

Investigation of Post-Flame Oxidation of Unburned Hydrocarbons in Small Engines

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ABSTRACT

The post-flame oxidation of unburned hydrocarbons released from the ring-pack crevice was investigated for a small, air-cooled, spark-ignition utility engine. Spark timing sweeps were performed at 50, 75 and 100% load and speeds of 1800, 2400 and 3060 RPM while operating at a 12:1 air-fuel ratio, which is typical for these engines. A global HC consumption rate (GCR) was introduced based on the temporal profile of the mass released from the ring pack; the mass release after CA90 and up to the point where the remainder of the ring pack HC mass is equal to the exhaust HC level was taken as the mass oxidized, and a rate was defined based on this mass and the corresponding crank angle period over which this took place. For all conditions tested, the GCR varied with the spark timing; advanced spark timing gave higher GCR. A threshold temperature, which corresponds to the bulk gas temperature at the end of the post-oxidation process, was found to vary with operating condition, and thus a simple model based on a kinetically defined critical oxidation temperature is insufficient to describe the process. A mixing-controlled model that assumes that the post oxidation is controlled by a mixing rate given by the maximum mass flow rate of the crevice mixture returning to the cylinder was found to describe the data well - a single linear correlation was able to fit the data. A kinetically controlled model that assumes that finite-rate chemistry controls the oxidation process also describe the data well, giving a good linear fit in an Arrhenius-type plot. The relative merits and weaknesses of both post-oxidation models were discussed.

INTRODUCTION

Small engines, which are typically considered to have a power output equal to or smaller than 19 kW, are found in a wide range of applications. The number of units sold every

year can be assessed in the order of tens of millions [1]. While the operation time of these engines is considerably shorter than automotive engines and their displacement is relatively small, because of the great number of units operating worldwide, they are considered a significant source of air pollution.

In spite of their similarities to automotive spark ignition (SI) engines, there are some unique attributes of small engines that make them perform differently and have pollutant emission behavior that differs from automotive SI engines. The main differences between small engines and automotive engines are: 1) they operate richer than stoichiometric for durability reasons, which leads to higher levels of carbon monoxide and unburned hydrocarbons emissions; 2) they are air cooled, which can produce an uneven bore distortion and affect the mechanism of gas storage in the ring-pack crevice; and 3) they use a carburetor, which provides poor fuel atomization and vaporization, leading to a buildup of liquid fuel films in the intake port.

The small engine industry faces emissions standards that, in the future, will be stricter. Due to production cost and space constraints (compact engine design), the small engine industry cannot directly adopt technologies like electronic fuel injection, exhaust gas recirculation (EGR), and aftertreatment, which have been successfully implemented in automotive engines to dramatically reduce the levels of pollutant emissions. Thus, the goal is to reduce engine-out emissions by developing low cost, but at the same time reliable technology. This motivates the need to understand the emissions production mechanisms under these unique operating conditions.

Background

HC emissions mechanism in SI engines

Hydrocarbon (HC) emissions have been extensively investigated for automotive engines, where there is a reasonable understanding of the different formation mechanisms. Estimates of the relative contribution of each HC mechanism for a fully warmed up automotive SI engine are roughly as follows [2]: combustion chamber crevices 38%; flame quenching 5%; oil film adsorption 16%; combustion chamber deposits 16%; liquid fuel 20%; and exhaust valve leakage 5%. The ring pack crevices are the greatest contributor to HC emissions, but depending on the operating condition, others mechanisms could be equally important [2, 3, 4, 5]. During the compression stroke, the ring-pack crevice is filled with the unburned air-fuel-residual mixture. Part of that mixture, which escapes the main combustion event, returns to the cylinder after the time of peak pressure. Depending on combustion characteristics, the early portion of gas that flows back to the cylinder can be consumed by the flame. However, the remaining unburned gas in the ring pack that is released after the flame extinguishes mixes with the burned gas and might partially or totally react during the expansion and exhaust strokes, this reaction process is known as post-flame oxidation. The portion of the unburned mixture stored in the ring-pack that escapes the flame and survives post-flame oxidation contributes to the engine-out HC emissions.

Salazar and Ghandhi [6] performed several studies in order to assess the relative contribution of each mechanism to the engine-out HC emissions in a 2 cylinder, air-cooled, V-twin, utility SI engine, which is representative of the small engine category. The effect of liquid fuel films in the intake port on HC emissions was studied by replacing the carburetor with a homogenous, pre-vaporized air-fuel mixture delivery system; a carburetor-mounted liquid fuel injector system, was used to estimate the liquid film mass. The results from the homogenous pre-vaporized system were compared to the standard carburetor system. A comparison of the steady-state and cycle-resolved HC emissions and heat release analysis showed that under steady-state operating conditions, the fuel delivery system did not have a significant effect on the HC emissions for all of the conditions tested. Carbon monoxide (CO) and nitrogen oxides (NO_x) were also not affected. The cycle-resolved HC emissions showed no significant differences between fuel systems, and the heat release analysis did not find significant differences either. Using stop-injection tests, the liquid fuel mass in the manifold was estimated to be equivalent to 60 cycles worth of liquid fuel. The conclusion for this study was that the liquid fuel film was not an important contributor of HC emissions in small engines.

In another study in the same experimental facility, Salazar investigated the relative contribution of the ring pack crevice on HC emissions [4, 5] using a simple ring pack filling and discharging model. It was found that under high load conditions, the maximum unburned mass of HC stored in the ring pack was significantly higher than the total mass of HC measured in the exhaust; this led to the conclusion that the main contributor to HC emissions at high load was the ring pack crevice. For the same engine running at low load, the results of the ring pack model showed that the mass stored in the ring pack crevice was less than the HC mass measured at the exhaust, which suggests that the ring pack crevice was not the main source of HC emissions and other mechanisms were contributing significantly to the total engine-out HC emissions. Heat release analysis and cycle-resolved HC data showed that in a significant fraction of the cycles, the main combustion event did not finish before exhaust valve opening (EVO). These findings suggested that late combustion was an important contributor to HC emissions at low load conditions.

The effect of fuel absorption-desorption in the lubricating oil in small engines was also investigated by Salazar [7] in the same experimental facility using two different fuels - a standard full-blend gasoline and propane, the latter having approximately one order of magnitude lower solubility in oil than standard gasoline. No significant differences in HC emissions were observed with both fuels tested, which suggests that fuel absorption-desorption was not a significant source of HC emissions in small engines.

Post-flame oxidation of HC

Post-oxidation is a complex process that involves fuel chemistry, mass transfer and fluid mechanics. As describe above, crevice HCs are one of the main sources of HC emissions from spark ignition engines. The unburned gas is stored in the ring-pack crevice during the compression stroke and early stages of combustion, then flows back to the cylinder starting after the time of peak cylinder pressure. Initially, a thin layer of unburned gas is built up at the cylinder liner, which later diffuses toward the burned gas. Depending on temperature and mixing parameters, the unburned gas can react totally, react partially, or not react at all; the latter two cases contribute to HC emissions.

Min and Cheng [8] investigated the effects of crevice size on engine-out HC emissions in a single cylinder research engine fueled with propane. Modifications to the piston were achieved by machining the top-land crevice to increase the crevice volume, and the resulting HC emissions were compared to the maximum HC emissions that could be obtained for each condition, i.e. the maximum mass trapped in the crevices at peak pressure. The results showed that a 2.4x increase in the crevice volume led to a modest 15 to 18% increase in HC emissions, following an approximately linear trend with crevice volume. For all the engine operating

conditions tested, a similar trend of HC emissions with crevice size was observed. As an explanation for this low sensitivity, the authors suggested that a compensation effect occurs between crevice size and post-oxidation, in other words, an increase in crevice size (which implies an increase in the maximum HC index) is coupled with an increase in post-oxidation rate within the cylinder.

To prove that hypothesis, the authors developed a model for the transport and chemistry of the ring-pack gases. The model results showed that a significant portion of the total mass trapped in the ring-pack crevice is released during the early part of the expansion stroke, right after peak pressure. Therefore, the distribution of unburned HC along the cylinder liner showed higher concentration at the beginning of expansion stroke (near TDC) and a lower concentration at the latter part of the expansion stroke (near EVO). Despite the fact that the majority of the unburned gas is released in the early stage of expansion, the concentration of HC at this position along the liner is zero at the time of EVO, which means that the unburned gas was completely oxidized before EVO. On the other hand, the crevice mass coming out later during the expansion stroke survives post-oxidation because of the relative low bulk gas temperature and the shorter time available to diffuse and react.

Wu and Hochgreb [9] studied the post-oxidation process using a one-dimensional reactive-diffusive model with detailed chemical kinetics. For all cases simulated, it was found that the higher the initial burned gas temperature, the higher the oxidation rate. The results showed that for crevice gas released when the core gas was 1800K or higher, complete HC oxidation occurred. For mass released when the core gas temperature was between 1800 and 1400K, the extent of oxidation was full or partial, and below 1300K, the chemistry was frozen. Most of the remaining HC that contribute to the engine-out emissions correspond to the unburned mass released when the core gas temperature was below 1400K.

Eng, *et al.* [10] developed a global HC consumption rate correlation to predict post-oxidation and explain HC emissions from an SI engine. The engine tested was a single-cylinder Waukesha Cooperative Fuel Research (CFR) engine operated over a range of speed, load, spark timing and air-fuel ratio. The fuels tested were n-butane and iso-octane. The correlation was able to predict HC emissions for both fuels within 15% over all operation conditions. In their analysis they assumed that the ring-pack crevice was the dominant mechanism of HC emissions. For this investigation, the main conclusions from the authors were: 1) the majority of the HC consumption took place in the high temperature gas region, when $T > 1500\text{K}$. 2) For bulk gas temperature higher than 1500K, the HC consumption rate depended on the mixing rate of the cold unburned gas in the boundary layer with the hot burned gas. Once mixed, the chemical kinetic rate (which

depends on the temperature of the mixture) dominates the rate of consumption. 3) the overall HC consumption rate scales almost linearly with engine speed due to an increase of turbulence of the burned gas with speed, and an increase in the diffusion rate of HC to the burned gas due to a thinner boundary layer. 4) The variation of HC emissions with fuel type correlates with the inverse of diffusion coefficient of the fuel into nitrogen. The latter two points demonstrate the importance of mixing on the overall consumption rate. In addition, results from their correlation showed an Arrhenius type behavior, which in turns demonstrated the importance of temperature in post-oxidation as well.

The effect of spark timing on HC emissions was further investigated by Eng [11] to understand the reason why HC emissions decrease with spark retard. Experiments were performed at constant speed and load using pre-vaporized and premixed gasoline in a steady-state condition. Two air-fuel ratios were tested: slightly lean, 15:1 ($\lambda = 1.03$), and slightly rich, 13.8:1 ($\lambda = 0.95$). The results showed that a considerable fraction of the crevice mass is released into the cylinder before the end of flame propagation (CA90) for the condition when spark timing was retarded, and this mixture can then be oxidized in the flame. The consequence of this was that the main source of engine-out HC emissions was the HC that returned to the cylinder after the end of flame propagation. The extent of post-flame oxidation was also evaluated. For rich operation, a reduction of HC emissions with retarded spark timing was observed until a certain point; further retard of spark timing did not lead to a further reduction of HC emissions. According to the author, the reason for this 'transition' point where no further reduction in HC occurs was believed to be due to the lack of oxygen in the bulk gas. For lean experiments, where there was always enough oxygen available in the bulk gas, the reduction of HC with spark timing retard was almost linear. It was found that post-oxidation can occur both within the cylinder and the exhaust port, due to the fact that the temperature after EVO was still high enough to support post-oxidation.

Objectives

The objective of this study was to investigate the post-flame oxidation of unburned hydrocarbons in the cylinder following their release from the ring-pack. A more complete understanding of the post-oxidation process will allow the prediction of the HC emissions. Chemical processes such as post-oxidation are strongly temperature sensitive, so the first step was to develop an engine model that accurately predicts temperature. This model was used along with a ring-pack filling and discharging model to investigate the phenomenology of the processes that control the HC post-oxidation. This study focuses on high load (5-10 bar IMEP) and modest speed (1800 - 3600 RPM), in contrast to the previously discussed studies. These operating conditions

represent real-world small engine conditions that are included in the emission standards for these engines.

EXPERIMENTAL SETUP

The engine test cell for this study was previously described fully by Salazar [4, 6, 12], and only the main features are given here. The engine tested was a Kohler CH23, 2 cylinder V-twin, air-cooled, utility spark ignition engine, that is representative of the small engine group. The intake system was modified by replacing the carburetor with a homogenous, pre-vaporized, air-fuel mixture system. The fuel was injected 1 meter upstream and two heaters were installed to control the temperature of the intake mixture to 50 °C to ensure fuel vaporization. The exhaust manifold was also modified; a separate exhaust system was installed for each cylinder and the exhaust gas was sampled from each cylinder individually. The engine was controlled using the MotoTron suite of software. Geometric specifications of the engine are given in [table 1](#).

Table 1. Engine specification

Type	Kohler CH23 two cylinder 90°V
Bore/Stroke	80 mm/67 mm
Displacement	674 cc (for both cylinder)
Compression ratio	8.15
Intake valve timing	IVO: 22 bTDC IVC: 134 bTDC
Exhaust valve timing	EVO: 130 aTDC/ EVC: 26 aTDC

Average CO, CO₂, HC, NO_x and O₂ emissions were measured in both cylinders separately using a Horiba standard 5 gas bench. Time-resolved pressure data were measured for both cylinders, both exhaust ports, the intake manifold and the crankcase. The fuel utilized was a standard full-blend gasoline US EPA TIER II EEE certification fuel. Air was supplied to the engine from the compressed air line of the building; the mass flow rate of air was controlled and measured by critical orifice plates.

Two-Zone model development

As mentioned above, HC post-oxidation is very temperature sensitive, thus an accurate estimate of the gas temperature is necessary. Although a single-zone heat release analysis, which is commonly used for analyzing pressure data, can provide a good estimate of the bulk gas temperature, it does not provide burned gas temperature which could be relevant to the post-oxidation process, so a two-zone approach was used. Moreover, the long-term goal is to incorporate the post-oxidation model into a thermodynamic combustion

simulation, so instead of performing a two-zone heat release analysis, a two-step procedure was undertaken. In the first step, a single-zone heat release analysis was performed to determine a first estimate of the heat release rate. In the second step, this heat release rate was utilized in a two-zone combustion simulation as described more fully below.

The model calculates the thermodynamic state of the in-cylinder contents during the compression, combustion, expansion and exhaust strokes, *i.e.* from IVC to EVC. The main assumptions of the model are listed as follows: 1) For the closed portion of the cycle (IVC to EVO) the trapped mass is constant. 2) For the exhaust stroke (EVO to EVC), the in-cylinder mass was calculated using a quasi-steady, one-dimensional compressible flow rate through the exhaust valve. 3) During combustion, the cylinder charge was divided in two zones separated by the flame front. The unburned gas ahead of the flame consists of fresh air-fuel mixture and residual gas, while the burned gas consists of combustion products at chemical equilibrium. Both gases obey the ideal gas law. 4) During compression, only unburned gas exists, and after combustion only burned gas is assumed to occupy the entire combustion chamber. 5) For both zones, it is assumed that the gas consists of a spatially homogenous mixture where thermodynamic and transport properties are averaged and vary only with time. 6) The in-cylinder pressure is spatially uniform throughout the combustion chamber. The chemical equilibrium composition, as well as thermodynamic and transport properties were calculated using the open-source CANTERA software [13]. The fuel utilized in the simulations was iso-octane. The heat transfer coefficient was modeled using the Annand correlation [15]. The NO concentration was calculated using the extended Zeldovich mechanism [14]. More details about the formulation of the two-zone model can be found in [15, 16, 17, 18, 19, 20].

Adjustment procedure

Heat transfer is not well understood in IC engines, and in zero-dimensional modeling the heat transfer term has the highest uncertainty of all parameters. Therefore, the approach taken here was to adjust the heat transfer coefficient using a multiplicative factor in order to match the calculated NO concentration at EVO to the measured NO_x emissions. There were also some other adjustments made to improve the agreement between the measured and simulated pressure trace. The in-cylinder trapped mass was adjusted to better match the peak pressure, and the Wiebe function parameters, *i.e.* the start of combustion and combustion duration, which were found by fitting the Wiebe function to the cumulative heat release curve, were slightly adjusted to match the location of the peak pressure and the width on the trace. Performing these adjustments, the extent of agreement between measured and calculated pressure trace was excellent for all condition tested. [Figure 1](#) shows a sample result of pressure traces calculated with the two-zone model

and the corresponding measured pressure curve. To validate the adjustment procedure, the results of the trapped mass of both cylinders were used to calculate the total delivered mass to the engine. This value was compared to the measured delivered mass, and the results showed an excellent agreement for all conditions tested [21]. It is assumed that since the model does such a good job of estimating the cylinder pressure, there should not be inaccuracies in the temperature determination.

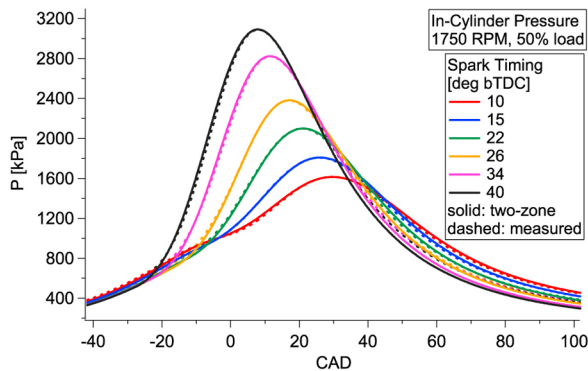


Figure 1. Measured and calculate in-cylinder pressure, spark timing sweep. Trapped mass and heat transfer coefficient multiplier tuned to match pressure and NOx emissions

Ring-Pack gas flow model

HC emissions from the ring-pack crevice depend on the mass flow rate into and out of the crevice region. A simplified ring-pack model was used to calculate mass storage in the crevice and the mass returning to the cylinder. The model characteristics have been described in detail by Salazar [4, 5, 12], and here only the main features will be provided. Similar ring-pack models have been successfully implemented in previous studies [8, 11, 22, 23, 24, 25].

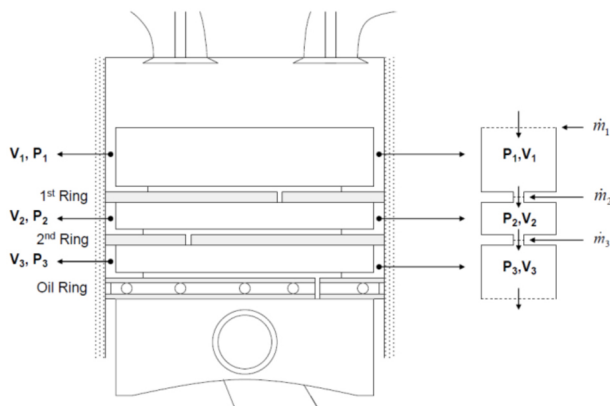


Figure 2. Schematic of the ring-pack configuration (taken from [12])

The ring-pack configuration is shown in Fig. 2. It consists of two compression rings and one oil control ring. The rings, liner and piston crown form three volumes that are connected through the ring end gap. The mass stored and released by the ring-pack was calculated with a one-dimensional, quasi-steady compressible gas flow model through an orifice [15, 22]. The results of the ring-pack model are: inter-ring pressure (P_2 in Fig. 2), mass flow rates (see Fig. 3), cumulative mass flow into the crevice (Fig. 4), cumulative mass returned to the cylinder (Fig. 5) and the blowby mass. All of these variables are a function of crank angle.

Figure 3, 4, 5 shows sample results of the ring-pack model for the baseline operating condition (3060 RPM, 50% load, air-fuel ratio 12)

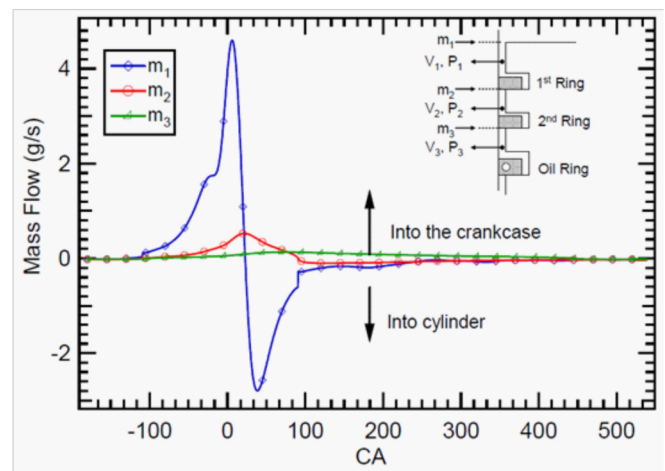


Figure 3. Mass flow rate of gas through the top-land crevice (m_1), first ring end gap (m_2), and second end ring gap (m_3). Operating condition: 3060 RPM, 50% load, air-fuel ratio 12:1

Figure 3 shows the mass flow rate of gas crossing the top-land crevice (m_1), the first ring end gap (m_2) and the second ring end gap (m_3), as function of crank angle degree. Positive values correspond to flow toward the crankcase while negative values are flow toward the cylinder. During compression, the ring-pack crevice is filled with gas at an increasing flow rate (a positive values of m_1 , blue curve in Fig. 3), reaching its peak a little after TDC (~ 6 CAD aTDC). In this case, peak cylinder pressure occurs at approximately 21 CAD aTDC (not shown here). Immediately after peak pressure, the flow reverses and the gas stored in the top-land starts to flow back to the cylinder, reaching its peak value at approximately 30 CAD aTDC. The discontinuities observed at ~ 110 CAD bTDC and 90 CAD aTDC are due to a change in position of the ring inside the groove (change in direction of net force on the ring).