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HYDROCARBON FORMATION AND OXIDATION

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IN SPARK-IGNITION ENGINES

Final Report on a Research Program Funded by General Motors Research Laboratories September 1976 to August 1979

Volume I: SUMMARY

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ABSTRACT

This report summarizes the key results and conceptual findings from a three year research program on hydrocarbon formation and oxidation mechanisms in spark-ignition engines. Research was carried out in four areas: laminar flame quenching experimental and analytical studies; quench layer studies in a spark-ignition engine using a rapid-acting gas sampling valve; flow visualization studies in a transparent engine to determine quench layer and quench crevice gas motion; studies of heat transfer, mixing and HC oxidation in the exhaust port. More detailed descriptions of the individual research activities in these areas can be found in the theses and publications completed to date which form Volumes II to XI of the final report on this program.

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1. BACKGROUND

From September 1976 through August 1979, the Engine Research Department at the General Motors Research Laboratories supported an extensive fundamental research program on hydrocarbon formation and oxidation in spark-ignition engines in the Sloan Automotive Laboratory at M.I.T. Three Ph.D. theses, six Master's degree theses and one Bachelor's degree thesis have been completed under this program; one Ph.D thesis and one Master's degree thesis initiated under the program are still in progress. This summary report describes the major findings of this research, and explains the importance of each of these pieces of research to developing our understanding of the overall hydrocarbon formation mechanism. The theses and publications completed to date on this program are listed in Appendix A. These were submitted to General Motors during the course of the program as they became available. To provide a complete record of this program, they are submitted with this summary as Volumes II through XI of the final report.

The study of spark-ignition engine hydrocarbon emissions mechanisms continues to be an important research problem. The latest hydrocarbon emission standards introduced in 1980 have brought with them a fuel economy penalty, which is likely to be made worse by the stricter 1981 NO_x standard. Evermore stringent fuel economy standards demand the most aggressive engine design and calibration strategy possible. Thus hydrocarbon emission control is likely to continue as an ever present constraint. Though the use of catalyst technology is now the major HC control strategy, materials

availability and pressures to reduce emission system cost, and in the longer term changing fuel composition, will insure that control of engine HC emissions will remain an important research and development activity.

Our conceptual understanding of the total hydrocarbon emissions formation mechanism is far from adequate. Prior to this current research program, the major insights into the basic mechanisms had come from work by Daniel and Wentworth at General Motors, who demonstrated the existence of quench layers in a spark-ignition engine, the importance of the crevice between the piston and cylinder wall, the influence of wall temperature and surface roughness, and the non-uniformity in hydrocarbon concentration within the engine exhaust gases. Work in the Sloan Automotive Laboratory at M.I.T. had shown that about half the mass of hydrocarbon emissions left the cylinder during the exhaust blowdown phase, and about half left the cylinder at the end of the exhaust stroke. It was hypothesized that the blowdown hydrocarbons came from quench layers on the cylinder head and upper part of the cylinder liner. It had been shown in water analog flow visualization studies that during the exhaust stroke the piston scraped the boundary layer fluid off the cylinder wall and rolled it into a vortex; it was suggested that this vortex could be the mechanism by which hydrocarbons quenched in the crevice between the piston and the cylinder wall eventually left the cylinder. Thus, at the start of this program, the major elements in a qualitative conceptual model of the total hydrocarbon emission mechanism had been proposed.

The sequence of steps which make up this complete hydrocarbon emissions formation and oxidation model is extremely complicated. The flame

quenches at the walls of the combustion chamber, leaving a quench layer of unburned and partially burned fuel-air mixture adjacent to the wall. The flame also quenches at the entrance to any crevices where the opening is too small to permit the flame to enter. During the expansion process, mixing at the outer edge of the quench layers is expected to occur as well as some oxidation of the unburned fuel species. As the cylinder pressure falls, gas will flow out of the crevices into the cylinder where mixing with the bulk cylinder gases and some oxidation of the unburned mixture would be expected. During the blowdown phase of the exhaust process, the rapidly exiting gas would entrain quenched gases from the boundary layers on the cylinder head and upper cylinder wall. During the exhaust stroke the piston scapes the cylinder walls of any gases laid there during expansion and pushes a large fraction of the hydrocarbons remaining in the cylinder after blowdown into the exhaust. Within the exhaust port, exhaust manifold and exhaust pipe, depending on the local oxygen concentration and temperature, additional oxidation of unburned hydrocarbons is expected to occur. There is considerable evidence to support this qualitative description.

The primary goal of the research program summarized here was to test, refine and quantify where possible these conceptual ideas and provide a more coherent model of the overall process. The following are key areas where data and predictive models have been lacking:

- 1) the effects of unburned mixture conditions and composition on the flame quenching process at the combustion chamber walls;
- 2) the effects of wall geometry, wall temperature, and thermal boundary layer structure on this flame quenching process;
- the effect of fuel composition on the quench layer thickness and its contents;

- the details of the quench crevice hydrocarbon generation mechanism and the influence of piston and piston ring geometry;
- 5) the motion of quench layer and crevice gas during the expansion and exhaust processes;
- 6) the oxidation of quench zone hydrocarbons subsequent to their formation, within the cylinder during the expansion and exhaust processes;
- 7) data which separates the in-cylinder formation and oxidation processes from mixing and oxidation processes in the exhaust port, manifold and tail pipe; and
- 8) the importance of hydrocarbon oxidation in the exhaust system as a function of engine operating conditions and exhaust system design.

The research carried out at M.I.T. and summarized in this report has contribued towards resolving several of these areas of uncertainty in two ways--first, by providing experimental data at selected intermediate stages in the overall hydrocarbon formation process which help define the role of the individual subprocesses in the total mechanism, and second, by developing quantitative scaling laws for key subprocesses where sufficient experimental data already existed or could be obtained. Work has been focused in four distinct areas:

- 1) Laminar flame quenching studies;
- 2) Engine quench layer studies with a rapid acting sampling valve;
- Flow visualization in a unique square cross section transparent engine;
- 4) Studies of heat transfer, mixing and hydrocarbon oxidation in the engine exhaust port.

The laminar quenching studies were carried out to define the flame quenching process in a simple geometry system, where precise experimental data and an analytic theory could be developed. The engine quench layer

studies had the goal of measuring quench layer properties in an operating engine, providing data on the variation of quench layer properties during the engine operating cycle as a function of major engine operation variables, and providing a test for the laminar flame quenching theory in the engine environment. The flow visualization studies were initiated to provide information on the motion of gas originating in quench regions, during the expansion and exhaust processes. Both qualitative and quantitative information on these flow processes was sought; this was regarded as a key area where conceptual ideas needed to be developed and substantiated. The exhaust port studies had the dual goal of separating in-cylinder and exhaust system mechanisms, and developing and validating a model which could be used to optimize exhaust system design. The major results in each of these four research areas will now be reviewed.

2. LAMINAR FLAME QUENCHING STUDIES

Although the combustion process in a spark-ignition engine is turbulent, we concluded that a laminar flame quenching study was relevant to the engine context and had substantial advantages as a starting point for a flame quenching analysis. In an engine, as the flame approaches the wall, it propagates into a viscous sublayer adjacent to the wall where turbulent fluctuations have negligible energy. Because the wall remains cold, the flame is extinguished a small distance away from the wall leaving unreacted fuel and carbon monoxide. The quenching distance is so small (50-500 μ m) that it is extremely difficult to study the process directly in the engine environment. A simpler geometry steady-flow system was chosen for study: the standoff of a laminar flame above a heat sink in a one-dimensional laminar premixed-flow. It was hypothesized that the standoff distance in this problem was analogous to the quench layer thickness in an engine. The details of this work are given in Volume II.

The problem for which a theoretical analysis was developed was a one-dimensional laminar flame with heat loss to an upstream cold boundary. The analysis relates the flame speed, the burned gas temperature and the standoff distance of the flame above the cold boundary. It was shown that there is both a high temperature and a low temperature solution for the standoff distance. Also, there is a minimum distance for which solutions exist. This minimum standoff distance is the quench distance for a transient flame propagating towards a wall, when the quasi-steady approximation

is valid. It was shown that a Peclet number based on laminar flame speed and standoff distance depends only on the ratio of the heat of combustion to the heat loss to the cold wall provided that: (i) the dimensionless activation energy $\beta = E/RT_b$ is greater than about 7, and (ii) that when hydrogen is a reactant it carries little of the sensible enthalpy. It was then shown that because so little heat is required to quench a flame, the minimum standoff distance is a good approximation to the quench distance for an unsteady flow. An expression was derived for the mass of fuel, per unit area of the wall, in a quench layer for use in engine quench layer calculations.

Experiments were carried out in a laminar porous-metal flat-frame burner to measure the flame standoff distance from the burner, as a function of fuel and unburnt mixture composition. A hot-wire pyrometer was developed to measure flame temperature and thus locate the flame front position relative to the porous-metal burner-surface. Acceptable quantitative agreement between the standoff Peclet number based on the measured standoff distance, as a function of the ratio of the heat of combustion to the heat loss, and the limiting Peclet number derived from the theory was obtained.

An analysis was also made of laminar flame quenching in flows parallel to a heat sink. The fundamental question examined was the appropriate characteristic length over which a flame in a tube loses heat. Two

^{*}The Peclet number is the ratio of convective to conduction heat transport. The standoff Peclet number used in this study was defined as Pe = $(\rho_u S_L c_p)/\lambda$ where ρ_u is the unburned gas density, S_L is the laminar flame speed, c_p the specific heat at constant pressure, D the standoff distance, λ the thermal conductivity.

possibilities were studied: the tube radius and the flame thickness. By using a functional form prescribed by the analysis, a correlation of laminar flame speed, quenching diameter, and lean limit flame temperature was developed. Nearly two orders of magnitude of quenching diameter and flame speeds were correlated by a Peclet number. The Peclet number is based on the quench distance, flame speed, unburnt gas density, frozen specific heat of the burned gas, and frozen thermal conductivity of the unburned gas at the adiabatic flame temperature.

These theories were used to compute quench distances in an engine. It was shown there is not much difference between the predictions with the correlation for perpendicular flow and four-tenths of the predictions for the parallel flow (0.4 is the accepted factor for relating the perpendicular and parallel flow quenching distances). This is also not much difference between using the free-stream unburnt-mixture temperature, or the wall temperature, as the temperature characterizing the unburnt gas. Quench layer thickness predictions were in approximate agreement with the engine layer thicknesses in the literature determined by Daniel. It was concluded that these laminar flame quenching models would therefore be useful in the engine context.

A critical parameter in these laminar quenching theories is the laminar burning velocity of the unburned mixture. Little reliable data was available for the laminar burning velocity of mixtures of air with fuels relevant to spark-ignition engines, under typical engine unburnt mixture conditions. A facility for measuring the laminar burning velocity of fuel-air residual gas mixtures had been constructed in the Energy and Chemical Dynamics Laboratory which is associated with the Sloan Automotive

Laboratory at M.I.T. Accordingly, an extensive program of experiments to develop laminar burning velocity data for mixtures of air with propane, isooctane, methanol and indolene was initiated. This work is described in detail in Volume III.

The facility consists of a spherical combustion bomb in an oven which can be heated up to 500 K. The bomb is equipped with ionization probes to measure the arrival time of the flame at the wall and check the spherical symmetry of the flame front. A piezoelectric pressure transducer to measure pressure during the combustion process, and a balanced pressure indicator to calibrate the transducer are built into the bomb. A laser shadowgraph system was used to measure the arrival time of the flame front at a known radius, and also to check the assumption of negligible pre-flame reaction. A thermodynamic model was developed and used to calculate the laminar burning velocity from the pressure time history obtained during the combustion process. The unburnt mixture properties were computed using thermdynamic data from the JANAF Tables, and the assumption of frozen composition; the burned gas properties were computed using an approximate equilibrium model for the burned gases. Allowance was made for heat loss to the bomb walls.

Laminar burning velocities for mixtures of propane-air, isooctane-air, methanol-air, and a multi-component hydrocarbon fuel (indolene)-air were measured in the pressure range 0.4 to 40 atm and temperature range 298 to 750 K, for fuel-air equivalence ratios from 0.8 to 1.5. Both power law and exponential relations were fitted to this data to permit easy estimation of laminar flame speed as a function of pressure, temperature and

fuel-air equivalence ratio. In addition, the effects of residual gases on the laminar burning velocity of stoichiometric isooctane-air mixtures were measured; the residual gases were simulated by mixtures of carbon dioxide and nitrogen to obtain the appropriate specific heat.

Methanol-air mixtures were found to have the highest laminar burning velocity amongst the fuel-air mixtures studied, followed by propane-air, isooctane-air and indolene-air mixtures. The difference between the isooctane and indolene values was small, however. The laminar burning velocity peaks at an equivalence ratio of about 1.1 and falls off rapidly as the mixture becomes both richer and leaner.

The burning velocity correlations developed under this program are based on a sufficiently extensive data set for us to conclude that this variable is no longer a major area of uncertainty in quench layer correlations. This data set and these correlations obviously have extensive application in other areas of combustion. In particular, they are proving extremely useful in spark-ignition engine flame propagation modeling.

3. ENGINE QUENCH LAYER STUDIES

To define the contribution from quench layers on the cylinder head and upper portion of the cylinder liner, to exhaust hydrocarbons, a program of engine experiments was undertaken. The goal of this part of the research program was to sample gases (including gases from the quench layer) after combustion, from the cylinder using a rapid-acting sample valve, and through use of a model for the flow into the valve develop more detailed information about the quench layer characteristics than has been available to date. By carrying out these experiments over a range of engine operating conditions, the variation of quench layer thickness and hydrocarbon content could be determined. Volumes IV and V describe the results of this activity.

For the engine experiments, a rapid-acting sampling valve supplied to the Sloan Automotive Laboratory by General Motors Research Laboratories was modified and inserted through the top of the cylinder liner in a single cylinder CFR engine. This sample valve, which had an open time of about two milliseconds, was used to extract a gas sample once per engine operating cycle at a pre-selected crank angle. A model was developed for a flow into the valve during the sample period, and was used to interpret the results of gas concentration measurements made on the sample valve flow. This model permitted an estimate to be made of mass of hydrocarbons in the quench layer, per unit wall area, and of the quench layer thickness.

The basis for the model of the flow into the sample valve was the following. The mass of hydrocarbons sampled per cycle is computed from the hydrocarbon concentration in the sample stream and the sample flow rate.

The mass of hydrocarbons sampled per cycle was then corrected for leakage which occurs while the valve is nominally closed. The leak rate with the valve closed was measured. The mass of hydrocarbons leaked was computed by assuming the leak rate to be proportional to the pressure difference between the cylinder and the valve sample line, and that prior to timeof-quench, the leaked gas is unburnt mixture while after time-of-quench the leaked gas is burned mixture with negligible hydrocarbon concentration. It was found necessary to modify the design of the valve and use a copper seat to keep the leakage correction to less than twenty percent. As a first approximation the flow into the sample valve was assumed radial and inviscid. The sample gas was assumed to occupy a hemispherical region concentric with the sample valve orifice. The mass of hydrocarbons per unit area on the cylinder wall (neglecting boundary layer effects) could then be computed. A viscous model for the flow into the sample valve was then developed, because it was clear that boundary layer behavior during portions of the engine cycle would significantly retard the entrainment of hydrocarbons on the wall. The axisymmetric boundary layer equations for flow into a point sink on a plane surface were solved, followed by the integration of an assumed quench layer profile over a volume specified by the flow field. It was found that the ratio of the thickness of the quench layer relative to the thickness of the viscous boundary layer is much larger during exhaust than during expansion, so that exhaust stroke estimates of quench layer hydrocarbons are likely to be much more accurate. Functions which relate the mass of hydrocarbons per unit area calculated from the inviscid model to the mass per unit area with the viscous model

were developed and computed for an appropriate range of engine conditions.

Two studies and sets of experiments were carried out. The first (by Wrobel, Keck and Woods; Vol. IV) developed the gas sampling methodology and model for flow into the valve, and investigated the effects of volume sampled per cycle by varying needle lift and sample duration, and time of sampling during the cycle. The second (by Weiss and Keck; Vol. V) improved the experimental technique, explored through a set of engine experiments the effect of variations in engine operating conditions on quench layer properties, set up the laminar flame quenching model of Ferguson and Keck (Vol. II) for predictions of quench layer properties in an engine, and compared predictions made with this quenching theory with the experimental engine data.

It was shown that the mass of hydrocarbons quenched per unit wall area was independent of the volume sampled, at constant sample duration, and only varied slightly with needle lift. In the studies where sampling occurred at different times during the engine cycle, it was found that the mass of hydrocarbons per unit area in the quench layer generally decreased during the expansion stroke. Peak value determined using the sample valve flow model described above occurred at about 180 degrees crank angle, during the exhaust blowdown process. The high gas velocities within the cylinder during blowdown violated the assumption made in the model that the radial flow velocity toward the valve orifice was the dominant velocity in the flow field; thus the model is not appropriate during blowdown. During the exhaust stroke, the mass of hydrocarbons per unit area remain essentially constant at the sample valve location used in this study

(close to the top of the cylinder wall).

Quench layer properties were determined in the CFR engine as a function of equivalence ratio, inlet manifold pressure, spark advance, percent exhaust gas recycle and coolant water temperature. The values of mass of hydrocarbons per unit wall area in the quench layer were relatively insensitive to operating conditions and varied between about 0.4 and 1 μ g HC/cm². The values of the quench layer thickness estimated from the mass per unit area data ranged from 0.05 mm early in the expansion process to 0.35 mm during the exhaust stroke. The mass of hydrocarbons per unit area showed a minimum at an equivalence ratio of 1.0, and showed a slight decrease with increasing inlet pressure, increasing spark retard and cylinder wall temperature, and a slight increase with increasing percentage EGR.

The laminar flame quenching theory described in the previous section was used to provide a theoretical estimate of quench layer properties to compare with the above experimental results. The laminar flame speed data of Metghalchi (Vol. III) were used in the Peclet number correlation which defines the minimum standoff distance, which was equated with the quench distance as explained previously. The predicted mass of hydrocarbons per unit area were comparable to the measurements, though higher by a factor of between 1.1 and about 2, and generally showed the same trends with the engine variables studied. Since entrainment from the quench layer during blowdown (see next section) is likely to have reduced the mass of the per unit wall area in the experimental results (which were evaluated during the exhaust stroke) the theoretical predictions would be expected to lie above the experimental data.

These results for mass of hydrocarbons in the quench layer, per unit wall area, have been used to estimate the contribution which quench layers on the cylinder head and upper portion of the cylinder liner could make to total exhaust hydrocarbons. Based on a mass of hydrocarbons per unit wall area of 1 μ g HC/cm², and a quench layer area swept into the exhaust during blowdown equal in magnitude to the piston area, the quench layer contribution would be of order 300 ppm C at wide-open-throttle and 600 ppm C at light load. These exhaust levels are small relative to CFR engine exhaust hydrocarbon levels, but are a significant fraction of exhaust levels typical of modern production engines.

The engine experiments in this program were carried out with relatively clean combustion chamber walls. The fuel used was isooctane, and deposit build up with this fuel under typical research engine usage is not significant. The effect of deposits on these surfaces, on the flame quenching process and quench layer properties has yet to be determined. Also, for extremely lean or dilute engine operating conditions, the quench layer contributions will be more substantial.

This study showed that the laminar quench correlations predict quench layer properties with reasonable accuracy. Thus, the flame quenching process with clean combustion chamber walls has, we believe, now been defined with sufficient accuracy, both experimentally and theoretically, for incorporation into an engine hydrocarbon model.

4. FLOW VISUALIZATION STUDIES

A substantial part of the effort in this program was devoted to the design, construction and use of a transparent engine to visualize the flow field within the engine cylinder from the time of flame quenching at the combustion chamber walls to the end of the exhaust stroke. Through qualitative descriptions of how unburnt hydrocarbons moved from quench layers and quench crevices at the outer edges of the combustion chamber to the exhaust valve had been proposed, there has been no direct confirmation of these conceptual ideas to date. It was anticipated that the motion of the thermal boundary layers on the combustion chamber walls, which contain the quench layers, and the flow out of crevices, during the expansion and exhaust strokes, could be observed by techniques such as Schlieren photography which identify regions where density gradients exist.

A square cross-section transparent engine was constructed for this purpose. The engine was built on a CFR engine crankcase using the CFR piston and cylinder as a crosshead for the square cross-section piston and cylinder assembly. A square cross-section cylinder assembly was chosen to permit optical access to the entire cylinder volume over the complete engine operating cycle. The square cross-section assembly had two parallel steel walls and two parallel quartz glass walls. The square cross-section piston was fitted with three sets of hard graphite rings, dovetailed at the corners and spring loaded, to seal against gas leakage. The CFR head and valve mechanism completed the assembly.

It was shown through a thermodynamic analysis of engine pressure data that the engine operates satisfactorily with propane fuel under typical engine operating conditions. The combustion efficiency determined from this analysis, and the cyclic variation in peak pressure are comparable in magnitude to conventional engine values. Spark-discharge short-time exposure photographs, and high-speed movies, were taken while the engine was operating, to define details of the flow and density fields in the engine cylinder throughout the engine cycle. A complete description of the engine, its operating characteristics, and an extensive set of photographs taken in this facility, with an interpretation of those features of the flow which were observable in the photographs and movies, are given in Volumes VI, VII and VIII. Those flow features which relate directly to the hydrocarbon formation mechanism are the following.

The turbulent flame front was observed to propagate into the thermal boundary layer on the combustion chamber walls. The quench distance was, as expected, too small to be observed directly. The thickness of the dark denser-gas layer adjacent to the wall (interpreted as the thermal boundary layer) did not change significantly from the time the front of the flame arrived at the wall to the time the back of the flame reached the wall. After time of peak cylinder pressure, early in the expansion process, denser gas was observed flowing out of the crevice around the spark plug electrode. Much later in the expansion process, gas was observed to flow as a jet out of the piston top-land region and the volume behind and between the piston rings. This piston crevice gas moved relatively rapidly into the bulk of the cylinder. During the exhaust blowdown process, the gas from the spark plug crevice exits the cylinder,

and a substantial portion of the boundary layer on the cylinder head and upper cylinder liner walls is entrained in the blowdown flow. The gas from the piston crevice reaches the exhaust valve during blowdown and some of it exits the cylinder. During the exhaust stroke, the piston pushes out much of this crevice gas with the bulk cylinder gases. As the piston travels up the cylinder during the exhaust stroke, the piston scrapes the boundary layer off the cylinder wall and rolls it into a vortex in the piston-crown cylinder-wall corner. In the square crosssection engine geometry, this vortex was not always stable. It was observed to lift off the piston crown at the end of the exhaust stroke and move towards the exhaust valve. Measurements of the size of this vortex show that it grows during the exhaust stroke at a rate described by the scaling law developed previously at M.I.T. by Tabaczynski and others from water analog piston-cylinder studies.

A preliminary model was developed for gas flow into and out of the crevice region between the piston and cylinder wall and behind the piston rings. These volumes can be regarded as linked to the cylinder volume through a set of flow restrictions. When the cylinder pressure is higher than the pressure behind and between the rings, gas flows into this crevice volume. During the expansion process, the pressure in the cylinder eventually falls below the pressure in the volume between and behind the rings, and the direction of gas flow reverses. Using volumes and flow areas estimated from the geometry of the piston and ring assembly, it was shown that this flow reversal should occur at about the point when jets issuing from the crevice are observed in the Schlieren movies.

We have estimated that the volume behind and between the piston rings (in the square cross-section engine) is about four times the equivalent volume in a conventional engine, and the flow area connecting this volume with the cylinder is also about four times that area in a conventional engine. Since this preliminary model predicts behavior approximately consistant with what was observed from the Schlieren movies, a more detailed model of the piston crevice volume, behind and between the rings, is under development.

If the flow into and out of the region between the piston and cylinder wall in a conventional engine is similar to that observed in this square cross-section engine, then our earlier suggestion that the vortex in the piston-crown cylinder-wall corner would contain most of the piston crevice gases would need to be modified. The jets of gas which issue from this crevice region, once the flow reverses direction and is from the crevice into the cylinder, may have sufficient velocity to penetrate a substantial distance towards the exhaust valve before the blowdown process is over. Note, however, that the gases in the crevice are likely to come out in approximately the order in which they entered. The first gas to enter the crevice, during the compression stroke and early part of the combustion process before the flame reaches the crevice entrance, should be unburned mixture. Following flame arrival at the crevice entrance, the gas entering the crevice will be burned gases until that point in the expansion stroke when the flow reverses.

In summary, we have observed and described a new process by which hydrocarbon rich gases from the crevice between piston, piston rings and cylinder wall could leave the cylinder. The gases in this crevice enter the cylinder as jets with substantial velocity. These jet flows provide a possible, though as yet unsubstantiated, mechanism for crevice gases to leave the cylinder during the blowdown process. At the same time, they add to the vortex mechanism by providing hydrocarbon rich regions, along the cylinder wall, above the piston, which would leave the cylinder much later in the exhaust process.

From the Schlieren spark-photographs and high speed movies, other features of the flow within the cylinder could be observed. These included the jet type flow through the intake valve and the in-cylinder motion this jet sets up, the turbulence scale and bulk motion during compression, the ignition, flame growth and flame propogation processes, details of the flame structure, examples of cycle-by-cycle variations, and additional details of the bulk gas motion during exhaust. These are described in more detail in Volume VIII.

To sum up this part of the total program, the use of a square cross-section transparent side-wall spark-ignition engine for flow visualization through the complete engine cycle has been successfully demonstrated, and the engine operating characteristics were shown to be sufficiently close to those of a conventional spark-ignition engine for the results to provide useful insights into the flow fields and the flame structure in real engines. Our observations and insights into both the hydrocarbon emissions mechanisms, and other aspects of the flow and combustion process can be summarized as follows:

- 1) For throttled operation, when the intake valve opens, the backflow from the cylinder into the intake system is evident and the bulk gas in the cylinder is drawn towards the valve.
- 2) The intake flow enters the cylinder as a connical jet which travels to and interacts with the cylinder wall.
- 3) A vortex type flow in the upper corners of the cylinder, set up by the intake jet, is visible in the Schlieren movies. This rotating motion in the upper corners persists through compression, combustion and expansion.
- 4) The turbulent flame which develops from the spark discharge propagates as an approximately spherical though irregular front. The flame zone is thick, the front to back distance being 10-15 mm, and a detailed internal flame structure is evident.
- 5) Only a fraction (of order one half during the earlier part of the burning process) of the mixture contained behind the propagating flame front is fully burned.
- 6) The characteristic burning time of mixture within the flame is of order a few milliseconds (average 1.8 ms). This gives a characteristic turbulent flame length scale of 14 mm (which is comparable to the observed flame thickness), and a characteristic laminar burning length scale of 1.3 mm.
- 7) The flame front shows both larger scale irregularities and a smaller scale structure. The larger scale irregularities are of order 10 mm in size (about 1/3 the clearance height). The smaller scale structure at the flame front appears to be burned gas elements of order 2.5 mm in dimension surrounded by a thin flame zone and then unburned mixture. This smaller scale is comparable to the laminar burning length scale. At the back side of the flame, the small scale structure is reversed: unburned mixture within a thin flame zone with burned mixture outside.
- 8) The spark discharge is observed as a thin column between the electrodes which then grows as a flame kernel develops around the spark. Once the kernel fills the electrode gap it develops irregularities. Once it extends beyond the electrodes (scale 5 mm or greater) its appearance is similar to that of a fully developed turbulent flame.
- 9) A comparison of pictures from different cycles shows different degrees of flame development at early times, and different flame center motion and front shape. These initial differences lead to substantial later differences in fully developed

flame front position and shape. The effect of cycle-bycycle variations in mixture motion on the flame can be observed. These differences in flame development and propagation can be related to the value and time of occurence of peak pressure.

- 10) During expansion (following time of peak cylinder pressure) flow of denser gas out of the spark plug crevice and the region between the piston and the cylinder walls was observed. Gas from the crevice volume behind and between the rings issued from the corners of the gap between the piston crown and the walls as a jet, late in the expansion process, when the cylinder pressure fell below the pressure in this crevice region. These crevices gases are expected to have a high unburned hydrocarbon concentration.
- 11) The blowdown flow was observed to entrain the denser thermal boundary layer gas off the cylinder head and upper part of the cylinder wall. Some of the gas from the crevice between the piston crown and cylinder wall also leaves the cylinder during blowdown.
- 12) During the exhaust stroke, the roll-up of a vortex in the corner between the cylinder-wall piston-crown-surface was observed, though the vortex was not always stable in this engine geometry. The growth of this vortex fits the scaling law developed previously by Tabaczynski, et al. in water analog piston-cylinder experiments.
- 13) Dark layers, interpreted as thermal boundary layers, of thickness between 0.2 and 2.2 mm were observed on the walls of the engine throughout the cycle. The boundary layers on the cylinder head and upper cylinder walls are thinnest when gas velocities are highest during intake and blowdown. The thickness grows to a maximum just before the exhaust valve opens.

The results obtained to date in the flow visualization engine at a single engine operating condition and with one engine combustion chamber geometry (square cross-section cylinder, uniform clearance height) have thus provided substantial insights into both the flow aspects of the hydrocarbon emissions mechanism, as well as details of the intake and compression flows, and the combustion process. This facility has tremendous potential for additional contributions in these areas.

5. EXHAUST PORT STUDIES

The motivation for devoting a significant fraction of the research effort to studies related to hydrocarbon oxidation in the exhaust port was the following. Engine experiments with exhaust port liners had indicated that significant additional burn up of hydrocarbons could be achieved through reductions in exhaust port heat transfer. Previous exhaust system models had focused primarily on the manifold. Our preliminary assessment indicated that most of the gas phase hydrocarbon burn-up outside of the cylinder occurred in the exhaust port. Yet no model was available, to our knowledge, for optimizing the design of the port to maximize the reduction in hydrocarbons. A major thrust therefore was the development of an exhaust port flow model which included heat transfer, mixing and hydrocarbon oxidation processes in adequate detail, and the validation of that model through engine experiments. An important additional reason for studying exhaust port processes was to provide information which separates the mechanisms governing hydrocarbon formation within the cylinder, from what happens to the hydrocarbons which exit the cylinder within the exhaust system. A program of engine experiments where the exhaust flow was quenched at selected locations within the port was also planned and carried out.

The development of the exhaust port model, and its use, are described in Volume IX. The modeling work first focused on heat transfer processes within the port to enable the gas temperature as a function of position and time to be determined. A series of heat transfer models were developed for different phases of the exhaust process: e.g., a jet

impingment model for the valve stem and valve guide heat transfer for small valve lift; a flow regime dominated by large scale fluid motion set up by the jet-type flow exiting the exhaust valve, again for small valve lift; a developing pipe flow model for the port during the high valve lift phase of the exhaust process. Visualization studies of the flow pattern in the exhaust port, described in Volume X, contributed to the definition of these flow regimes.

To assist in developing these heat transfer correlations, experiments were carried out in a CFR engine to measure the decrease in exhaust gas temperature in the exhaust port, on a time and space resolved basis during the exhaust process. The gas temperature at cylinder exit during exhaust was estimated from cylinder pressure measurements using a thermodynamic model to determine the state of the gases within the cylinder. To measure the gas temperature at exhaust port exit, a fine wire resistance thermometer probe was developed, which could be traversed across the exhaust-port exit-plane. Gas temperatures as a function of time were determined with the resistance thermometer as a function of position at port exit, engine load, speed, equivalence and spark advance.

The heat transfer models were coupled with a one-dimensional quasisteady, though time varying, model of the flow through the port, and were developed to give good agreement with the experimentally determined gas temperatures at port entrance and exit. A simple correlation based on the gas velocity at the valve seat was found to give an adequate estimate of the heat transfer in the port. A four time period heat transfer correlation was also developed, based on two distinct flow regimes for low and high valve lift, which provided the best overall agreement with the measured gas-temperature data.

A mixing model was added to this flow model to approximate the mixing which takes place between gas at the end of one exhaust pulse and the beginning of the next pulse. An analysis of overall hydrocarbon oxidation rate expressions in the literature relevant to exhaust system hydrocarbon oxidation identified a suitable oxidation rate expression which was coupled with the flow, heat transfer and mixing models. Several possible hydrocarbon concentration profiles at the exhaust port inlet were tested in conjunction with the model to provide port exit concentration profiles for comparison with available time-resolved experimental hydrocarbon concentration data. A two level concentration profile was found to give reasonable agreement. A sensitivity analysis indicated the detailed shape of hydrocarbons concentration profile at port inlet was not important to the fraction reacted in the port. An analysis of various mixing volumes within the port showed that the precise choice of mixing volume was not important either.

A model study of the effect of changes in key engine operating variables on the percentage reduction in cylinder exit hydrocarbons which occurs in the exhaust port was then carried out. The base point for this study was an indicated mean effective pressure of 345 kPa and speed of 1400 rev/min. The predicted percent hydrocarbon reacted in the port varied between about ten and forty percent. Percent reacted decreased with increasing engine load, increased with increasing engine speed, increased as the spark was retarded, and showed a maximum at an equivalence ratio of 1.0, decreasing slightly as the mixture is made leaner, and more rapidly as the mixture is made richer.

The model was then used to explore the effect of engine design variables. It was shown that changes in average temperature at cylinder exit significantly affected the percent reacted (higher cylinder temperatures giving higher percent reacted). Thus increases in engine compression ratio would be expected to decrease percent reacted significantly. Increases in port wall temperature (for example through the use of port liners) showed substantial increases in percent reacted. Increasing the cross-sectional area of the port increased percent reacted by increasing port residence time and decreasing the impact of heat transfer. An analysis of the degree of oxidation occurring in a pipe downstream of the port exit showed that the reaction rate steadily decreased with increasing distance from the valve; by port exit about two thirds of the total percent reacted had occurred. These studies illustrated the utility of this model for improving exhaust port design, and identified the key design variables. The percent hydrocarbon which reacts in the port, under typical engine operating conditions, is sufficiently large for this to be a fruitful development area.

To provide confirmation of these predicted levels of hydrocarbon reaction in the port, and the trends with major engine operating variables, and also provide data which defines cylinder exit hydrocarbon emission levels, an additional experimental activity was initiated. A CFR engine set-up was developed where the exhaust gas flow could be cooled by dilution with a cold gas stream, at a selected plane within the exhaust port to quench the exhaust hydrocarbon oxidation reactions. By differencing exhaust concentrations with and without quenching, the reduction

in hydrocarbons downstream of the quenching plane could be determined. In the test set-up, the quench gas, carbon dioxide, could be injected via a hollow-stemmed exhaust-valve through thirty-two holes drilled in the back of the valve head to provide uniform quenching just downstream of the valve seat, or through an injector probe which could be traversed axially into the exhaust port along the port axis from the port exit plane. It was shown that a quench-gas flow equal to the exhaust flow was sufficient to quench the hydrocarbon oxidation reactions in the port. This quench flow had no effect on indicated mean effective pressure at typical engine operating conditions, and reduced NO_x emissions by less than ten percent.

The experimental set-up was designed, fabricated and tested within the grant period. Since that time, a program of experiments to measure the percent hydrocarbon reacted in the port has been completed, and the results are described in Volume XI.

Experiments were carried out over a matrix of engine operating conditions comparable to those studied by Caton (Volume IX) in the exhaust port modelling program. It was shown that the reaction rate decreased rapidly as the quenching plane was moved downstream of the cylinder exit, thus confirming that the upstream portion of the exhaust port is the critical design area. Trends and magnitudes in percent hydrocarbon reacted in the port, with indicated mean effective pressure, speed, equivalence ratio, and spark retard were comparable with model predictions, and values up to 40 percent were measured. That the maximum percent reacted occurs at stoichiometric operating conditions, as predicted by the model, was con-

firmed. These experiments also defined the variation of cylinder exit hydrocarbon level with indicated mean effective pressure, engine speed, equivalence ratio, spark retard and compression ratio. The trends with indicated mean effective pressure, speed, equivalence ratio and compression ratio, at cylinder exit compared to exhaust system exit, are sufficiently different for this data to be extremely valuable in future studies of in-cylinder hydrocarbon formation mechanisms.

6. SUMMARY

A concise summary of the major achievements of the program is pro-

a) Laminary Quenching Studies

- 1) Correlations for the flame stand-off distance for a laminar flat-flame burner, and for critical tube diameter for extinguishment of a laminar flame in a tube have been developed and verified with laminar flame-quenching data. It was shown that these correlations are relevant to flame quenching in the SI engine context.
- 2) A combustion bomb and method of analysis for measurement of laminar flame speeds of fuel-air mixtures under conditions relevant to engines, have been developed. This facility has been used to measure laminar flame speeds for propane, methanol, isooctane and indolene fuel-air mixtures under conditions appropriate to spark-ignition engine operation. The laminar flame speed characterizes the combustion chemistry in the correlations developed for flame quenching as well as in other engine combustion problems.

b) Quench Layer Studies in an Engine

- 1) An experimental technique based on the GM fast-acting valve for efficient sampling of gases from the engine cylinder at any point in the entire engine cycle, with an acceptably low leak rate for quench layer studies, has been developed and tested successfully.
- 2) A model for flow into the sampling valve, which permits an estimate of the mass of hydrocarbons per unit area of combustion chamber surface in the quench layer and the thickness of the quench layer to be estimated from sampling valve data, has been developed. The model allows for viscous boundary layer effects.
- 3) With these experimental and analytical techniques, estimates of quench layer composition and thickness in an operating CFR engine have been made. At typical engine operating conditions the mass of hydrocarbons per unit area is about 1 μ g HC/cm². The effects of variations in equivalence ratio, inlet pressure, spark advance, exhaust gas recycle and coolant temperature on quench layer properties have been quantified.

4) The laminar quenching theory has been applied to the engine context, over the above range of engine variables, and has been shown to be in reasonable agreement with the quench layer mass of hydrocarbons per unit area determined experimentally.

c) Flow Visualization Studies in the Transparent Engine

- 1) A square cross-section transparent engine for Schlieren photography flow visualization has been designed, constructed and operated successfully to produce spark-photographs and highspeed movies which illustrate flow features in the engine cylinder through the complete engine operating cycle.
- 2) Flow of denser gas out of the spark plug crevice during expansion, and flow of this gas out of the cylinder during the exhaust blowdown process has been observed.
- 3) Measurements were made from these movies of thermal boundary layer thickness on the cylinder head and upper cylinder wall. The thickness varied over the operating cycle between 0.2 and 2 mm. A substantial part of the boundary layer in these regions was entrained by the exhaust blowdown flow.
- 4) A jet-type flow out of the crevice volumes between the piston, piston rings and cylinder wall late in the expansion process has been defined. This jet penetrates to the exhaust valve (and maybe beyond) during blowdown, and is pushed out of the cylinder during the exhaust stroke. It represents a possible alternative mechanism to the previously proposed for crevice hydrocarbons leaving the cylinder: the vortex formed by the piston motion during the exhaust stroke.
- 5) The vortex generated in the piston-crown cylinder-wall corner by the piston motion during the exhaust stroke was observed in the Schlieren movies, and its dimensions were shown to correlate with previously developed scaling laws. This vortex lifts off the piston at the end of the exhaust stroke and moves towards the exhaust valve.
- d) <u>Studies of Heat Transfer, Mixing and HC Oxidation in the Exhaust</u> Port
 - 1) Experiments were carried out in a CFR engine to measure the gas temperature at exhaust port exit, to provide data for developing an exhaust-port heat-transfer model. A fine-wire resistance-thermometer was developed for this purpose.

- 2) A model for the flow in the exhaust port, which includes new correlations for the exhaust-port heat-transfer process, includes gas mixing due to the jet-type flow through the valve seat at the start of the exhaust blowdown, and incorporates a kinetic model for hydrocarbon oxidation has been developed to match this gas temperature data.
- 3) The model has been used to define the degree of HC reaction in the exhaust port as a function of engine load, speed, spark advance and equivalence ratio. Percent HC reacted in the exhaust port varied from 10 to 40 percent.
- 4) The model was used to predict the effect of changes in key design variables--port wall-temperature, port area, port length--on percent HC reacted.
- 5) An experiment to quench the exhaust flow in a CFR engine within the exhaust port, to determine directly the percent HC reacted in the port, was planned. The measured percent HC reacted in the port confirmed the magnitude and trends predicted by the model. The data also defined several engine variables for which cylinder exit HC and exhaust exit HC showed different trends.

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HYDROCARBON FORMATION AND OXIDATION IN SPARK

IGNITION ENGINES

A research program in the Sloan Automotive Laboratory at MIT funded by the Engine Research Department, General Motors Laboratories.

The following theses and papers have been published or are in progress:

1. Theses Completed:

B.S. Degree

John Harrington, "Visualization Studies of Flow through an IC Engine Exhaust Valve" May 1976

Masters Degree

- Stephen P. Hansen, "The Design and Testing of a Flow Visualization Engine" January 1978
- Mohamad Metghalchi, "Laminar Burning Velocity of Isooctane-Air, Methane-Air, and Methanol-Air Mixtures at High Temperature and Pressure" October 1976
- Andrej K. Wroebel, "Experimental Study of Quench Layer Hydrocarbons During the Expansion Stroke of a Spark-Ignition Engine, Using a Fast Sampling Valve" February 1978
- Joachin Sanchez-Barssé, "Schlieren Flow Visualization of Combustion and Quench Zone Motion in an Internal Combustion Engine" March 1979
- Paul Weiss, "A Parametric Study of Quench Layer Properties by Rapid Sampling in a Spark-Ignition Engine" January 1980
- John Mendillo, "Quenching Studies to Determine Hydrocarbon Oxidation in the Exhaust Port of a Spark-Ignition Engine" February 1980

Ph.D. Degree

Colin Ferguson, "Standoff Distances on a Flat Flame Burner" February 1977 Jerry Caton, "Heat Transfer, Mixing and Hydrocarbon Oxidation in an Engine Exhaust Port" September 1979

Mohamad Metghalchi, "Laminar Burning Velocity of Mixtures of Air with Indolene, Isooctane, Methanol and Propane"

October 1979

2. Theses in Progress:

Masters Degree

Edward Lyford-Pike, "Boundary-Layer Studies in the MIT Square Cross-Section Flow Visualization Engine" 1980

Ph.D. Degree

Mehdi Namazian, "Quench Gas Motion Within the Cylinder of a Spark-Ignition Engine" 1980

3. Publications to Date

- Colin R. Ferguson and James C. Keck, "Hot-wire Pyrometry," J. Appl. Phys. 49(6), June 1978, 3031-2.
- Colin R. Ferguson and James C. Keck, "Stand-Off Distances on a Flat Flame Burner," Combustion and Flame 34, (1979), 85-98.
- P. Weiss, A. K. Wroebel and J.C. Keck, "A Parametric Study of Quench Layer Hydrocarbons Using a Fast Sampling Valve," Paper No. CSS/CI 79-16 presented at Spring Meeting of Central States Section, The Combustion Institute, April 9-10, 1979 in Columbus, Indiana.
- M. Metghalchi and J.C. Keck, "Laminar Burning Velocity of Propane-Air Mixtures at High Temperature and Pressure," Paper No. CSS/CI-79-04 presented at Spring Meeting of Central States Columbus, Indiana. Submitted to Combustion and Flame.
- J.A. Caton and J.B. Heywood, "Models for Heat Transfer, Mixing and Hydrocarbon Oxidation in an Engine Exhaust Port," SAE Paper 800290 presented at SAE Automotive Congress, February/March 1980.
- M. Namazian, S. Hansen, E. Lyford-Pike, J. Sanchez-Barsse, J.B. Heywood and J.M. Rife, "Schlieren Visualization of the Flow and Density Fields in the Cylinder of a Spark-Ignition Engine through the Complete Operating Cycle", SAE Paper 800044 presented at SAE Automotive Congress, February/March 1980.
- 4. Publications in Preparation

- J.C. Caton and J.B. Heywood, "An Experimental and Analytical Study of Heat Transfer in an Engine Exhaust Port," to be submitted to <u>International Journal of Heat and Mass Transfer</u>.
- J. Mendillo and J.B. Heywood, "Quenching Studies of Hydrocarbon Oxidation in the Exhaust Port of an SI Engine" to be presented at SAE meeting, 1980.