Post-Flame Oxidation of Unburned Hydrocarbon in Spark Ignition Engines

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1. MOTIVATION

It is known that a major contributor to the unburned hydrocarbons (HC) emissions from an SI engine is the storage of fuel in the ring-pack crevice, where it escapes the main combustion event, and its subsequent return to the cylinder. A substantial fraction of this fuel mass can react within the cylinder after its release from the crevice. This process is known as post-flame oxidation, and this process needs to be fully understood in order to develop a predictive HC emission model.

2. THE POST-FLAME OXIDATION PROCESS

During compression and early combustion, unburned mixture is stored in the crevices. After peak pressure, the mixture flows back into the cylinder. The portion released early might be consumed by the flame. After the flame extinguishes, the burned gas can still be hot enough to support HC oxidation. During exhaust, the temperature of the bulk gas is lower, so the chemistry is frozen.

Post-flame oxidation is controlled by both the mixing and chemistry rates.

3. RING-PACK GAS FLOW MODEL

HC emissions depend on the amount of mass stored in the ring-pack. Mass flow into and out of the ring-pack crevice is calculated. The flow rate back into the cylinder is higher in early expansion stroke. During the late expansion and exhaust strokes, the mass flow rate decreases.

Engine Tested

- Two cylinder 90º V-twin Utility engine.
- Air cooled.
- Bore/stroke: 80 mm/67 mm
- Displacement: 674 cc
- Compression ratio: 8.15
- Intake Valve Timing: IVO: 22º bTDC, IVC: 134º bTDC
- Exhaust Valve Timing: EVO: 130º aTDC, EVC: 386º aTDC
- Normalized mass of HC within the unburned gas parcel

4. FRACTION OF CREVICE GAS POST-FLAME OXIDIZED

Not all the unburned crevice gas that returns to the cylinder contributes to engine-out HC emissions.

- The first fraction of gas released from the crevice is consumed by the flame.
- The following fraction is exposed to a high temperature environment, thus post-flame oxidation takes place.
- The last fraction to be released does not react because of the lower burned gas temperature; it leaves the engine as HC emission.

5. DETAILED CHEMICAL KINETIC, ZERO-D MODEL

The model follows the oxidation process of a small parcel of unburned crevice gas from the time it is released until EVC. Burned gas is injected at a fixed rate.

- As the gases are mixed, the parcel warms up.
- If the temperature is high enough, reaction takes place.
- The parcel’s gas composition evolves with time. The final fraction of HC at EVC is quantified: \( w_{\text{HC,EVC}} \)

Models specification

- Cantera (open-source toolkit for MATLAB)
- ERC-PRF mechanism with 45 species and 155 reactions.
- Iso-octane as raw fuel

6. NEW METRIC TO QUANTIFY EXTENT OF HC POST-OXIDATION

- Normalized mass of HC within the unburned gas parcel
- THCE: Total Hydrocarbons: EVC: Exhaust Valve Closing time
- Mass of HC at EVC
- Max THCE post-oxidation

Sample case: parcel released at 270 CA\(^\circ\) aTDC
- Parcel is fully consumed by the time of EVC.
- Less than 50% of THC is consumed by EVC.
- Approx. 57% of the unburned crevice HC survives post-oxidation (i.e. \( w_{\text{HC,EVC}} = 0.57 \)).
- This 57% contributes to the engine-out HC emission.

7. KINETICALLY CONTROLLED HC EMISSION CALCULATION

- The results of the kinetic model described above are affected by the mixing rate (\( w_{\text{mix,opt}} \)).
- For a given release time, there is an ‘optimum’ mixing rate that provides the minimum HC emissions.
- Knowing the mass of crevice HC returning to the cylinder and its extent of oxidation, the engine-out HC emission is calculated.

8. PRELIMINARY RESULTS

- For a given operating condition, a “theoretical” minimum of HC emission can be estimated using the optimized mixing rate in the chemical kinetic model for each release time.
- The majority of the crevice HC returns during expansion stroke.
- This fraction is completely oxidized.
- Engine-out HC emissions comes from crevice HC that are released during exhaust stroke.

9. FUTURE WORK

- The effect of the oxygen level in the mixture (air-fuel ratio) will be investigated.
- Air-fuel ratio affects the engine operating condition in multiple ways. The goal is to isolate the effect of the oxygen concentration by fixing variables such as in-cylinder pressure and temperature.
- Is it possible to obtain zero engine-out HC emission? If not, what is the minimum possible? This study aim to answer these questions. The idea is to identify theoretical boundaries for how much post oxidation can actually take place, therefore establishing the minimum engine-out HC emission for a given operating condition.