

Determination of Cycle Temperatures and Residual Gas Fraction for HCCI Negative Valve Overlap Operation

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ABSTRACT

Fuel injection during negative valve overlap offers a promising method of controlling HCCI combustion, but sorting out the thermal and chemical effects of NVO fueling requires knowledge of temperatures throughout the cycle. Computing bulk temperatures throughout closed portions of the cycle is relatively straightforward using an equation of state, once a temperature at one crank angle is established. Unfortunately, computing charge temperatures at intake valve closing for NVO operation is complicated by a large, unknown fraction of residual gases at unknown temperature. To address the problem, we model blowdown and recompression during exhaust valve opening and closing events, allowing us to estimate in-cylinder charge temperatures based on exhaust-port measurements. This algorithm permits subsequent calculation of crank-angle-resolved bulk temperatures and residual gas fraction over a wide range of NVO operation. Validation methods are employed to assess both accuracy and precision of the temperature calculations. Measured iso-octane ignition temperatures and combustion phasing sensitivity are compared with published experimental trends. Computed bulk temperatures throughout the main compression stroke are compared with core temperature measurements using tracer-based laser-induced fluorescence imaging. For a range of motored and fired operating conditions, computed temperatures are also validated using a 1-D full-engine model. The algorithm-computed temperatures follow trends

closely in all validation tests lending confidence in its intended use as a tool for analyzing NVO-HCCI combustion.

INTRODUCTION

HCCI combustion offers the potential of high combustion efficiency and low engine-out emissions, but remains limited by high pressure-rise rates and knock-induced engine noise at high loads, and misfire caused by low charge temperature at low-loads. Because of the kinetically-limited nature of HCCI, proposed solutions for these problems typically rely on various temperature control strategies. Thermal stratification has been shown to decrease pressure-rise rates at high load [1], while various exhaust-gas-retention strategies have been employed facilitate low-load operation. In both cases, knowing temperatures throughout the cycle is an invaluable aid to understanding HCCI combustion and developing strategies for alleviating problems at the operation limits.

Negative valve overlap (NVO) is one such strategy for extending low-load limits. NVO retains large residual fractions through early closing of the exhaust valve(s) and late opening of the intake valve(s). In addition, recompression provides an opportunity to control charge temperature and reactivity through reacting and reforming fuel injected during NVO. NVO fueling can both elevate temperatures and alter chemical composition of the charge prior to main compression. The extent of thermal versus chemical effects is a current research topic [2] that requires accurate cycle temperature measurements. Accuracy and precision of

temperature measurements are particularly important for the study of HCCI combustion since it is highly sensitive to charge temperatures.

BACKGROUND

Various investigators [3,4,5,6,7,8,9,10] have developed algorithms for computing in-cylinder temperatures and residual gas fractions (RGF) based on measured pressures. Nearly all algorithms employ some form of mass conservation with an ideal gas equation of state to compute average temperatures once trapped mass is determined. Accurately determining trapped mass can be particularly challenging for NVO operation since the amount of retained residuals is often on the same order as the inducted mass.

Estimates of in-cylinder temperature are commonly based on port-measured temperatures during the intake or exhaust processes. Assumptions made may have a significant impact on accuracy and precision. Therefore, validation is needed to assess the impact of assumptions over the range of operating conditions for which in-cylinder temperatures are computed.

Several investigators have focused on the intake mixing process to determine in-cylinder mass and temperatures. Caton *et al.* [6] computed RGF for rebreathing and reinduction strategies by employing a control volume energy analysis of the combustion chamber throughout the cycle. The authors assume that the intake mixing process is adiabatic and that measured intake and exhaust temperatures are equal to those at system boundaries. Estimated errors in RGF are reported as $\sim 5\%$. A similar approach to compute RGF and in-cylinder temperatures was employed by Gazis *et al.* [9]. The authors assume that internal energy is conserved (by neglecting heat loss and any P-V work) during intake mixing with residuals, so that measured exhaust and intake temperatures can be related to in-cylinder temperature at intake valve closing (IVC). Sensitivities of the computational algorithm to pressure pegging (used to offset transducer drift) and thermal shock of the transducer were carefully assessed to correct for deleterious effects. The authors estimated an error of 4-6% due to the assumption that temperatures at exhaust valve closing are *equal* to measured exhaust port temperatures.

Although many investigators assume that specific internal energy of the intake stream is conserved, Sjöberg *et al.* [5] demonstrate that heat transfer and dynamic heating (i.e., kinetic energy dissipation) significantly affect charge temperature after mixing. The authors develop an algorithm for their low RGF conditions to compensate for these effects by accounting for measured changes in volumetric efficiency with intake temperature. Residual mass and charge temperature are computed, to reveal mixture temperatures at BDC diverging from intake temperature by as much as 20 K ($\sim 5\%$).

To escape some of the inherent difficulties in relating intake temperatures to in-cylinder temperatures, some investigators instead focus on the exhaust process. Yun *et al.* [3] assume a simple isentropic exhaust process in order to compute RGF from ratios of pressure and volume at exhaust valve opening (EVO) and closing (EVC) using the specific heat ratio (γ). Although this technique does not require an external temperature measurement, neglect of heat exchange during exhaust prevents the capture of subtle trends in trapped mass with changing EVC temperatures. Consequently, the precision of computed in-cylinder temperatures suffers. Zhao *et al.* [4] compute trapped mass by assuming in-cylinder temperatures at EVC *equal* measured exhaust-port temperatures. The authors compared computed values of RGF with predictions from a one-dimensional gas dynamic code tuned to match measured experimental parameters, revealing differences of 5-10% between the two approaches.

Wildman *et al.* [11] also equate EVC temperatures and port thermocouple measurements to compute trapped mass. The authors compare computed RGF using this approach to values obtained from a more direct CO₂ measurement approach. A simple measurement of the ratio of CO₂ concentration before and after combustion using a fast-response time-resolved in-cylinder gas analyzer can be directly related to RGF. Comparisons of the two approaches showed nominal agreement with data scatter on the order of 4-5%.

For all of these techniques, errors in RGF translate to errors in calculated temperatures since the latter are computed from trapped mass using an equation of state. For example, under our experimental conditions, errors in trapped mass of 5% translate to temperature errors of 25 K at 500 K (early in compression) and 45 K at 900 K (prior to ignition). Such large uncertainties impede the study of thermal effects of residuals on HCCI combustion. To address this challenge, we develop a new algorithm for computing trapped mass and in-cylinder temperatures throughout the NVO cycle. To evaluate performance, we test assumptions and validate results over a range of operating conditions.

COMPUTATIONAL APPROACH

Key to our approach is estimating in-cylinder temperatures at EVO and EVC based on exhaust gas temperatures measured in the exhaust port. The fact that mean exhaust-port temperatures vary little during our tests, despite wide variation of intake temperatures and NVO fueling parameters, facilitates this approach.

Intake-port temperatures are measured in the experiments but are not used directly for our in-cylinder temperature computations. As already mentioned, measured intake temperature must be corrected to reflect heat loss and dynamic heating during induction. These effects may vary

significantly over a wide range of intake temperatures, complicating accurate computation. Furthermore, calculating in-cylinder charge temperature at IVC requires summing the sensible energies of both the intake and residual fractions. For all of these reasons, we instead use the measured intake temperatures as boundary conditions for a GT-Power 1-dimensional engine model [12]. This model's results serve as a consistency check on our computations, but only for experiments with no NVO fuel injection-GT-Power currently does not accommodate combustion during the NVO period.

GOVERNING EQUATIONS

In-cylinder mass is related to cylinder volume, pressure, and temperature using the ideal-gas equation of state:

$$m = \frac{PV}{RT} \quad (1)$$

For the whole cycle, we possess measured pressures, calculated volumes, and estimated gas constants (determined by composition as described later), so that only temperature and total mass are unknown. Knowledge of temperature at any single crank position during a closed portion of the cycle allows the fixed mass to be determined from Eq. (1), so that temperatures throughout the closed portion can be computed.

Our operating conditions provide steady performance (coefficients of variation of residual fraction for example are less than one percent), so we can assume that the same mass of air and fuel that enters the cylinder during intake, exits during exhaust. As a result, for NVO operation during which the exhaust and intake valve events do not overlap, the difference in trapped mass between the two closed portions¹ of the cycle is given simply by:

$$m_1 - m_2 = m_{ex} = m_{air+fuel,in} \quad (2)$$

in which m_1 is the trapped mass during main compression and expansion, m_2 is that during the NVO period, and m_{ex} is the mass that is exhausted from the cylinder each cycle. As a result, knowledge of the trapped mass during one closed portion of the cycle allows that in the other portion to be computed from Eq. (2) using measured intake air and fuel masses. From m_1 and m_2 , mass-averaged temperatures are then readily determined for both closed portions of the cycle using Eq. (1). Residual gas fraction is computed as:

$$RGF \equiv \frac{m_2}{m_1} \quad (3)$$

To summarize, knowing pressures, volumes, gas constants, inducted mass, and a single closed-system temperature is sufficient to compute RGF and temperatures throughout the closed portions of the cycle using Eqs. (1), 2, (3). Accurately determining a single closed-system temperature is a crucial step.

When in-cylinder gas temperature cannot be practically measured, *e.g.*, using PLIF [13] or CARS [14], it is often inferred from a temperature measurement made outside of the cylinder. We adopt this approach, using a thermocouple placed in the exhaust port just downstream of the exhaust valve. The important detail is how gas temperatures inside the cylinder during the closed portion of the cycle can be determined from the external measurements.

Our algorithm uses the following two-step procedure. T_{EVO} and T_{EVC} are defined as temperatures at either end of the exhaust process, *i.e.*, T_{EVO} represents cylinder contents *just before* the exhaust valve opens, and T_{EVC} represents contents *just after* the valve closes. Thus both are closed-system temperatures.

Accordingly, our first step requires relating T_{EVO} and T_{EVC} to a reference temperature during the middle of the exhaust process. Figure 1 indicates that the reference temperature, $T_{cyl, 1atm}$, is selected at a CAD² at the end of exhaust *blowdown* and the start of *recompression*, when cylinder and port pressures are both approximately 1 atm. (Here the term *recompression* refers to the pressurization that takes place between bottom dead center and EVC-not to be confused with *NVO recompression* which begins at EVC.) The blowdown and recompression processes are assumed reversible but not adiabatic, and represent only the mass that remains in the cylinder, not the exhausted mass.

The obvious second step of our algorithm is to relate $T_{cyl, 1atm}$ to the measured exhaust-port temperature, T_{ex} . T_{ex} is measured external to the cylinder and so is shown in Fig. 1 as a solitary square below the cycle-temperature curve.

¹By definition, a closed portion of the cycle has no change in trapped mass. For simplicity, the equations presented here are simplified for cases in which all fuel is added prior to valve closing. To account for fuel added after valve closing (*e.g.*, during NVO), an additional term is needed. Our computational algorithm properly accounts for fuel addition after valve closing.

²Relative crank angle degree (CAD) values are used in this paper. Such values are labeled, for example, as CAD aTDC-main = crank angle degrees after top dead center of main compression, or CAD bTDC-NVO = crank angle degrees before top dead center of the NVO period. In some unambiguous circumstances the aTDC and bTDC suffixes are omitted.

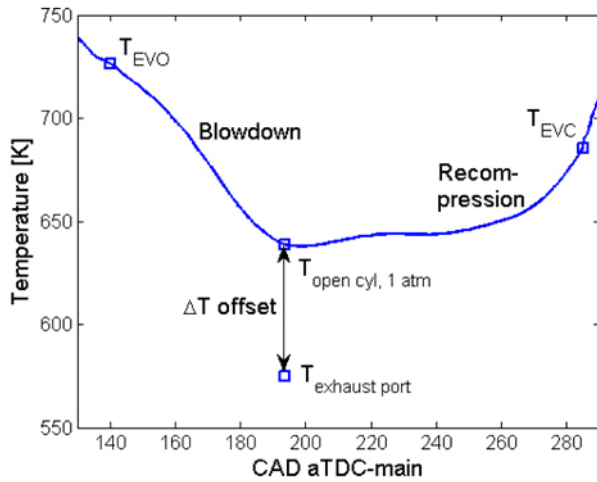


Figure 1. Calculated cycle temperatures from EVO to IVC. The in-cylinder contents undergo blowdown and recompression processes including heat transfer to the cylinder walls. T_{ex} is the measured exhaust port temperature.

RELATING T_{EVO} AND T_{EVC} TO $T_{CYL,1ATM}$

In step 1, estimating heat loss during blowdown and recompression provides a key constraint needed to solve for unknown temperatures, T_{EVO} and T_{EVC} . The development of this constraint follows.

For an ideal gas undergoing a reversible process, the differential heat loss per unit mass may be expressed as:

$$\delta q = T ds = c_p dT - \frac{RT}{P} dP \quad (4)$$

Integrating Eq. (4) for the blowdown process beginning at EVO and ending when cylinder contents reach ambient pressure ($cyl,1atm$), gives heat loss per unit mass during blowdown:

$$q_{blowdown} = \int_{EVO}^{cyl,1atm} c_p dT - R \int_{EVO}^{cyl,1atm} \frac{T}{P} dP \quad (5)$$

Similarly, integration during recompression gives:

$$q_{recompression} = \int_{cyl,1atm}^{EVC} c_p dT - R \int_{cyl,1atm}^{EVC} \frac{T}{P} dP \quad (6)$$

For convenience, we define the ratio of heat loss per unit mass for blowdown and recompression:

$$C_{BD/RC} \equiv \frac{q_{blowdown}}{q_{recompression}} \quad (7)$$

$C_{BD/RC}$ is determined iteratively for each test (as described in the next section). Substitution of Eqs. (5) and (6) into Eq. (7) gives:

$$\int_{EVO}^{cyl,1atm} c_p dT - R \int_{EVO}^{cyl,1atm} \frac{T}{P} dP = C_{BD/RC} \left(\int_{cyl,1atm}^{EVC} c_p dT - R \int_{cyl,1atm}^{EVC} \frac{T}{P} dP \right) \quad (8)$$

To simplify Eq. (8) we assume constant specific heats since, in this study, temperatures vary by less than 150 K. Consequently, the first integral on each side may be expressed in terms of temperature differences at EVO and EVC. Average values of temperature are used to evaluate the remaining integrals (with little consequence to accuracy), so that Eq. (8) becomes:

$$c_p (T_{cyl,1atm} - T_{EVO}) - R \frac{(T_{cyl,1atm} + T_{EVO})}{2} \ln \left(\frac{1}{P_{EVO}} \right) = C_{BD/RC} \left[c_p (T_{EVC} - T_{cyl,1atm}) - R \frac{(T_{cyl,1atm} + T_{EVC})}{2} \ln(P_{EVC}) \right] \quad (9)$$

This expression relates T_{EVO} and T_{EVC} to $T_{cyl,1atm}$. Once $T_{cyl,1atm}$ and $C_{BD/RC}$ are known (as described in the next sections), T_{EVO} and T_{EVC} are computed from Eq. (9) using one additional constraint formulated by combining Eqs. (1) and (2):

$$m_1 - m_2 = m_{EVO} - m_{EVC} = \frac{P_{EVO} V_{EVO}}{R_{EVO} T_{EVO}} - \frac{P_{EVC} V_{EVC}}{R_{EVC} T_{EVC}} = m_{air+fuel,in} \quad (10)$$

Equations (9) and (10) are the means by which in-cylinder temperatures during the closed part of the cycle can be determined using our reference in-cylinder temperature from the exhaust period. Together they incorporate the relationship between breathing, heat exchange, cylinder pressures, and cylinder temperatures during exhaust. We emphasize that the accuracy of this formulation depends on an accurate estimate of the heat-transfer ratio $C_{BD/RC}$, and not necessarily on accurate knowledge of the *absolute amount* of heat transfer during exhaust.

RELATING $T_{CYL,1ATM}$ TO T_{EX}

As described earlier, the second step in our analysis requires relating $T_{cyl,1atm}$ to our measured exhaust port temperature.

T_{ex} . Both temperatures correspond to the open, exhaust part of the cycle, but the temperatures are not normally equal. $T_{cyl, latm}$ represents a calculated in-cylinder reference temperature, while T_{ex} is a thermocouple measurement affected both by temporal averaging and by heat transfer to cooled port walls [15]. We have found that a simple temperature offset ($\Delta T_{cyl/ex}$) is adequate to relate these temperatures:

$$T_{cyl, latm} = T_{ex} + \Delta T_{cyl/ex} \quad (11)$$

The measured T_{ex} for our range of fired experiments is 555-580 K, and a value of $\Delta T_{cyl/ex} = 65$ K performs well for predicting cycle temperatures over this range—predicted temperatures agree within 1% with our GT-Power model as discussed in a later section. Note that $\Delta T_{cyl/ex}$ is the single adjustable parameter in our algorithm.

DETERMINING $C_{BD/RC}$

$C_{BD/RC}$ is determined by an iterative process in which an initial guess is made (e.g., unity) and Eqs. (9) and (10) are solved to determine T_{EVO} and T_{EVC} . Pressures and temperatures at EVO, EVC, and the reference state ($cyl, latm$) are then used to compute the polytropic coefficients n_{BD} and n_{RC} :

$$\begin{aligned} T_{EVO} &= T_{cyl, latm} \left(\frac{P_{EVO}}{P_{latm}} \right)^{n_{BD}} \\ T_{EVC} &= T_{cyl, latm} \left(\frac{P_{EVC}}{P_{latm}} \right)^{n_{RC}} \end{aligned} \quad (12)$$

Next, in-cylinder gas-temperatures (T_{cyl}) throughout blowdown and recompression are computed using the polytropic coefficients. Finally, the heat-transfer ratio $C_{BD/RC}$ is calculated from the convective heat-transfer equation:

$$C_{BD/RC} = \frac{\int_{blowdown} h_c A (T_{cyl} - T_w) dt}{\int_{recompression} h_c A (T_{cyl} - T_w) dt} \quad (13)$$

where h_c is the convective heat-transfer coefficient, A is the instantaneous cylinder surface area, and T_w is the temperature of the surrounding walls. Heat-transfer coefficients are computed using a Woschni correlation [16] that accounts for effects of fluid motion due to differences in pressure between fired and motored values during expansion (blow-down) and recompression. Once $C_{BD/RC}$ is recomputed, the procedure is repeated to obtain convergence of $C_{BD/RC}$ for each test.

For the entire range of tests in this work, the ratio of heat lost during blowdown and recompression ($C_{BD/RC}$) is between 1 and 1.2. A sensitivity assessment reveals that a 20% error in $C_{BD/RC}$ affects T_{EVO} and T_{EVC} by less than 0.5% (3-4K).

DETERMINING R AND C_p

Accurate computation of in-cylinder temperatures requires accurate determination of specific heat (C_p) during exhaust and the gas constant (R) during the entire cycle. Both require knowledge of in-cylinder composition.

Charge composition required for specific heat (C_p) and gas constant (R) values is estimated using chemical kinetics simulations correlated to our experimental data using combustion efficiency. Efficiencies of both main and NVO combustion are determined from experimental heat-release analysis, and overall cycle combustion efficiency comes from emission measurements. The kinetics simulations (based on Lawrence Livermore National Laboratory's iso-octane kinetics mechanism [17]) employ initial conditions from experiments, with some tuning to match combustion efficiencies. For all tests in this work, main combustion efficiency was greater than 90% so that experimental main efficiency fluctuations have little impact on R and C_p . Since NVO fuel mass comprises a small fraction of the total, variations in NVO combustion efficiency also have little effect.

VALIDATION APPROACH

ENGINE EXPERIMENTS

The engine is a single-cylinder 0.63L optical engine configured for NVO operation, with specifications listed in Table 1. Short dwell (145 CAD) cams are phased symmetrically to give 150 CAD of NVO. A GM prototype pent-roof head houses two intake valves and a single exhaust valve. Iso-octane fuel is direct-injected at 10 MPa using a vertical, 8-hole injector that is centrally located in the head. Injector delivery is measured with a positive displacement flow-meter placed in the high-pressure fuel line. For PLIF experiments (described below), 3-pentanone tracer is evaporated and premixed in the intake air 1-m upstream of the intake plenum. Average delivered tracer mass per cycle is computed using a precision scale and stop-watch.

Table 1. Engine Specifications

Displacement (single-cylinder)	0.633 L
Bore	92 mm
Stroke	95.25 mm
Effective Compression Ratio	10.6*
Intake Valve Opening	75 CAD aTDC-NVO*
Intake Valve Closing	220 CAD aTDC-NVO
Exhaust Valve Opening	220 CAD bTDC-NVO
Exhaust Valve Closing	75 CAD bTDC-NVO
Valve Lift	3 mm

*The engine's nominal geometric compression ratio is 11.5. However, 1-dimensional engine modeling and analysis of motored pressure data reveal that the effective compression ratio is 10.6. This value is used for all computations in this study.

Airflow to the engine is measured with a sonic orifice upstream of the engine while maintaining manifold pressure at 100 kPa to simulate naturally aspirated conditions. Temperature of the intake air flow is controlled with a series of heaters on the air line and components between the sonic orifice and the engine.

A primary purpose of this work is to accurately estimate cycle temperatures needed for a companion study analyzing thermal and chemical effects of NVO fuel reactions [2]. Thus, engine operating conditions are the same for both studies. Two modes of operation are examined: *main-fuel* tests with a single fuel injection during the intake stroke, and *NVO-fuel* tests with an additional fuel injection during NVO. Intake temperatures are elevated for the main-fuel experiments to match the phasing of the NVO-fuel cases. The experiments cover a wide range of main-combustion phasing, NVO fuel amount, and NVO fuel injection timing. Further details are listed in [Table 2](#).

ENGINE OPERATION FOR PLIF MEASUREMENTS

Slightly different operating conditions ([Table 3](#)) are required for experiments we perform using a 2-wavelength PLIF technique to measure in-cylinder core temperatures [18]. In these experiments 3-pentanone is premixed with the intake air to serve as a fluorescent tracer. When the tracer is used, an equivalent amount (in lower heating value) of iso-octane is removed from the main injection, maintaining IMEP near 190 kPa.

Measurements of core temperature are made by passing a horizontal laser sheet through a quartz ring integrated at the top of the cylinder. The sheet is located about 4 mm below

the firedeck. Resulting tracer fluorescence is imaged through a quartz window in the Bowditch piston. Centered on the cylinder axis, the interrogation region is 25×65 mm and 1 mm thick. Spatially averaged core temperatures are computed by ensemble-averaging 50 consecutive cycles over the entire field of view. Further details of the application of 2-line PLIF to temperature measurement in our engine are described in [18].

Table 2. Engine Operating Conditions for Experiments with Iso-Octane Fuel

	Main-Fuel Experiments	NVO-Fuel Experiments
Intake Temperature	420 – 470 K	335-360 K
Coolant Temperature	363 K	353-363 K
Main Fuel Amount	7.9 mg/cyc	7.9 mg/cyc
Main Start of Injection	270 CAD bTDC-main	270 CAD bTDC-main
NVO Fuel Amount	NA	1 – 2 mg
NVO Start of Injection	NA	100 – 15 CAD bTDC-NVO
Fuel Injection Pressure	10 MPa	
Manifold Pressure	100 kPa	
Engine Speed	1200 RPM	

Table 3. Engine Operating Conditions for Experiments with Iso-octane Fuel and 3-Pentanone Tracer

	Main-Fuel Experiments	NVO-Fuel Experiments
Intake Temperature	420 – 470 K	335-360 K
Coolant Temperature	363 K	363 K
Main Fuel Amount	6.5 mg	6.5 mg
Main Start of Injection	270 CAD bTDC-main	270 CAD bTDC-main
NVO Fuel Amount	NA	0.9 – 1.4 mg
NVO Start of Injection	NA	100 – 30 CAD bTDC-NVO
Fuel Injection Pressure	10 MPa	
3-Pentanone Tracer Amount	2.1 mg	
Manifold Pressure	100 kPa	
Engine Speed	1200 RPM	

DATA ACQUISITION

Cylinder pressure measurements are acquired every ¼ CAD using a piezo-electric pressure transducer. Manifold pressure measured near the intake plenum is used to peg cylinder pressure during intake. This process is crucial for accurate results and is evaluated in more detail in a later section.

Strategically placed thermocouples provide mean gas temperature measurements in the intake port and exhaust