ANALYSIS OF COMBUSTION PRODUCT FOR MODIFIED HIGH-SPEED DIESEL COMBUSTION MODEL PCI ENGINE OF AFTER-TREATMENT SYSTEM

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ABSTRACT

Recent development of diesel engine attracts the automotive manufacturers due to its high thermal efficiency and load carrying capacity compared to other internal combustion engines. To design diesel engine adapted to future exhaust gas emission regulations, it would be advantageous to have a driving mode simulator for vehicle performance and exhaust emission, including after-treatment systems. The authors have developed a diesel combustion model, which is called Tsururushima model based on the Hiroyasu model. In this study, the result is compared to that of the previous model, called Schreiber model and with the experiment also. And finally, the model is expanded for calculating ethylene and CO in the exhaust emissions. Tsurushima reduced kinetic model has been introduced together with characteristic mixing time scale. And analysis shows the better simulation result and also it is possible to calculate the intermediate species of combustion. The modified model is applicable for the both combustions of spray diffusion flame and of homogeneous charge compression ignition.

Key Words: Diesel Engine, Premixed Compression Engine (PCI), After Treatment, Ignition Delay, Reaction Scheme.

1. INTRODUCTION

To design diesel engines complying with future regulations of exhaust emissions, it is necessary to optimize combinations of combustion chamber configurations, common rail injection patterns, EGR, and after-treatment technology such as urea selective catalytic reaction (SCR) systems and diesel particulate filter (DPF). It is also necessary to control the optimum-operating mode of the engine system during transient operation. However, considerable time and costs are necessary to develop an optimization and control logic for the total engine systems by experiments with real engines. One of the development goals would be establishing a total engine simulation system, which can predict the emission characteristics and engine performance including the after-treatment with real time processing speed (Shimazaki et al., 2006; Saidur et al., 2008). For such a simulation system, a combustion model is required to possess both processing speed and prediction accuracy. This study develops a combustion model for use in high-speed total engine simulation. The model is based on the combustion analysis program HTB-DECS with a phenomenological model developed by Hiroyasu et al. (1982a; 1982b) due to its high speed computational characteristics. The paper improves the models by introducing Tsurusrushima reduced reaction scheme. The present model has also been extended to deal with premixed compression ignition combustion, and this paper provides details of the formulation to solve the Tsurushima reaction sets with large time step, and a characteristic mixing time concept to take into account the local heterogeneity of the mixture. And compare with previous combustion model among experimental and calculated results of a single cylinder engine for present developed model.

The Tsurushima reaction model, as it has a possibility of simulating ethylene and CO in the exhaust, which may be important for after treatment simulation.

2. BASIC ENGINE COMBUSTION MODEL OF HTB-DECS

The basic model developed by Hiroyasu et al. (1982a) is based on the free spray structure indicated in Figure 1. Fuel spray is divided into packages, which contains same amount of fuel mass, and air is entrained into the package. The local velocity of the package determines the air entrainment rate. Initial velocity at the nozzle exit is given by injection rate, and it follows the history of free spray velocity profile. The air entrainment rate is influenced by wall impingement and turbulence in the cylinder, and it changes the package velocity to maintain the spray momentum in next time step. This causes deviation of local velocity of the package from the free spray velocity profile and the air entrainment of the next time step jumps to the corresponding spray position with the same local velocity in the free spray. The mixture in the package is treated uniform and chemical reaction takes place for the mixture.

In the previous work the authors have modified the program to take into account the combustion gas re-entrainment, approaching to the uniform gas state in the cylinder with time. Modification is also made to keep the momentum of the package even for different air entrainment rate due to local turbulence and entrainment of combustion gas. In order to extend the original model to PCI combustion Schreiber model was introduced for the chemical reaction of the fuel. This allows the

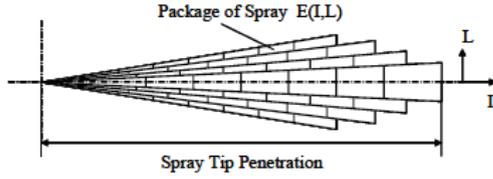simulation of low temperature combustion typically seen in the PCI.

Figure 1 Schematic outline of the spray distribution in the base model; HTB

3. INTRODUCTION OF THE SCHREIBER MODEL

Table 2 shows the model of Schreiber et al. (1994) The F represents a fuel, n-dodecane was the fuel in their model. Reactions 1 and 2 are high temperature oxidation reactions and reactions 3 to 5 are low temperature oxidation reactions. P expresses the end product, and X, Y, and I are chemical species, which represent intermediate products forming in the process of the oxidation. The X is compounds which form by thermal decomposition of the fuel, Y is intermediate product such as OH radicals which appear in the reaction process, and I is also an intermediate product mainly the peroxides of the fuel. Five steps reaction steps of Schreiber as shown in the following:

Table 1 Chemical properties of Schreiber model

	Reaction	$H^{\cdot}_{300}$ (kJ/mol)	A (mol m3 s)	E/R (K)
1	$F \rightarrow X$	709.9	5.0×10^{8}	18050
2	$X + 18.5O_2 \rightarrow P$	-6709.9	7.0×10^{6}	7200
3+	$F + 2O_2 \rightarrow I$	-53.9	3.5×10^{9}	19500
3-	$I \rightarrow F + 2O_2$	53.9	6.0×10^{27}	37500
4	$I \rightarrow 2Y$	-60.0	6.0×10^{7}	5000
5	$Y + 0.5F + 17.5O_2 \rightarrow P$	-5943.1	1.0×10^{9}	16500

The reaction rate of each reaction is as follows (Schreiber et al., 1993).

$$R_1 = K_1[F](p/p_0)^{0.5}$$
$$R_2 = K_2[X][O_2][M]$$
$$R_{3+} = K_{3+}[F][O_2][M](p/p_0)^{-2.2} C_{3+}$$
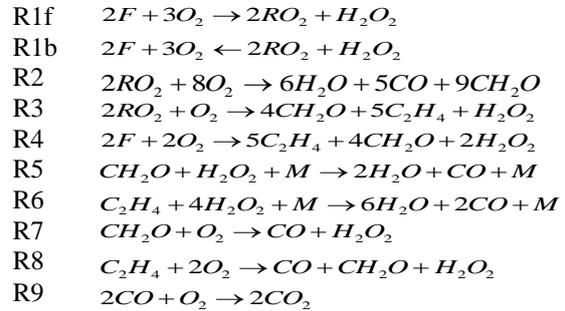$$R_{3-} = K_3[I](p/p_0)^{-3.5}$$
$$R_4 = K_4[I]C_4$$
$$R_5 = K_5[O_2][Y]$$

Table 2 Reaction constant of Schreiber model

Reaction	A Mol.m3.Sec	Modified A Mol.m3.Se	H_{298} (KJ/mol)	E/R [K]
1	5.0E08	1.5E09	709.9	18050
2	7.0E06	7.0E06	-6709.9	7200
3+	3.5E09	3.0E08	-53.9	19500
3-	6.0E27	1.5E27	53.9	37500
4	6.0E07	6.0E07	-60.0	5000
5	1.0E09	1.0E13	-5943.1	16500

4. TSURUSHIMA REACTION MODEL AND MIXING TIME SCALE

Tsurushima model consists of nine reaction steps (Takashima et al., 2008) including several intermediate species as follows (Arato. et al., 2006):

R1f $\quad 2F + 3O_2 \rightarrow 2RO_2 + H_2O_2$
R1b $\quad 2F + 3O_2 \leftarrow 2RO_2 + H_2O_2$
R2 $\quad 2RO_2 + 8O_2 \rightarrow 6H_2O + 5CO + 9CH_2O$
R3 $\quad 2RO_2 + O_2 \rightarrow 4CH_2O + 5C_2H_4 + H_2O_2$
R4 $\quad 2F + 2O_2 \rightarrow 5C_2H_4 + 4CH_2O + 2H_2O_2$
R5 $\quad CH_2O + H_2O_2 + M \rightarrow 2H_2O + CO + M$
R6 $\quad C_2H_4 + 4H_2O_2 + M \rightarrow 6H_2O + 2CO + M$
R7 $\quad CH_2O + O_2 \rightarrow CO + H_2O_2$
R8 $\quad C_2H_4 + 2O_2 \rightarrow CO + CH_2O + H_2O_2$
R9 $\quad 2CO + O_2 \rightarrow 2CO_2$

The F represents a fuel, n-dodecane in the original model. Reactions 1, 2 and 3 are low temperature oxidation reactions and reactions from 4 to 9 are high temperature oxidation reactions. The M is the total concentration of all species, and is obtained from the state equation as $[M] = p/(RT)$.

The reaction rates are expressed as follows (Tsurushima et al. 2007):

$$R_{1f} = k_{1f}[F][O_2] \quad R_5 = k_5[CH_2O][H_2O_2][M]$$

$$R_{1b} = k_{1b}[RO_2] \quad R_6 = k_6[C_2H_4][H_2O_2][M]$$

$$R_2 = k_2[RO_2][O_2] \quad R_7 = k_7[CH_2O][O_2]$$

$$R_3 = k_3[RO_2][O_2] \quad R_8 = k_8[C_2H_4]^{0.1}[O_2]^{1.65}$$

$$R_4 = k_4[F][O_2]^2 \quad R_9 = k_9[CO][H_2O]^{0.5}[O_2]^{0.25}$$

Table 3 Reaction constants of Tsurusima model
(Tsurushima et al., 2008)

Reaction	Ai (mol.cc.Sec)	Modified Ai (mol.cc.Sec)	H^-_{298} (kJ/mol)	n	Ei/R [K]
1f	5.000E+20	0.227E+20	-652	0.0	23000
1b	6.000E+27	0.150E+27	652	0.0	44000
2	6.000E+19	36.00E+19	-2211	0.0	23000
3	6.000E+19	36.00E+19	448	0.0	23000
4	3.000E+18	0.200E+18	-204	0.0	15000
5	6.000E+21	6.000E+21	-291	0.0	22896
6	6.000E+21	0.750E+21	-974	0.0	22896
7	2.200E+15	52.80E+15	-183	0.0	19624
8	1.100E+11	1.100E+11	-467	0.0	15097
9	4.440E+07	4.440E+07	-566	1.0	20129

The reaction rate k in the equation is given by $k = AiT^n exp(-Ei/RT)$, whose constants are given in Table 3. To solve the reaction sets with large time step, we introduced the following relationship for average values:

$$\overline{x_i} = \frac{x_i(t) + x_i(t+\Delta t)}{2} = x_i(t) + \frac{1}{2}\left\{\sum \nu_j R_j(\overline{x_k})\right\}\Delta t \quad (1)$$

The second term in the right hand side is the produced mole of the species in the above reaction rate, which is a function of the average concentration during the time step. This means that the reaction takes place with the rate for the average concentration, and it must satisfy the definition of the average concentration. We assumed that the following four intermediate species are numerically unstable to be solved, and that the other species such as fuel, oxygen, and CO can be solved Eulerian manner i.e. we do not need to use Eq. (1) for these stable species. Then we obtained the following equations from Eq. (1) for the unstable intermediate species:

$$[\overline{RO_2}] = \frac{[RO_2]_t + k_{1f}[F]_t[O_2]_t\Delta t}{1 + \{k_{1b} + k_2[O_2]_t + k_3[O_2]_t\}\Delta t}$$

$$[\overline{H_2O_2}] = \frac{2[H_2O_2]_t + \{R_1([\overline{RO_2}]) + R_3([\overline{RO_2}]) + 2R_4 + R_7([\overline{CH_2O}]) + R_8([\overline{C_2H_4}])\}\Delta t}{2 + \{k_5[\overline{CH_2O}][M] + 4k_6[\overline{C_2H_4}][M]_t\}\Delta t}$$

$$[\overline{C_2H_4}] = \frac{2[C_2H_4]_t + \{5R_3([\overline{RO_2}]) + 5R_5([\overline{CH_2O}],[\overline{H_2O_2}]) - R_8([\overline{C_2H_4}])\}\Delta t}{2 + k_6[\overline{H_2O_2}][M]_t\Delta t}$$

$$[\overline{CH_2O}] = \frac{2[CH_2O]_t + \{9R_2([\overline{RO_2}]) + 4R_3([\overline{RO_2}]) + 4R_4 + R_8([\overline{C_2H_4}])\}\Delta t}{2 + \{k_5[\overline{H_2O_2}][M]_t + k_7[O_2]_t\}\Delta t}$$

As the above equations are nonlinear for the average concentrations, iteration scheme was applied using relaxation coefficient. This scheme allowed large time step to solve the concentration change, which was not possible with ordinary Runge-Kutta method.

In order to take into account the heterogeneity of the species during mixing process (Arato et al., 2006; Song-Charng et al., 2001; Jahirul et al, 2007), R_{mix} is the reaction rate (Golovithev et al., 2000) corrected by a characteristic time scale of mixing, τ_{mix}. We introduced

the following reaction speed modified by mixing time scale, τ_{mix}

$$R_{mix} = \frac{dt}{dt + \tau_{mix}} R_{chem} \quad (2)$$

The dt is the computational time step, and when the time step is large compared with the mixing time scale, the element can be regarded as having a uniform mixture. The mixing time scale was correlated with local air entrainment rate and velocity as detail described by Hiroyasu et al. ((1982) :

$$(\tau_{mix})_{spr} = A_{spr} \frac{\dot{m}_{spr}}{u^{,3}_{spr}}$$

$$(\tau_{mix})_{cyl} = A_{cyl} \frac{\dot{m}_{cyl}}{u^{,3}_{cyl}}$$

$$\frac{1}{\tau_{mix}} = \frac{1}{(\tau_{mix})_{spr}} + \frac{1}{(\tau_{mix})_{cyl}} \quad (3)$$

The turbulent velocities are correlated with the local velocity of the spray package and piston speeds are explained by Hiroyasu et al. (1982).

5. RESULTS AND DISCUSSIONS

Figure 2 shows a result comparing rates of heat release and pressure curves for Tsurushima model, Schreiber model, and experiment. Engine specification used for the experiment is shown in Table 4. The engine is operated at 1350 rpm, 50 Mpa injection pressure, injection timing -21 deg. CA, (Hiroyasu and Arai, 1985) injection quantity 20 mm³/st, and EGR rate 55%. It shows that without adjustment of reaction rates both of the reaction models do not simulate the experimental result well. The both of the models show higher heat release rates and the low temperature reaction is smaller than the experiment. Tsurushima model gives good ignition point but the high temperature combustion starts too early compared to the experiment.

In similar manner to the previous paper (Hiroyasu et al., 1982) for Schreiber model, we tried to adjust the reaction coefficient of

Table 4 Engine specification of the tested engine (Kikuta and Tabay, 2008)

Engine Type	4 stroke, single cylinder
Bore×Stroke	103 mm×99 mm
Compression ratio	16.5
Combustion Chamber	ϕ60 mm Reentrant
Swirl ratio	2.1
Nozzle type	Mini-sac, 7 holes

Tsurushima model to fit the experimental result. The modified Ai values are shown in Table 3, and the result is shown in Figure 3 for different injection timings; -27, -21, and -15deg. ATDC.

It is seen that reasonably good simulation is possible by the modified reaction coefficients.
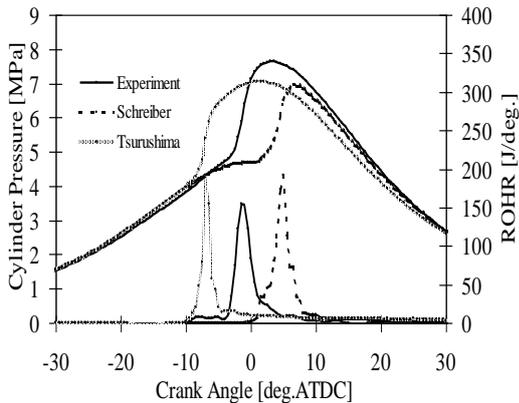

Figure 2 Comparison of Schreiber, Tusurishima and experimental result: 1350 rpm and injection timing at −21.CA

Considering that the reaction coefficients for the both models were established by the homogeneous charge reaction experiments, it may not be an appropriate way to adjust the reaction constants, although it gave a good simulation results for several conditions as shown above. It suggests that the difference between the simulation results with original coefficients and the experimental results may be due to the local heterogeneity of the mixture. To accomplish the simulation it should use very fine packages of the spray, but it is unrealistic for this kind of model (Narayanaswamy and Rutland, 2004). Thus this effect was taken into account in the next by introducing mixing time scale as explained in the previous section.

Figure 3 is the result with adjustment of coefficient relating to τ_{mix} values; $A_{spr}=11.6E3$ and $A_{cyl}=1.5E3$ in Eq. (3) based on theory of free jet as shown in reference (Rajaratnam and Turbulent, 1976). For Tsurushima model and $A_{spr}=1.7E6$ and $A_{cyl}=6.0E4$ (Murakami, 1990) used for Schreiber model. In this case the reaction coefficients are set original values before modification shown above.

The experimental result for 1350 rpm is shown in Figure 3. The figure indicates that good simulation results are obtained in case of Tsurushima for 1350 rpm .The coefficient may be different depending on the conditions, but it may be unique for an engine because it is correlated to the local mixing strength based on the air entrainment and turbulence consideration (Leppard, 1990). Figure 4 shows rate of heat release for Tsurushima model (Tsurushimna et al., 2007) and it also gives good simulation accuracy when it is compared with the experiment result.
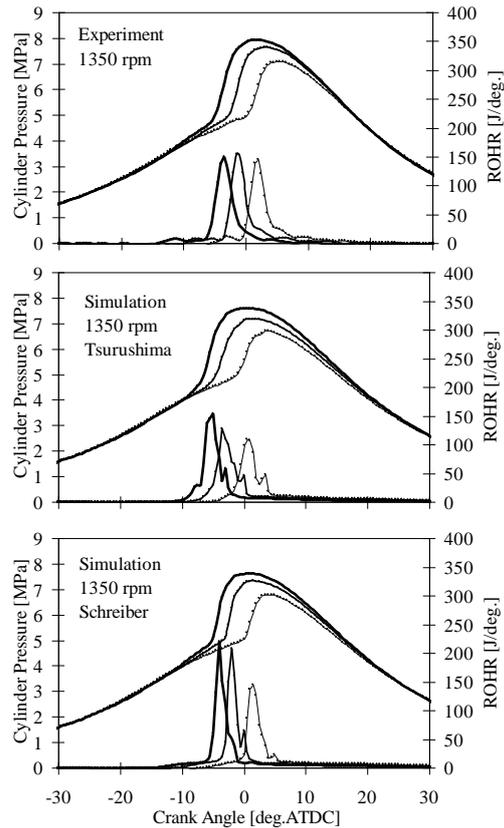

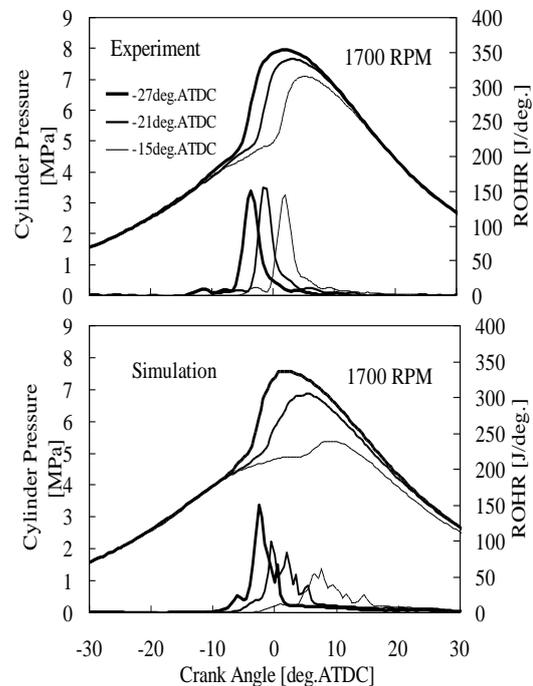Figure 3 Comparison of Schreiber, Tusurishima and experimental result: 1350 rpm and injection timing at −15°CA, -18°CA and −21°CA.

Figure 4 R.O.H.R for Tusurishima model and compare with experimental result at 1700 rpm injection timing at −15°CA, -18°CA and −21°CA.
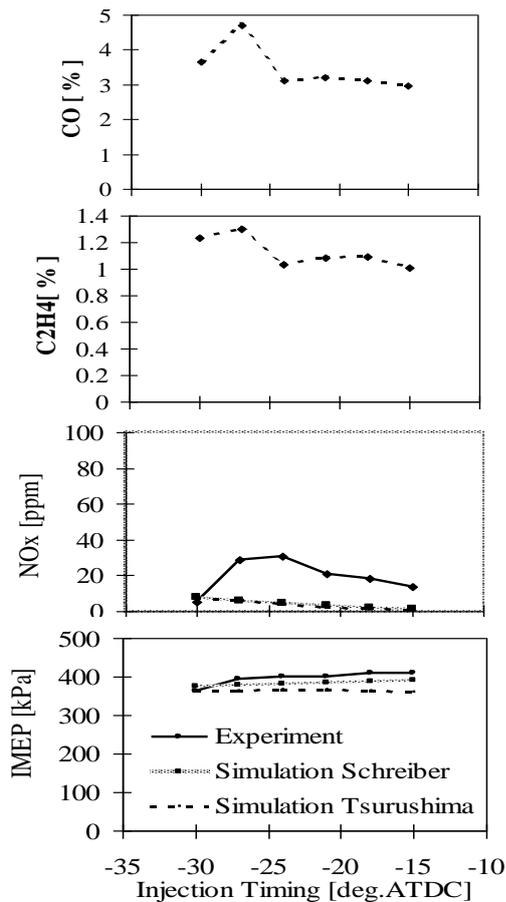
Figure 5 IMEP, emissions for the Schreiber and
Tsurushima model and experiment.

In this type of simulation model, it may have empirical constants, which are determined by simple experiment at a specific condition, as far as the constants are available for different operating conditions. The availability of the above discussion should be confirmed in the next experiment.

Figure 5 shows an example of this simulation model for IMEP, NO_x , CO and C_2H_4 with various injection timings at 1350 rpm. It compares the simulation results Schreiber, Tsurushima with experiment. For NOx both models show almost similar result, but Tsurushima gives percentage change of CO and C_2H_4. As the experimental result was not available for the emissions, this should be investigated in the future research.

6. CONCLUSION

The phenomenological model devised by Hiroyasu et al. (1982) is further developed by including Tsurushima reaction model to simulating ethylene and CO in the exhaust, which may be important for after treatment simulation. It is confirmed that good simulation appears to be possible by applying Tsurushima reduced chemical kinetics scheme instead of Schreiber model, and combustion prediction is more stable than previous. But the proposed scheme allows large computational time

step, resulting in about 10 seconds with a personal computer with a Pentium 4 and 2.8 GHz.

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