# Modeling of NOx Formation in Natural Gas Fueled Diesel Combustion

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### **ABSTRACT**

A model for predicting the formation and destruction of nitrogen oxides and their emissions from a natural gas fueled diesel engine has been developed by taking chemical kinetics into account. The stochastic approach was used to model fluid dynamic behavior in the combustion chamber by assuming the turbulent mixing is a random mixing processes among fine fluid particles.

The calculations were made under the same conditions as the experiments. The mixing rate or collision frequency was chosen to fit the pressure and heat release rate with those of the experiments. It is shown that the model reproduces the pressure history of the experiments well and the predicted NO concentration at exhaust coincides with that of the experiments within a factor of 1.5. The results also show that most NO is formed locally at temperatures higher than 2500 K under a range of fuel-air equivalence ratios,  $0.8 < \phi < 1$  and that the NO, once formed, is hardly destroyed through combustion.

## INTRODUCTION

Reducing nitrogen oxides emitted from a diesel engines requires urgent attention to prevent further worldwide air pollution. At present, however, reduction methods that do not sacrifice heat efficiency are still unclear. To obtain a solution, there is a need to clarify the origin of the nitric oxide generation and its destruction during diesel combustion. Almost all nitric oxide in the exhaust can be formed locally at the region having the highest temperature and fuel lean equivalence ratio in the combustion chamber. The generation from such regions may strongly depend not only on turbulent mixing but also on slow chemical reactions such as ignition processes. Furthermore, as is well known, NO formation itself, under the high temperature, is controlled by a slow chemical mechanism. Therefore,

it is important for modeling the NO formation during diesel combustion, to take both the turbulent mixing and the detailed chemical kinetics into account. However, the multidimensional model for diesel combustion (1-3) does not seem practical at present, because long computation time will be required if detailed chemical mechanism is taken into account. On the other hand, the stochastic model for diesel combustion (4) developed by Ikegami et al., seems suitable for this problem. This model relies on the concept that combustion evolves by random collision and coalescence of individual fluid particles. This allows the description of heterogeneity of the fuel concentration without relying upon the concept of space that is indispensable to the deterministic approach. Therefore, it is easy for this model to introduce detailed chemical kinetics with reasonable increase of computation time. As for ignition processes, unfortunately, the original model does not take the detailed chemical kinetics into account and, with regard to NO formation, considers only the Zeldvich mechanism. In a practical system such as diesel combustion, it is not known whether the destruction of NO is controlled by the Zeldvich mechanism only or not.

In the present study, the stochastic model was extended, taking into consideration a detailed chemical mechanism for both processes of the initiation and the NO formation, to test the origin of NO emission. We carried out a computer simulation of NO formation for natural gas fueled, high-speed direct-injection diesel engines under the condition of an actual experiment (5).

### STOCHASTIC MODEL

A stochastic approach for diesel combustion (4) was employed in the present study. In this model the heterogeneity and its devolution are described using the Curl collision-redispersion model (6) and thermodynamic states of fluid are expressed by probability density functions. The turbulent mixing is

described by random collision and coalescence of individual fluid particles. These collision and coalescence occurred at the intervals related to turbulent intensity between two individual fluid particles chosen at random. The composition of each fluid cell is homogeneous and changes continuously with time under the control of chemical kinetics.

### **Basic** equations

The state of a fluid is described by assigning the pressure p, the specific enthalpy h, and the mole number of species  $y_j$ , (j=1,n). According with the stochastic model mentioned above, since pressure is uniform at every moment, the probability density function is defined f=f(x,t), where  $x=(h,y_1,...,y_j,...,y_n)$  denotes state vector and the master equation is given by

$$\frac{\partial f}{\partial t} + \frac{\partial \dot{h}f}{\partial h} + \sum_{j} \frac{\partial \dot{y}_{j}f}{\partial y_{j}} = \omega \phi(\mathbf{x}, t) \tag{1}$$

$$\phi(\mathbf{x}, t) = \iint 2f(\mathbf{x}^{(1)}, t)f(\mathbf{x}^{(2)}, t)\delta\left\{\frac{h^{(1)} + h^{(2)}}{2} - h\right\}$$

$$\prod_{j} \delta\left\{\frac{y_{j}^{(1)} + y_{j}^{(2)}}{2} - y_{j}\right\} d\mathbf{x}^{(1)} d\mathbf{x}^{(2)} - 2f(\mathbf{x}, t) \tag{2}$$

where  $\phi(x,t)$  denotes the extended Curl collision function,  $\omega$  the collision frequency or the probability of collision for a fluid particle during a unit time, and  $\delta$  the Dirac's delta function. Eq.(1) shows that the change of the probability density function with time is given from the changes of state vector due to collision.

To describe the probability density function, a large amount of fluid particle having the same mass is taken into account in the calculation. From the first law of thermodynamics and equation of state for ideal gas, pressure change is given as the function of the cylinder volume Vc and composition of each particle as follows.

$$\frac{dp}{dt} = \frac{m\sum_{i} T_{i} \frac{dR_{i}}{dt} - m\sum_{i} R_{i} \frac{\sum_{j} h_{j} y_{ij} + \dot{q}_{i}}{\sum_{j} c_{pj} y_{ij}} - p \frac{dV_{c}}{dt}}{V_{c} - m\sum_{i} \frac{R_{i} V_{i}}{\sum_{j} c_{pj} y_{ij}}}$$
(3)

Where m is the mass of particle,  $R_i$  the gas constant for i-th particle,  $h_i$  the enthalpy of i-th particle,  $y_{ij}$  the mole number of j-th species in i-th particle,  $c_{pj}$  the specific heat at constant pressure for species j, and  $q_i$  the heat loss for i-th particle. Since  $dy_{ij}/dt$  can be determine by kinetics, we can get dp/dt from Eq.(3).  $dT_i/dt$  is given from the first law of thermodynamics as the function of dp/dt.

$$\frac{dT_i}{dt} = \frac{V_i \frac{dp}{dt} - \sum_j h_i \frac{dy_{ij}}{dt} - \dot{q}_i}{\sum_j c_{pj} y_{ij}}$$
(4)

In summary, the diesel combustion model based on the stochastic approach results in solving Eqs.(1)-(4) simultaneously.

### Reactions

At the present stage of this study, the diesel engine fueled natural gas was studied in place of the engine fueled commercial gas oil since the detailed chemical mechanism of natural gas has been developed and NO formation in natural gas fueled diesel engine is not far from that in normal diesel engines. Although the primary concern of the present study is the NO formation, accurate prediction for the initiation or ignition process is critical for quantitative modeling of NO formation. considerations underlie our interest in maintaining this chemical model as realistic as possible, while keeping its size to the minimum possible. initial, "full" reaction mechanism for methane combustion was taken from Ref. (7). It was reduced in size at the conditions typical of diesel combustion to a 21-species mechanism, listed as reaction 1-74 in Table 1. This mechanism includes chemistry for  $C_2H_6$ but excludes that for C3H8. Usually, natural gas contains a small amount of propane and butane in addition to methane and ethane. Therefore, the set of reactions 1-74 was augmented with dissociation of propane, reactions 75 (Table 1). The butane in the fuel was incorporated into propane, in order to restrict the size of the reaction set.

For NO formation, the Skeletal mechanism (8) was used in the present study. This mechanism includes the Zeldvich mechanism, prompt NO mechanism and destruction of NO by  $NH_2$ .

# Computational Procedure

We present computer simulations of NO formation for the combustion of natural gas in a glow-assisted direct-injection diesel engine. The computations were carried out under the conditions of an actual experiment(5): engine speed 1800 rpm, cylinder, water cooled, naturally-aspirated, four cycle, swirl ratio 2.7, compression ratio 16, fuel-air equivalence ratio 0.65. When the equivalence ratio was 0.65, a total 197 cells of equal mass, 190 of air and 7 of fuel, were considered. The collision frequency, which depends on the total number of particles considered in the calculation, was obtained by fitting the rate of heat release. In the present study, collision occurred with a constant frequency, 2.5 µs during the fuel injection and 10 us after injection. Heat losses were estimated with Annand and Ma's empirical formula (9).

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Table 1 Mechanism of methane oxidation and NO formation						Table 1 (continued)					
$k = AT^n exp($			AT <sup>n</sup> exp(-	-E/RT)			k = AT <sup>n</sup> exp(-E/RT)				
No.	Reaction <sup>a</sup>	Α	n	E	<del></del>	No. Reaction <sup>a</sup>	A	n	E		
,,,,,		(cm, mol,		$(kJ mol^{-1})$			(cm, mol,		$(kJ mol^{-1})$		
1	H + O2 = OH + O	5.33D+16	750	72.000		58 CH3O + CO = CO2 + CH3	4.68D+02	3.160	22.500		
2	O + H2 = OH + H	3.87D+04	2.700	26.200	!	59 CH3O + M = CH2O + H + M	1.00D+14	.000	105.000		
_	OH + H2 = H2O + H	2.16D+08	1.510	14.350		ETBE <sup>b</sup> H2=2.9 CO2=4.3 O2=1.2	N2=1.2 H2	0=18.5	0=2.1		
	OH + OH ≈ O + H2O	2.10D+08	1.400	~1.660		60  C2H3 + H = C2H2 + H2	3.00D+13	.000	.000		
	H + O2 + M = HO2 + M	7.00D+17	800	.000		51  C2H3 + 02 = CH2O + CHO	3.98D+12	.000	-1.000		
	ETBE <sup>b</sup> H2=0.0 CO2=0.0 O2=0.0					52 C2H4 + H = C2H3 + H2	3.16D+11	.700	33.500		
	H + O2 + H2 = HO2 + H2 H + O2 + O2 = HO2 + O2	2.80D+18	860	.000 .000		53 C2H4 + O = C2H3 + OH 54 C2H4 + OH = C2H3 + H2O	7.11D+08 3.00D+13	1.550	31.340		
	H + O2 + O2 = HO2 + O2 H + O2 + N2 = HO2 + N2	3.00D+20 3.75D+20	-1.720 -1.720	.000		55  C2H4 + CH3 = C2H3 + CH4	3.92D+12	.000 .000	12.500 54.500		
	H + O2 + C0 = HO2 + C0	2.10D+18	860	.000		56  C2H4 + M = C2H3 + H + M	3.80D+17	.000	410.700		
	H + O2 + CO2 = HO2 + CO2	4.10D+18	860	.000		ETBE H2=2.9 CO2=4.3 O2=1.2					
11	H + O2 + H2O = HO2 + H2O	9.40D+18	760	.000	(	57  C2H5 + O2 = C2H4 + HO2	2.00D+12	.000	20.900		
	HO2 + H = OH + OH	1.50D+14	.000	4.200	(	$58 \text{ C2H5 (+M)} = \text{C2H4} + \text{H (+M)}^{\text{C}}$	4.97D+10	.730	154.228		
	HO2 + H = H2 + O2	2.50D+13	.000	2.900		LOW PRES. LIMIT	6.24D+39	-6.800	177.800		
	HO2 + O = O2 + OH	2.00D+13	.000	.000 .000		SRI DATA.	0.667	653.88	8733.74		
	HO2 + OH = H2O + O2 HO2 + HO2 = H2O2 + O2	6.02D+13 1.06D+11	.000	-7.100	(	59 C2H6 (+M) = CH3 + CH3 (+M) <sup>C</sup>		-2.792	389.670		
	H2O2 + M = OH + OH + M	1.00D+17	.000	190.000		LOW PRES. LIMIT	2.23D+61		414.847		
	ETBE <sup>b</sup> H2=2.9 CO2=4.3 O2=1.2					SRI DATA.	0.805	302.71	10730.56		
	H2O2 + OH = H2O + HO2	7.00D+12	.000	6.000	7	$^{70}$ C2H6 (+M) = C2H5 + H (+M) <sup>C</sup>		-1.230	427.777		
	$HOCO (+M) = H + CO2 (+M)^C$	1.74D+12	.310	137.825		LOW PRES. LIMIT SRI DATA.	1.27D+46 0.603	-7.810	450.854		
	LOW PRES. LIMIT	6.44D+29	-4.440	149.559	-	71  C2H6 + H = C2H5 + H2	5.40D+02	759.32 3.500	10869.84 21.800		
	SRI DATA.	0.683	534.32	10777.07		$^{2}$ C2H6 + 0 = C2H5 + OH	1.40D+00	4.300	11.570		
20	$HOCO (+M) = CO + OH (+M)^C$	5.89D+12	.530	142.226		$^{7}3$ C2H6 + OH = C2H5 + H2O	2.20D+07	1.900	4.700		
	LOW PRES. LIMIT	6.16D+26	-3.310	150.459	7	74 C2H6 + CH3 = C2H5 + CH4	5.50D-01	4.000	34.700		
	SRI DATA.	0.467	454.32	8483.82		75 C3H8 = CH3 + C2H5	7.90D+22	-1.790	371.000		
	CO + OH = CO2 + H	1.22D+07	1.350	-2.640		76  NH3 + H = NH2 + H2	6.40D+05	2.390	42.470		
	CO + HO2 = CO2 + OH CO + O + M = CO2 + M	1.50D+14 3.01D+14	.000	98.700 12.600		77  NH3 + O = NH2 + OH $78  NH3 + OH = NH2 + H2O$	1.10D+06 4.70D+06	2.100 1.900	21.760 2.090		
	ETBE <sup>b</sup> H2=0.0 CO2=7.0 O2=12.0					79 NH2 + H = NH + H2	4.00D+13	.000	15.270		
	CO + O2 = CO2 + O	2.50D+12	.000	200.000		30 NH2 + 0 = NO + H + H	6.60D+14	500	.000		
	CHO + H = H2 + CO	7.23D+13	.000	.000	8	31  NH2 + 0 = NH + OH	7.00D+12	.000	.000		
26	CHO + OH = H2O + CO	1.00D+14	.000	.000		32  NH2 + OH = NH + H2O	4.00D+06	2.000	4.180		
	CHO + O2 = HO2 + CO	4.20D+12	.000	.000		33  NH2 + NO = N2 + H2O	1.30D+16	-1.250	.000		
	CHO + M = H + CO + M	1.86D+17	-1.000	71.100		34 NH + H = N + H2 35 NH + O = NO + H	3.20D+13 7.80D+13	.000	1.360		
	$ETBE^{b}$ H2 = 1.9 CO2=1.0 O2=1					35 NH + OH = NO + H + H	2.00D+13	.000 .000	.000 .000		
	CH2S + H2 = CH3 + H	7.23D+13	.000	.000		37  NH + OH = N + H2O	5.00D+11	.500	8.370		
	CH2S + O2 = CO + OH + H CH2S + M = CH2 + M	3.10D+13 6.00D+12	.000	.000 .000		18  NH + NO = N2O + H	4.30D+14	500	.000		
	ETBE <sup>b</sup> H2=2.4 CO2=3.6 O2=1.0					89 N + OH = NO + H	3.80D+13	.000	.000		
	CH2 + O2 = CO2 + H + H	1.60D+12	.000	4.180		10  N + 02 = NO + 0	6.40D+09	1.000	27.280		
	CH2 + O2 = CH2O + O	5.00D+12	.000	37.700		01  N + NO = 0 + N2	3.30D+12	0.300	.000		
	CH2O + H = CHO + H2	1.26D+08	1.620	9.100		02 O + N2 + M = N2O + M 03 N2O + H = N2 + OH	1.40D+08 1.90D+06	1.430 2.420	74.100 56.530		
35	CH2O + O = CHO + OH	3.50D+13	.000	14.700		14  N2O + 0 = NO + NO	1.00D+14	0.000	117.990		
	CH2O + OH = CHO + H2O	7.23D+05	2.460	-4.060		15  N2O + 0 = N2 + O2	1.00D+14	0.000	117.990		
	CH20 + 02 = CH0 + H02	1.00D+14	.000	167.000		06 CN + H2 = HCN + H	3.00D+05	2.450	9.360		
	CH20 + H02 = CH0 + H202 CH20 + CH3 = CH0 + CH4	1.00D+12	.000 7.400	33.500		7  HCN + O = NCO + H	1.40D+04	2.640	20.790		
	CH2O + CH3 = CHO + CH4 CH2O + M = CHO + H + M	8.91D-13 5.00D+16	.000	-4.000 320.000		18  HCN + OH = CN + H2O	1.50D+13	0.000	45.610		
	ETBE <sup>b</sup> H2=2.9 CO2=4.3 O2=1.2					9 HCN + OH = NH2 + CO .00 CN + O = CO + N	4.40D+02	2.980	39.140		
	CH3 + H = CH2 + H2	1.80D+14	.000	63.200		.01 CN + OH = NCO + H	1.80D+13 6.00D+13	0.000 0.000	.000 .000		
	CH3 + O = CH2O + H	8.43D+13	.000	.000		02 CN + 02 = NCO + 0	2.60D+14	-0.500	.000		
	CH3 + OH = CH2O + H2	8.00D+12	.000	.000		03  NCO + H = NH + CO	5.00D+13	0.000	.000		
44 (	CH3 + OH = CH2 + H2O	1.13D+06	2.130	10.200		.04  NCO + H2 = NH2 + CO	8.60D+12	0.000	37.660		
	CH3 + O2 = CH3O + O	4.30D+13	.000	128.900		05  NCO + NO = N2O + CO	1.00D+13	0.000	-1.670		
	CH3 + O2 = CH2O + OH	5.20D+13	.000	146.000		06  CO2 + N = NO + CO	8.60D+11	0.000	9.250		
	CH3 + HO2 = CH3O + OH	2.28D+13	.000 500	.000		07 CH3 + N = HCN + H + H	7.10D+13	0.000	.000		
	CH3 + CHO = CH4 + CO CH3 + CH3 = C2H5 + H	3.20D+11 4.90D+12	. 500 . 000	.000 49.100		08 CH2 + NO = NCO + H2	3.50D+12	0.000	-4.600 92.050		
	CH3 + CH3 = C2H3 + H	5.00D+12	.000	.000		09 CH + N2 = HCN + N 10 CH + NO = HCN + O	4.40D+12 1.00D+14	0.000 0.000	92.050 .000		
	$CH4 (+M) = CH3 + H (+M)^{C}$	7.05D+16	558	438.909		11 C + N2 = CN + N	6.30D+13	0.000	192.460		
	LOW PRES. LIMIT	1.19D+35	-4.911	447.562		12 C + NO = CN + O	1.90D+13	0.000	.000		
	SRI DATA.	0.555	405.62	4580.86	1	13 C + NO = N + CO	2.90D+13	0.000	.000		
	CH4 + H = CH3 + H2	7.80D+06	2.110	32.400	_1	14 HCCO + NO = HCN + CO2	2.00D+13	0.000	.000		
	CH4 + 0 = CH3 + OH	1.90D+09	1.440	36.300	a	Reactions wih sign "=" were					
	CH4 + O2 = CH3 + HO2	8.00D+13	.000	234.300	b		-				
	CH4 + OH = CH3 + H2O CH4 + HO2 = CH3 + H2O2	1.50D+06 1.12D+13	2.130 .000	10.200 103.100	C	<ul> <li>The pressure dependence of treated based on the SRI for</li> </ul>		verticie	ncs were		
	CH30 + 02 = CH3 + H202 CH30 + 02 = CH20 + H02	4.28D-13	7.600	-14.760		created based on the SKI TO	n ui.				
					-						

Calculations were carried out by a step-by-step numerical integration. An implicit manner was used for chemical kinetic calculation. Pressure and temperature of each particle was calculated in an explicit manner. When the mole fraction of OH in a particle exceeds  $10^{-5}$  and that of CH<sub>4</sub> was below  $10^{-2}$ , a state of partial equilibrium was assumed to save computation time. The NO and intermediates, whose formation was controlled by slow kinetics, :HCN, CN, NCO, N, NH, NH<sub>2</sub>, N<sub>2</sub>O were calculated kinetically at any given moment. To check if the partial equilibrium assumption gives accurate results, several preliminary calculations regarding single particles has been carried out under constant temperature and pressure. Fig. 1, an example of those calculations, shows the concentration of some major species and temperature in an ignition process of natural gas-air mixture obtained by the full kinetic calculation and by the method of present study assuming a state of partial equilibrium after ignition. As for the full kinetic calculation, immediately after OH concentration reaches 10-5 in mole fraction, heat is released instantaneously and the state reaches equilibrium. The calculations done under various initial temperature T<sub>0</sub> and fuel-air equivalence ratio φ show the same tendency. From these results, therefore, it is noted that the assumption of partial equilibrium used in the present study is likely.

# **RESULTS AND DISCUSSION**

Figure 2 shows a comparison of predicted pressure history and heat release rate with those at the experiment. The Runs 1 and 2 were performed under identical conditions except for different stochastic sequence of fluid particle collisions, originating from different "seed" numbers for the random number generator These two runs test the "reproducibility" of the stochastic simulations. The difference of pressure and heat release rate obtained in these runs shows that 197 particles are not statistically sufficient to describe heterogeneity. (The number of particle considered in a calculation is restricted by the CPU time. The typical run using a workstation (HP-715/32) took about 12 hours of CPU time.) In the actual engine, however, cycle to cycle variation shows several percents of difference in pressure history. Although, of course, these variations can not be explained by the low number of particles used in this study, the difference in pressure history due to statistical variance nevertheless appears to be at an acceptable level.

Furthermore, the close proximity to the experiment indicates that the parameters used in the calculation seems likely. It should be noted that the predicted heat release rate indicates shorter ignition time lag than that at the experiment. One is an overestimate of the glow assistance, the other is the

constant collision frequency. The collision frequency depends on turbulent characteristics such as turbulent intensity and dissipation rate, should be treated as a function of a time for a precise prediction. In the present study, however, these treatments were not chosen on account of focusing on NO formation rather than precise prediction.

The space averaged NO concentrations in Runl and Run2 and these mean values are shown in Fig. 3. The NO concentration obtained by the calculation taking into account only the Zeldvich mechanism as the NO formation is also displayed by the curve marked Run3. The collision sequence is the same as that in Run1. The variance of NO concentration between two runs, as mentioned above, comes from the low number of particles used in this study. However, the mean value of those at 60° ATDC., where NO formation freezes, is very close to the experimental

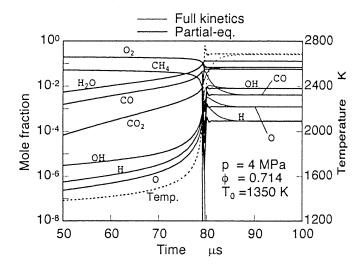


Fig. 1 Concentration of some major species in a ignition process of natural gas-air mixture

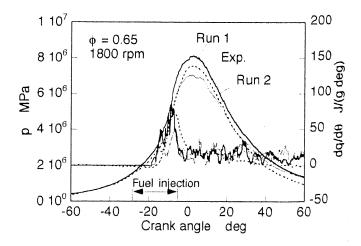


Fig. 2 Pressure history and heat release rate

value of 1020 ppm (5) at exhaust. By comparing Run3 with Run1, it is apparent that the Zeldvich mechanism is not sufficient to predict real NO formation during diesel combustion. The results also suggest that the destruction of NO in a deoxidization circumstance, which is realizes by the collision between fuel-lean and fuel-rich particle, is not controlled by only the Zeldvich mechanism

The calculated average concentration of some major species in the case of Run1 is displayed in Fig. 4, versus crank angle. The average temperature and its deviation are shown in Fig. 5. Inspection of these results indicates that most NO is formed around the early stage of the diffusive combustion where the deviation of temperature is high and that NO, once formed, is hardly destroyed through expansion stroke. Fig. 6 shows the correlation between NO and temperature at 1.6° ATDC where NO formation becomes intensive, and Fig. 7 shows that between NO and equivalence ratio. These results indicate that most NO is formed in a small number of particles, having higher temperatures than 2500 K and fuel lean equivalence ratio in the range of  $0.8 < \phi < 1$ . The above results also suggest that the turbulent mixing process during ignition time lag and explosive combustion strongly depends on NO formation which occurs subsequently during the early stage of the diffusive combustion.

To see the effects of fuel injection timing on NO formation, the calculations have been performed under the same collision sequence as Run 1. It is noted that the results calculated under the same collision sequence are comparable to each other even in the case of having different injection timing. The space averaged NO concentrations and temperatures are displayed in Fig. 8. Early fuel injection elevates the NO level due to the increase of average temperature. In comparison with the experiments, the present model well explain the real tendency of NO increment at early injection, though absolute value does not coincide with that in experiments exactly owing to the low number of particles used in this study mentioned above.

### CONCLUSIONS

Stochastic simulations of NO formation were performed for the combustion of natural gas in a glow-assisted direct-injection diesel engine. The simple fluid dynamic method of Curl (6) was employed, which describes turbulent mixing by random collision and coalescence of individual fluid particles. The composition of each fluid particle is homogeneous and changes with time under the control of the chemical kinetics.

It is shown that the predicted NO concentration at exhaust coincides with that of the experiments within a factor of 1.5. The results also show that

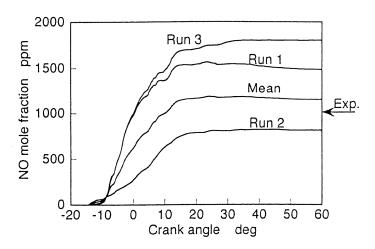


Fig. 3 The space averaged NO concentrations

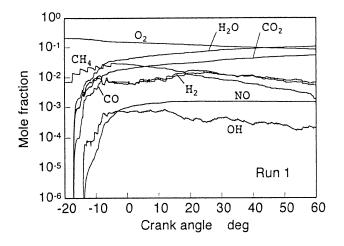


Fig. 4 The calculated average concentration of some major species (Run1)

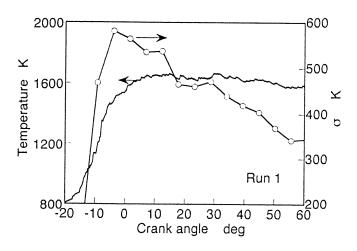


Fig. 5 The average temperature and its deviation (Run1)

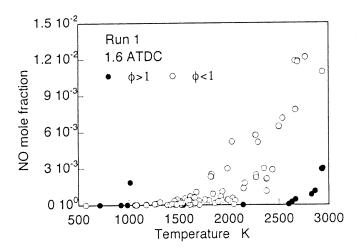


Fig. 6 Correlation between NO and temperature at 1.6° ATDC

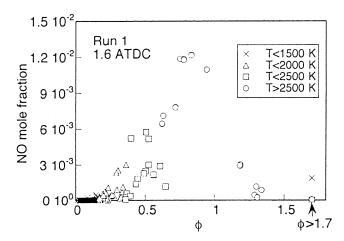


Fig. 7 Correlation between NO and equivalence ratio at 1.6° ATDC

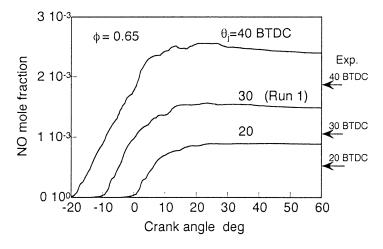


Fig. 8 Space averaged NO concentrations and temperatures at various injection timing

most NO is formed locally at temperatures higher than 2500 K under a range of fuel-air equivalence ratios,  $0.8 < \phi < 1$  and that the NO, once formed, is hardly destroyed through combustion. Analysis of NO formation channels suggest that the destruction of NO in a deoxidization circumstance, which is realizes by the collision between fuel-lean and fuel-rich particle, is not controlled by only the Zeldvich mechanism.

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