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Reduction of NO in Reheat Combustor of Compound Engine

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ABSTRACT

The authors investigate a Diesel-Brayton Compound engine to improve efficiency and to reduce NOx and soot. This paper shows the deoxidization of NOx in a reheat combustor with non-equilibrium calculations which consist of the Zeldovich reactions and other six reactions. H radical mainly causes the decomposition of NO. In case of higher temperature than 2,000K, the reduction of NO is advanced because O radical decreases by CO. The experimental research to check the reduction of NOx showed the good accordance with the simulation.

INTRODUCTION

High thermal efficiency and reduction of NOx and soot are very important for internal combustion engines. The reference (1) indicates well these research tendency. The authors proceed a Diesel-Brayton compound engine system which comprises a diesel engine and a gas turbine. The engine system, as a basis of the heat insulated diesel engine, burns fuel in the reheat combustor with the exhaust gas from diesel engines, and recollects power using the turbine.

In the reheat combustor, the recombustion of soot and the reduction of NOx at the early stage of combustion are expected. A simulation of the formation and decomposition of NO using computer was carried out with non-equilibrium calculations using the Zeldovich reactions and other six reactions considering the effects of CO. As the result, it became clear that the reduction of NO was mainly caused by H radical having deoxidizing effects. The reduction of NO was accelerated at the reaction temperature of 2,000K or more by the reduction of O radical caused by the effects of CO. Moreover, the experimental research on the reheat combustor to recirculate combustion gas showed much amount of deoxidization of NO in fuel rich condition.

OUTLINE OF NON-EQUILIBRIUM CALCULATIONS

This engine system is structured to advance the deoxidization of NO and the recombustion of soot from the diesel engine in the reheat combustor. The simulation method is below.

First of all, equilibrium compositions of the combustion gas are obtained by chemical equilibrium calculations. The program described in references (4) et al. were used to ensure the equilibrium calculations. The components are CO, CO2, O2, H2, O, OH, H2O, H, NO, and N2. Six chemical formulas were used.

Second, when a constant amount of NO comes into these equilibrium compositions, non-equilibrium calculations were used to investigate the formation and decomposition of NO. Fig.1 shows the chemical reaction formulas used for non-equilibrium calculations. Three Zeldovich reaction formulas from (1) to (3) and other six reactions considering the effects of CO were used to clarify the formation mechanism of NO. In this research, the two kinds of simulation were carried out using only the Zeldovich reaction formulas and the nine formulas including Zeldovich. The constants of reaction speed were selected from the references (5) and (6).

$$N_2 + O \rightleftharpoons NO + N \qquad (1)$$

$$N + O_2 \rightleftharpoons NO + O \qquad (2)$$

$$N + OH \rightleftharpoons NO + H \qquad (3)$$

$$CH_2 + N_2 \rightleftharpoons HCN + NH \qquad (4)$$

$$HCN + OH \rightleftharpoons CN + H_2O \qquad (5)$$

$$CN + O_2 \rightleftharpoons CO + NO \qquad (6)$$

$$CN + O \rightleftharpoons CO + N \qquad (7)$$

$$NH + OH \rightleftharpoons N + H_2O \qquad (8)$$

$$N_2 + OH \rightleftharpoons NO + NH \qquad (9)$$

Fig.1 Reaction Formulas
for Non-equilibrium Calculations

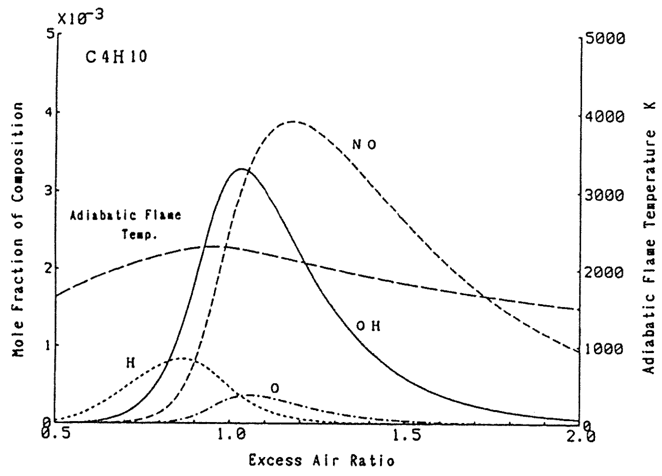

Fig.2 Equilibrium Calculations-1 (Butane)

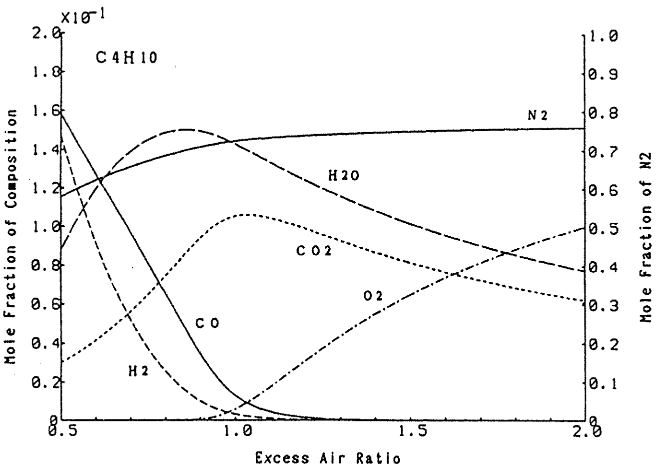

Fig.3 Equilibrium Calculations-2 (Butane)

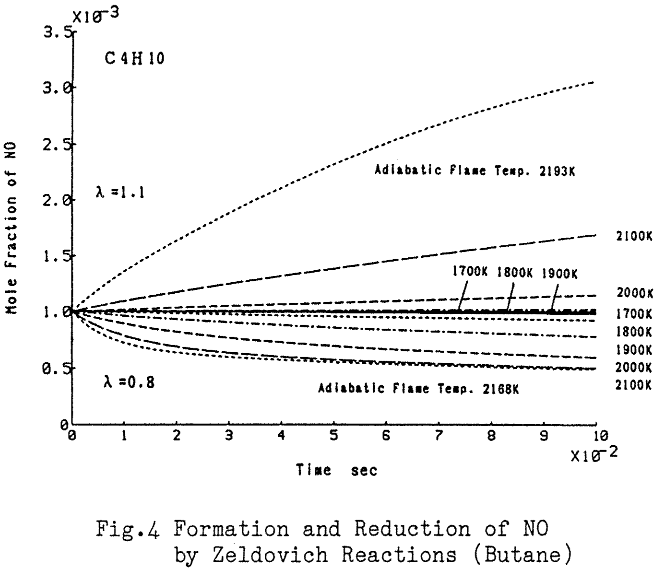

Fig.4 Formation and Reduction of NO
by Zeldovich Reactions (Butane)

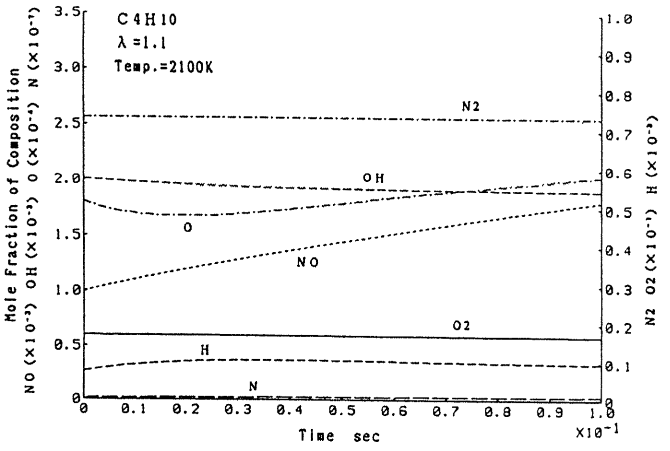

Fig.5 Mole Fractions by Zeldovich Reactions
(Excess air ratio = 1.1)

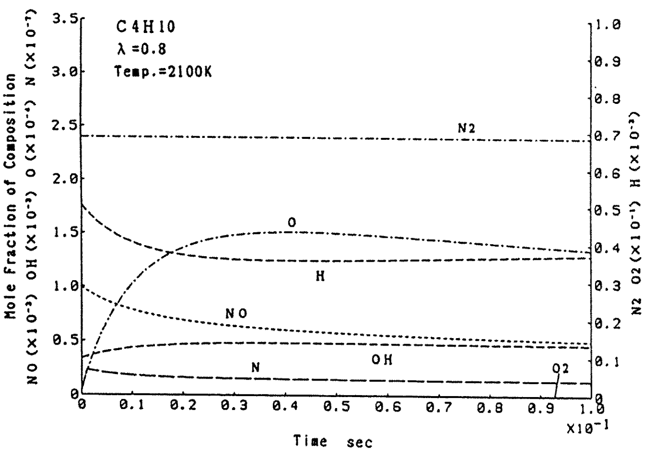

Fig.6 Mole Fractions by Zeldovich Reactions
(Excess air ratio = 0.8)

SIMULATION WITH THE ZELDOVICH REACTIONS

Fig.2 and 3 show the results of the equilibrium calculation of each fraction in adiabatic flame temperature when butane is used as fuel. This calculation was carried out at the excess air ratio of 0.5 to 2.0. The formation of NO reaches approximately 4,000ppm at the excess air ratio of 1.2. NO can be identified with O radical. The residual O2 can also be identified at the excess air ratio of 0.9 and increases with higher excess air ratio, and H2 and CO decreases in reverse fashion. The maximum value of H radical showing deoxidization is obtained at the excess air ratio of 0.85. According to H radical, NO decreases. This is because H radical accelerates the deoxidization of NO.

Fig.4 shows the results of non-equilibrium calculations using the Zeldovich reaction formulas (1) to (3). As described above, the figure shows the results of the formation and decomposition of NO with the elapse of time when the concentration of NO becomes 1,000 ppm after the equilibrium combustion has been finished. The calculations were processed under the condition of various temperatures and the excess air ratio of 0.8 and 1.1.

When the reaction temperature is 1,900K or less at the excess air ratio of 1.1, the formation of NO can not be identified and the reaction is still frozen. On the other hand, when the reaction temperature is 2,000K or more, the formation of NO increases exponentially. This means that the simulation of thermal NO is made possible. For example, when the adiabatic temperature is maintained for 0.1 second, the concentration of NO becomes 3,000ppm.

When the reaction temperature is 1,700K at the excess air ratio of 0.8, the concentration of NO is mostly kept unchanged. However, if it is 1,800K or more, the decomposition of NO will proceed. For example, when the temperature of 2,100K is maintained for 0.1 second, the concentration of NO is reduced to approximately 500ppm. At the initial stage of reactions, the substantial decomposition of NO can be identified. This is because the decomposition of NO is accelerated by H radical. The higher the reaction temperature is, the higher the decomposition of NO is. The decomposition of NO proceeds faster at a longer retaining time. However, the concentration of NO is curved at a constant value after a certain period of time.

Fig.5 and 6 show the variation of each component to produce with non-equilibrium calculations. When the formation and decomposition of NO was distinguished at the reaction temperature of 2,100K, each component is investigated at the excess air ratios of 1.1 and 0.8.

When the excess air ratio is 1.1 as shown in Fig.5, the concentration of H radical is lower than that of 0.8, and OH and O radical are higher. It is found that O radical is used for formation of NO because O radical decreases with the formation of NO. When the excess air ratio is 0.8 as shown in Fig.6, O radical is produced with decomposition of NO. H radical decreases substantially at the initial stage of the reaction and its behavior is similar to that of NO. The decomposition of NO is accelerated by H radical. The reverse reaction of the Zeldovich formula (3) can be identified mainly with the reduction of NO.

Fig.7 shows the results of the simulation when cetane is used as fuel. The results are mostly similar to those obtained when butane is used as fuel, except that the formation of thermal NO is higher.

SIMULATION CONSIDERING THE EFFECTS OF CO

In order to investigate what components affect the formation and decomposition of NO in such a way other than use of the Zeldovich reaction formulas, the nine reaction formulas including Zeldovich were programmed considering the effect of CO.

Fig.8 shows the results when butane is used as fuel. The results are mostly similar to those using the Zeldovich reaction formulas when the reaction temperature is 2,000K or less at the excess air ratio of 0.8. It is found that CO does not affect the reduction of NOx at this temperature. However, when the reaction temperature is 2,000K or more at the excess air ratio of 0.8, the decomposition of NOx considering the effects of CO proceeds faster. In particular, the decomposition ratios of NO are higher at the initial stage of the reaction.

For the more detailed research of the

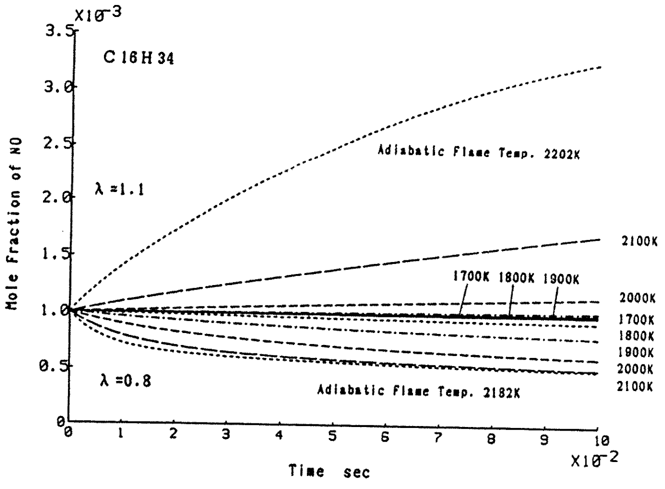

Fig.7 Formation and Reduction of NO by Zeldovich Reactions (Cetane)

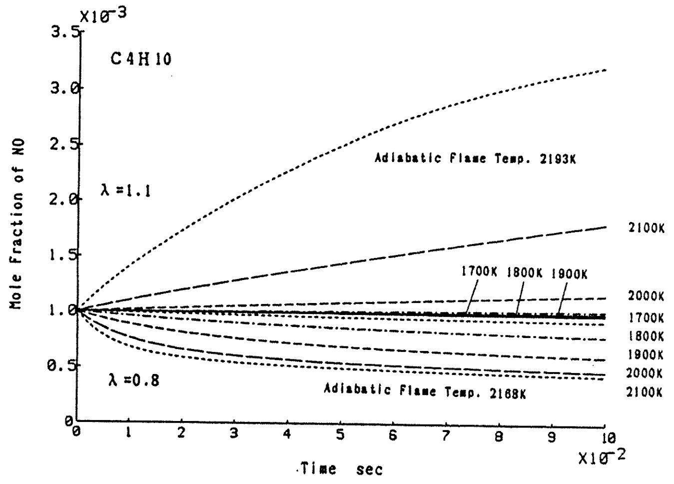

Fig.8 Formation and Reaction of NO by Nine Reactions

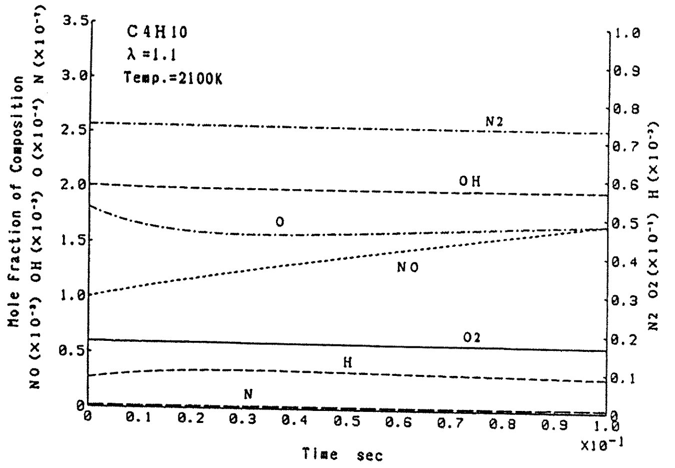

Fig.9 Mole Fractions by Nine Reactions-1 (Excess air ratio = 1.1)

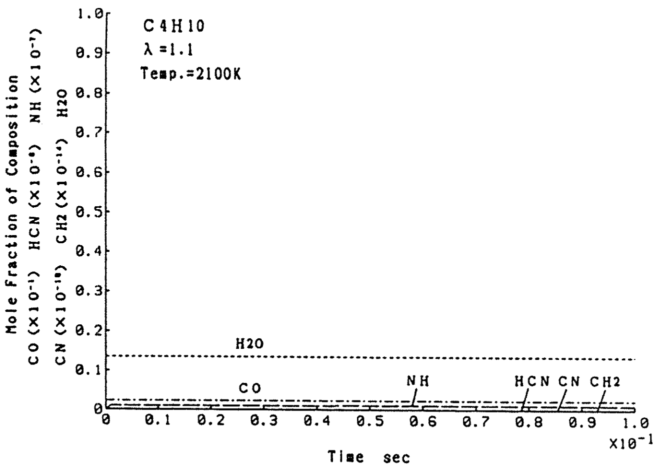

Fig.10 Mole Fractions by Nine Reactions-2
(Excess air ratio = 1.1)

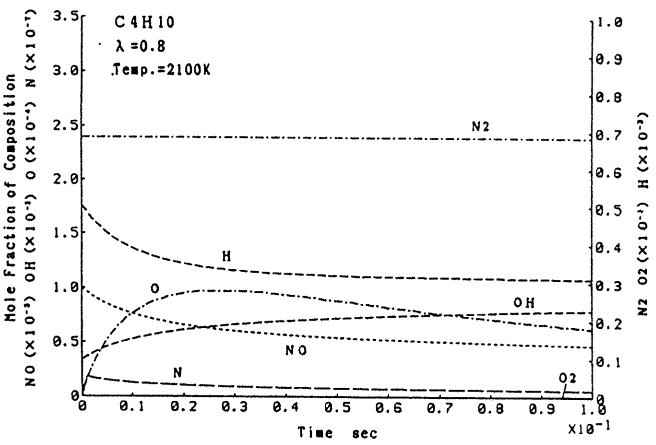

Fig.11 Mole Fractions by Nine Reactions-3
(Excess air ratio = 0.8)

decomposition processes, Fig.9 and 10 show the behavior of each fraction at the temperature of 2,100K when the excess air ratio is 1.1. CO does not affect the decomposition of NO in such a condition because only small amounts of HCN, NH, CN, and CH2 have been produced and kept at a constant value.

Fig.11 and 12 show the results of the calculation when the reaction temperature is 2,100K at the excess air ratio of 0.8. When these results are compared with the results using the Zeldovich reaction formulas, O radical decreases, while the formation of OH is larger. As shown in Fig.12, the fractions of HCN, CN, and CH2 correspond to each other. The formation of CN is accelerated with NO and CO by the reverse reaction of formula (6). This is because the formation of OH and HCN increase by the reverse reaction of formula (5), resulting in the production of CH2 by the reverse reaction of formula (4). Under such conditions, it is found that CO greatly affects the reduction of NO in high temperature.

EXPERIMENTAL RESEARCH OF THE CONTINUOUS COMBUSTOR

An experimental research was conducted using the continuous combustor to investigate the actual decomposition of NO. Fig.13 is the layout of the continuous combustor used for the experimental research. As shown in Fig.14, the combustor has a combustion gas recirculator to reduce NO and soot from the combustor itself. The combustor has a plate at the outlet of the combustion chamber to increase the internal pressure a little, and the recirculator accelerates the recirculation of the combustion gas. The combustor has a window to observe the combustion status and to photograph.

To investigate the decomposition of NOx, the NO cylinder was provided in the downstream of the air flow as shown in Fig.13 to supply a certain amount of NO. The gas sampling ports of the exhaust gas analysis and the Bosch smoke meter were provided 10 mm away from the outlet of the combustor. For the measurement of exhaust gas fractions such as NOx, CO, CO2, O2, and THC, the exhaust gas analyzer (Horiba Co. Ltd.; MEXA-8120D) was used. The bullet type fuel consumption meter was used to measure the fuel. The laminar air flow meter was used for measurement of the air. During the experimental research, fuel was supplied with a constant pressure of 5kgf/cm2. The fuel used is kerosene. The Delavan nozzle used has the flow rate of 0.75 gal/h and the cone angle of 60 degrees.

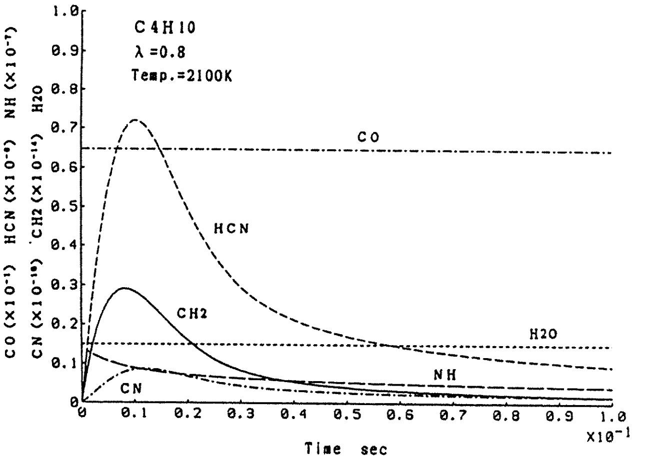

Fig.12 Mole Fractions by Nine Reactions-4
(Excess air ratio = 0.8)

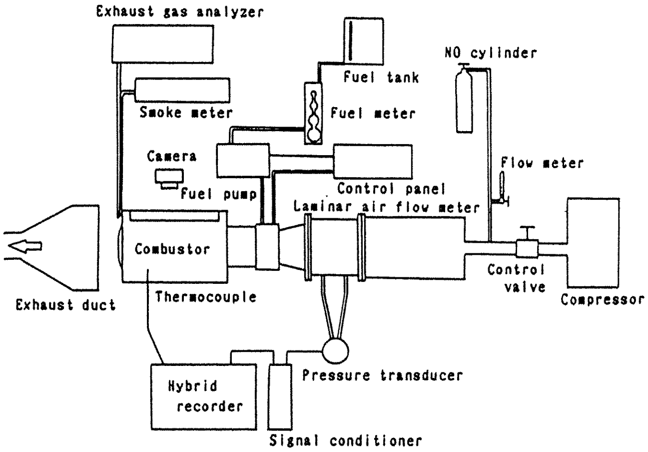

Fig.13 Layout of the Continuous Combustor

RESULTS OF THE EXPERIMENT

Fig.15 shows the characteristics of the exhaust gas when kerosene is used as fuel. If the excess air ratio is too low, the fraction of O2 in exhaust gas is low, and those of CO, CO2, NOx, THC, are high. This is caused by the low rate of air supplied to the combustor. The fraction of THC and CO become very high in this situation, however, they decrease according to the excess air ratio. The residual O2 tends to be mostly proportional to the rate of air supply. The maximum value of NOx becomes approximately 35ppm at the excess air ratio of 1.0 and decreases with the increase of the excess air ratio. The fraction of NOx is substantially low because of recirculation of combustion gas. Soot is not generated at the excess air ratio of 1.0 or more.

Fig.16 shows the results for the fraction of NOx when a constant amount of NO is supplied in advance in the combustion air. As shown in the figure, when NO fraction of 500ppm supplies in the combustion chamber at the excess air ratio of 0.8, NOx in exhaust gas was deoxidized and decreases to 300ppm. The simulation results of cetane close to kerosene prove that approximately 50% of NO has been decomposed. The above results tend to be very similar to the results of fundamental research.

At the excess air ratio of 1.0, NOx of 300ppm in exhaust gas is found to be reduced from the NO supply of 400ppm. If the air excess ratio becomes higher than 1.0, the reduction of NO decreases. Only 10% of NO is found to be decomposed from the total NO supply at the excess air ratio of 1.4 or more. This is because the decomposition of NOx is restricted at the excess air ratio. At the excess air ratio of 1.0 or less, the recirculating combustion can be performed efficiently in the combustion chamber and the decomposition of NOx is accelerated by the deoxidizing fractions produced by combustion.

CONCLUSIONS

The conclusions are summarized below:

(1) The reduction of NO is accelerated by the deoxidizing fractions produced by combustion such as H radical and CO. The higher the reaction temperature is and the longer the retention time is, the higher the reduction of NO is.

(2) When the reaction temperature is 2,000K or more at the excess air ratio of 1.0 or less, the reduction of NO can be identified by the effects of CO. However, when it is 2,000K or less, the simulation is made possible using the Zeldovich reaction formulas.

(3) The reduction of NO can be identified at a lower excess air ratio at the experiment to use the combustor with a combustion gas recirculator. These experimental results are similar tendency to the simulation.

ACKNOWLEDGEMENT

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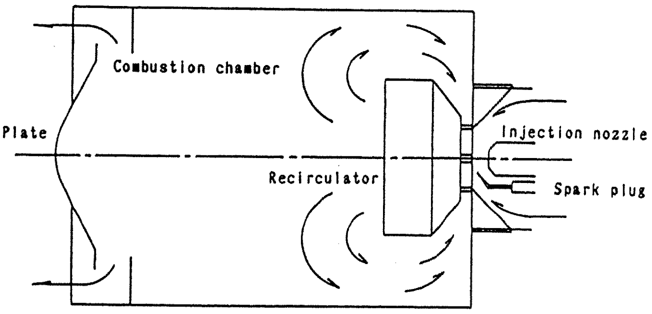

Fig.14 Combustion Chamber

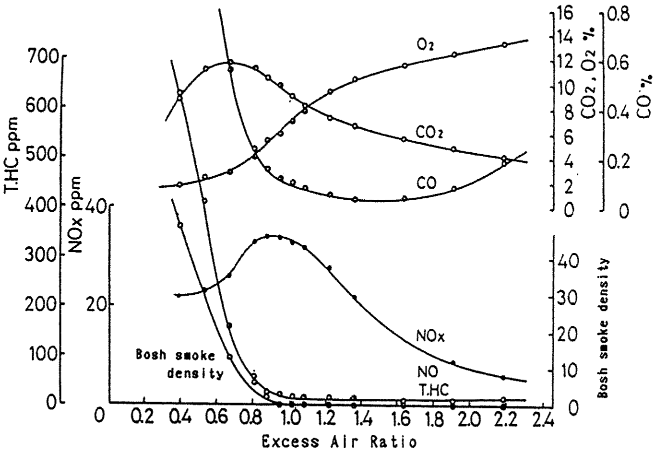

Fig.15 Emission of Exhaust Gas (Kerosene)

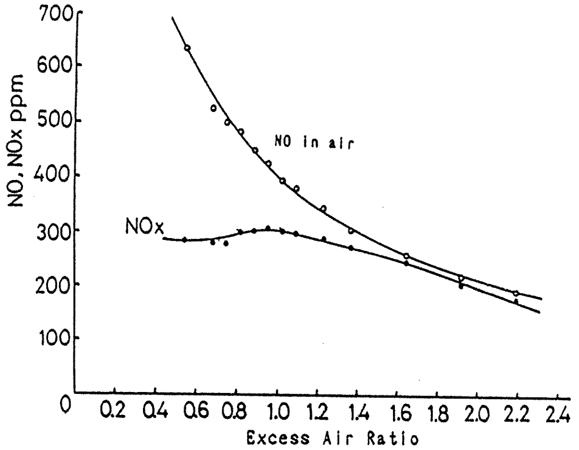

Fig.16 Reduction of NO

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