

# Computational Simulation of Diesel Combustion with High Pressure Fuel Injection

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## ABSTRACT

Computational simulation for the combustion process in a DI diesel engine was performed through the KIVA code. Two conditions of different injection pressure were examined in the simulation. The injection pressures are 150 MPa and 50 MPa. A model for the combustion process was added to the KIVA code. The combustion phenomenon was modeled as a combined process of formation of a combustible mixture and a chemical reaction. The rate of mixture formation was assumed to be dependent on the turbulence characteristics and the concentration of species in each computational cell. The rate of chemical reaction is described as an Arrhenius equation. The result of the simulation agrees with the experimental result qualitatively, and the effect of injection pressure on the combustion process is well predicted.

## INTRODUCTION

Computational simulation for the diesel combustion is an active area of research. Several sub-models for the combustion process and the spray behavior have developed. For practical applications, there are some requirements in the computational code. They are accuracy of the simulation, ability of dealing with several input variables such as geometry of the combustion chamber, operating conditions, and fuel specifications. In addition, it is also required that the simulation is able to be performed with a practically allowable CPU time and available computer resources. In so far, however, computer simulation codes seem not necessarily have enough ability, and so, the developments of useful sub-models are open problems. In the present study, the authors used the KIVA<sup>(1)</sup> code and simulated the effect of injection pressure on the combustion process.

## SUB-MODELS OF FUEL SPRAY AND COMBUSTION

The authors found that the size of the computational grid have a substantial effect on the simulating result for the penetration and the shape of spray as shown in Fig. 1. Figure 1 shows the parcels of fuel spray in a quiescent inert gas at the end of the injection. In these simulations, an axial symme-

try is assumed and two dimensional cylindrical coordinates are used. The size of the grid for the radial and the axial coordinates are the same. The process of vaporization of fuel is not included in the simulation for Fig. 1. It is obvious that the penetration and the shape of the spray is not correctly predicted when the grid size is greater than 1 mm.

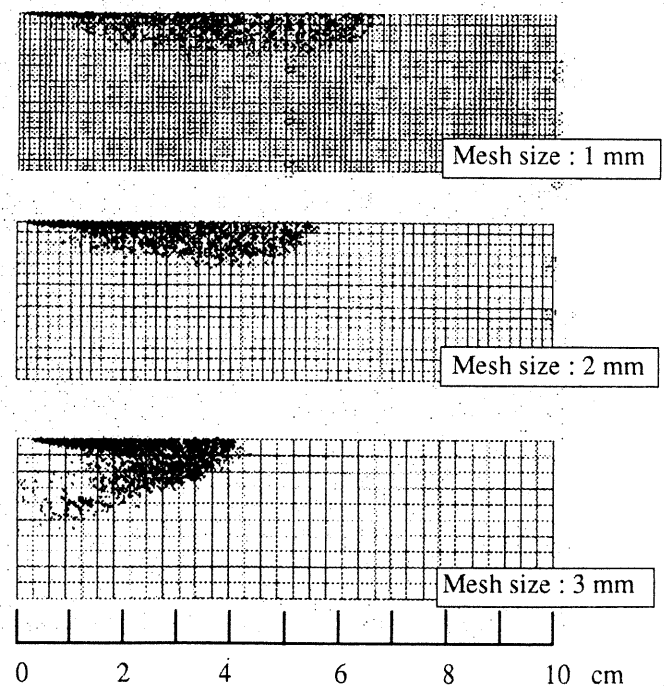


Fig. 1 The effect of computational grid on the penetration and shape of spray

The sub-model for fuel spray is one of those given in the original KIVA code. In the sub-model, fuel droplets of which diameters are smaller than that of nozzle holes emerge from the nozzle. The initial diameter of the droplet is determined by empirical equation of Kuo, T. W. et. al.<sup>(2)</sup> as

$$SMR_0 = B[4\pi(\sigma_1/\rho_g V_0^2)2/3] \quad (1)$$

where B is a constant,  $\sigma_1$  the surface tension,  $\rho_g$  the density of air, and  $V_0$  the velocity of the fuel jet.

Another model was also tested. In the later case, the initial diameter of droplets was assumed to be equal to the diameter of the nozzle hole, and a breakup process of droplets was considered. From the comparison of two sub-models for a fuel spray, it was found that the former model well predicts the observed penetration and the shape of the fuel spray. Therefore, the former sub-model was used in the simulation of the combustion process.

In the simulation, the injection rate was assumed to be constant during the injection period. This assumption is reasonable for an accumulator type fuel injection system used in the experiment<sup>(3)</sup>.

A sub-model<sup>(4)</sup> for the combustion process is added to the KIVA code. The model consists of two equations for the rate of mixture formation and the rate of chemical reaction. The rate of mixture formation  $R_m$  is determined from turbulence kinetic energy (TKE) and dissipation rate ( $\epsilon$ ) as

$$R_m = (1+S)(A\rho\epsilon/k)\min(m_{fu}, m_{ox}/S) \quad (2)$$

where  $S$  is theoretically required mass of oxygen to make a stoichiometric mixture with a unit mass of fuel,  $A$  is an empirical constant which is assumed to be 1 in the present study, and  $\rho$  is the density of gas.  $m_{fu}$  and  $m_{ox}$  are the mass fractions of fuel and oxygen respectively. TKE and  $\epsilon$  are calculated in the KIVA code through a  $k$ - $\epsilon$  turbulence model. The rate of chemical reaction  $R_f$  is determined from an Arrhenius's type equation as

$$R_f = (S/(1+S))(\rho^2 m_{mi}^2 / M_{O_2}) F \exp(-D/T) \quad (3)$$

where  $m_{mi}$  is the mass fraction of combustible mixture,  $M_{O_2}$  the molecular weight of oxygen,  $F$  is a frequency factor and  $D$  is the activation temperature.  $F$  and  $D$  are assumed to be  $10^{10}$   $m^3/skmol$  and  $1.2 \times 10^4$  K. For the most part of the present study, chemical species considered were fuel,  $O_2$ ,  $N_2$ ,  $CO_2$ , and  $H_2O$ . The fuel was treated as  $C_{12}H_{26}$ , with properties of its vapor pressure, critical temperature, latent heat, and liquid viscosity equal to that of hexadecane, and remaining properties equal to that of dodecane. In a case for the condition of high pressure fuel injection, a chemical equilibrium was also tested. When the chemical equilibrium was counted, the species added to the computational code were N, O, OH, CO,  $H_2$ , and H.

## TEST ENGINE SPECIFICATIONS AND COMPUTATIONAL CONDITIONS

The engine specifications are shown in Table 1. The calculating conditions are shown in Table 2. The difference of injection pressure is given through the input parameters of fuel injection shown in Table 3. The engine has a centrally located 6-holes nozzle and an accumulator type fuel injection system<sup>(3)</sup>. A periodicity was assumed. So, the calculation was performed for a part of the combustion chamber which includes one fuel spray. The number of computational grids is 25 for the radial coordinate, 33 for the tangential coordinate, and 33 for the axial coordinate. The total number of grids is

Table 1 Test engine specifications

Bore	mm	135
Stroke	mm	140
Compression ratio		16.5
Combustion system		Direct injection
Diameter of the piston bowl	mm	90
Injection nozzle		6 holes, diameter=0.17 mm.

Table 2 Calculating conditions

Engine speed	rpm	1000
Injection quantity	mm <sup>3</sup> /st	110
Injection timing	ATDC degree	-5
Injection pressure	MPa	150, 50

Table 3 Initial value of fuel spray

Injection pressure MPa	Injection duration degree	Sauter mean radius mm	Initial velocity m/s
150	12.7	0.025	411
50	19.8	0.065	257

27225. The authors think that these grids are not necessarily enough to predict the penetration and the shape of the spray precisely, however, the available computer resource does not allow much computational grids. The computer system used in the present study is TITAN 3000 with 96 Mbyte memories. The CPU time for a simulation from -90 ATDC degree to 40 ATDC degree for one condition is about 1200 hours (50 days).

## RESULTS AND DISCUSSION

Figure 2 and Fig. 3 show concentrations of fuel and products (only carbon dioxide is shown as representative species), profiles of temperature and TKE. In the Figures, the side view shows a section includes the axis of fuel injection. The top view show the section locates 17 mm above the bottom of the combustion chamber except squish area where the picture shows the section locates at the top of the piston.

The concentration of fuel increases in the injection duration only near the fuel spray axes, and is low at the wall. After the end of injection, the concentration of fuel decreases rapidly. The concentration of product species increases around the fuel spray. Strong turbulence is formed along the

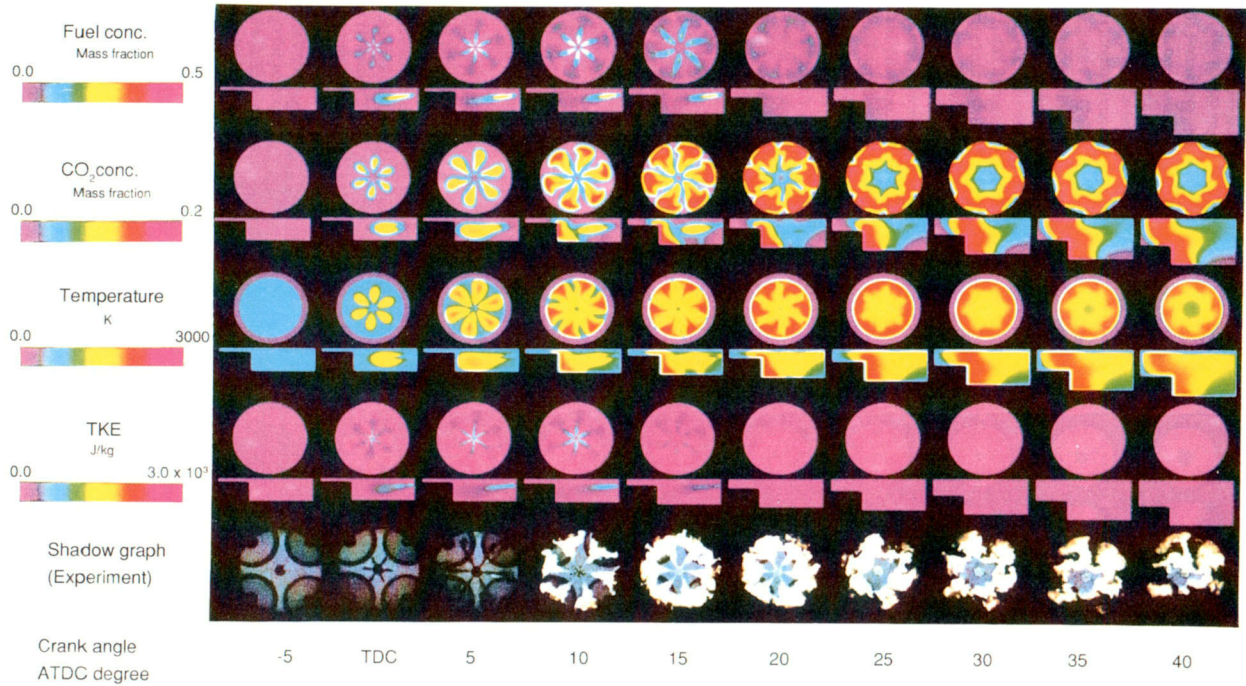


Fig. 2 Profiles of concentration, temperature, TKE, and shadowgraph (injection pressure : 50 MPa)

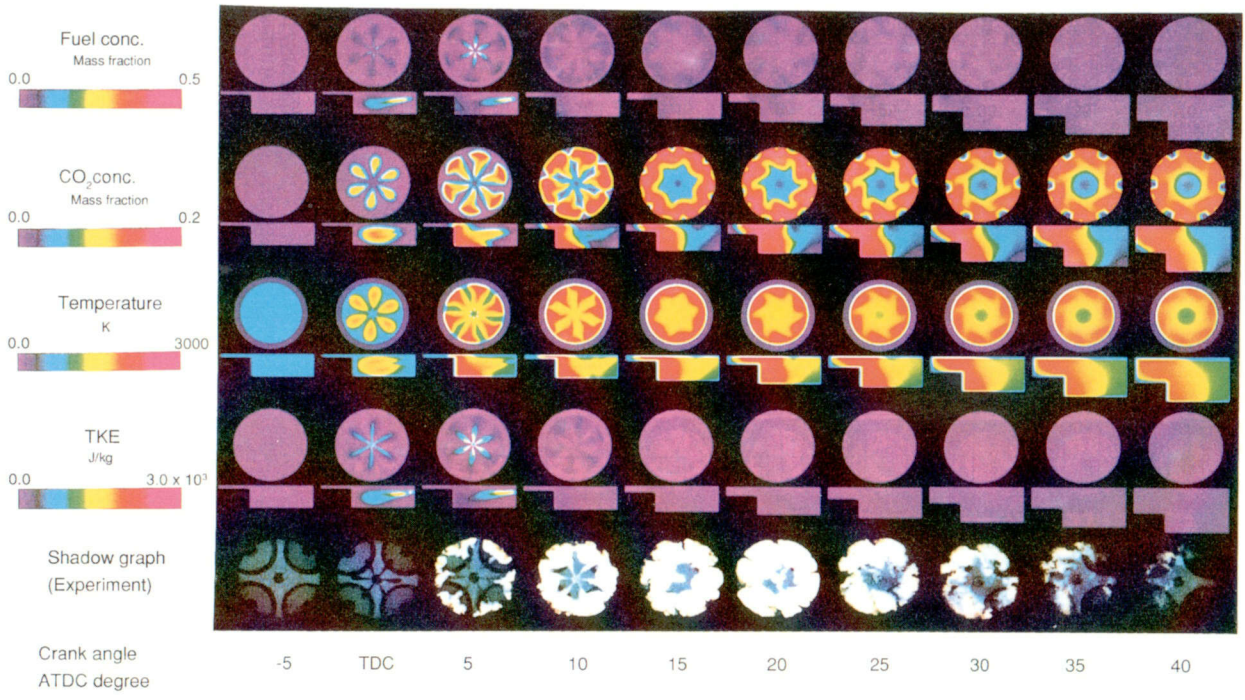


Fig. 3 Profiles of concentration, temperature, TKE, and shadowgraph (injection pressure : 150 MPa )

axes of fuel spray in the injection duration (from -5 to 14.8 ATDC degree for 50 MPa, from -5 to 7.7 ATDC degree for 150 MPa). From these observations, the combustion process seems to occur mainly around the axes of fuel spray. Therefore, the fuel spray characteristics such as the penetration and the shape have essential effects on the combustion process in this kind of simulation for DI diesel engines.

Figure 2 and Fig. 3 also show the shadow graphs<sup>(3)</sup> of the combustion process in a DI diesel engine. The specifications and the operating conditions of the engine are that used in the simulation (Table 1 and Table 2). An Ar-ion laser (wave length is 488.8 nm) was used as a light source. The laser beam was expanded with a couple of lenses and introduced through a quartz window attached at the bottom of the piston. The light is then reflected at a plane mirror attached at the under surface of the cylinder head. The valve surfaces were coated with platinum and polished for the mirror surface reflection. A half mirror was used to introduce the shadow image into a high speed camera system. As the optical system does not have band-pass filter, the spontaneous emission from the flame was also recorded on the film.

The result of the simulation well agree with the observed combustion process qualitatively, and the simulation well predicts several features of the effect of high pressure fuel injection on the combustion process. When the fuel injection pressure is high, the flame develops more rapidly than that in the ordinary pressure condition. In the high pressure condition, the flame development near the wall starts at 5 ATDC degree; in the ordinary injection pressure, it starts at 10 ATDC degree.

Figure 4 shows the predicted pressure in the combustion chamber. Corresponding result of the experiment is shown in Fig. 5. The high pressure condition gives a higher peak pressure and an earlier peak pressure timing. These features are commonly found in both the simulation and the experiment.

Quantitatively, the simulation agree with the experiment in the peak pressure timing, however, the peak pressure in the simulation is higher than that observed in the experiment. The predicted pressure is about 0.4 MPa higher than experimental result at injection timing (-5 ATDC degree). At first, the authors thought the cause of higher peak pressure was due to simplified model for chemical reaction without thermal dissociation. However, it was found that the peak pressure was not varied even if the chemical equilibrium is counted, though the peak temperature decreases about 150 K when chemical equilibrium is counted. In addition, the simulation gives higher pressure in the combustion chamber before the combustion process initiates. Therefore, there will be other causes of the discrepancy in the predicted pressure and the observed pressure. One possible cause is a blow-by gas in the compression stroke. In the simulation, the effect of blow-by gas was simply neglected. However, there is some blow-by gas in real engine systems.

Figure 6 and Fig. 7 show the predicted rate of heat release (ROHR) and the experimentally obtained ROHR respectively. There are some fluctuations on the ROHR curves Fig. 7. The experimentally obtained ROHR curves

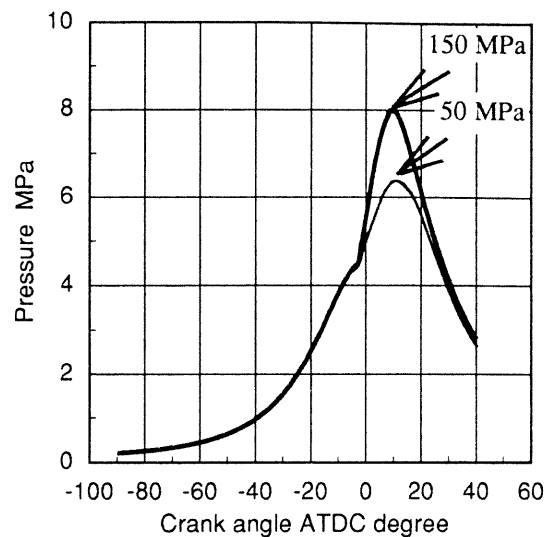


Fig. 4 Pressure diagram. (calculation)

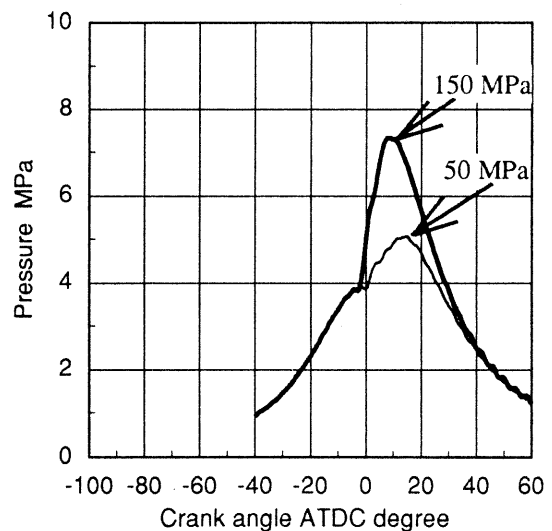


Fig. 5 Pressure diagram. (experiment)

were calculated from the pressure indicator obtained in only one cycle of the engine operation, and the fluctuations in Fig. 7 is not essential. Due to these fluctuations, it is difficult to discuss precisely about the propriety of the combustion model, however, the essential effect of the injection pressure on the ROHR seems to be well predicted at least qualitatively. The ROHR in the injection duration increases when the fuel injection pressure increases. In general, the constants used in the equation (2) and (3) must be optimized through the comparison of the prediction and the observation. This kind of optimization will be the next step of the study.

For the condition of high pressure fuel injection, a chemical equilibrium was also tested. The ROHR was not significantly varied whether the chemical equilibrium is counted or not.

Figure 8 shows the integrated TKE in the combustion chamber. Before the fuel injection starts, the increase of TKE is moderate. After fuel injection starts, TKE increases rapidly and reaches maximum in the injection duration, and then TKE decreases after fuel injection finishes. These features well



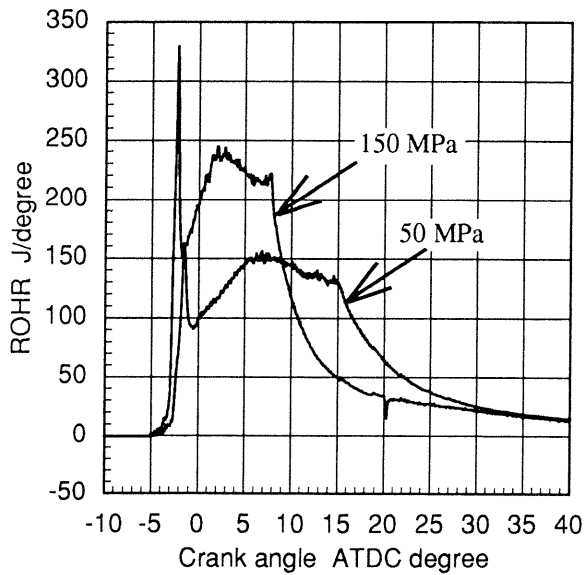


Fig. 6 Rate of heat release. (calculation))

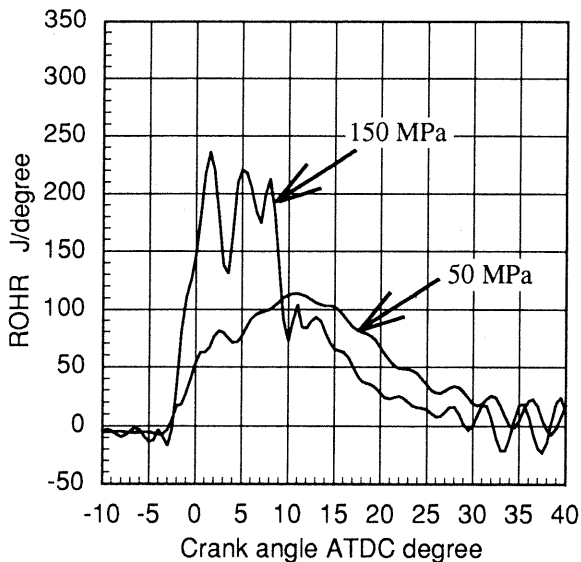


Fig. 7 Rate of heat release. (experiment)

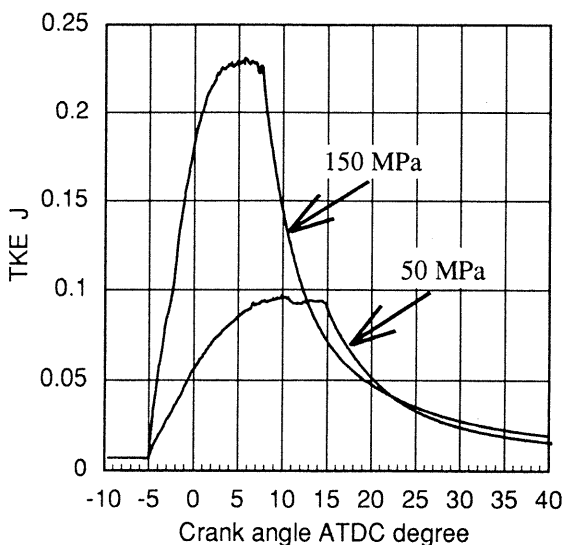


Fig. 8 TKE. (integrated)

correspond to the ROHR curve. This is natural from the nature of the sub-model for the combustion process used in the present study. The simulation for the combustion process in DI diesel engines essentially depends on the model of mixing rate, sub-models for the turbulence and the combustion process.

## CONCLUDING REMARKS

A computational simulation for a DI diesel engine was performed through the KIVA code. Two conditions of the fuel injection pressure were tested. The difference of the fuel injection pressure is given in the input parameters of diameter and velocity of initially injected fuel droplets. From the comparison of the results of experiment and simulation, it was concluded as follows.

- (1) As fuel injection pressure increases, flame develops rapidly, and the timing of flame development near the wall becomes earlier. These are well predicted by the simulation.
- (2) It was suggested that the combustion process in the injection duration of DI diesel engines is strongly dependent on the behavior of the fuel spray and the characteristics of the turbulence formed by the fuel spray.
- (3) When injection pressure increases, the peak pressure in the combustion chamber increases and the timing of the peak pressure becomes earlier. Qualitatively, the simulation well predicts these observed effects of high pressure fuel injection. Quantitatively, predicted pressure in the combustion chamber is higher than that observed in the experiment.

As mentioned above, the simulation well predicts the effect of high pressure fuel injection in many aspects qualitatively. Fine computational grids and appropriate sub-models for the fuel spray is essentially important in this kind of simulation.

## REFERENCES

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