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Influence of the Cyclic Parameters on the Nitric Oxide Formation in the Diesel Engine

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ABSTRACT

This study describes the influence of combustion parameters on the nitric oxide emission, such as injection timing, air flow rate, injected amount of fuel, and compression ratio of engine. In order to determine the influence factors on the nitric oxide emission, the experiment were investigated with various parameters of engine cycle. According to the results of this study, the retardation of injection timing and the increases of airflow rate, and the decreases of fuel injection amount reduce the nitric oxide concentration in the exhaust emissions. Also, the increases of compression ratio of engine increase in the concentration of nitric oxide formation in the combustion chamber. The results of this study give a guideline to decrease the nitric oxide formation by using the simulation program.

Keywords : Nitric Oxide formation, Combustion Characteristics, Exhaust Emission, Combustion Simulation, Direct Injection type Diesel Engine

1. Introduction

Increasing environmental concerns and regulations of government have intensified the need for the clean emission from diesel automotive engines, which are nitric oxide and particulate emission. In fact, a direct injection

diesel engine causes high level of nitric oxide emission compare with the indirect injection diesel engine. The reduction of nitric oxide is one of the important goals of the design of combustion chamber in the direct injection type diesel engine. The cycle conditions and the structure of combustion chamber have influence upon the nitric oxide, carbon monoxide, and the other harmful component for human body and environment. The formation

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of nitrogen oxide of exhaust gas in diesel engine depends on the various engine parameters.

Combustion process of a direct injection type diesel engine is closely related to the behaviour of fuel-air mixing, involving atomization and vaporization of spray droplets. The formation of nitric oxide depends on many different parameters such as fuel-air ratio, temperature of combustion chamber, load, injection timing, compression ratio, engine speed and fuel injection pressure. Especially the engine speed, fuel injection timing, and compression ratio of engine have influence on the nitric oxide in engine emission.

The higher cylinder pressure and temperature have influenced on the formation of higher nitric oxide emission. In order to reduce the nitric oxide of engine emission, it is necessary to decrease the gas temperature because the generation of the nitric oxide is a function of temperature. The various studies of theoretic and experiment on the combustion characteristics and exhaust emission of diesel engine are investigated by several authors.^{1)~4)} But the studies of cyclic parameters on the nitric oxide formation in the engine are necessary to investigate the reduction factors of nitrogen oxide and exhaust emissions.

The aim of this study is to present the results of the effect of engine cyclic parameters on the exhaust emission of direct injection diesel engine. In this simulation, the effects of various factors on the nitric oxide and combustion characteristics of engine were analyzed by using the theoretical investigation.

2. Method of Investigation

2.1 Thermodynamic system of engine

The principle of the simulation models is based on the first law of thermodynamics with the attention being focused on the combustion process^{5)~10)}. The analysis assumes that the cylinder contains a mixture of fuel-air and residual combustion gas at any time in the cylinder at the control volume is in equilibrium. In order to investigate the effect of processes on engine performance and nitric oxide emission, the conservation equations of energy are used to describe change in the working substance.

$$\frac{dm u}{d\theta} = -P \frac{dV}{d\theta} + \frac{dQ}{d\theta} + \sum_i \dot{m}_i h_i \quad (1)$$

where P , V , θ , u and m are the pressure, volume, crank angle, internal energy and mass of the cylinder charge respectively.

Differentiating the equation of ideal gas equation gives

$$PV = mRT \quad (2)$$

$$V \frac{dP}{d\theta} + P \frac{dV}{d\theta} = RT \frac{dm}{d\theta} + mT \frac{dR}{d\theta} + mR \frac{dT}{d\theta} \quad (3)$$

Considering the convection heat transfer and radiant heat transfer from the combustion of fuel-air mixture in the combustion chamber, the term of $dQ/d\theta$ is given by

$$\frac{dQ}{d\theta} = h_o A (T_g - T_{ws}) + \xi A \sigma (T_g^4 - T_{ws}^4) \quad (4a)$$

where,

- h_c : gas to wall heat transfer coefficient
 T_g : gas temperature
 T_{ws} : surface temperature of cylinder wall
 A : total area for heat transfer
 ξ : emissivity depending on the engine speed and load ($\xi=0.576$)¹¹
 σ : Stephan-Boltzmann constant

Woschni³ proposed the following equation for the heat transfer coefficient as a function of the pressure rise due to the combustion, that is

$$h_c = \frac{C_1 P^{0.8}}{B^{0.2} \bar{P}^{0.53}} \left[C_2 V_p + C_3 \frac{V_s T_r}{P_r V_r} (P - P_{mot}) \right]^{0.8} \quad (4b)$$

where,

- V_s : swept volume
 V_p : mean piston speed
 V_r, T_r, P_r : cylinder volume, temperature and pressure at reference condition
 P_{mot} : motoring pressure

The C_1 , C_2 and C_3 are empirical constants that can be adjusted for local variation due to intake swirl, combustion chamber geometry and radiation effect.

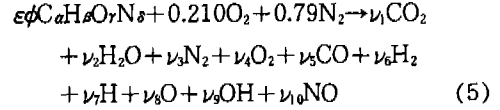
where, $C_1=0.13$, $C_2=2.28$, $C_3=3.24 \times 10^{-3}$

2.2 Chemical equilibrium

During combustion process, the calculation of thermodynamic properties requires the values of mole fraction of the combustion products. The composition of the combustion products depends upon the properties of fuel, pressure, temperature and fuel-air equivalence ratio.

The mole fraction equation for $C_a H_b O_r N_s$ and air at equivalence ratio ϕ react and the combustion products subject to temperature T

and pressure P can be expressed as,



Atom balancing yields the following four equations

$$C : \varepsilon \phi \alpha = (\nu_1 + \nu_5) N \quad (6)$$

$$H : \varepsilon \phi \beta = (2\nu_2 + 2\nu_6 + \nu_7 + \nu_9) N \quad (7)$$

$$\begin{aligned} O : \varepsilon \phi \gamma + 0.42 = (2\nu_1 + \nu_2 + 2\nu_4 + \nu_5 + \nu_8 + \nu_9 \\ + \nu_{10}) N \end{aligned} \quad (8)$$

$$N : \varepsilon \phi \delta + 1.58 = (\nu_1 + \nu_3) N \quad (9)$$

where $N = \sum_{i=1}^{10} \nu_i$ is the total number of moles and mole fraction of constituent i .

From the six equilibrium among product species constants will yields eleven equations for ten unknown mole fractions y_i and the number of moles N .

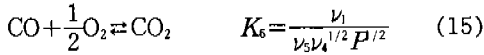
Reaction	Partial Pressure Equilibrium constant
$\frac{1}{2} H_2 \rightleftharpoons H$	$K_1 = \frac{\nu_7 P^{1/2}}{\nu_6^{1/2}}$ (10)

$\frac{1}{2} O_2 \rightleftharpoons O$	$K_2 = \frac{\nu_8 P^{1/2}}{\nu_4^{1/2}}$ (11)
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$\frac{1}{2} H_2 + \frac{1}{2} O_2 \rightleftharpoons OH$	$K_3 = \frac{\nu_9}{\nu_4^{1/2} \nu_6^{1/2}}$ (12)
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$\frac{1}{2} O_2 + \frac{1}{2} N_2 \rightleftharpoons NO$	$K_4 = \frac{\nu_{10}}{\nu_4^{1/2} \nu_3^{1/2}}$ (13)
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$H_2 + \frac{1}{2} O_2 \rightleftharpoons H_2O$	$K_5 = \frac{\nu_2}{\nu_4 \nu_6^{1/2}}$ (14)
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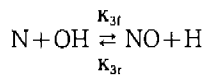
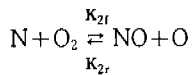
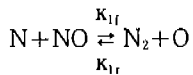
The calculation of the nitric oxide formation requires knowledge of pressure, temperature, and equivalence ratio dependent upon the combustion parameter in the combustion chamber.

2.3 Kinetics model of the nitric oxide

There are two sources of nitric oxides in the combustion chamber such as fuel oxidation due to the atmospheric nitrogen and oxidation of nitrogen containing compound in the fuel. The nitric oxide formations in the combustion chamber are due to reactions of molecular oxygen and nitrogen with oxygen atoms. The temperature, pressure and air-fuel ratio in the premixed and diffusion combustion were used as input data for the empirical equation used to calculate the nitric oxide.

The extended Zeldovich mechanisms⁵⁾ are known to describe the nitric oxide formation in the diesel engine process. This mechanism is described briefly as follows :

First the following three reactions are considered,



where the constant of reaction rate of positive and negative direction K_{1f} , K_{1r} , K_{2f} and K_{3f} are given respectively as follows,

$$K_{1f} = 7.6 \times 10^{13} \times \exp(-3,800/T)$$

$$K_{1r} = 1.6 \times 10^{13}$$

$$K_{2f} = 6.4 \times 10^9 \times T \times \exp(-3,150/RT)$$

$$K_{3f} = 4.2 \times 10^{13}$$

Next, the equilibrium rate R_1 , R_2 and R_3 of positive direction is written by,

$$R_1 = K_{1f}[\text{NO}]_e[\text{N}]_e$$

$$R_2 = K_{2f}[\text{N}]_e[\text{O}]_e$$

$$R_3 = K_{3f}[\text{N}]_e[\text{OH}]_e$$

where the subscript e refers to equilibrium conditions.

To explain the steady-state approximation for the concentration of nitrogen atom and assuming equilibrium oxygen and OH concentration, the rate of change nitric oxide formation is given by equation below,

$$\frac{d(\text{NO})}{d\theta} = \frac{2R_1(1-X^2)}{X \frac{R_1}{R_2+R_3} + 1} \quad (16)$$

$$\text{where } X = \frac{[\text{NO}]}{[\text{NO}]_e}$$

3. Simulation procedures

The above equations are solved numerically using a predictor corrector iterative technique to obtain gas temperatures, pressure, rate of the release, rate of pressure rise, and the other combustion characteristics as a function of crank angle. The gas properties and the combustion characteristics of fuel-air mixture in the combustion chamber were calculated at each crank angle increment.

In general, the nitric oxide emission appears during the mid-period of combustion.

The combustion characteristics and the formation of nitrogen oxide are calculated by using the above equations under the various engine input data and initial condition of engine cycle.

4. Experimental apparatus and procedures

The basic engine used in this work is a four stroke cycle, single cylinder, and naturally aspirated direct injection type diesel engine with displacement of 1425cc. The engine has a 17.4 compression ratio and a rated power output of 7.36kW at 1,200 rpm. The specifications of engine are as shown in Table. 1.

An experimental apparatus is shown schematically in Fig.1. The tests were conducted on a single cylinder diesel engine coupled to an eddy current dynamometer system. Combustion analyzer was composed of pressure measuring device and crank angle detecting system. The cylinder pressure of engine cylinder was obtained by using high pressure

transducer and crank angle detecting system.

In order to obtain the variation of combustion characteristics of diesel engine, the engine was investigated under the following conditions;

- Engine speed; 800~1,500rpm
- Opening pressure of fuel injection; 170bar
- Cooling water temperature; 50°C, 60°C, 70°C
- Injection timing; 22°, 15°, 10°, 5° BTDC

5. Results and discussion

5.1 Combustion characteristics

Figure 2 shows the cylinder pressure and the rate of pressure rise in the engine. As shown in pressure-crank angle diagram, the predicted result is coincided with the experimental results. The cylinder pressure, and rate of pressure rise, as a function of crank angle for simulation and experiment at 1,000rpm of engine speed.

Figure 3 shows the gas temperature and the rate of heat release in the engine. It was found that the trend of the experimental temperature variation due to crank angle was same with the results of predicted tempera-

Table 1 Engine specification

Engine type	4 stroke cycle diesel engine
Number of cylinder	1
Combustion chamber	Direct injection type
Bore × Stroke	110mm × 150mm
Compression ratio	17.4 and 14.1
Connecting rod length	300mm

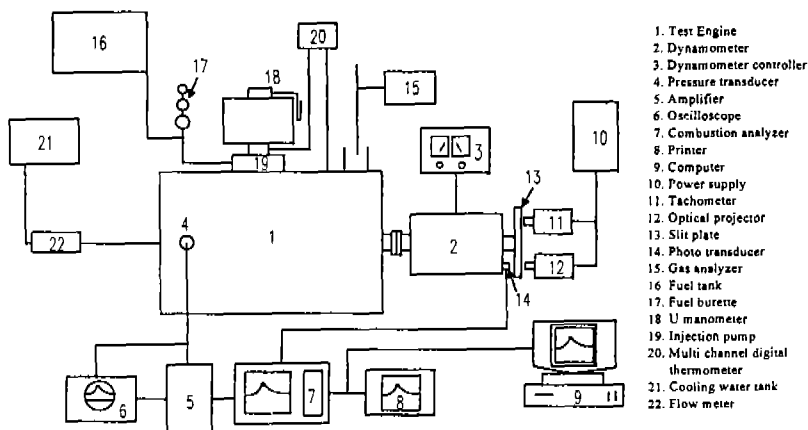


Fig.1 Schematic Diagram of Experimental Apparatus

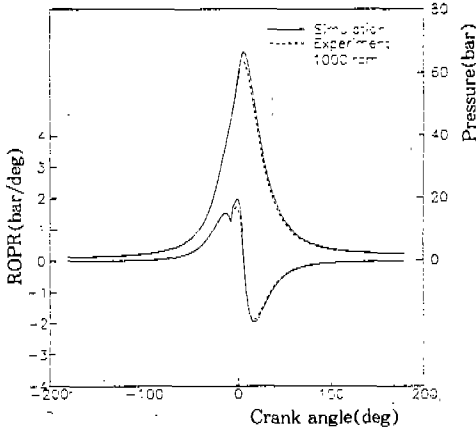


Fig.2 Comparison between Simulation and Experimental Results of Cylinder Pressure and Rate of Pressure Rise

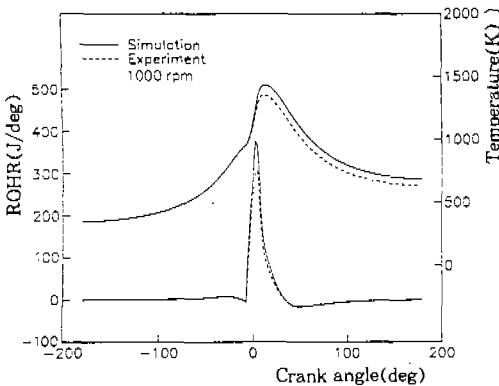


Fig.3 Comparison between Simulation and Experimental Results of Cylinder Temperature and Rate of Heat Release

ture. These results illustrated the experimental and theoretical results at the engine speed of 1,000rpm, the fuel amount of 40mg/cycle, and the injection timing of 15° before TDC. The small difference between the experimental results and simulation results may be due to the various assumption, approximation of the simulation, uncertainty of experiment and inconsistent matching of operating conditions. The rate of pressure rise value depends on the rapid increase of cylinder pressure.

In all combustion process there are two phase combustion, such as the premixed and diffusion burning region as shown in Fig. 3. The comparative analysis rate of heat release showed that the premixed process is an important controlling factor in diesel combustion engine. In operating condition of engine speed, rates of fuel injection and injection pressure have direct influence on the mixing process between fuel and air in combustion chamber.

As the beginning of combustion, the gas temperature increases sharply. The reason for this change significantly is due to the storage amount of the fuel injected in combustion chamber during the ignition delay period. In this period, the increase of temperature of combustion products is very sensitive to nitric oxide formation in the engine.

5.2 Effect of injection timing on the formation of nitric oxide

Figure 4 shows that the injection timing plays an important role in the formation of nitric oxide in combustion chamber. Nitric oxide concentrations are reduced with the retardation of injection timing. As regard of advanced injection timing, it can be seen a longer delay time for fuel-air mixing in the combustion chamber before the combustion process. The advance of injection timing brings about the increase of gas temperature causes by the rapid combustion of the large amount of fuel mixture. But the late start of combustion due to retarding injection timing reduced the peak combustion temperature level. As the retard of injection timing the combustion process progressively moves into the expansion process. This related to the decrease of local temperature in cylinder. Therefore, the variation of injection timing is an important factor that determines the level of ni-

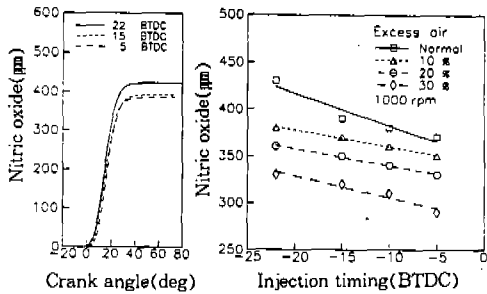


Fig.4 Effect of Injection Timing on the Nitric Oxide Emission at 1,000rpm

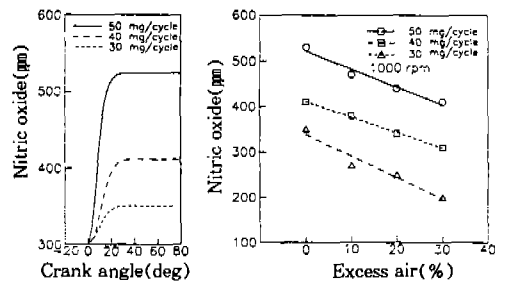


Fig.5 Effect of Fuel amount on the Nitric Oxide Concentration at 1,000rpm

tric oxide concentration of exhaust emission.

5.3 Effect of fuel injected amount on the nitric oxide formation

Figure 5 shows the effect of fuel injection amount on the nitrogen oxide formation. As shown in this figure, the nitrogen oxide emission increases in accordance with the increase of injection amount. Especially the increase of fuel amount results in the increase of earlier formation of nitric oxide in the engine. The large amount of fuel injection results in the increase of nitric oxide emission because of large reaction amount of fuel. Also the increase of fuel amount into the cylinder increases the amount of combustion fuel in the duration of ignition delay. The ignition delay, the time between the start of injection and the start of combustion is essentially constant in this experiment.

The increase of fuel amount brings results increase in the combustion duration of fuel injected in the engine. Also, it is a factor of increases not only the rise the cylinder pressure but also to increase in the heat release in the combustion chamber. The changes in the combustion duration according to the amount of fuel injection have an effect on the changes in the premixed burning and heat release in the combustion duration. Therefore, increase of

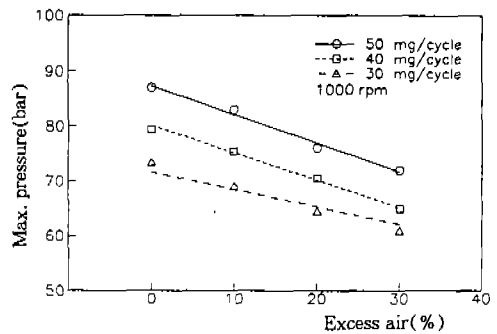


Fig.6 Effect Fuel Injection amount on the Maximum Cylinder Pressure

the fuel injection amount increase in the nitric oxide emission.

As shown in Fig.6, the increase of fuel amount brings about the higher maximum pressure in cylinder because of higher gas temperature. The peak pressure increased with the increase of the amount of fuel injection and also due to the increase of heat release in the combustion chamber.

5.4 Effect of compression ratio on the formation of nitric oxide

Figure 7 show the influence of two compression ratios on the nitric oxide concentration of exhaust emission. A retard in injection timing reduces the nitric oxide formation. Nitric oxide formations of exhaust emissions decrease as the injection timing is retarded, but

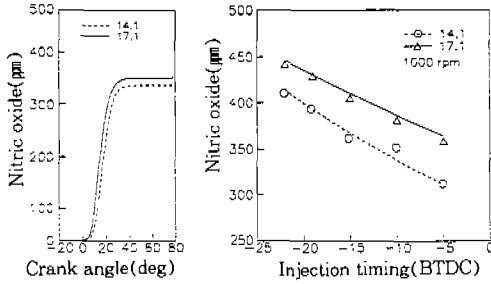


Fig.7 Effect of Compression Ratio on the Nitric Oxide Concentration

the nitric oxide increase with an increase of the compression ratio. It appears that the higher compression ratio represents the higher nitric oxide emission than the case of lower compression ratio of engine.

5.5 Effect of Fuel Properties on the formation of nitric oxide

Figure 8 shows the effect of fuel properties on the nitric oxide concentration of exhaust emission. The fuel properties have direct influence on the mixing process between fuel and air. When the different fuel properties are used such as the fuel density the nitric oxide concentration was reduces with the decreasing of the fuel density in the combustion process. The lower fuel density has potential to reduce the retention time of the temperature

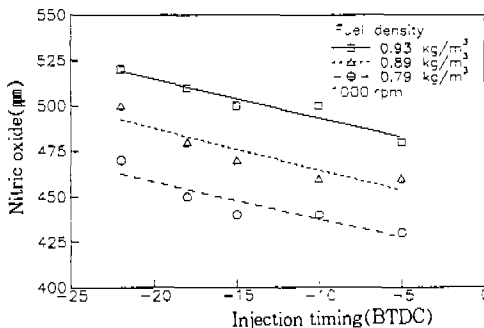


Fig.8 Effect of Fuel Density on the Nitric Oxide Concentration

and pressure conditions in the combustion chamber. These were results reduction in the cylinder gas temperature and pressure in the combustion chamber of direct injection type diesel engine. Therefore the fuel density provide some benefit in term to reduced the concentration of nitric oxide formation in the engine.

6. Conclusions

The combined effects of injection timing, fuel injection, compression ratio and combustion process were investigated using a single cylinder direct injection type diesel engine. From the results of this investigation in diesel engine, the following conclusions were obtained.

- 1) A retard of fuel injection timing brings about the decrease of cylinder pressure and the reduction of nitric oxide concentration in the engine.
- 2) The nitric oxide concentration and gas pressure increase in accordance with the increase of fuel amount of engine cycle.
- 3) Increase of the compression ratio of engine results in the improvement of combustion performance, but increases the nitric oxide emission.
- 4) The increase of excess air ratio and the fuel density show the decrease of nitric oxide and the temperature of combustion gases in the engine.

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