In-Cylinder Oxidation of Piston-Crevice Hydrocarbon in SI Engines

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ABSTRACT

Engine-out HC emissions were measured in SI engine experiments in which the piston top-land crevice size was changed systematically. For a warmed-up engine, the HC emissions were found to be modestly sensitive to the crevice size — a 10% change in size results in approximately a 2% change in HC emissions. This low sensitivity is explained in terms of a crevice HC diffusion/oxidation model in the expansion process.

INTRODUCTION

The pathway by which fuel escapes the in-cylinder combustion and oxidation processes is an essential element of the hydrocarbon (HC) emissions mechanism in spark ignition engines. A recent study [1] suggests that 8.4 percent of the fuel inducted into the cylinder escapes primary combustion even though the vehicle-out HC emissions are 0.4 percent. This "escaped" fuel contributes to significant loss of fuel economy as well as to high exhaust HC emissions. The major sources of unburned HC emissions and their contribution to engine-out HC emissions at part load in a warmed-up engine are as follows [1]: crevices, about 40 percent; oil layers and deposits, about 20 percent each; flame quenching and in-cylinder liquid fuel effects, about 10 percent each; and exhaust valve leakage, less than 5 percent. Because of its major role as a HC source, the crevice mechanism, in particular, the in-cylinder oxidation of the crevice HC, is the subject of this paper.

Crevices are "narrow" regions of the combustion chamber into which the flame can not penetrate. The largest crevice volume is the piston ring pack crevice volume. In compression and in the first part of the combustion process during which the cylinder pressure rises, cylinder gas flows into the crevice volumes. The fraction of the total cylinder charge trapped in the crevices is about 4 to 6 percent at the time of peak cylinder pressure; the fuel in this trapped charge escapes the primary combustion process [2]. (When the engine is cold, the crevice dimensions are larger and the crevice gas is denser. Therefore the trapped amount is larger in a cold engine.) As the cylinder pressure decreases in the expansion process, a major part of the crevice gas flows back into the cylinder. When this crevice gas is not oxidized completely and escapes the cylinder in the exhaust process, it contributes to the engine-out HC emissions.

This paper will focus on the role of the piston top-land crevice on HC emissions because it is the largest and most important crevice volume in a spark ignition engine [3-5]. The objective is to quantify and explain the crevice mechanism contribution. There are two parts to this paper: the experimental part reports on the changes in engine-out HC emissions when the piston top-land crevice is modified systematically[1]; then a model for in-cylinder piston crevice gas transport and oxidation in the expansion process is discussed to explain the observed dependence of the HC emissions on the top-land crevice volume.

EXPERIMENT

The details of the experiment have been presented elsewhere [6], and they are described briefly in the following for completeness. The engine used in the experiments was a Ricardo Hydra Mark III single cylinder research engine. Specifications for this engine are summarized in Table 1. All the data to be presented in this paper were obtained with propane fuel. Only the data for the fully warmed-up engine at steady-state conditions are presented here. (Results during the warm-up process and results obtained with liquid fuel may be found in Ref. [2].) Propane fuel was used to minimize engine oil layer, deposit, and liquid fuel effects on the exhaust hydrocarbon emissions. The experimental conditions were 900 rpm, 1.0 bar inlet pressure; 1600 rpm, 0.4, 0.7, and 1.0 bar inlet pressure; 2500 rpm, 1.0 bar inlet pressure; and air-fuel equivalence ratio (λ): 1.05 to 1.1. A slightly lean value of λ was used because then the HC emissions are not sensitive to the exact values of λ. All experiments were done with MBT timing.

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[1] Much of the experimental results were reported in a previous paper [6]. The results presented here are for comparisons to the oxidation model.

Table 1 Ricardo Hydra MK III engine specification.

Type:	Single cylinder, iron block and liner (wet), alloy head, two valve, separate overhead cams
Chamber:	Hemispherical, central ignition
Compression ratio:	8.3
Bore x stroke:	85.67 mm x 86.00 mm
Clearance volume:	68 cm^3
Displacement:	496 cm^3
Valve timings:	IVO: 4° BTC IVC: 49° ABC EVO: 54° BBC EVC: 16° ATC

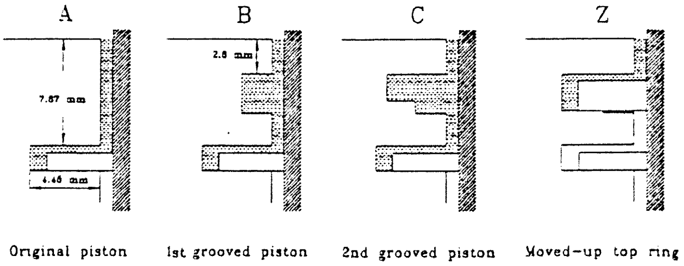
The instantaneous HC emissions at ~15cm downstream from the exhaust valve (measured by a Fast-Response Flame Ionization Detector) and the cylinder pressure were recorded at every other crank angle degree for a large number of consecutive cycles. From these measurements, the cycle-averaged HC emissions were obtained. (In principle, it would suffice to use a steady-state HC analyzer for the steady-state results; the cycle-resolved data were used because the data presented here are part of a large set which includes engine warm-up behavior.)

Piston Modification

To investigate the sensitivity of the exhaust hydrocarbon emissions to the piston crevice size, the piston of the Ricardo engine was modified in several steps, shown schematically in Fig. 1. Emissions data were obtained from each configuration. From the original piston (Configuration A, with a top-land plus first ring region volume of 0.939 cm^3), the piston top-land was first grooved to increase the piston crevice volume by 43 percent (Configuration B). In order to prevent flame propagation into the piston top-land crevice, the piston was grooved 2.8mm below the top so that the crevice entrance geometry was preserved. The second step was to groove the piston top-land further to increase the top-land crevice volume by 0.4 cm^3 (Configuration C). The last step of the piston modifications was to move the first ring up (Configuration Z) to decrease the piston crevice volume by 31 percent of its original value.

Data Analysis

Since the crevices are characterized as a "source" of hydrocarbon, it is appropriate to specify its "strength". The "strength" is defined as the maximum amount of unburned mixture that is trapped in the crevices and this amount was calculated as follows. The total crevice volume consists of the piston top-land, the first ring region, the spark plug, and the other threads in the cylinder head. For the Hydra engine the head gasket and valve seat crevices are negligible. (The second-land and the ring region volume were not included in the above because the pressure there is significantly lower than the top-land region; therefore the trapped mass in these regions is comparatively much smaller.)



Cold top land plus first ring groove crevice volume

A	B	C	Z
V = 0.939 cm^3	V = 1.339 cm^3	V = 1.737 cm^3	V = 0.650 cm^3

Normalized volume change

A	B	C	Z
0 %	+43 %	+85 %	-31 %

Fig. 1 Piston modification procedure.

The gas temperature in the piston top-land and the first ring region was assumed to be the average of the piston and the cylinder wall temperature, and the crevice gas temperature in the threads was assumed to be the same as the cylinder head temperature. We assumed that the crevices were filled with fuel/air mixture and residual gas and that the mixture in the crevices was an ideal gas. To a very good approximation, the pressure in the crevices defined in the above is in pressure equilibrium with the cylinder. Therefore the maximum trapped mass occurs at peak cylinder pressure which was obtained from the experiments. The maximum mass trapped in the crevices is then:

$$m_{cr} = \frac{p_{max} V_{cr}}{R T_{cr}} \tag{1}$$

The crevice volume at steady state was calculated from the values of the cold engine by using a component temperature simulation program [7].

The above procedure is necessary for the proper interpretation of experimental results because the experimental matrix covers a range of load and speed operating conditions. Therefore simply comparing the results according to the cold crevice volume only would not include the effects of the different peak pressures, wall temperatures, and actual crevice volume sizes at the operating conditions. Because the flame geometry was unknown, it was not possible to assess precisely how much of the trapped mass was unburned gas. For comparison purposes, we assumed that all the trapped mass is unburned gas. Then, using the total in-cylinder mass, air/fuel ratio, and residual fraction which was estimated using the correlation of Ref. [8], the maximum trapped fuel was normalized by the fuel delivered per cycle to obtain a maximum trapped HC index. We will compare this maximum trapped fuel index with the measured unburned hydrocarbon emissions at the exhaust port to estimate how much of the unburned fuel in the crevices survives the in-cylinder oxidation and escapes the cylinder.

EXPERIMENTAL RESULTS AND DISCUSSION

Typical engine-out HC emissions as a function of crevice volume are shown in Fig. 2. Two sets of data are shown, for 900 rpm WOT and 1600 rpm 0.4 bar intake pressure conditions. For a substantial variation in piston crevice volume from configuration Z to C, by which the total crevice volume increased from 0.7 to 1.65 cm^3 (a factor of 2.4), the engine-out HC emissions increased modestly and approximately linearly, by ~15 to 18% for the two operating conditions.

The above trends, that the engine-out HC emissions were modestly sensitive to the piston crevice volume, were generally observed for all the test conditions. The results are summarized in a normalized way in Fig. 3. In this figure, the x axis is the maximum crevice HC value as discussed in the Data Analysis section. The y axis is the engine-out HC emissions value. Both axes are normalized by the corresponding reference values which are defined to be those of Configuration B at the same engine operating conditions. In this manner, the data from all the operating conditions (900 rpm WOT; 1600 rpm, intake pressure 0.4, 0.7, and 1 bar) and all the crevice configurations collapse onto a single line. The slope of the linear fit to the data may be interpreted as the sensitivity derivative of the engine-out HC emissions to the crevice size. This value is 0.2, meaning that a 10% change in piston top-land crevice size would lead to a 2% change in the HC emissions.

That the size of the piston top-land crevice has only modest effect on the steady state HC emissions (sensitivity derivative ~0.2) needs explanation. The exhaust HC may be interpreted with the framework that it is a result of both the source strength of the HC mechanism, and the pathway connecting the source to the exhaust [1], whence:

$$HC_{ex} = \sum_i S_{HC,i}(1 - f_{cyl\_ox,i})(1 - f_{cyl\_ret,i})(1 - f_{exh\_ox,i}) \quad (2)$$

Where $S_{HC,i}$ are the source strength of the crevices, $f_{cyl\_ox,i}$, $f_{cyl\_ret,i}$, and $f_{exh\_ox,i}$ are the fraction of the HC from these crevices that is oxidized in the cylinder, that is retained in the cylinder in the exhaust process, and that is oxidized in the exhaust port. Under the same engine operating condition, it is reasonable to assume that the factors $f_{cyl\_ret,i}$ and $f_{exh\_ox,i}$ are the same, irrespective of the crevice size. Since the source term $S_{HC,i}$ is proportional to the crevice size, the explanation of the insensitivity of the engine-out HC should lie in the in-cylinder oxidation term.

The in-cylinder oxidation of the crevice gas may be divided into three phases: during the expansion process; during the blow-down period when the exhaust valve is open; and during the displacement process in the exhaust stroke. In the following, we shall discuss the transport and oxidation of the crevice gas in the expansion process. We have left the oxidation in the other two phases out of our discussion because of our ignorance rather than for good reasons. Fortunately we have devised a mechanism for explaining the insensitivity of the engine-out HC emissions to the piston crevice size by using only the crevice gas transport and oxidation in the expansion process.

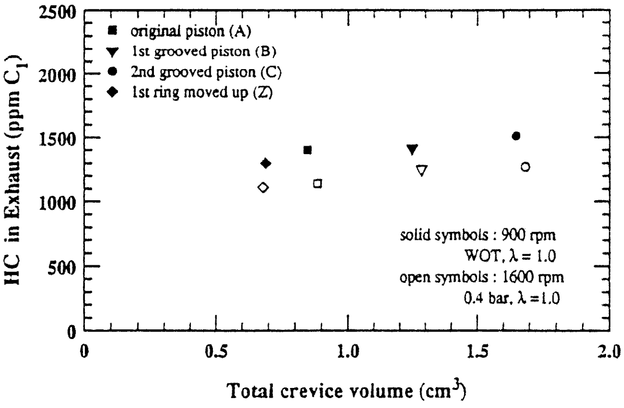


Fig. 2 Effect of piston crevice on steady state exhaust HC emissions at 900 rpm, WOT and 1600 rpm, 0.4 bar.

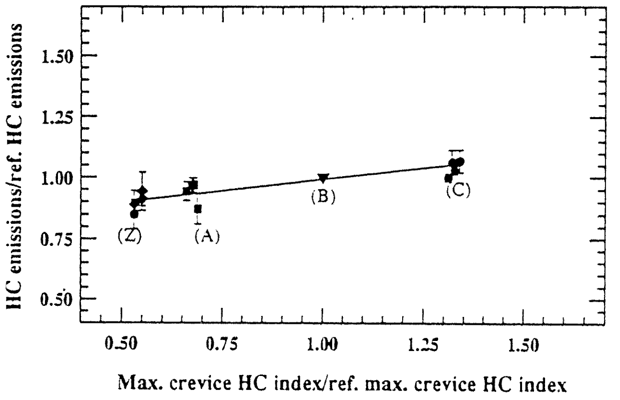


Fig. 3 Effect of piston crevice volume changes on steady state exhaust HC emissions.

MODELING OF PISTON CREVICE GAS TRANSPORT AND OXIDATION

The model of the transport and oxidation of the crevice gas during the expansion process consists of two parts: a lump parameter model of the filling and emptying of the piston crevices [9] was used to calculate the mass outflow from the crevice based on the measured cylinder pressure; then this outflow was distributed along the liner as the piston descends, and a one dimensional diffusive/reactive model was used to calculate the oxidation of the HC content of each mass element along the liner.

Piston Crevice Gas Flow

Using the crevice flow model, the distributions of the out-flow mass as the piston descends are shown in Fig. 4. The x-axis is the position from the top of the liner normalized by the piston stroke (86mm). The piston crevice gas flow scales with the piston crevice size (piston top land+first ring region). Also shown in Fig. 4 is the percent piston crevice gas out flow during the expansion process, irrespective of the crevice size. The majority of the piston crevice gas flows out during the early expansion process. At exhaust-valve-open, more than 86 percent of the total crevice gas trapped in the piston crevice has already been discharged into the combustion chamber. Less than 14 percent of the maximum piston crevice gas comes into the cylinder during the blowdown period.

The nature of the crevice out-flow [6] is that the Reynolds number is below ~100, and the piston is descending faster than the outflow velocity so that the out-flow mass is stretched in a laminar manner along the liner into a layer thinner than the piston-liner clearance which is ~0.1mm. Because of the thinness of the layer, the diffusive transport into the cylinder bulk gas is much more important than the convective transport along the liner. Therefore a useful perspective is that adjacent to the liner there is a stationary layer of crevice gas which diffuses out to the cylinder bulk gas.

Modeling of Transport and Oxidation

The model calculates the transport and oxidation of individual segments of crevice gas which flow out of the piston crevice for each two crank-angle interval. A one dimensional model describing the diffusion and expansion processes of the crevice gas normal to the liner wall is used. The model assumes that:

1) There is no axial transport between segments.
2) Each segment is stationary in the axial direction and may expand in the direction normal to the cylinder liner as the piston descends.
3) The transport process is laminar.
4) Temperature of the cylinder wall is constant during the expansion process.
5) The core gas temperature during expansion is obtained from a thermodynamic cycle simulation.

A one-step kinetic mechanism for the oxidation of propane is employed.

$$\frac{d[C_3H_8]}{dt} = -1.0\text{x}10^{23}\text{x}[C_3H_8]\,[O_2]\,\exp(\frac{-25000}{T}) \tag{3}$$

where [ ] denotes concentration in moles per cubic centimeter, t is in seconds, and T in Kelvins. This oxidation model was obtained from fitting the results detailed of kinetics calculation based on the hydrocarbon oxidation mechanism developed by Dagaut [10].

For the one-dimensional model, the governing equations are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \tag{4a}$$

$$\frac{\partial Y_i}{\partial t} + u\frac{\partial Y_i}{\partial x} = \frac{1}{\rho}\frac{\partial}{\partial x}(D\frac{\partial Y_i}{\partial x}) + \frac{\dot{\omega}_i}{\rho} \quad (i = 1, 2) \tag{4b}$$

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} - \frac{1}{\rho C_p}\frac{dp}{dt} = \frac{1}{\rho C_p}\frac{\partial}{\partial x}(k\frac{\partial T}{\partial x}) - \frac{1}{\rho C_p}\Delta h_r\,\dot{\omega}_1 \tag{4c}$$

where x is the direction in normal to the liner, ρ is the gas density, Y_i, the species mass fractions, D, the binary diffusivity, ω_i, the reaction rate, k, the thermal conductivity, C_p, the specific heat and Δh_r, the heat of reaction of the hydrocarbon oxidation. The indices 1 and 2 refer to fuel and oxygen.

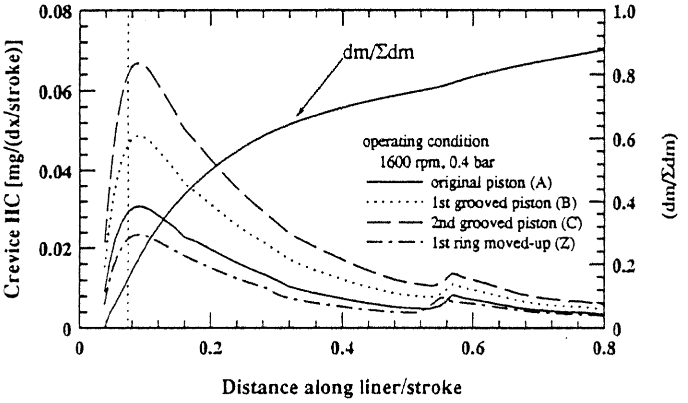


Fig. 4 Piston crevice gas distributions along the liner during the expansion process.

Because the crevice out-flow emerges into the thermal boundary layer of the "bulk" gas, the initial temperature profile (for each crevice gas mass segment at the crank angle when it emerges) needs to be specified. Outside the crevice gas region (the extent of which is obtained from the crevice out-flow mass), the temperature is based on the measurements of Ref. [11]; this is

$$T(x) = T_{core} + \frac{(T_{core} - T_{wall})}{2.6}\log(\frac{x - \delta_o}{\delta_{t0}})$$

$$10^{-2.6} < x - \delta_o < \delta_{to} \tag{5}$$

Where T_{core} is core gas temperature (K), from engine simulation, T_{wall} is wall temperature (K), δ_{to} is the initial thickness of thermal boundary layer (1mm), and x is distance from wall. A typical initial temperature profile is shown in Fig. 5. The value of 1mm for δ_{to} is based on the data from Ref. [12]. As the thermal boundary layer develops in time, the boundary condition at the core gas side is specified as temperature equals to T_{core} (calculated by the cycle simulation) at x equals to δ_t, which, according to Ref. [12]:

$$\delta_t = \delta_{to} + 0.6(\alpha t)^{0.5}\,\text{Re}^{0.2} \tag{6}$$

The above set of equations were solved by the Crank-Nicolson method using a cell size (Δx) of 0.01mm and a time step (Δt) of $1.3\text{x}10^{-6}$ sec.

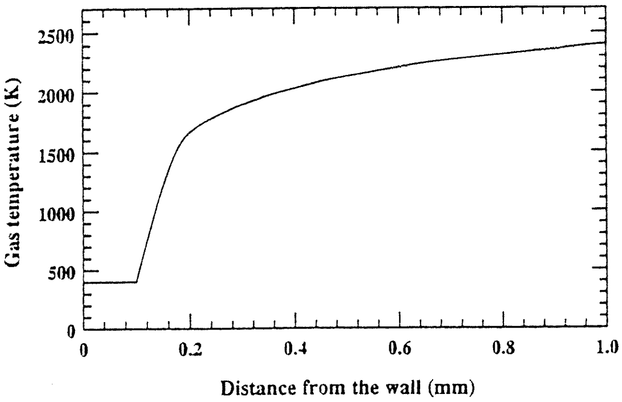


Fig. 5 A typical initial boundary layer temperature profile.

Results from the Model and Discussion

The calculations of piston crevice gas transport and oxidation were conducted until EVO after which the gas motion in the cylinder changes dramatically and the above model no longer applies. Figure 6 shows the crevice gas that survives the in-cylinder oxidation at EVO as a function of the position at which the crevice gas is released from the piston crevice. Compared to Fig. 4, it is seen that although a large portion of the crevice gas comes out early in the expansion cycle (~the first quarter of the cycle), almost all of this is oxidized because of the high bulk gas temperature. Only the crevice gas coming out later (~ beyond the first quarter of the cycle) persists till EVO.

The fraction of crevice gas remaining at EVO (i.e., the ratio of the quantities in Fig. 6 to those in Fig. 4) is shown in Fig. 7. Towards EVO, a high percentage of the crevice gas remains; this is because of the lower bulk gas temperature and of the shorter time available for diffusion and reaction.

An interesting trend is observed in Fig. 7: as the piston crevice size increases, the point at which a significant fraction of the emerged HC survives in-cylinder oxidation moves towards the later part of the expansion cycle. Since the amount of HC that survives is the product of the source (i.e., the quantities in Fig. 4) and the fraction that survives (Fig. 7), a self regulating mechanism is evident and is simply stated as follows. Only the crevice gas that comes out later than a certain point in the expansion cycle survives in-cylinder oxidation. When the crevice size increases, this point of "transition" moves to later in the expansion cycle, thus nullifying the effect of the crevice size increase on HC emissions. With this regulating effect, therefore, the sensitivity derivative of the HC emissions to crevice volume becomes much less than 1.

The explanation for the later "transition" point with a larger crevice volume has to do with the sensitivity of the chemical reaction to temperature, see Eq. (3). As the piston descends, the gas temperature in the boundary layer will drop so that there is a "transition" point after which the oxidation becomes ineffective. This "transition", however, depends on the local gas temperature, which, in turn, depends on the heat release from the oxidation of the HC. With the larger crevice volume, there is a higher concentration of HC so that the heat release is higher, resulting in a later "transition" point.

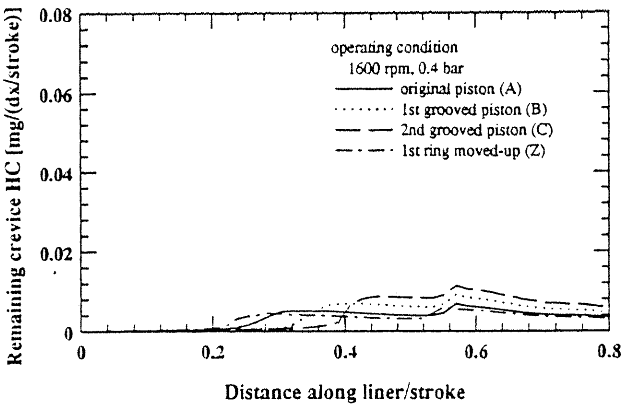


Fig. 6 The remaining unburned hydrocarbons at EVO.

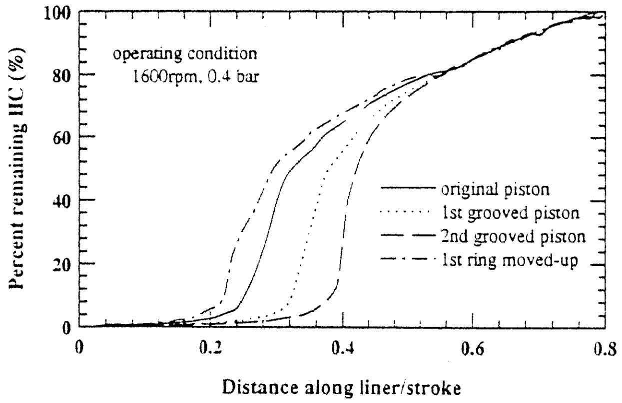


Fig. 7 Percent remaining unburned HC.

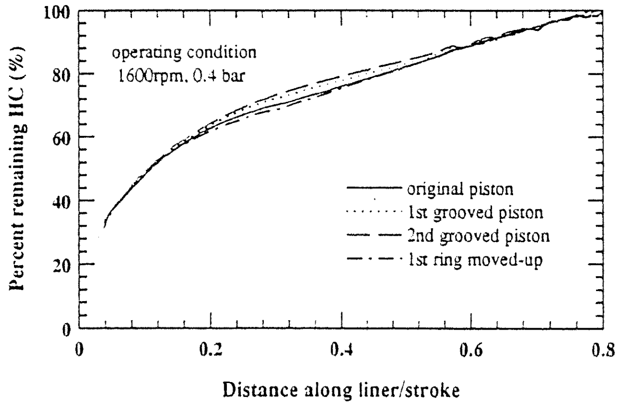


Fig. 8 Percent remaining HC without heat release.

To confirm the above explanation, the crevice gas oxidation model was exercised with the heat release turned off, i.e., Δh_r was set to zero. The fraction of HC remaining at EVO is shown in Fig. 8. In this figure, there is no significant difference between the cases with different crevice volumes. Thus for the hypothetical case with the heat release switched off, the sensitivity of the engine-out HC emissions to crevice volume should be 1.

If we assume that the HC emissions are proportional to the value calculated by the above model at EVO, we could compare the model results to the experimental values. This is shown in Fig. 9., which is drawn in the same normalized manner as in Fig. 3. The slope of the calculated points is much less than one. It is comparable to the experimental value and lends support to our explanation. The difference between the experimental and the model values may be a result of oxidation in the exhaust process.

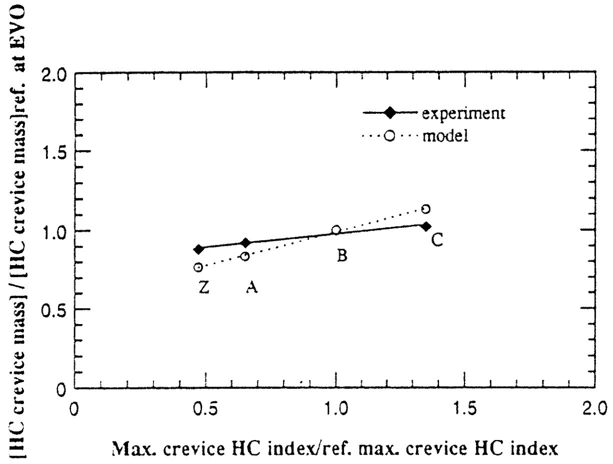


Fig. 9 Comparison of experiments with calculation results.

CONCLUSIONS

The effects of crevice size on HC emissions were measured in a single-cylinder research engine at steady state by systematically changing the piston top-land crevice size. The engine-out HC emissions was found to be modestly sensitive to the top-land crevice size, with a sensitivity derivative of ~0.2. A diffusion and oxidation model was formulated to calculate the evolution of the crevice HC in the expansion process. Results of the model show that the crevice gases that come out during the early part (~first quarter) of the expansion cycle are almost completely oxidized. There is a "transition" point in the cycle after which the oxidation is not effective and much of the emerging HC survives. This "transition" point depends on the local temperature, which, in turn, depends on the heat release from the HC oxidation. With a larger crevice volume, the higher HC concentration leads to a higher heat release and the "transition" occurs later in the expansion cycle. Thus the higher HC from the larger crevice is offset by a later "transition" point to ineffective oxidation, and the HC emissions level is only modestly sensitive to the piston crevice size.

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