the heat release is not generated. Thus the high mixture fraction region indicates low temperature due to the latent heat of droplet evaporation. The heat release is not confirmed before 0.20 ms and the diesel spray region is below temperature of 900 K which is the initial ambient gas temperature. The mixture fraction is below 0.80. The ignition cell is the mixture fraction of approximate 0.20.

Premixed phase(*t*= 0.25-0.40ms)

The premixed flame is enveloped whole diesel spray, and the high temperature region is generated rapidly.

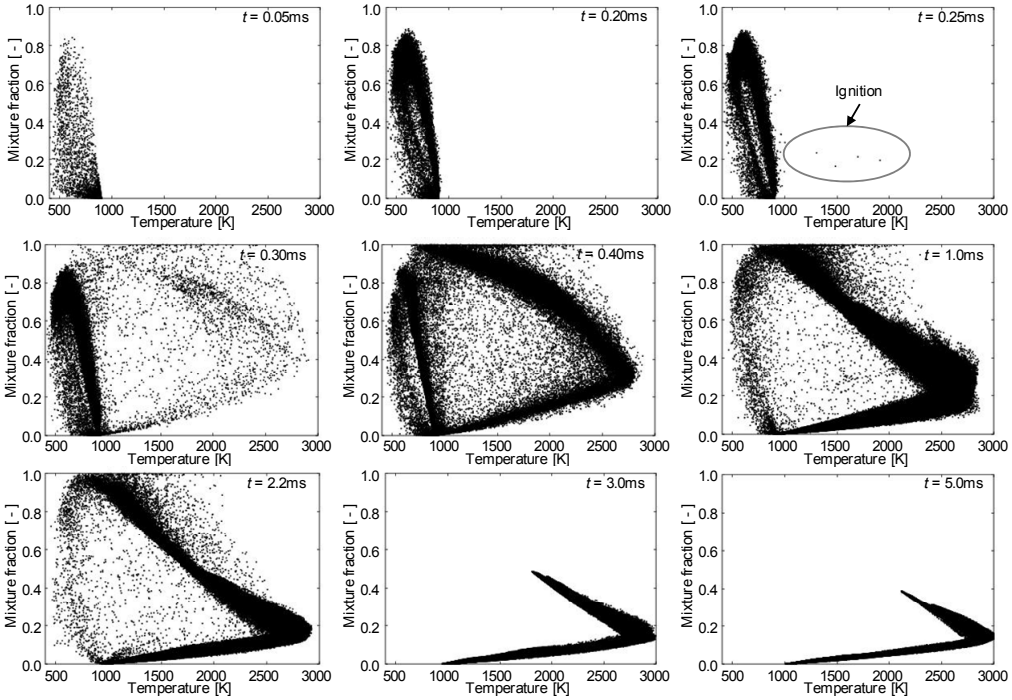

Fig. 4 Temporal change in mixture fraction temperature map simulated in LES approach.

The mixture fractions over temperature of 1000K is mainly located in separated high and low mixture faction zone on the boundary of 2800 K. Low temperature and high temperature zones are corresponding to the internal and the periphery of diesel spray flame, respectively. Furthermore high mixture fraction zone of approximate unity is confirmed in premixed phase, because the droplet evaporation is prompted within diesel spray flame in which oxygen is consumed due to the premix burn. In this zone, the soot precursor and soot would be generated.

Mixing control phase (*t*= 0.40-2.2ms)

In this phase, the high mixture fraction branch is decreased in the range of temperature between 1000K and 2800 K due to the transition from the premixed burn to the diffusion burn. The highest temperature is increased, and the highest mixture fraction is also decreased to 0.20 at 2.2 ms with increasing the time.

Late combustion phase(*t*= 2.2-5.0ms),

After 2.2ms, the highest mixture fraction is decrease, since all fuel droplets are already evaporated. The spray flame structure is significant simple like the jet flame. The almost diesel spray flame is located in the high temperature and low mixture fraction zone where the NO_x would be generated.

CONCLUSION

The LES spray simulation using FTS model was conducted to improve the description of the diesel spray flame. The ignition reaction is modeled using Shell model, while the premixed and diffusion burn is modeled by FTS model. The following conclusions are obtained,

(1) FTS model with the characteristic time scale using laminar time and turbulent time predicts the diesel spray flame well.

(2) Using mixture fraction and temperature map, it is confirmed that the diesel spray flame is complicated significantly due to fuel vapor supply and cooling related to the droplet evaporation.

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