Computational Prediction of NO_x Reduction Characteristics of Premixed Lean Diesel Engine*

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Three-dimensional computations were carried out to study the effects of engine operating conditions on NO_x emissions from premixed lean diesel combustion in a DI (Direct fuel Injection) engine. A modified version of the KIVA II computer code was used for numerical simulations. Qualitatively good agreement between computational and experimental results of the spatial distribution of impinging fuel sprays, the heat release rate, and the relative NO_x mass have been achieved. The computational results demonstrate that NO_x emissions are significantly influenced by intake air temperature, fuel injection timing, and fuel ignitability. It was also shown that fuel droplets which enter the squish region can later contribute to unburned fuel emissions.

Key Words: Diesel Engine, Premixed Combustion, Computational Fluid Dynamics, Fuel Spray, NO_x Reduction

1. Introduction

Research on a low-NO_x diesel engine combustion strategy involving lean mixture formation by early fuel injection and autoignition combustion has been carried out^{(1)–(3)}. Takeda et al.⁽¹⁾ called this particular low-NO_x combustion method “PREDIC” (PREmixed lean Diesel Combustion). An extensive engine testing program has shown that premixed lean combustion can result in very low-NO_x combustion, if the operation conditions are properly chosen^{(1)–(3)}. These NO_x levels are not achievable with conventional diesel engines. However, from a practical point of view, several problems remain to be solved: for example, the operating range is limited, and HC emissions are too high.

In order to discuss the practical use of PREDIC, it is necessary to understand the mixture formation process under each set of operating conditions, and the relationships between combustion and emission characteristics. Numerical simulations including combustion and emission are an effective means of achieving these goals, but to date, none have been published for PREDIC. At this point, it is not known if realistic results can be obtained from computations.

This research program was thus undertaken in order to start accumulating computational results for PREDIC. The KIVA II⁽⁴⁾ code was used with modifications, as described later, to simulate this case of lean compression ignition combustion with early fuel injection. Then, comparing the computational results with past experimental results, we looked for factors which influenced the heat release rate and NO_x emission levels.

2. Computational Methodology

2.1 Outline of computational method

The computations used n-dodecane (C₁₂H₂₆) as the fuel, and NO was taken to be representative of NO_x. Twelve chemical species and ten reactions

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were considered, as shown in Table 1. Of the chemical reactions, four kinetic reactions involved fuel oxidation and NO formation via the extended Zeldovich mechanism. The remaining six reactions involved chemical equilibria. Other important equations included those on the conservation of chemical species (mass), conservations of mass, momentum and energy for the fuel droplets and fluid mixture, and gaseous equations of state. The main improvements to the original KIVA II code that were adopted here are the spray/wall collision submodel and turbulent combustion submodel. These points are now explained in more detail.

2.2 Spray wall collision submodel

In the original KIVA II code, a simplistic model is used wherein every colliding spray droplet adheres to the wall. In this research, the Naber and Reitz⁽⁵⁾ submodel was used, which allowed droplet reflection and motion along the wall.

2.3 Turbulent combustion submodel

A mass fuel consumption rate per unit volume is simply called the fuel consumption rate. Following Gosman and Harvey⁽⁶⁾, the slower one of the mixing and reaction rates was assumed to control the combustion rate. Thus, the following model was used. First, when the chemical reaction time scale (τ_c) is larger than the turbulent mixing time scale (K/ϵ), it is assumed that combustion proceeds via chemical reactions following the Arrhenius equation. When the time scale, τ_c , is small, the fuel consumption rate based on the Arrhenius equation is compared with the fuel consumption rate governed by the turbulent mixing rate (proposed by Magnussen and Hjertager⁽⁷⁾), and the lower of the two is chosen. In the original KIVA II code, the fuel consumption rate can only be based on a generalized Arrhenius equation.

Table 1 Chemical reactions

$2C_{12}H_{26} + 37O_2 \rightarrow 24CO_2 + 26H_2O$	(R1)
$O + N_2 \rightleftharpoons NO + N$	(R2)
$N + O_2 \rightleftharpoons NO + O$	(R3)
$OH + N \rightleftharpoons NO + H$	(R4)
$H_2 \rightleftharpoons 2H$	(R5)
$O_2 \rightleftharpoons 2O$	(R6)
$N_2 \rightleftharpoons 2N$	(R7)
$O_2 + H_2 \rightleftharpoons 2OH$	(R8)
$O_2 + 2H_2O \rightleftharpoons 4OH$	(R9)
$O_2 + 2CO \rightleftharpoons 2CO_2$	(R10)

The fuel consumption rate based on the chemical reaction and turbulent mixing rates, Γ_{CHEM} and Γ_{MIX} , and the chemical reaction time scale (τ_c) can be described as follows.

$$\Gamma_{CHEM} = 2W_F [C_{12}H_{26}]^{0.25} [O_2]^{1.5} A \exp\left(-\frac{E}{RT}\right) \quad (1)$$

$$\Gamma_{MIX} = B \left(\frac{\epsilon}{K}\right) \min\left\{\rho_F, \frac{\rho_{O_2}}{r}, \frac{C\rho_P}{r+1}\right\} \quad (2)$$

$$\tau_c = (D\rho_G)^{-1} \exp\left(\frac{E}{RT}\right) \quad (3)$$

Using Eqs. (1)–(3), the fuel consumption rate Γ_{COMB} is obtained by

$$\Gamma_{COMB} = \Gamma_{CHEM} \quad \text{if } \tau_c \geq \frac{K}{\epsilon} \quad (4)$$

$$\Gamma_{COMB} = \min\{\Gamma_{CHEM}, \Gamma_{MIX}\} \quad \text{if } \tau_c < \frac{K}{\epsilon} \quad (5)$$

where A =frequency factor, B , C , and D =empirical constants, E =activation energy, K =turbulence kinetic energy (TKE in KIVA II), T =temperature, W =molecular weight, r =oxygen required to stoichiometrically burn 1 kg of fuel, ϵ =turbulent dissipation rate, ρ =gaseous density and subscripts, F , G , O_2 , and P indicate fuel, entire gas phase, oxygen, and combustion products, respectively.

The criterion was used so that the combustion was started by the chemical reaction. Without this criterion, when there are no combustion products, the mixing-controlled combustion rate becomes zero according to Eq. (2). This means that the combustion does not progress, because the zero-rate mixing-controlled combustion is chosen as the combustion with the lower rate initially.

3. Computational Conditions

Figure 1 shows the combustion chamber shape

Fig. 1 Combustion chamber and fuel spray layout

Table 2 Engine specifications and basic test conditions

BORE x STROKE	135 mm x 140 mm
DISPLACEMENT	2004 cc
COMBUSTION CHAMBER	98 mm DIAMETER
COMPRESSION RATIO	16.5
SWIRL RATIO	0.5
ENGINE SPEED	1000 rpm
EXCESS AIR RATIO	2.7
INJECTION NOZZLE	0.17 mm x 2 x 2
INJECTION PRESSURE	100 MPa
INJECTION START θ_{INJ}	- 70 deg. ATDC
FUEL (GAS OIL)	Diesel (JIS#2) Cetane number = 62

and spray location. Table 2 shows the engine specifications and basic test conditions corresponding to the calculation conditions. Under these conditions, the same amount of NO_x is emitted as from conventional diesel combustion.

In this work, the initial condition was at the compression bottom dead center (BDC). The initial temperature in the cylinder was 355 K, and the initial air quantity was calculated using the experimental data (under baseline conditions) on pressure before ignition. The cylinder and piston walls were assumed to be at a temperature of 400 K.

The constants in Eqs. (1)–(3) were determined so that the computed and experimental heat release rates were in the best agreement. The resulting values were $A=1.0 \times 10^{11}$, $B=8.0$, and $D=1.0 \times 10^{10}$. $E/R=1.51 \times 10^4$ K has previously been used for $E^{(8)}$. Constants in the reaction rate equations (except for combustion reaction (R1)) were the same as in the original KIVA II code. Moreover, the fuel injection velocity was 387.8 m/s, as determined from the relationship between the experimentally obtained discharge coefficient ($C_d=0.79$) and the measured injection pressure (100 MPa). A 15 μ m Sauter mean diameter (SMD) and χ^2 -diameter fuel droplet distribution were assumed for the modeled spray. Since relatively small droplet sizes were assumed for the initial droplets, an aerodynamic breakup submodel was not used; however, the original droplet collision and coalescence model was used unaltered.

In order to examine the most promising low- NO_x conditions based on the standard conditions mentioned above, some parametric calculations were conducted, as shown in Table 3. STD indicates stan-

Table 3 Computation case

CASE	DIFFERENCE FROM THE BASELINE TEST CONDITION
STD	NO DIFFERENCE (BASELINE CONDITION)
TUR	HIGHER INITIAL TURBULENT KINETIC ENERGY: $TKE=2TKE(STD)$
TEMP	INITIAL TEMPERATURE LOWER: $T_{IN} = T_{IN}(STD) - 20 [K] = 335 [K]$
INJ	INJECTION TIMING 60 [DEG] EARLIER: $\theta_{INJ} = -130 [DEG. ATDC]$
INJ + T	BOTH INJ AND TEMP
EV	FUEL EVAPORATION RATE HIGHER: DROP-AIR HEAT TRANSFER COEFFICIENT $K_H = 3.9K_H(STD)$
IGN	LOWER FUEL IGNITABILITY: $A = 0.1A(STD)$ IN EQ.(1)
IGN + I	IGN + 8 [DEG] EARLIER INJECTION TIMING: $\theta_{INJ} = -78 [DEG. ATDC]$
IGN + I + S	IGN + I + HIGHER SWIRL RATIO ($S/R = 2.1$)

Number of grid points = $22 \times 36 \times 16$,
Number of spray parcels = 4000×4

dard (or baseline) conditions. Other codes indicate alterations of the baseline conditions. The first series of computations was carried out to examine the individual effects of the initial temperature (TEMP), initial turbulent energy (TUR), injection timing (INJ), fuel ignitability (IGN), and fuel evaporability (EV). The other series of computations was carried out to examine the effects of multiple condition changes, e.g., INJ+T, IGN+I, and IGN+I+S. Constants A , B , C , D , and E under all conditions in the table, were the same values as given above, except for fuel ignitability A , which was changed to 0.1×10^{11} . In addition to the parametric table, other computations were carried out to allow comparison with visualization engine results (discussed in the following section).

4. Computational Results and Discussion

4.1 Comparison with experimental results

Figure 2 shows computational and experimental results in terms of fuel spray shape. The experimental results (bottom row) show a shadowgraph-type image of the fuel spray, obtained in a bottom-view visualization engine. The upper row shows calculated spray parcel distributions in the combustion chamber, also viewed from the bottom. The calculated spray is described by plotting a semitransparent sphere at the location of each droplet parcel. In the computational results shown in Fig. 2, it is clear that the fuel sprays collide with one another, and disperse widely in the cylinder. These results indicate that with a proper

Fig. 2 Comparison between computation and experiment in terms of fuel spray shape (Injection start : -80 deg. ATDC)

Fig. 3 Rate of heat release (R.O.H.R.) and cylinder pressure (Left : computation, right : experiment)

choice of the fuel droplet diameter distribution, and the use of the droplet collision and coalescence model, it might be possible to obtain results which are not significantly different from the observed spatial droplet distribution.

Figure 3 shows a comparison of heat release rate, cylinder pressure, and NO production. Note that the experimental heat release rate was obtained from the measured pressure, while the computed heat release

rate was obtained from the energy released by the reactions. The calculated NO production under the baseline condition was about four times higher than the measured result, a fairly large quantitative difference. Therefore, values are shown relative to the value under the baseline condition. In order to perform a quantitative prediction of NO_x production, it seems necessary to more precisely understand the initial temperature. Moreover, it also seems

necessary to carry out reaction calculations in which temporal and spatial variations in temperature and chemical species concentration are taken into consideration. The results shown in Fig. 3 include experimental factors which cannot be quantitatively reflected in the computations, such as the cetane number (CN). In this paper the cetane number difference is expressed by altering the frequency factor A in Eq. (1).

As understood from Fig. 3, the computed heat release rate and cylinder pressure reproduce the experimental trends very well. In particular, the fact that the computed NO production decreases markedly under certain parametric conditions corresponds well to the experimental data. The measured heat release rate shows a second peak corresponding to main combustion, after a relatively low initial heat release rate. In the computations, however, only the heat release rate corresponding to the main combustion event can be expected, because the fuel oxidation reaction is described only by an overall reaction (R1).

Fig. 4 Calculated relative in-cylinder NO mass (STD case = 100%)

In order to predict a two-stage heat release rate, it is necessary to include a low-temperature oxidation mechanism in addition to reaction (R1).

4.2 Possible methods of NO_x reduction

Figure 4 shows the parametric effects of NO_x production. The calculated results shown in Fig. 4 strongly indicate that a reduced initial temperature (by charge cooling, for instance), earlier injection timing, and lower fuel ignitability, are all effective for NO_x reduction.

4.3 Relationship between heat release and NO_x reduction characteristics

Figure 5 shows the cylinder pressure and heat release rate under the baseline condition and six other parametric conditions. As understood from Figs. 4 and 5, a better NO_x reduction effect is associated with a lower peak cylinder pressure. In addition, a lower cylinder pressure corresponds to a later combustion timing. When the combustion timing is delayed, NO production decreases. The reason seems to be that when the combustion timing is delayed, postcombustion compression is lower, and the cylinder pressure at TDC is lower, that is, the temperature is also lower. In particular, in the IGN case, most combustion occurs after TDC, as with conventional diesel combustion, and compared to other cases, the cylinder pressure is lower. As shown in Fig. 4, the NO_x reduction effect is considerable. However, in conventional diesel combustion, the fuel air mixture is not lean, so low-NO_x combustion is not possible^{(1),(2)}. It can thus be understood that in compression autoignition combustion with early fuel injection, not only the amount of mixture leaning, but also differences in combustion timing, significantly influence NO_x production. Moreover, Fig. 5 indicates that the combustion timing is greatly influenced by not only the fuel ignitability but

Fig. 5 Computational results of rate of heat release (R.O.H.R.) and cylinder pressure

Fig. 6 Mass of NO and fuel vs crank angle in STD and INJ cases

also the initial in-cylinder temperature.

It should be noted that in case INJ the location of the peak heat release rate is almost the same as in the baseline case, but the peak rate is lower. In this case, since the total heat release is slightly less, the cylinder pressure is lower than in the baseline case. Why the total heat release is less will be explained in the next section. Because the total heat release is less, the residual gas and wall temperatures (after the exhaust cycle) become lower than the baseline values. This should lead to a lower cylinder temperature at the start of compression. If the influence of the previous combustion cycle is considered, the earlier injection computation, case INJ, should be investigated further, in addition to the effects of the lower initial temperature. Case INJ+T includes such initial temperature effects, and the results show that a lower initial temperature causes delayed combustion timing. The measured data (Case 2) shown in Fig. 3 indicate that when the injection timing is earlier than in the baseline case, the peak heat release rate location is delayed, and at the same time the peak value drops. Thus, based on the measured data it can be concluded that both the lower total heat release, along with earlier fuel injection, and a lower initial in-cylinder gas temperature contribute to a reduction in NO_x emissions.

4.4 Required spray characteristics for early fuel injection

Figure 6 shows fuel evaporation, combustion, and NO production processes for the baseline and earlier injection (INJ) cases. This figure indicates that when fuel injection occurs earlier, NO_x production is halved, but the amount of unburned fuel remains unchanged. Figures 6 and 7 can be examined together to gain a quantitative and spatial understanding of the injected fuel. It is apparent that liquid fuel droplets collide with the cylinder walls and remain in the squish region. This fuel remains as unburned fuel. Figure 8 shows the cross-sectional equivalence ratio distribu-

Fig. 7 Fuel sprays in STD and INJ cases

Fig. 8 Equivalence ratio distribution in section A-A after combustion (INJ case, bottom view at TDC)

tion after combustion for case INJ. It can be seen that most of the fuel remains (equivalence ratio approaching 3) in the squish region, where it is deprived of oxygen. The region roughly corresponds to that in which droplets concentrate before combustion (Fig. 7). That is, in this particular case, the main cause of the lower overall heat release is that the fuel spray droplets impinge on the cylinder walls, and later congregate in the squish region, where they remain due to a lack of oxygen. With early fuel injection, it is important to not only widely disperse the spray droplets to form a lean mixture, but also to not allow the impingement on the cylinder walls, in order to avoid high levels of unburned hydrocarbons.

5. Summary

Using an improved version of the KIVA II engine modeling code, transient three-dimensional numerical simulation of PREDIC was carried out. The numerical simulation qualitatively reproduced experimentally observed trends in the heat release rate and NO emissions according to the operating variables. From parametric calculations, it was shown that the initial in-cylinder temperature, injection timing, and fuel

ignitability significantly influenced the heat release rate and NO production. In addition, it was found that the spatial fuel spray distribution had a notable influence on the heat release rate, and NO and unburned fuel emissions.

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References

- (1) Takeda, Y., Nakagome, K. and Niimura, K., Emission Characteristics of Premixed Lean Diesel Combustion with Extremely Early Staged Fuel Injection, *Trans. Jpn. Soc. Mech. Eng.*, (in Japanese), Vol. 62, No. 599, B (1996), p. 2887-2894.
- (2) Takeda, Y., Nakagome, K. and Niimura, K., Emission Characteristics of Premixed Lean Diesel Combustion with Extremely Early Staged Fuel Injection, SAE Paper 961163, (1996).
- (3) Yanagihara, H., Simultaneous Reduction of NO_x and Soot in Diesel Engines Using a New Mixture Preparation Method, *Trans. Jpn. Soc. Mech. Eng.*, (in Japanese), Vol. 63, No. 606, B (1997), p. 724-729.
- (4) Amsden, A.A., O'Rourke, P.J. and Butler, T.D., KIVA-II: A Computer Program for Chemically Reactive Flows with Sprays, Los Alamos National Laboratory Report LA-11560-MS, (1989).
- (5) Naber, J.D. and Reitz, R.D., Modelong Engine Spray/Wall Impingement, SAE Paper 880107, (1988).
- (6) Gosman, A.D. and Harvey, P.S., Computer Analysis of Fuel-Air Mixing and Combustion in an Axisymmetric D.I. Diesel Engines, SAE Paper 820036, (1982).
- (7) Magussen, B.F. and Hjertager, B.H., On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion, 16th (Int.) Symp. on Combust., The Combustion Institute, (1976), p. 719-729.
- (8) Westbrook, C.K. and Dryer, F.L., Chemical Kinetic Modeling of Hydrocarbon Combustion, *Prog. Energy Combust. Sci.*, 1984-10, (1984), p. 1-57.
- (9) O'Rourke, P.J., Collective Drop Effects in Vaporizing Liquid Sprays, Ph. D. Thesis 1532-T, Princeton Univ., (1981).