Piston Crevice Hydrocarbon Oxidation During Expansion Process in an SI Engine

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Combustion chamber crevices in SI engines are identified as the largest contributors to the engine-out hydrocarbon emissions. The largest crevice is the piston ring-pack crevice. A numerical simulation method was developed, which would allow to predict and understand the oxidation process of piston crevice hydrocarbons. A computational mesh with a moving grid to represent the piston motion was built and a 4-step oxidation model involving seven species was used. The sixteen coefficients in the rate expressions of 4-step oxidation model are optimized based on the results from a study on the detailed chemical kinetic mechanism of oxidation in the engine combustion chamber. Propane was used as the fuel in order to eliminate oil layer absorption and the liquid fuel effect. Initial conditions of the burned gas temperature and in-cylinder pressure were obtained from the 2-zone cycle simulation model. And the simulation was carried out from the end of combustion to the exhaust valve opening for various engine speeds, loads, equivalence ratios and crevice volumes. The total hydrocarbon (THC) oxidation in the crevice during the expansion stroke was 54.9% at 1500 rpm and 0.4 bar (warmed-up condition). The oxidation rate increased at high loads, high swirl ratios, and near stoichiometric conditions. As the crevice volume increased, the amount of unburned HC left at EVO (Exhaust Valve Opening) increased slightly.

Key Words : Unburned Hydrocarbon, Piston Crevice, Oxidation Model, SI Engine

1. Introduction

During the SI engine start and warm-up, a substantial amount of exhaust HC (hydrocarbon) is emitted because of the low conversion efficiency of the catalytic converter, poor mixture preparation, and cold combustion chamber surface. Also, the fuel enrichment which is necessary to achieve good driveability contributes to high-level of unburned HC emissions (Son S. G. et al., 2000).

The major sources of unburned HC emissions and their contributions to HC emissions in a

warmed-up engine are as follows (Cheng et al., 1993): crevices, about 40%; oil layers and deposits, about 20% each; flame quenching and in-cylinder liquid fuel effects, about 10% each; and the exhaust valve leakage, less than 5%. All of the above mechanisms result in high HC concentrations near the combustion chamber wall. When normal combustion process ends, the unburned HCs mix with hot burned gases and become oxidized quickly during the expansion process or within the exhaust port. The in-cylinder oxidation of the crevice HC during the expansion process was studied, because it was one of major HCs sources.

Crevices are narrow regions of the combustion chamber, into which the flame cannot penetrate. The largest crevice is the piston ring pack crevice. During compression and the first stage of the combustion process when the cylinder pressure is

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increasing, the cylinder gas flows into the crevices. For a warmed-up engine, 4 to 6 percent of the total cylinder charge is trapped in the crevices at the peak cylinder pressure (Min. K., 1994). The fuel trapped in the crevice escapes the primary combustion process. As the cylinder pressure decreases during the expansion process and the piston descends, most of the crevice gas flows back into the combustion chamber. If this crevice gas that has entered the combustion chamber is not oxidized completely and escapes the cylinder during the exhaust process, it will contribute to the engine-out HC emissions.
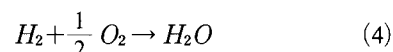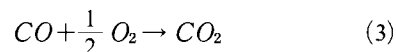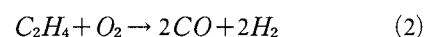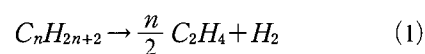
At present, there is not much knowledge of HC emissions mechanisms during starting and warm-up. This work aims to quantify and explain the contribution of crevice mechanisms on HC emissions in terms of the crevice outflow and the oxidation process during the expansion stroke with numerical simulation. Because experimental examinations are difficult to quantify the process and other phases (blow down, exhaust stroke) was not exaimined in that they contribute less to the HC oxidation than the high-temperature and high-pressure expansion phase does, and major concerns in this work are about HC oxidation during the expansion stroke.

Since an analysis that incorporates a detailed chemical reaction model is complex, a 4-step oxidation model of Hautman et al. (Hautman et al., 1981) was used. The coefficients of the 4-step oxidation model were optimized based on the results from the study of detailed mechanisms (Dagaut et al., 1987), because the development conditions of the 4-step oxidation model are different from those of the engine cylinder (high temperature and high pressure). Only the piston top-land crevice was considered because it is the largest and the most important crevice volume in SI engines. Propane was used as the fuel because its oxidation process is better known than those of other fuels and is free from oil layer absorption and liquid fuel effects.

2. Modeling of the Piston Crevice Gas Oxidation and Flow

2.1 Unburned HC oxidation model

A simulation with detailed chemical kinetic mechanisms costs exhaustive computing time and efforts. Thus, in this work, a 4-step HC oxidation model involving seven species was used (Hautman et al., 1981). The proposed overall mechanism follows the form:

$$C_nH_{2n+2} \rightarrow \frac{n}{2} C_2H_4 + H_2 \qquad (1)$$

$$C_2H_4 + O_2 \rightarrow 2CO + 2H_2 \qquad (2)$$

$$CO + \frac{1}{2} O_2 \rightarrow CO_2 \qquad (3)$$

$$H_2 + \frac{1}{2} O_2 \rightarrow H_2O \qquad (4)$$

The corresponding rate expressions are

$$\frac{d[C_nH_{2n+2}]}{dt} = -10^{x_1} \exp\left(-\frac{E_1}{RT}\right)[C_nH_{2n+2}]^{a_1}[O_2]^{b_1}[C_2H_4]^{c_1} \qquad (5)$$

$$\frac{d[C_2H_4]}{dt} = -10^{x_2} \exp\left(-\frac{E_2}{RT}\right)[C_2H_4]^{a_2}[O_2]^{b_2}[C_nH_{2n+2}]^{c_2} \qquad (6)$$

$$\frac{d[CO]}{dt} = \left\{-10^{x_3} \exp\left(-\frac{E_3}{RT}\right)[CO]^{a_3}[O_2]^{b_3}[H_2O]^{c_3}\right\} \times S \qquad (7)$$

$$\frac{d[H_2]}{dt} = -10^{x_4} \exp\left(-\frac{E_4}{RT}\right)[H_2]^{a_4}[O_2]^{b_4}[C_2H_4]^{c_4} \qquad (8)$$
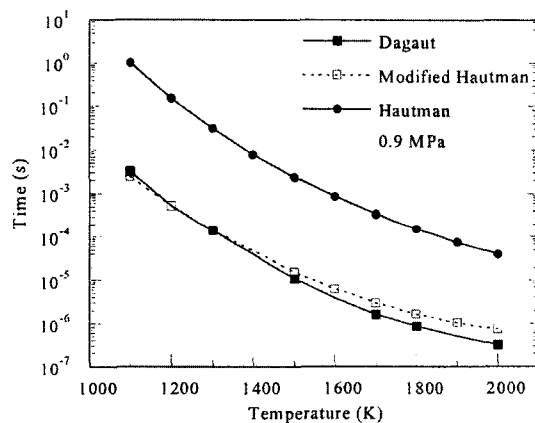
$$S = \min(7.93 \exp(-2.48\Phi), 1) \qquad (9)$$

The original HC oxidation model was designed for 960 K to 1146 K and for initial fuel equivalence ratio of 0.12~2.0 and atmospheric pressure (Hautman et al., 1981). But, the HC concentrations and cylinder gas temperature of SI engines are different from Hautman's experimental conditions. In general, the fuel mass fraction and the burned gas temperature are in the range of 0~0.05 and 1,000~2,500 K, respectively. Moreover, the pressure in the combustion chamber is much higher than atmospheric pressure. Hence, the coefficients of Hautman et al.'s oxidation model were modified based on the results obtained from a study using the detailed chemical model of Dagaut et al. (1987) and adjusted for typical in-cylinder conditions in SI engines.
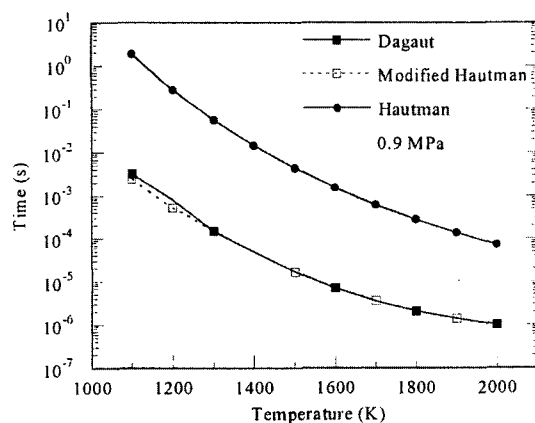
The 16 coefficients in the rate expressions except for the four activation energy terms were adjusted, so that the differences in oxidation rates of the two-oxidation models became minimal (Kim, 2000). And The 50% fuel oxidation time and 50% and 90% total hydrocarbon oxidation times were calculated to compare the mechanisms at constant pressure and homogeneous and adiabatic conditions using the Chemkin library (Kee et al., 1989). Propane (C_3H_8) was selected as a fuel in this study. Only one non-fuel HC species, ethylene, was in the 4-step oxidation mode, and thus, the ethylene represented the intermediate HCs in the detailed model. The direction-set method was used to find the optimized coefficients. Subsequently, libraries of coefficients sets

(a) THC 50% burning time

(b) THC 90% burning time

Fig. 1 THC burning times at 9 bar for the detailed, 4-step model with original and modified coefficients

are obtained for pressures between 3~13 bars and temperatures from 1100 to 2000 K (William et al., 1992).

Figure 1 shows the graphs of 50% and 90% burning times of THC vs. temperature at 9 bar from several HC oxidation models-Dagaut's mechanism, the original 4-step oxidation model of Hautman et al., and the modified 4-step model. The original Hautman et al.'s model predicts the THC oxidation time to be one hundred times longer than that predicted by Dagaut's detailed mechanism. Thus, the original coefficients of the Hautman's 4-step model are not appropriate to model the in-cylinder condition. In Figure 1, the prediction of the modified 4-step oxidation model agrees well with the results of the detailed mechanism.
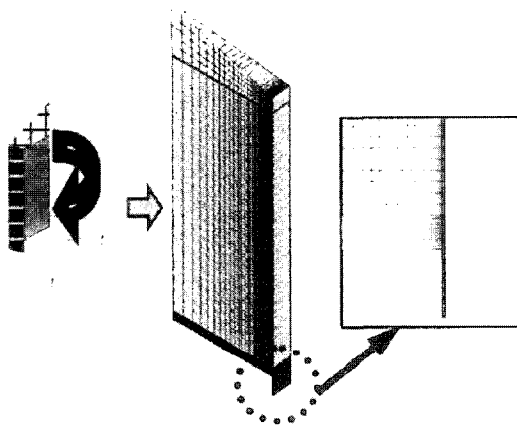
2.2 Mesh configuration

The computational mesh with moving grids was constructed to represent the piston motion in the combustion chamber for a commercial four-cylinder SI engine, as specified in Table 1. The cylinder was axisymmetric so that the mesh was constructed as 2-dimensional cross section as shown in Figure 2. Each section was defined as a cyclic boundary. To observe the behavior of HCs near the piston, the piston crevice region mesh was refined and the mesh size was gradually increased toward the center of the cylinder. The crevice dimensions were 6×0.35 mm, and its volume was 1.09% of the cylinder clearance volume. To maintain good mesh quality during the

Table 1 Specifications of computational engine

Engine type			Inline 4 cylinder
Bore			82 mm
Stroke			84 mm
Connecting rod length			141 mm
Compression ratio			10.0
Displacement volume			1795 cc
Valve timing	Intake	Open	BTDC 6°
		Close	ABDC 46°
	Exhaust	Open	BBDC 50°
		Close	ATDC 10°

Table 2 Computational base engine condition

Engine speed	1,500 rpm	
Fuel/air equivalence ratio	1.0	
Intake pressure	0.4 bar	
Exhaust pressure	1.0 bar	
		Warm up	Cold start
Temperature	Cylinder liner	373 K	293 K
	Piston surface	450 K	300 K

Fig. 2 Computational mesh configuration at BTDC

calculation, cell layers in the cylinder were added as the piston descended. The chamber shaped grid was constructed by a maximum of 4375 cells at EVO and a minimum 1200 of cells at TDC.

2.3 Simulation

A multipurpose thermofluid analysis package STAR-CD was used, and the HC oxidation model was added as a subroutine. The standard k-ε model was used with the algebraic 'law of the wall' to simulate flow, heat and mass transfer within boundary layers. Thermodynamic and transport properties such as the viscosity, thermal conductivity, specific heat, diffusion coefficients, and Schmidt numbers were obtained from the Chemkin thermodynamic database and the transport property database. The wall heat transfer coefficient proposed by Launder and Spalding was used to simulate the heat transfer to the wall (Launder et al., 1972). Initial burned gas temperature and in-cylinder pressure were obtained from a 2-zone cycle simulation (Poulos, 1982).

The calculation was carried out at the engine speed of 1,500 rpm and 0.4 bar intake pressure (base condition) from the end of combustion to the exhaust valve opening. The results are compared to those obtained at other operating conditions. Table 2 shows the base simulation condition.

3. Results and Discussion

3.1 Oxidation at base engine operating condition

At the base engine operating condition, crevice gas oxidation was calculated from the end of combustion to the exhaust valve open. The calculation results for the base engine condition in which the engine is warmed up are presented in Figures 3 and 4. The velocities of the piston and the crevice gas are shown in Figure 3. The velocity of the downward-moving piston is faster than the crevice outflow gas velocity thus, the piston crevice gas stretches into a thin laminar layer (of a thickness thinner than the piston-liner crevice) along the liner. The fuel, which is laid along the liner, diffuses into the hot burned gas, and the heat from the combustion gas diffuses into the piston crevice gas. The unburned hydrocarbons that mix with the hot burned gas start to get oxidized and increase the temperature of the thermal boundary layer; the increasing temperature accelerates the oxidation of the unburned hydrocarbons. The unburned fuel exists within 0.5 mm from the wall (Figure 4). Figure 4 shows a high concentration of C_3H_8 near the liner, and intermediate substances such as C_2H_4, CO and H_2 surrounding the C_3H_8's high concentration region.

As the temperature and pressure of the burned gas drop during the expansion stroke, however, the oxidation rate of crevice HC decreases and the unburned HCs from the piston crevice regions remain along the wall. Some of the unburned HCs next to the cylinder liner diffuse out into the cylinder hot bulk gas and are then oxidized (Min. K., 1994).

The mass fraction profiles of the fuel (C_3H_8) and ethylene (C_2H_4) during the expansion pro-
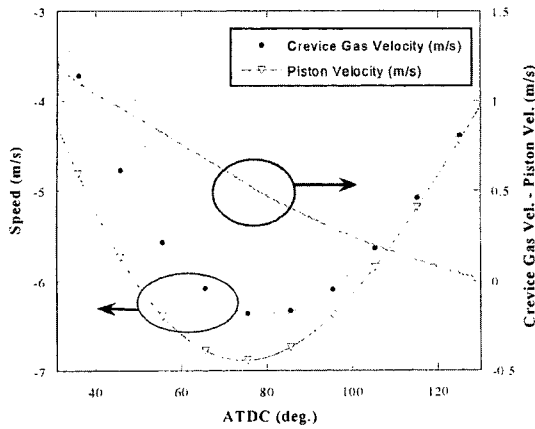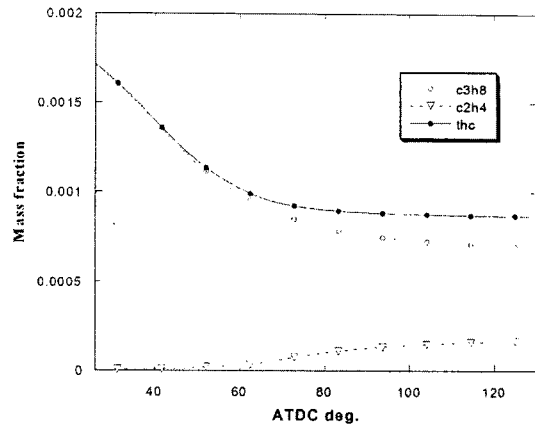
Fig. 3 Crevice gas velocity vs. piston velocity

Fig. 5 Mass fraction of C_3H_8, C_2H_4 and THC 1500 rpm, 0.4 bar

Thus, at constant load and MBT timing, the HC oxidation rate decreased at low wall temperature conditions. At cold start under the base engine condition, 51.9% of the fuel and 38.9% of the THC oxidized but under the warmed-up condition, 67.1% of fuel and 54.9% of THC oxidized.

3.2 Effect of engine operating conditions on oxidation rate

To investigate the effect of engine load on crevice HC oxidation rate, two engine load conditions (0.4 bar, 0.8 bar) were considered. An engine at high volumetric efficiency condition (high load : 0.8 bar) emits large amounts of unburned HC when the exhaust valve opens but HC oxidation rate is also enhanced in such a high temperature and high pressure condition. And the high pressure increased the amount of HC in the crevice. The more HCs outflow from the crevices, the more heat is released ; as a result, the temperature of the oxidation region increases and this increases the oxidation rate. The oxidation rate at 1500 rpm and high load condition (0.8 bar) is 44.7% higher than that at 1500 rpm and the base condition (0.4 bar).

The effect of engine speed at 1500 rpm and 2500 rpm on oxidation rate is examined. The effect of speed on the peak cylinder pressure is minimal but the effect on burned gas temperature is significant, primarily because of the reduced time per cycle available for heat transfer (at 0.4 bar intake
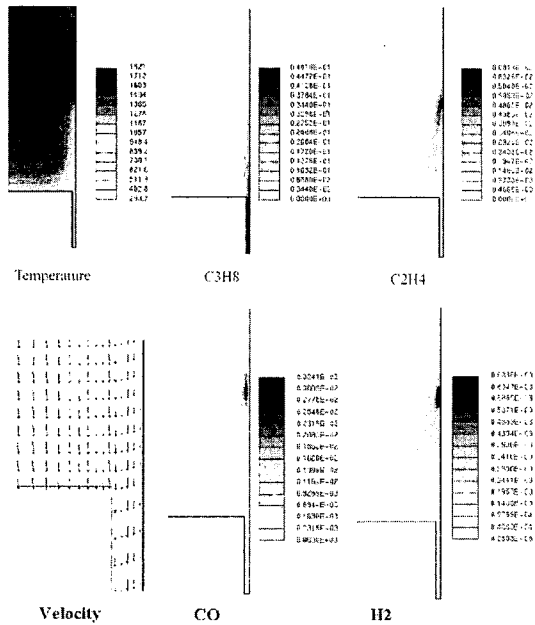

Fig. 4 Temperature, concentration, velocity profiles at 100 deg. ATDC, 1500 rpm, 0.4 bar

cess are shown in Figure 5. The crevice HC was oxidized rapidly in the first stage of the expansion process, but as the piston descends, the oxidation rate decreased because the gas temperature rapidly decreased. The simulation results showed that ethylene, which represents the non-fuel HC components, only contributed to 24% of the unburned THC at the exhaust valve opening.

During cold start and warm-up the cold cylinder wall prevents the oxidation of crevice HCs.

Table 3 Crevice HC oxidation rate vs. Engine Speed

Condition	Fuel	THC
1500 rpm	67.1%	54.9%
2500 rpm	66.9%	53.3%

Table 4 Crevice HC oxidation rate vs. Swirl Ratio

Swirl Ratio	Fuel	THC
1.0	67.1%	54.9%
3.0	74.6%	64.6%

Table 5 Crevice HC oxidation rate vs. Equivalence ratio

Equivalence ratio	Fuel	THC
0.9	45.7%	30.4%
1.0	67.1%	54.9%
1.1	64.8%	53.8%

pressure, the burned gas temperature is 2275 K at 1500 rpm, and 2340 K at 2500 rpm). Therefore, the increased temperature promotes the oxidation of HC. However, despite the increased temperature of the burned gas, the reduced in-cylinder residence time of HC lowers the oxidation rate during the expansion stroke. As shown in Table 3 at 1500 rpm, the crevice fuel and THC oxidation rates are 67.1% and 54.9%, respectively, and at 2500 rpm, they are 66.9% and 53.3%.
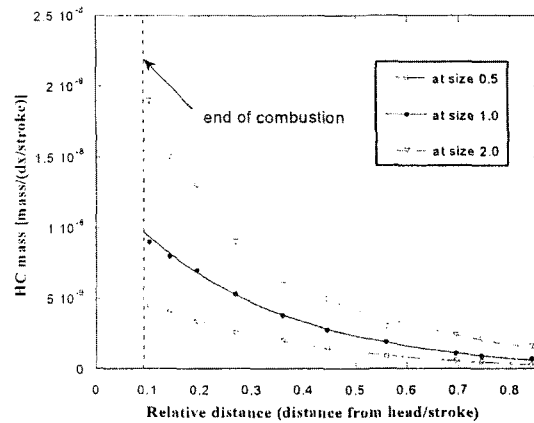
The simulations were performed at two swirl conditions ; swirl ratios of 1.0 and 3.0. The swirl motion is modeled by the Bessel function to consider the velocity decaying effect due to the wall (Wahiduzzaman, 1986). As shown in Table 4, a higher swirl ratio shows a higher oxidation rate which results from the enhanced mixing of the crevice outflow gas and high-temperature burned gas. At the swirl ratio of 1.0 and the base condition, 67.1% of the fuel is oxidized and 54.9% of THC and at the swirl ratio of 3.0, the 74.6% of the fuel is oxidized and 64.6% of THC.

Changes in fuel/air equivalence ratio at constant load and MBT spark timing (1500 rpm, 0.4 bar) have little effect on the peak cylinder pressure but greatly affect the in-cylinder temperature. Thus, the oxidation rate of the crevice HC is the highest at the stoichiometric condition, because at the end of combustion, the temperature of the burned gas at the 1.0 fuel/air equivalence ratio condition is higher than that at non-stoichiometric condition. Table 5 represents the effect of the equivalence ratio on the crevice HC oxidation rate.
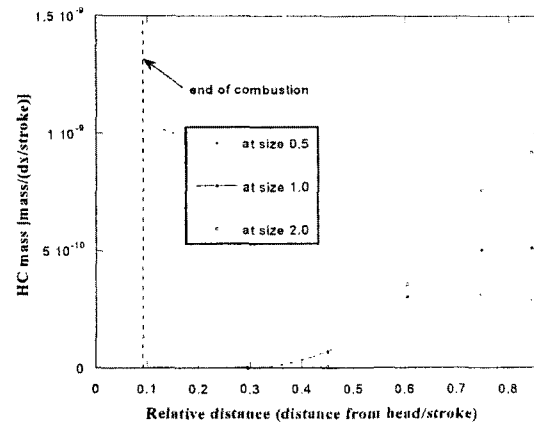
The sensitivity of the crevice HC oxidation rate

(a) Out from the crevice

(b) Remaining along the liner

Fig. 6 Unburned HC flow out from the crevice and remaining along the liner at EVO, 1500 rpm, intake pressure 0.4 bar

to crevice size was evaluated by doubling the crevice volume and reducing the crevice volume in half at the base condition. The results are shown in Figures 6 and 7. The amount of unburned hydrocarbons surviving oxidation in the cylinder increases as the piston crevice volume increased, because the crevice gas layer was very thin as it came out from the piston crevice, and
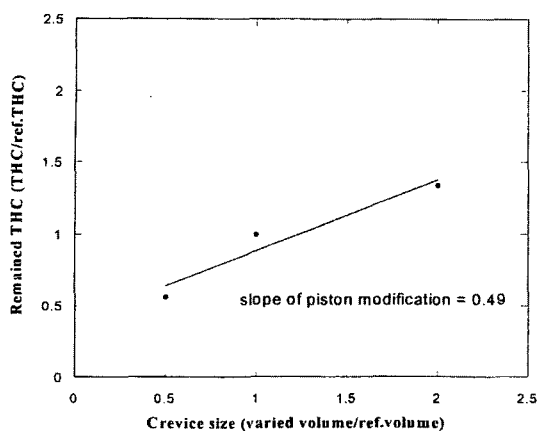
Fig. 7 Sensitivity of the amount of unburned hydro-
carbons left at EVO to piston crevice volume
size

the temperature of this crevice gas increased
slowly due to large heat transfer to the wall.
However, as more unburned HC came out of the
piston crevice, the temperature near the crevice
rose because HC oxidation released more heat.
Thus, the oxidation rate of unburned HC from
the crevice rose because of the volume increase
while the modest increase in the amount of
unburned HC remained in the cylinder. Figure 7
shows the sensitivity of the unburned HC left
at EVO to piston crevice volume. The slope is
0.49.

4. Conclusions

A 4-step oxidation model was used to simulate
the crevice HC oxidation process from the time
when main combustion ended to the time when
exhaust valves opened. The coefficients of the
4-step HC oxidation model's rate expressions to
describe the engine conditions were modified
based on the results of analysis using the detailed
chemical kinetics model.

The HC which escaped from the crevice during
the early part of the expansion process, almost
completely and rapidly oxidized as long as the gas
temperature in the cylinder remained high. At
1500 rpm and at cold start condition, 38.9% of
HC from the crevice was oxidized during expan-
sion stroke, and 54.9% of the HC was oxidized

at the warmed-up condition. Engine operating
conditions greatly affected the crevice HC oxi-
dation rate. The oxidation rate at the high load
condition (0.8 bar) increased from that at the low
load condition (0.4 bar) by 44.7%, and the crev-
ice HC oxidation rate was the highest at the 1.0
fuel/air equivalence ratio. More swirl motion in
the combustion chamber promoted the oxidation
rate. As the crevice volume increased, the amount
of unburned HC left at EVO increased slightly.

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