Understanding the dynamic evolution of cyclic variability at the operating limits of HCCI engines with negative valve overlap

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ABSTRACT

An experimental study is performed for homogeneous charge compression ignition (HCCI) combustion focusing on late phasing conditions with high cyclic variability (CV) approaching misfire. High CV limits the feasible operating range and the objective is to understand and quantify the dominating effects of the CV in order to enable controls for widening the operating range of HCCI. A combustion analysis method is developed for explaining the dynamic coupling in sequences of combustion cycles where important variables are residual gas temperature, combustion efficiency, heat release during re-compression, and unburned fuel mass. The results show that the unburned fuel mass carries over to the re-compression and to the next cycle creating a coupling between cycles, in addition to the well known temperature coupling, that is essential for understanding and predicting the HCCI behavior at lean conditions with high CV.

INTRODUCTION

It was early noted that homogeneous charge compression ignition (HCCI) combustion can have low cyclic variability (CV) compared to spark ignited (SI) combustion [1]. However, at certain operating conditions, even if all inputs are held constant, the combustion phasing can alternate between early and late timing in a oscillatory manner or run away towards increasingly advanced conditions. The process can exhibit significant oscillations at late phasing [2, 3] and runaway-knock phenomena at high loads [4]. This behavior points to the fact that there is considerable nonlinear feedback between cycles that can stabilize or destabilize the process. The coupling has been attributed to the fast variations from cycle to cycle in combustion inefficiency and residual gas temperature [5, 6] and the slower variation of the cylinder wall temperature [4, 7, 8].

HCCI can be achieved with variable valve timing and the focus here is on the negative valve overlap (nvo) strategy. This re-compression strategy is also known as controlled autoignition (CAI) and means that autoignition is induced by raising the charge temperature of the next cycle by trapping and compressing residual gases from earlier cycles through an early closing of the exhaust valve [9].

To investigate the nature of CV, we perform a set of experiments and then analyze the data in order to arrive at an interpretation of the dynamical behavior of the process. To enable the analysis, standard combustion analysis methods are extended with a novel method for determining the unburned fuel mass and combustion efficiency on cycle basis. The main contribution in our work is this thermodynamic analysis of the experimental data which explains and quantifies the dominating effects governing the process. Specifically, the analysis show that lean HCCI combustion with high CV is mainly the result of the recycled thermal energy in the residual gas and the unburned fuel passing over to the re-compression and to the next cycle.

Experiments with the re-compression strategy at conditions with noticeable CV were performed and analyzed in [5, 10]. Linear correlation coefficients were also computed to study the relationships between subsequent cycles. Control of valve timings and injection timings for reducing the CV was developed in [11, 12] based on model linearizations. Our analysis corroborate the trends found in [5, 10] and used in [11, 12] but also show that, for high CV, the relationships are more complicated than can be captured with a linear analysis. Specifically, there are sequences of cycles, characterized by combustion phasing and heat release, that occurs with increasing probability when the CV increases.

The focus here is on understanding lean HCCI combustion operated with nvo. Wagner et al. [13, 14] report experimental observations and analysis of transitions, using variable valve timing, between SI and spark-assisted HCCI combustion with stoichiometric mixtures where the process transitions through regions with high CV. These conditions give qualitatively different dynamical behavior than the lean case without spark assist.
HCCI engines operating with intake heating and a low amount of residuals also show different behavior, as shown in [15].

Experimental work investigating the effect of different mixtures of primary reference fuels on CV in HCCI are found in [16–18]. An analysis of the stability of HCCI with large amounts of residual gas was done in [19] where, by studying the thermal dynamics of the charge, unstable behavior with limit cycles at late phasing and runaway knock at early phasing were predicted. Similar analysis is also shown in [20]. Our work show that, for higher CV, the effect of unburned fuel creates an additional coupling that must be taken into account. The use of injecting fuel during the nvo period for control was mentioned in [9] and experimentally investigated in [21, 22] and used in [23, 24] to extend the low load limit of HCCI. In the present work, the injection parameters are constant for each operating point and the effect of the unburned fuel, recycled from incomplete combustion in previous cycles, is investigated.

The objective here is to identify, understand, and quantify the most influential properties for the CV to enable control-oriented modeling. A simulation model for studying misfire in HCCI using chemical kinetics with 31 species and air flow model was developed in [25] and reduced to a eight state model in [26]. Our aim is to find the dominant factors and a minimum set of variables for describing CV.

The paper is organized as follows. The experimental setup is described first and the data analysis method used is outlined. After that, the results from the methodology are interpreted in order to explain the dynamic behavior of the combustion process. Finally, the conclusions from the work are summarized.

**EXPERIMENTAL SETUP**

Experiments were performed at the Automotive Laboratory at University of Michigan on a single-cylinder gasoline direct-injected engine with a Ricardo Hydra crankcase. The engine is equipped with an electro-hydraulic fully-flexible valve actuation (FFVA) system from Sturman Industries, which allows lift, timing, and duration of each valve event to be controlled independently. Fuel is delivered via a gasoline injector mounted between the two intake valves and aimed into the piston bowl. The engine geometry is listed in Table 1, while a detailed schematic of the engine setup is seen in Fig. 1. More details for the experimental setup can be found in [27]. The usable range of HCCI for the engine was determined by Manofsky et al. [27] and is shown by the shaded region in Fig. 2. Experiments were performed at various fueling rates, indicated by lines in Fig. 2, and nvo was varied to control combustion phasing. Fuel was delivered with a single injection, starting at a crank angle 330° before top dead center combustion (TDCm). The fuel used was research-grade gasoline (90.5 RON, 82.6 MON). The usable HCCI operating range was limited by high CV (measured by the coefficient of variation, CoV, of IMEP) at late phasing and high ringing intensity (RI) at early phasing. In [27], these limits were chosen to a CoV of IMEP of 5% and a RI of 4 MW/m². Note that the focus in the current work is on individual engine cycles and that these values are averages over many cycles only used to depict the feasible operating range. As indicated in Fig. 2, at low loads, a large range of nvo could be spanned before the limits of combustion were reached. However, at higher loads, slight changes in nvo had a greater effect on combustion. As fueling was increased, the limits of ringing intensity and CV converged and the operating range became narrower.

The analysis in the present work is focused on the two square points in Fig. 2, at fuel injection of 9.6 mWcycle, that transition from acceptable CV to higher CV. These conditions are a typical medium load operating point corresponding to net IMEP is approximately 2.8 bar with $\lambda = 1.7$. To fully observe and analyze the patters of cycle–to–cycle coupling, in-cylinder pressure

<table>
<thead>
<tr>
<th>Component</th>
<th>Characteristic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinders</td>
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</tr>
<tr>
<td>Displaced volume</td>
<td>550 cm³</td>
</tr>
<tr>
<td>Stroke</td>
<td>94.6 mm</td>
</tr>
<tr>
<td>Bore</td>
<td>86.0 mm</td>
</tr>
<tr>
<td>Connecting rod</td>
<td>152.2 mm</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>12.5:1</td>
</tr>
<tr>
<td>Number of valves</td>
<td>4</td>
</tr>
<tr>
<td>Piston shape</td>
<td>Shallow bowl</td>
</tr>
<tr>
<td>Head design</td>
<td>Pent-roof</td>
</tr>
<tr>
<td>Fueling method</td>
<td>Direct injection</td>
</tr>
</tbody>
</table>

Table 1: FFVA engine geometry.
The definitions of the engine cycle and important variables are given in Fig. 4 together with typical curves of measured pressure $p(\theta)$, calculated heat release $Q(\theta)$, and known valve lift (dashed line).

Figure 3: Block diagram for the iterative estimation routine using measurements of $\lambda, m_i, p(\theta)$, and $T_{ex}$.

Figure 4: Definition of the engine cycle and important variables for typical curves of measured pressure $p(\theta)$, calculated heat release $Q(\theta)$, and known valve lift (dashed line).

was sampled at each crank angle degree for 3000 consecutive cycles. Nominal operating conditions for the experiments were 2000 rpm, controlled by a hydraulic dynamometer, and a coolant temperature that was controlled at 90°C. Analysis of points at lower and higher load were also done revealing that the same characteristics appear at these loads with the addition of runaway knock phenomena at higher loads.

DATA ANALYSIS

To analyze the experimental data an iterative estimation routine, depicted in Fig. 3, based on conservation of mass and energy is used. A novel method for estimating the mass of unburned fuel on a cycle basis is developed and combined with standard combustion analysis methods. The goal is to calculate the thermal-mechanical state, pressure and temperature, as well as variables important for explaining CV, such as unburned fuel and combustion efficiencies. The process is iterated until the values of combustion efficiencies converge at which point the governing relations of mass and energy conservation are satisfied.

The definitions of the engine cycle and important variables are given in Fig. 4 together with typical curves of measured pressure $p(\theta)$, calculated heat release $Q(\theta)$, and known valve lift. Note that the heat release is calculated for both the main combustion event, between intake valve closing (ivc) and exhaust valve opening (evo), and the nvo period, between exhaust valve closing (evo) and intake valve opening (ivo). Top dead center main combustion is 0° and a new cycle starts at ivc. The total heat release in cycle $k$ during main combustion and the nvo period are denoted by $Q_m(k)$ and $Q_n(k)$ respectively. In cycle $k$, the 50% burn angle where half the $Q_m$ has occurred during main combustion is denoted by $\theta_{50}^m(k)$ and the corresponding angle during the nvo period is denoted by $\theta_{50}^n(k)$.

In the remainder of this section, the method for estimating the mass of unburned fuel on a cycle basis is derived. The other steps shown in Fig. 3 are based on standard methods and are described in detail in the Appendix.

UNBURNED FUEL In order to model the mass of unburned fuel on cycle basis, a difference equation is derived for the unburned fuel mass that depends on known quantities and an initial unburned fuel mass. It is observed that the equation converges to the correct value given any initial guess. The model is subsequently used to estimate the combustion efficiencies.

The main combustion consumes a fraction $\eta_m(k)$ of the fuel mass and after the exhaust phase a fraction $x_r(k)$ of the residual gases is trapped. During re-compression a fraction $\eta_n(k)$ is further consumed so that, with homogeneous residuals, the unburned fuel mass carried over to the next cycle $k+1$ is

$$m_u(k+1) = x_r(k) (1 - \eta_m(k)) \left( 1 - \eta_n(k) \right) m_i(k)$$

where the fuel mass $m_i(k)$ in the beginning of cycle $k$ is

$$m_i(k) = m_i(k-1) + m_u(k)$$

with $m_i(k-1)$ being the injected fuel mass. The unknown combustion efficiencies in (1) are now related to the accumulated heat release. The gross heat released during main combustion $Q_m$ is modeled by

$$Q_m(k) = m_f(k)\eta_m(k)q_{lhv}$$

with $q_{lhv}$ as the lower heating value for the fuel. As explained above, the fraction $\eta_m(k)$ of the fuel mass is consumed during main combustion and then the fraction $x_r(k)$ of the residual gases is trapped. Thus, the gross heat released during re-compression $Q_n$ is given by

$$Q_n(k) = m_f(k)(1 - \eta_m(k)) x_r(k) \eta_n(k) q_{lhv}.$$
factor of $0.4^k < 1/1000$ after 8 cycles. The results are practically indistinguishable after this number of cycles for all cases starting from different initial conditions. This is demonstrated in Fig. 5 which shows the first iterations, starting from a range of initial conditions, for two cases. The approach adopted here is to guess $m_u(0) = 0$ and discard the first cycles in the analysis. Finally, when the unburned fuel mass is computed, (3) and (4) give

$$
\eta_m(k) = \frac{Q_m(k)}{q_{lhv}} m_i(k)
$$

(5a)

$$
\eta_n(k) = \frac{Q_n(k)}{x_r(k) (m_i(k) - Q_m(k)/q_{lhv})}
$$

(5b)

as approximations for the efficiencies which depends on the total gross heat releases ($Q_m, Q_n$) and residual gas fraction $x_r$. The computation of these quantities are based on standard methods and are described in the Appendix.

The proposed estimation of unburned fuel, based on the model (1), includes possible heat release during re-compression, the term $Q_n(k)$, which is neglected in previous low-order models associated with higher CV in HCCI–SI transients [28]. Simulation models with higher fidelity, including the effect of unburned fuel, are used in [25, 26] to study the effect of misfire in HCCI. In contrast, the aim here is to estimate the unburned fuel mass from experimental pressure data.

RESULTS

Observations from the data processing described in the previous section, applied on the measurements, are interpreted here. Results are shown for different nvo settings transitioning from lower to higher values of CV. The observations show that lean HCCI combustion with high CV is the result of unburned fuel passing over to the re-compression and to the next cycle which is supported by the following three important findings:

- There is a strong coupling and complementarity of the fuel burned during the main combustion and the re-compression events.
- Despite the complementarity, the available fuel does not necessarily burn during one cycle meaning that unburned fuel may carry over to the next cycle.
- Following a partial misfire, injection after TDC of re-compression does not necessarily cause combustion.

To explain and quantify these findings we highlight results from experiments with two nvo settings.

All the measured cylinder pressure traces for the two cases are shown in the upper half of Fig. 6. The lower part of the figure shows the charge temperatures computed from the heat release analysis. When reducing the overlap from 153° to 147° the average residual gas fraction reduces from 46% to 44% (see Fig. 17 in the Appendix). The average combustion phasing $\theta_m^{50}$ is pushed from 7.4° to 9.7° and the standard deviation is increased from 0.9° to 2.4°. The CoV of IMEP raises from a moderate 2.4% to a value of 13.3% which is typically considered above the acceptable limit. A few consecutive cycles are marked in Fig. 6, with the numbers 6 to 9, for the high CV case with nvo of 147°. These show, in the upper part of the figure, the peak pressure locations and, in the lower half, they identify the corresponding temperature traces. The same cycles are also shown in Fig. 7, 9, and in more detail in 13–15.

The spread of the attained pressures and temperatures generally increases when reducing nvo as shown in Fig. 6. Both lower and higher peak pressures and pressure rise rates are seen. The temperature during the re-compression does, however, mostly increase which suggests that if the temperature at evo is low,
The estimates of the residual gas fraction \( x_r \) were found to be close to normally distributed (see the normal probability plot in Fig. 18 in the Appendix) indicating that the variability in \( x_r \) is random and without deterministic structure. The result in Fig. 8 further indicates that the variability in \( x_r \) has no clear influence on the heat release during main combustion \( Q_m \). For the high CV case the cloud of points is moved to the left, since the mean \( x_r \) is reduced, and stretched vertically, due to the higher variability in \( Q_m \), but no trends appear.

In Fig. 9(a)–(d) the phasing \( \theta_{50}^m(k) \) of main combustion, the temperature \( T_{evo}(k) \) at evo, the heat release \( Q_m(k) \) during the nvo period, and the temperature \( T_{ivo}(k) \) at ivo are all plotted versus the heat release \( Q_m(k) \) during main combustion in the same cycle \( k \). Additionally, Fig. 9(e) and (f) show the phasing of the next cycle \( \theta_{50}^m(k+1) \) and the unburned fuel in the next cycle \( m_u(k+1) \) versus \( Q_m(k) \). Figures 9(a)–(b) show that as \( Q_m \) decreases and CV increases, late burns with low values of \( Q_m \) occur. These late cycles are associated with a lower temperature at evo and thus, here, the low combustion efficiency dominates the effect of late phasing on \( T_{evo} \). With a lower \( Q_m \) there is a higher heat release \( Q_u \) during the subsequent nvo period as shown in Fig. 9(c). The end result is that a low \( Q_m \) is correlated with a higher temperature at ivo which is seen in 9(d). Figure 9(e) also shows that the increased residual charge temperature, through increased \( T_{ivo} \), tends to advance the phasing of the next cycle \( \theta_{50}^m(k+1) \). Figure 9(f) shows that, for the case with lower CV, the unburned fuel is approximately 0–6% of the injected fuel. For higher CV and particularly cycles with low \( Q_m(k) \), the unburned fuel can reach up to higher values of approximately 10% of the injected fuel. Values up to 14% of the injected mass have been seen in an operating point with nvo of 145\(^\circ\) and CoV of IMEP of 17.8\%. In summary, \( T_{ivo}(k) \) decreases with decreasing \( Q_m(k) \) but this effect is offset by \( Q_u(k) \) leading to an increase in \( T_{ivo}(k) \) and thus, the residual charge temperature of the next cycle increases and \( \theta_{50}^m(k+1) \) advances. In addition, the unburned fuel mass carrying over to the next cycle is increased when the main combustion has a poor efficiency even though there is heat release during the re-compression. This chain of events is also evident for the sequence of cycles \( k = 6, . . . , 9 \) marked in Fig. 9. The seventh cycle burns late with a low \( Q_m \) causing low \( T_{evo} \). Some of the unburned fuel burns during nvo giving a high \( Q_u \) and increased \( T_{ivo} \). The following cycle, number 8, has an early phasing and an unburned fuel of about 8% of the injected fuel mass, as shown in the bottom two plots. The bottom right plot also shows that during the eighth cycle with a high \( Q_m \) all the unburned fuel is depleted.
Note that the trends in Fig. 9(a) and (f) are reversed. A low $Q_m(k)$ in cycle $k$ is correlated with a late phasing $\theta_{50}^m(k)$ but, as explained above, correlated with an early phasing $\theta_{50}^m(k+1)$ of the next cycle. It is thus crucial to have a clearly defined engine cycle when studying data from operating conditions with high CV.

The calculated $\eta_m(k)$, through Eq. (5a), versus combustion phasing $\theta_{50}^m(k)$ in main combustion is shown in Fig. 10. The spread in ($\theta_{50}^m, \eta_m$) becomes larger with increasing CV and the mean of $\eta_m$ has a negative trend with a sharp falloff when phasing is retarding. The peak combustion efficiency, the combustion timing where the efficiency starts to drop, and the rate with which the efficiency drops are features that are expected to vary and primarily depend on equivalence ratio and engine speed according to the experimental results in [29] and the computational fluid dynamics studies in [30]. These conditions are fairly constant for the operating conditions here but the relationship between efficiency versus phasing has the expected qualitative trend.

The computed $\eta_n(k)$, see Eq. (5b), are shown in Fig. 11 versus phasing during nvo $\theta_{50}^n(k)$ and in Fig. 12 versus the main combustion efficiency $\eta_m$ (5a). Since $\eta_n$ is undefined when there is negligible unburned fuel mass, only points where noticeable heat release occurs are plotted. Because of this, there are no points in Fig. 11 or 12 for the low CV case. For the combustion efficiency during the nvo period, there is no clear correlation with phasing in Fig. 11. Most of the cycles with significant heat release during re-compression have a rather early phasing of 4 to 10 degrees before top dead center and an efficiency of 50% to 80%. In Fig. 12, the majority of the points lies under the diagonal which shows that, when heat release occur during nvo, the efficiency $\eta_n$ is typically lower than during the main combustion $\eta_m$. Note that more accurate estimates of the efficiencies can be obtained by analyzing gas samples on a cycle basis but with the current experimental setup we are limited to pressure-based analysis. Moreover, it is noted that the value of $\eta_n$ is more challenging to estimate than $\eta_m$ due to a lower signal (the heat release during re-

![Figure 9: Heat release $Q_m(k)$ during main combustion versus combustion phasing $\theta_{50}^m(k)$ during main combustion, temperature $T_{evo}(k)$ at evo, heat release $Q_n(k)$ during the nvo period, temperature $T_{nvo}(k)$ at ivo, combustion phasing $\theta_{50}^n(k+1)$, and unburned fuel $m_u(k+1)$.](image9)

![Figure 10: Combustion efficiency $\eta_m$ and scaled averaged pressures for high and low CV. The efficiency decreases quickly with late combustion phasing $\theta_{50}^m$.](image10)

![Figure 11: Combustion efficiency $\eta_n$ versus the phasing $\theta_{50}^n$ during re-compression and a scaled averaged pressure.](image11)
Figure 12: Combustion efficiency $\eta_n$ during nvo versus efficiency $\eta_m$ during main combustion for high CV.

Figure 13: Gross heat release for consecutive cycles in conditions when the CV is high. The markers identify the corresponding cycles in 14. Cycles 6–9 are also shown in Fig. 6, 7, 9.

compression) to noise ratio (noise in the pressure measurements and the accuracy of the heat transfer model).

CYCLE EVOLUTION To study how the cycles evolve, when the CV is high, in some detail a few illustrative cycles are selected from the condition corresponding to an nvo setting of 147°. After that, return maps are used to show that this qualitative behavior is indeed typical for this operating condition. Out of the 15 selected cycles, 6–9 were discussed also in the previous section, in connection with Fig. 6, 7, and 9. That perspective suggested that the sequence started and ended with seemingly regular cycles and in between there were two extreme ones with low and high heat release. However, studying the dynamical behavior in more detail reveals that there is a sequence of several cycles leading up to the extreme ones.

The gross heat releases for the 15 selected cycles are shown in Fig. 13, the combustion phasing and net IMEP are shown in Fig. 14. From the IMEP and the heat release traces it is seen that the first six cycles have approximately a period-2 cycle. All odd cycles have lower heat release during main combustion and higher during re-compression compared to the even cycles.

This leads to oscillations in the initial temperature which are transferred to the phasing and efficiency of the combustion. The combustion phasing oscillates with an increasing amplitude as seen in Fig. 14. Due to the fact that the combustion efficiency drops sharply when the phasing is late, as shown in Fig. 10, the increasing amplitude eventually leads to a particularly poor burn in the seventh cycle, marked with bold lines in Fig. 13–14. This leads to a heat release and a peak pressure, see Fig. 6, during nvo that are higher than previously. The following cycle has an early phasing due to the elevated initial temperature. Cycle 8 also has the largest heat release of all cycles which indicates an efficient burn, due to earlier phasing, of the injected fuel plus unburned fuel from previous cycles. The following cycle has an average heat release but an early phasing indicating that the initial temperature is elevated after the high heat release in the eight cycle. The two extreme cycles, 7 and 8, cause the combustion to recover and then, at least temporarily, continue with average values of phasing and heat release.

Figure 15 shows the return maps for the combustion phasing $\theta_m$ and the total gross heat release $Q_m$ for all cycles at the operating point studied. The return map is a plot of the variable at cycle $k$ versus the value at the next cycle $k + 1$ and so reveals relationships between subsequent cycles. The 15 cycles from Fig. 13–14 are marked and the evolution of cycle 5–9 is traced with arrows.
The observations collectively show that quantifying the unburned chemical energy in the unburned fuel mass are very important to explain the behavior of CV. These nonlinear couplings between cycles, in addition to the known coupling effect of temperature, that is essential to take into account in order to understand, predicting, and eventually controlling HCCI combustion smoothly. Ongoing efforts have also shown that if these dominating mechanisms are modeled, the observed behavior can be reproduced.

**ACKNOWLEDGMENTS**

Laura Manofsky in the Automotive Laboratory at University of Michigan is thanked for all help acquiring the measurements.

This material is based upon work supported by the Department of Energy (National Energy Technology Laboratory) under award number DE-EE0003533. This work is performed as a part of the ACCESS project consortium (Robert Bosch LLC, AVL Inc., Emitec Inc.) under the direction of PI Hakan Yilmaz, Robert Bosch, LLC.

**REFERENCES**


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The properties $\gamma(\theta)$ and $R(\theta)$ are first assumed to be constant and equal to the values for unburned gas. Solving (6) and (7) gives the accumulated heat release $Q(\theta)$. The cylinder temperature is $T_{cyl} = pv/mR$ where $m$ is $m_c$ for the main combustion and $m_r$ for the nvo period. The thermodynamic properties are then updated based on the mass fractions $y(\theta)$,

$$y(\theta) = (1 - x_b(\theta))y_u + x_b(\theta)y_b(\theta)$$

where $x_b(\theta)$ is the mass fraction burned curve defined by

$$x_b(\theta) = \frac{\eta Q(\theta)}{\max Q(\theta)}$$

with $\eta$ being $\eta_m$ for main combustion and $\eta_n$ for nvo combustion. The fractions $y_u$ and $y_b(\theta)$ represent the compositions of the unburned and burned gas respectively. The composition $y_b(\theta)$ is computed for chemical equilibrium at $(p(\theta), T(\theta))$. The equilibrium and the thermodynamic properties for a given composition can be found by chemical equilibrium software, e.g., [35]. This process is iterated until the values of the properties change less than a given tolerance. Finally, the total gross heat release during the main combustion and re-compression, denoted by $Q_m$ and $Q_n$ respectively, are given by

$$Q_m(k) = \max_{\theta \in (ivc,evo)} Q(\theta)$$

$$Q_n(k) = \max_{\theta \in (evo)} Q(\theta)$$

when the process has converged.

CHARGE MASS

The computation of the fresh charge mass uses the relative air-fuel ratio $\lambda$, determined from exhaust species measurements, and injected fuel mass $m_i$, measured by a flow meter, together with the estimate of unburned fuel $m_u$, see Fig. 3. The accurate determination of the fresh charge on a cycle basis is complicated and the most accurate method available for this work is relying on exhaust measurements sampled once every second. With lean combustion, small cyclic variations in air charge should have minor influence on the combustion in comparison to, e.g., the mass of unburned fuel. For these reasons, the fresh air charge inducted $m_a(k)$ is assumed to be equal for all cycles $k$ and computed from the relative air-fuel ratio $\lambda$, which correspond to an averaged value, according to

$$m_a(k) = \bar{\lambda} \bar{m}_i AF_{i}$$

where $AF_i$ is the stoichiometric ratio and $\bar{m}_i$ is the average value of the injected fuel mass.

The residual charge mass is determined from measurements of pressure $p$ and exhaust temperature $T_{ex}$ together with the estimate of combustion efficiency during main combustion $\eta_m$, see Fig. 3. The calculation follows the method in [36], with a few changes, described below. For a discussion about the accuracy and sensitivity of this method, please see [36, 37].

The mass flowing out from the cylinder in a cycle is the difference between the total charge mass $m_t$, trapped in the cylinder during main combustion, and the residual charge mass $m_r$, that remains trapped during the nvo period,

$$m_{out} = m_t - m_r.$$
The mass flow out of the cylinder is assumed equal to the flow in
\[ m_{in} = m_a(k) + \bar{m}_t \]  
(10)
during stationary conditions and neglecting blow-by. Using the ideal gas law for \( m_t \) and \( m_r \), we have the equation
\[ m_{in} = \frac{p_{evo}V_{evo} - p_{evc}V_{evc}}{RT_{evo}} \]  
(11)
with the unknowns being the temperatures \( T_{evo} \) and \( T_{evc} \). In addition to the mass conservation (11), the exhaust process is approximated by an ideal gas undergoing a reversible process so that the heat lost per unit mass \( q_l \) is
\[ q_l(\theta_0, \theta_1) = \int_{p(\theta_0)}^{p(\theta_1)} \frac{RT}{p} dp \]  
(12)
and the exhaust process is divided at a reference point \( \theta_{ref} \) into a blow-down phase (BD) and a compression phase (CO). The ratio between the heat losses during the two portions of the exhaust phase, divided by \( \theta_{ref} \), is denoted by \( r_{ex} \).
\[ r_{ex} = \frac{q_l(\theta_{evo}, \theta_{ref})}{q_l(\theta_{ref}, \theta_{evc})} \]  
(13)
The point \( \theta_{ref} \) is chosen in [36] as the point where cylinder pressure reaches 1 atm during the exhaust phase in between evo and evc. To ascertain that there always is a \( \theta_{ref} \), it is here instead chosen as the point of minimum pressure, denoted by \( p_{ref} \), during the exhaust phase. With simplifications outlined in [36], Eq. (12) is written as
\[(c_p + a)T_{evo} + (c_p - b)r_{ex}T_{evc} = T_{ref}(c_p - a + (c_p + b)r_{ex}) \]  
(14)
where \( a = \frac{1}{2}R\log \frac{p_{ref}}{p_{evc}} \) and \( b = \frac{1}{2}R\log \frac{p_{evo}}{p_{ref}} \). The temperature \( T_{ref} \) at \( \theta_{ref} \) is offset by \( \Delta T \) from the measured average exhaust temperature \( T_{ex} \).
\[ T_{ref} = T_{ex} + \Delta T \]  
(15)
where \( \Delta T \) is selected based on comparisons, in previous work, between results from the algorithm with simulation results from a GT-Power model of the engine [37]. The ratio \( r_{ex} \) is estimated based on convective heat transfer, governed by Eq. (7), where the cylinder temperature \( T_{cyl} \) is obtained by assuming polytropic processes. The coefficients \( h_c \) is taken from the modified Woschni relation derived in [33] and the wall temperature \( T_w \) is assumed constant. Combining (7) with (15) yields \( r_{ex} \) as a function of \( T_{evo} \) and \( T_{evc} \).
\[ r_{ex} = f(T_{evo}, T_{evc}) \]  
(16)
The thermodynamic properties \((c_p, R)\) in (11) and (14) are computed based on the mass fraction \( y_r \)
\[ y_r = (1 - \eta_m)y_{re} + \eta_my_{pr} \]  
(17)
where \( \eta_m \) is the combustion efficiency during main combustion and \( y_{re} \) and \( y_{pr} \) are the mass fractions for the reactants and products, respectively, calculated for each operating point.

In summary Eq. (11), (14), and (16) are three equations containing the three unknowns \( T_{evo}, T_{evc}, \) and \( r_{ex} \) that can be solved iteratively. The computed \( r_{ex} \) for each cycle are plotted in Fig. 16 showing that the mean is slightly decreasing and the spread increases somewhat as nvo decreases and CV increases. A sensitivity analysis by Fitzgerald et al. [36] showed that 20% error in \( r_{ex} \) causes errors less than 0.5% in the temperatures and thus, the influence on the estimates of \( T_{evo} \) and \( T_{evc} \) from the variability in \( r_{ex} \) shown in Fig. 16 is low.

When the solution \((T_{evo}, T_{evc}, r_{ex})\) is found, the charge mass \( m_t \) and residual charge mass \( m_r \) are computed from the ideal gas law and the residual gas fraction is approximated by
\[ x_r(k) = m_r/m_t = \frac{p_{evc}V_{evc}T_{evo}}{p_{evo}V_{evo}T_{evc}} \]  
(18)
The estimates of \( x_r \) are shown in Fig. 17. The mean value \( \bar{x}_r \) decreases with nvo and the standard deviation is approximately 0.8% for both cases. In the normal probability plot in Fig. 18 the values cluster close to a straight line implying that the estimates are close to a normally distributed and, hence, that there are almost no deterministic relationships between values of \( x_r \).