

LES Analysis of Mixture Formation and Combustion Processes in a Diesel Spray

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ABSTRACT

Numerical calculations based on large eddy simulation were performed in order to investigate mixture formation, ignition, and combustion processes in a diesel spray formed by fuel injection into a constant-volume vessel under high-temperature and high-pressure conditions. Fuel concentration distributions in a spray and local non-homogeneous mixture distributions were compared with experimental results to verify the accuracy of the calculations. In addition, calculations were carried out to examine the effect of injection parameters, namely, injection pressure and nozzle orifice diameter. Ignition and combustion processes were also investigated using Schreiber's model for calculating the progress of oxidation reactions.

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INTRODUCTION

In recent diesel engines, exhaust emissions and thermal efficiency have been remarkably improved using the latest technologies, such as high-pressure and multi-stage injection, exhaust gas recirculation, supercharging, and exhaust aftertreatment. However, the demand for further improvements in emissions, fuel economy, and engine output continues to grow. As such, the development of advanced technologies is required in order to accurately control in-cylinder combustion processes, which contributes to the simplification and cost-reduction of engine systems. The formation process of harmful substances such as nitrogen oxides (NOx) and soot, and heat release rate, which directly influences thermal efficiency and combustion noise, are strongly affected by not only the average mixture concentration but also non-homogeneity, i.e., the microscopic variation of the mixture concentration[1]. However, the non-homogeneous mixture distribution in a spray and its influence on ignition and combustion processes have not been sufficiently clarified. It is important to fundamentally investigate the mechanism from the viewpoint of combustion control.

In addition to experimental approaches, computational fluid dynamics (CFD) is an effective means of analyzing combustion processes. Since ignition and combustion are very complicated phenomena, in which the fuel-air mixture is formed by an unsteady turbulent flow and chemical reactions

progress simultaneously, Reynolds-averaged Navier-Stokes-based (RANS-based) CFD has frequently been used in the calculation of diesel combustion, due to its relatively low computational load. However, since RANS is a time-averaged model, calculated concentration distributions do not reproduce the existence of locally rich and lean mixtures in a spray, which are actually observed in the instantaneous mixture distributions[2]. Therefore, calculation based on large eddy simulation (LES) is thought to be more suitable for the purpose of analyzing the behavior of turbulent flow, the formation of non-homogeneous mixtures, and its influence on ignition and combustion. For example, in order to develop a spray breakup model, Apte et al. calculated the development of a spray using LES for gas phase[3]. In this calculation, LES contributes to providing accurate predictions of turbulent transport, which affects the maximum stable diameter of droplets. In addition, Jhavar et al. used LES-based CFD for the calculation of in-cylinder mixture formation and combustion[4]. The results indicate that LES is able to capture more detailed flow structures than RANS and to predict some cycle-to-cycle variations. Furthermore, Jhavar et al. performed the calculation starting from the intake process through to the combustion process by coupling LES with KIVA-CHEMKIN code and showed that the results match the experimental data better than the results obtained through RANS-based calculation. As a fundamental study on spray development, Hori et al. calculated the development of a diesel spray in a constant-volume vessel using KIVA-LES

code. The calculation reproduces the intermittent behavior around the spray boundary region, which is observed in experimentally visualized images, and well predicts the spray tip penetration[5]. However, few reports have compared calculated mixture distributions and experimental results for a high-temperature and high-pressure condition, and no quantitative evaluation has been reported for local non-homogeneous distributions of mixture.

In the present study, numerical calculation based on LES was carried out for a fuel-air mixture formation process in a spray formed by injecting n-heptane into a constant-volume vessel under high-temperature and high-pressure conditions. In order to evaluate the results, mixture concentration distributions and local non-homogeneous distributions obtained by the calculation were quantitatively compared with the experimental results obtained by the planar laser-induced fluorescence (PLIF) method[2]. In addition, the effect of injection pressure and nozzle orifice diameter were examined. Furthermore, the ignition and combustion processes were investigated considering oxidation reactions in mixtures by Schreiber's model[6].

NUMERICAL SCHEME AND METHOD

CONDITION AND METHOD

Large eddy simulation (LES) calculations were performed for the mixture formation and ignition processes of a diesel spray, which is formed in a constant-volume vessel under a pressurized high-temperature condition. The calculation results are compared with the distribution of fuel concentration measured by PLIF[2]. Figure 1 shows a schematic diagram of the constant-volume vessel used in (a) the PLIF experiment[2] and (b) its calculation grid system, which consists of $123 \times 68 \times 90$ cells. The results of calculations using neither a finer grid system nor a uniform grid system were confirmed to be significantly different from the results presented in the present paper. The origin of the coordinate system is set at the nozzle exit, which is located 6 mm away from the top wall, and the x-axis coincides with the spray axis. The distance from the nozzle exit to the bottom wall is 74 mm. The initial thermodynamic temperature in the vessel is $T_i = 900$ K and the pressure is $p_i = 2$ MPa and 4 MPa. The surrounding fluid is nitrogen for non-combustion calculations and air with an oxygen mole fraction of 21% for combustion calculations.

The liquid phase of fuel was described by the discrete droplet model (DDM). The initial fuel temperature is 338 K and the initial velocity of the droplet was determined such that the spray tip penetration corresponds to that of a visualized image obtained by the shadowgraph method. The initial direction of the fuel droplet was given by the angle from the x-axis, which is determined using normal random numbers with a standard deviation of $\sigma_\theta = 4.5$ degrees. This value was determined by comparing the width of spray in the

upper region ($x < 30$ mm) and images visualized by the shadowgraph and PLIF techniques. The injection duration is set to 3.85 ms and approximately 25,000 parcels are injected in total during this period. The drag force on a droplet from the surrounding fluid was calculated by assuming the droplet to be a rigid sphere. For a break-up model of a spray droplet, the WAVE model[7] proposed by Liu et al. was used and the empirical constants B_0 and B_1 were determined to be 0.61 and 15, respectively. These constants were adjusted based on a visualized image obtained by the Mie-scattering method and measurement results for the mixture distribution obtained by the PLIF method. The change in the radius of a droplet due to evaporation and the temperature change caused by heat transfer were calculated by diffusion equations under forced convection[8].

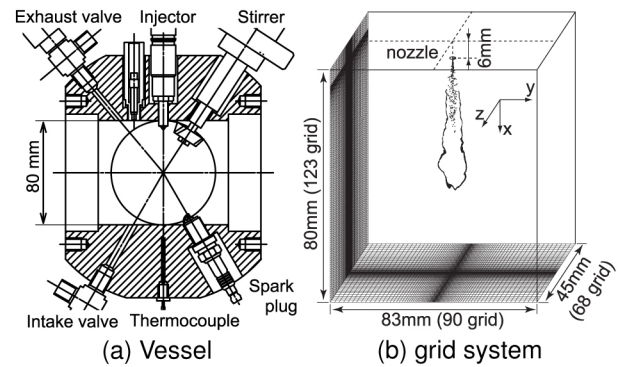


Fig. 1. Schematic diagram of the constant-volume vessel and calculation grid system

The flow and turbulent diffusion processes were calculated based on spatial Favre-filtered continuity, Navier-Stokes, mass transport, and enthalpy transport equations. The volume ratio of the fluid and the cell V_f is introduced in order to take into account the excluded volume in a calculation cell by droplets. The governing equations are expressed as follows:

$$\frac{\partial \bar{\rho} V_f}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = \bar{\rho}^s, \quad (1)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{u}_j + \tau_{ij}^{SGS})}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \bar{F}_i^s, \quad (2)$$

$$\frac{\partial \bar{\rho} \tilde{t}_m V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{t}_m \tilde{u}_j + j_{j,m}^{SGS})}{\partial x_j} = -\frac{\partial}{\partial x_j} \tilde{j}_{j,m} + \bar{\omega}_m + \bar{\rho}_m^s, \quad (3)$$

$$\frac{\partial \bar{\rho} \tilde{h} V_f}{\partial t} + \frac{\partial (\bar{\rho} \tilde{h} \tilde{u}_j + q_j^{SGS})}{\partial x_j} = \frac{\partial p_0 V_f}{\partial t} - \frac{\partial}{\partial x_j} \tilde{q}_j + \bar{Q}^s, \quad (4)$$

where $\bar{\cdot}$ denotes a spatial filtered quantity, and $\tilde{\cdot}$ denotes the Favre-average. The sub-grid scale (SGS) Reynolds stress τ_{ij}^{SGS} in equation (2) is given by the Smagorinsky model, and the constant C_s is fixed to 0.11[9]. The SGS mass flux $\tilde{j}_{j,m}^{SGS}$ in equation (3) and the SGS heat flux $\tilde{q}_j^{SGS}$ in equation (4) were also modeled by the gradient diffusion model, and the turbulent Schmidt number and turbulent Prandtl number are assumed to be unity. Here, p_0 is the mean pressure in the vessel. In addition, $\bar{\rho}^s$ and $\bar{\rho}_m^s$ are source terms due to the evaporation of fuel droplets, and $\bar{F}_i^s$ and $\bar{Q}^s$ are source terms for momentum and heat transfer from fuel droplets. Finally, $\bar{\omega}_m$ represents the production rate of each species by chemical reactions. The effect of SGS turbulence on ω_m is not considered. The implicit method was used for the temporal integration, and the SIMPLER method was applied to pressure correction and a staggered system was used. For the momentum equation, a fourth-order Adams-Moulton scheme and a fourth-order central scheme were applied. For the convection terms of the mass and enthalpy equations, the QUICK scheme was applied. However, for a region with a large density gradient, a first-order upstream scheme was applied in order to avoid under-shoot and over-shoot of scalar variables[10]. For other spatial differences, a second-order

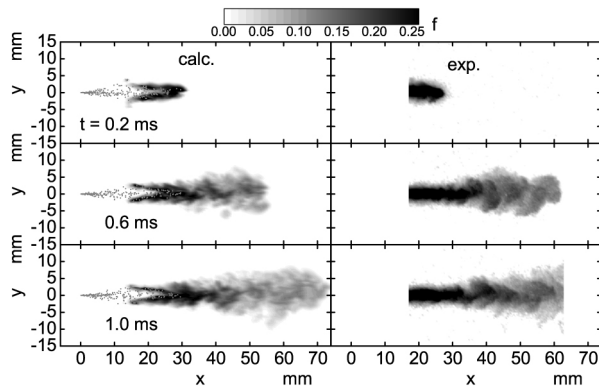
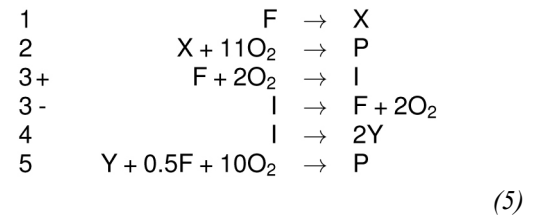


Fig. 2. Distributions of fuel mass fraction f ($p_{inj} = 120$ MPa, $d_n = 0.141$ mm)

central scheme was used. The calculations were performed from the start of injection $t = 0$ ms until $t = 6.0$ ms. The time step was 50 ns, and the maximum Courant number was approximately 0.15 at the very fine grids below the nozzle exit. On all of the wall boundaries, a slip wall boundary condition and an adiabatic wall boundary condition were applied, and there was no inlet or outlet of gas. In addition, the influence of SGS components on fuel droplets was ignored.

CHEMICAL REACTION MODEL

Schreiber's five-step reduced mechanism[6] was used to predict the progress of chemical reactions in mixture. The reaction scheme for n-heptane is as follows:



where F is the fuel, X are the products of fuel pyrolysis, Y and I are the intermediates in a low-temperature reaction pass, and P are the final products, which are composed of CO_2 and H_2O . Since the original reaction rates provide a much shorter ignition delay than the full kinetics calculation under the conditions relevant to the present study, the frequency factors A_i were modified. The details are described in the Appendix.

RESULTS

FUEL DISTRIBUTION IN A SPRAY

Based on these models and procedures, the mixture formation process of a diesel spray was calculated, and the results were compared with experimental data. Here, the injection pressure and nozzle orifice diameter were set to be $p_{inj} = 120$ MPa and $d_n = 0.141$ mm, respectively. The initial condition of the surrounding gas was assumed to be homogeneous with a pressure of $p_i = 2$ MPa and a temperature of $T_i = 900$ K. Figure 2 shows the distributions of the fuel mass fraction f on the x-y plane at the

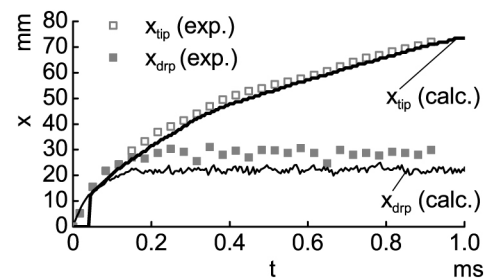


Fig. 3. Temporal change of spray tip penetration x_{tip} and liquid length x_{drp}

time of injection $t = 0.2$ ms, 0.6 ms, and 1.0 ms after injection along with those measured by the PLIF method[2]. The calculation results generally agree with the experimental data. The calculated mixture distributions reproduce a corrugated boundary between the fuel and the surrounding fluid due to an unsteady flow, which is observed in the measurement results. The values of f for the experimental data ranging from $x = 20$ mm to 30 mm are higher than those for the calculated data. Based on the calculation results, fuel droplets