

Primary Reference Fuel Behavior in a HCCI Engine near the Low-Load Limit

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ABSTRACT

In a previous study, a wide range of gasolines with RON~90 were tested in a single cylinder engine operated in HCCI mode using negative valve overlap, and all were found to have very similar behavior near the low-load limit. Here we broaden the range of gasolines to include PRF90 and PRF60. At high engine speed, both PRF60 and PRF90 behave similarly to all the other gasolines tested. However, at 1000 RPM, PRF90 is very different from all the other gasolines: it ignites very late, and the engine cannot be operated at low load. Simulations using a popular fuel chemistry model cannot distinguish PRF60 and PRF90 under these conditions. However, a new fuel chemistry model correctly shows the onset of fuel sensitivity at low engine speed. Sensitivity analyses indicate the low-load limit at low engine speed strongly depend on both the chemistry parameters and on the heat-transfer parameters.

INTRODUCTION

Research on homogenous-charge, compression-ignition (HCCI) engines has experienced explosive growth over the last decade. HCCI engines have the potential to provide a significant improvement in fuel economy (~15 – 20%) relative to spark ignition (SI) engines. The NO_x and particulate emissions from HCCI engines are extremely low compared to those from Diesel engines [1]. Consequently, HCCI engines are viewed as a possible alternative to conventional SI and Diesel technology.

One of the greatest challenges facing HCCI engines is its limited operating range relative to SI or Diesel engines [1]. The HCCI operating range lies in the low speed, low load portion of the SI operating range. Under these conditions, SI engines suffer large efficiency losses due to the throttling process. However, HCCI engines generally operate unthrottled, and consequently they

have significantly higher (~25%) efficiencies than SI engines at light loads [2]. Unfortunately, the HCCI operating range does not extend down to idle operation. Therefore, developing an understanding of the limiting mechanism for the low-load limit (LLL) is crucial to future HCCI engine development. This work focuses on explaining the phenomenon that cause an HCCI misfire and how this affects the HCCI LLL.

There is a consensus that chemical kinetics is critical to HCCI combustion [1]. Several studies have been presented in the literature in which researchers examined how fuel ignitability affects combustion phasing and/or operating range in HCCI engines [3-8]. For example, Lü et al. [5] tested a broad range of PRF octane numbers (0 – 90) and found that the start of ignition was more delayed for higher octane PRFs. In addition, their results showed that combustion duration decreased with increasing PRF octane number. Yao et al. [7,8] examined the effect of PRF octane number on the size of the HCCI operating range. Yao et al. observed that higher RON fuels could operate over a smaller range of fuel/air ratio ϕ than lower RON fuels at a fixed speed.

Substantial insight to the chemical origin of the LLL may be gained by augmenting the experimental studies with chemical kinetics simulation. A HCCI engine simulator could provide detailed species information and identify the key chemical pathway that controls the LLL. For example, Dec [9] and Sjöberg and Dec [10-12] used a combination of simulations and experiments to investigate HCCI operation at the LLL. In [9], Dec used a single-zone kinetic model to examine how reducing the fueling rate affected quenching of the bulk-gas reactions. In these simulations, the fueling rate was reduced by decreasing ϕ . At the low limit of equivalence ratios, the bulk gas reactions were quenched due to low combustion temperatures. Sjöberg and Dec [10] investigated how fuel chemistry and engine speed

affected the onset of incomplete combustion in HCCI engines. They found that fuels with minimal cool-flame chemistry (e.g., iso-octane, gasoline) reach the onset of incomplete bulk-gas reactions at the same ϕ independently of engine speed. However, for fuels that exhibit significant cool-flame chemistry (e.g., n-heptane), engine speed influenced the onset of incomplete bulk-gas reactions; larger ϕ were required at lower engine speeds to maintain complete combustion.

In the works of Dec [9] and Sjöber and Dec [10-12], and several other studies in the literature (see, for example, [13-15]), the lower load limit was reached by varying the equivalence ratio. However, if HCCI engines are hybridized with SI engines, stoichiometric operation diluted with residual will likely be required for current 3-way catalyst technology. Very likely this dilution with residual will be accomplished by using negative valve overlap (NVO). To the authors' knowledge, no studies exist in the literature that examine the cause of an HCCI misfire at stoichiometric operation. Therefore, the goal of this work is to establish the mechanism that governs the LLL of an HCCI engine operating with a stoichiometric fuel/air ratio using NVO, and to understand how fuel chemistry and engine operating conditions affect the engine stability.

In our previous work [16], market-typical variations in commercial gasolines were shown to have little effect on the HCCI operating range, particularly at the LLL. However, the impact of fuel chemistry on the LLL was examined only over the range of market-typical variations in gasolines. In this study, the sensitivity of the LLL to a much broader range of fuels (with regards to fuel ignitability) was investigated to examine the basis of the conclusions reached in [16]. The current experiments were performed with two well-characterized fuels with very different ignition behaviors, primary reference fuel 90 (PRF90) and PRF60. A full- (or multi-) cycle simulation of a single cylinder HCCI engine [17] is used to study the misfire limit phenomenon. Detailed chemistry models embedded in the cycle simulation are used to establish trends describing how fuel chemistry and engine speed affect the LLL of HCCI operability. Finally, these trends are used to explain the experimental LLL data with primary reference fuels.

EXPERIMENTAL SETUP

The experimental setup used in this work was reported previously [18]. Only the essential features of the experimental setup are described here. The experiments were performed on a production Mazda 2.3L, 4-cylinder, 16-valve engine, modified for single-cylinder operation. The intake and exhaust manifolds of the production engine were modified to keep the intake air and exhaust gases of the firing cylinder separate from the rest of the cylinders. This was done to ensure accurate fuel/air ratio measurements. Other modifications to the production engine included: increasing the compression ratio from 9.7 to 11.1, using cams with reduced durations and lifts, and adding continuously variable cam phasing to the

exhaust valve train. The final engine configuration is presented in Table 1, and a schematic of the experimental apparatus is shown in Figure 1.

Table 1. Engine specifications

Displacement (cm ³)	565
Bore (mm)	87.5
Stroke (mm)	94.0
Connecting Rod Length (mm)	154.8
Compression Ratio	11.1
Intake Cam Duration (° crank angle)	120
Exhaust Cam Duration (° crank angle)	120
Intake Valve Maximum Lift (mm)	2.0
Exhaust Valve Maximum Lift (mm)	2.0
Equivalence Ratio (ϕ)	1.0

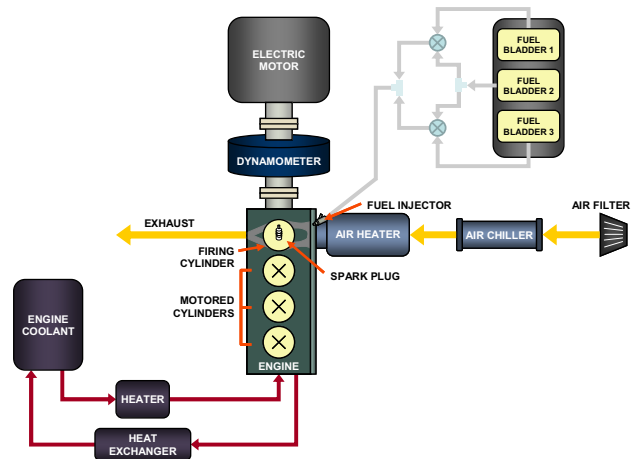


Figure 1. Schematic of the experimental apparatus

A heater and heat exchanger were included in the coolant loop to maintain the engine block at 90°C $\pm$ 2°C throughout all the experiments. A desktop computer controlled the fuel injection pulse width, spark timing, and intake and exhaust cam phasing; changes to each could be made in real time as desired. The cam phasing control was accurate to within $\pm$ 1 crank angle degree (CAD), and the cam position was recorded once per cycle; the resolution on cam position was $\pm$ 1 CAD.

PRFs 60 and 90 were chosen for this study. The LLL of HCCI operability was obtained at 3 engine speeds: 1000, 1500, and 2000 RPM. The intake air was dehumidified to a dew point of 4°C (corresponding to a water vapor mole fraction of approximately 0.7%) and then reheated to 40°C before entering the engine. All experiments were performed at stoichiometric fuel/air equivalence ratios and at wide open throttle (naturally-aspirated).

HCCI combustion was achieved by negative valve overlap (NVO), i.e. the exhaust valve was closed early during the exhaust stroke to trap hot exhaust gas residuals. The thermal energy of the exhaust gases was used to induce auto-ignition on the subsequent cycle. Cam phasing was used to vary the engine load.

When approaching the LLL, the exhaust cam phasing was advanced (i.e. exhaust valve closing, EVC, occurred earlier during the exhaust stroke). Since the equivalence ratio was held constant, increasing the residual fraction resulted in a lower fresh charge fraction. At the LLL, the EVC timing could not be advanced without producing a misfire. In contrast, the intake cam phasing was generally set to the position that maximized flow into the cylinder and kept constant as EVC was varied. Intake cam phasing had only minor effects on load near the LLL in the present engine [18]. All experiments were performed at fixed intake and exhaust cam durations, 120 CAD.

HCCI ENGINE SIMULATOR

The HCCI simulator used here combines a user-defined, detailed chemistry model of the engine combustion with a commercial engine simulation software, Ricardo WAVE [19]. The coupled model is referred to as the MIT Engine Simulator (MITES). MITES was previously used to model transient behavior in HCCI engines [17]. In that work, MITES was able to accurately predict transient time constants and relative changes in engine load for experimental transients in fueling rate and engine speed. A detailed description of MITES is given in [17]. However, a brief review of the model methodology is given here.

GAS EXCHANGE MODEL

The engine simulation software (WAVE) models the flows to and from the cylinder using 1-D fluid mechanics. During the gas exchange portions of the engine cycle (i.e., exhaust and intake valve opening to valve closing), WAVE models the flows across the cylinder valves, and thus is responsible for calculating the trapped mass and residual mass fraction. Valve flows are calculated using isentropic compressible orifice flow equations [20]. Backflow for the inlet valve was also calculated. The correlation between flow coefficient and L/D (ratio of valve lift/valve diameter) was provided by Ford Motor Co. WAVE also calculates the mass of fuel to inject in order to maintain the correct fuel/air equivalence ratio within the cylinder. Unlike the version reported in [17], a constant pressure ambient block is used for the intake process. This approach led to greater simulation stability.

CHEMISTRY MODEL

Modeling of the auto-ignition process requires an accurate representation of the in-cylinder chemical reactions. The closed-cycle and full-cycle simulations were performed using the full mechanism for primary reference fuels (PRFs) developed at the Lawrence Livermore National Laboratory (LLNL) [21]. This

mechanism is used broadly and has been validated against many experimental results. This detailed chemical mechanism contains 1036 species undergoing 4238 elementary reactions. A second chemistry model developed at the University of Tokyo (UT) [22] was used to check the sensitivity to chemistry. This mechanism has similar structure to the LLNL model, but can simulate combustion characteristics of PRF mixtures more accurately.

The model divided the cylinder content into two regions: a boundary layer zone and a core zone. Here, the "boundary layer" zone represented the mass in the colder volumes of the cylinder (i.e., the true boundary layer plus the crevice volumes). The boundary layer zone contained a user-specified fraction, $x_{boundary}$, of the mass in the cylinder. In the present work $x_{boundary} = 0.05$. The mass in the boundary layer was assumed to be non-reactive due to the low temperature. Therefore, reactions occurred in the core zone only. Each zone was assumed to be spatially uniform in temperature and composition, and the pressure in the cylinder was uniform throughout both masses.

The chemical kinetic model consists of a system of differential-algebraic equations (DAEs). It includes equations for species conservation, energy conservation (with heat losses), and the ideal gas equation of state. The resulting set of equations has a sparse Jacobian matrix [23]. The detailed model equations are given in [17]. The equations are solved using the JACOBIAN software package [24], which contains a computationally efficient numerical solver, DSL48S, for sparse systems of DAEs [25]. Additional computational speed-ups were obtained by using analytical expressions for the Jacobians, which were obtained a priori using automatic differentiation [26]. Fast accurate numerics are crucial for modeling HCCI with NVO near the misfire limit, since a large number of cycles must be simulated to determine stability, and the equations are very sensitive to small numerical errors.

HEAT TRANSFER MODEL

Due to the sensitivity of the auto-ignition process in HCCI engines, it was necessary to model accurately the heat transfer processes between the cylinder walls and the charge. Despite its widespread use in HCCI engine simulations, the Woschni and reduced Woschni heat transfer correlations [27] were developed for a direct-injection, four-valve diesel engine without swirl, which is an operating regime quite different than that of HCCI engines. Chang et al. [28] proposed a global heat transfer correlation that is appropriate for HCCI simulations. This correlation, which is being used in the present study, includes a term that involves the difference between the pressure in the cylinder and the motored pressure. The present work used motored pressures that were computed using WAVE. As noted by Chang et al. and discussed below, there is significant uncertainty in the heat transfer coefficient.

NUMERICAL PROCEDURE

CLOSED-CYCLE SIMULATIONS

MITES was first used to determine the minimum temperature required to induce auto-ignition of a stoichiometric fuel/air mixture at a fixed residual fraction for one engine cycle only. Because the conditions sought simply needed to guarantee combustion for a single cycle, only the closed-portion of the engine cycle was simulated (i.e., from intake valve closing (IVC) to exhaust valve opening (EVO)). Note that thermal conditions sufficient for auto-ignition on one cycle do not guarantee sustained combustion for multiple cycles. Often it is observed both in the simulations and in experiments that the engine will fire for dozens of cycles before misfiring.

In order to specify the thermodynamic state of the cylinder at IVC, the residual mass fraction had to be specified. Given the residual mass fraction, equivalence ratio, and the molecular weight of the fuel, and assuming the residual is composed of H_2O , N_2 , and CO_2 , the composition of the in-cylinder mixture can be determined [20]. The pressure at IVC (P_{IVC}) was always set to 1.115 bar; it is consistent with the pressure at IVC from the full-cycle simulations. The θ_{IVC} chosen was consistent with the valve timing at the LLL in experimental work; 141 CAD before top center (BTC) at 1000 RPM, or 138 CAD BTC at 1500 RPM.

The fire/misfire line was constructed in the following manner. For a specified residual fraction, the temperature at IVC (T_{IVC}) was increased by 1 °C until a simulation resulted in auto-ignition. This temperature was recorded as the fire/misfire temperature. Repeating this procedure for a range of residual fractions yielded the fire/misfire line. This line is very helpful in understanding how an increase of residual fraction increases the minimum temperature required to burn a mixture. In this work, a cycle was defined as a misfire if the first derivative of the cylinder pressure with respect to time was never positive after top center (i.e., zero CAD).

FULL-CYCLE SIMULATIONS

In the context of a real engine, the residual fraction and in-cylinder temperature are directly linked. Therefore, in order to gain an understanding of how the in-cylinder temperature correlates with residual mass fraction, full- (or multi-) cycle simulations were required.

The full-cycle simulations were performed in a manner consistent with the experimental approach used to obtain the LLL. For a fixed set of operating conditions which produce stable operation (e.g., θ_{IVC} , engine speed, intake air temperature), a simulation was run over 50 cycles to achieve steady-state. Once steady-state was achieved with the initial configuration, the exhaust valve timing (θ_{EVC}) was advanced by 1 CAD (effectively increasing the residual fraction), and the simulation was allowed to achieve steady-state at the new valve timing. θ_{EVC} was repeatedly advanced until the simulation misfired. The

transition in valve timing occurred without terminating the original simulation. Therefore, MITES captured the cycle-to-cycle dynamics of changing the valve timing. It is recognized that the above procedure approaches the LLL along a selected trajectory (namely, via the advancement of EVC with fixed IVC) and the LLL may be trajectory dependent. Nevertheless, the LLL obtained in this manner should be representative of the engine operation.

For all the simulations, the following variables were fixed at the values used experimentally: fuel/air equivalence ratio ($\phi = 0.99$), intake air temperature ($T_{INT} = 40^\circ C$), and θ_{IVC} (141 CAD BTC at 1000 RPM, 138 CAD BTC at 1500 RPM). Defining a misfire cycle in the context of a full-cycle simulation was straight forward. On cycles that misfired, the NIMEP was negative, i.e., no work was produced from the combustion process.

EXPERIMENTAL RESULTS AND DISCUSSION

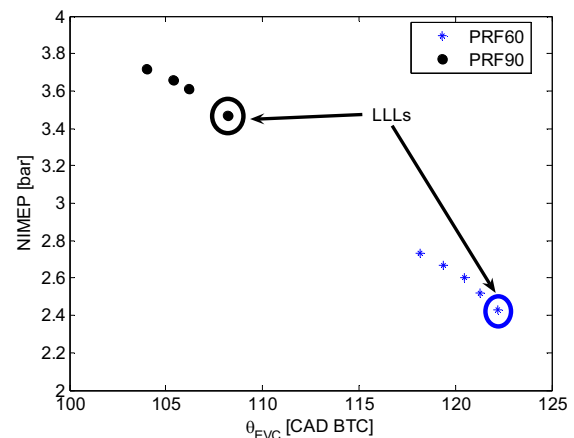


Figure 2. Experimental LLL trajectories for PRFs 60 and 90 at 1000 RPM

The experimental LLL trajectories for PRFs 60 and 90 at 1000 RPM are shown in Figure 2. Each point on the plot represents the steady-state load for a fixed set of engine operating conditions: θ_{EVC} was advanced to lower the NIMEP values. The intake cam phasing at the LLL for both fuels was very similar: θ_{IVC} for PRF90 was 141 CAD BTC, and θ_{IVC} for PRF60 was 144 CAD BTC. As the exhaust valve timing was advanced, more residual gases were trapped in the cylinder. This decreased the available cylinder volume for fresh fuel and air, and the reduction in fueling resulted in a lower engine load. The LLL was reached when the θ_{EVC} could not be advanced without producing a misfire. At this engine speed, the LLL of PRF60 was 1.04 bar (~30%) lower than that of PRF90.

Furthermore, as shown in Figure 3, the combustion phasing of PRF60 at the LLL was significantly advanced relative to that of the PRF90. The difference of 50% burned location (CA50) was 4.7 CAD. The LLL measurement for a single fuel was repeatable to 0.11 bar