

Dynamic Modeling of HCCI Combustion Timing in Transient Fueling Operation

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Abstract

A physics-based control-oriented model is developed to dynamically predict cycle-to-cycle combustion timing in transient fueling conditions for Homogeneous Charge Compression Ignition (HCCI) engines. The model simulates the engine cycle from the intake stroke to the exhaust stroke and includes the thermal coupling dynamics caused by the residual gases from one cycle to the next cycle. A residual gas model, a modified knock integral model, a fuel burn rate model, and thermodynamic models for the gas state in combustion and exhaust strokes are incorporated to simulate the engine cycle. The gas exchange process, generated work and completeness of combustion are predicted using semi-empirical correlations. The resulting model is parameterized for the combustion of Primary Reference Fuel (PRF) blends using 5703 simulations from a detailed thermo-kinetic model. Semi-empirical correlations in the model are parameterized using the experimental data obtained from a single-cylinder engine. The dynamics of fuel transport from intake port into the cylinder is described using the wall wetting fuel dynamic model. Step Air Fuel Ratio (AFR) excursions are used to excite the HCCI engine to determine

the parameters for fuel dynamics using methods of system identification. In addition, the dynamics of exhaust gas transport and AFR sensor are included to correctly interpret measurements from the AFR sensor.

Step fueling transient tests of the equivalence ratio and octane number are used to validate the model. Compared to the experimental measurements the model captures the ignition timing (CA50) transient dynamics with a maximum offset less than 2 degrees of crank angle. The model developed in this work seems promising for HCCI control as: all of its inputs can be relatively easily measured or estimated on an engine; has low computation requirements, and seems to have sufficient accuracy for control applications.

INTRODUCTION

Ignition timing affects different aspects of the operation of HCCI engines including the operating range, the combustion stability, the engine performance and emission characteristics [1, 2, 3, 4, 5]. The operating range is influenced by ignition timing as late ignitions lead to high cyclic variation which determines the instability limit [2]. Conversely,

early ignitions lead to high peak pressure and high pressure rise rate which determine the knock limit [1]. Combustion efficiency depends on ignition timing [6] and completeness of combustion deteriorates by shifting the ignitions later in the expansion stroke [4] which increases the potential of partial burn and misfired cycles. This can influence Carbon Monoxide (CO) and Hydrocarbons (HC) emissions [3, 5]. Ignition timing also affects the peak combustion temperature which has a direct impact on NOx (Oxides of Nitrogen) emissions [5]. The thermal efficiency and the engine work output are also affected by ignition timing and less work is produced by releasing energy part-way down the expansion stroke for late ignitions [4].

Ignition timing is the main control parameter in HCCI engines and the quality of HCCI operation depends on the quality of the system used to control ignition timing [3, 7]. But control of ignition timing, particularly for a wide range of load and speed, has been recognized as the most challenging problem in HCCI engines [8, 9]. This is because of the absence of a specific event to initiate the combustion and high sensitivity of HCCI to the variations in the charge properties [10]. Influential charge properties are gas thermodynamic properties (temperature and pressure), mixture AFR, Exhaust Gas Recirculation (EGR) rate, fuel composition/octane number, compression ratio, thermal and compositional inhomogeneities and the residual gas from the previous cycles [3, 10]. Disturbances in any of these factors can disturb the HCCI ignition timing. HCCI becomes even more sensitive to these disturbances for the late ignitions [4, 11]. If one of the charge variables is used as the parameter to control ignition timing, both the dynamics of changing the charge variable on combustion timing and the actuator dynamics should be considered. Three main techniques to control HCCI ignition timing during transients are: 1) Variable Valve Actuation (VVA) by changing the amount of retained residual gas and by changing the effective compression ratio [12, 13]; 2) Vari-

able Compression Ratio (VCR) to change compression temperature and pressure [14, 15]; 3) Dual Fuel Modulation (DFM) for changing the fuel octane number and the fuel composition [16, 17]. To apply each of these methods, the corresponding dynamics should be considered. For instance, the dynamics of thermal coupling between cycles by the residual gases from one cycle to the next cycle becomes important for the residual affected HCCI using VVA. DFM is another means for control of HCCI combustion and the problem of carrying two fuel tanks can be solved by generating two fuels from one fuel using a reformer [7]. Applying DFM to control ignition timing requires the consideration of fueling transient dynamics.

This paper focuses on modeling the dynamics affecting the combustion timing particularly for transient fueling conditions where AFR and fuel octane number are changed to control HCCI ignition timing. Model-based control of HCCI requires computationally efficient control models of the dynamics affecting the combustion timing. These models can also be used in an off-line simulation bed to design and evaluate the combustion timing controller.

The two main categories of control-oriented models used to predict combustion timing for HCCI engines are: I) steady-state models, II) cycle-to-cycle (transient) models. The first category includes the models that provide mean-value combustion timing. These models are helpful for control of ignition timing in steady-state conditions and include 1) simple look-up table approach [18], temperature threshold method [19] or double-Wiebe function combustion model [20]; 2) Shell model [21, 22]; 3) Arrhenius-type rate threshold models [23, 24, 25]; 4) knock integral models [26, 27, 28, 29]; 5) Modified Knock Integral Models, MKIM [30, 31, 32].

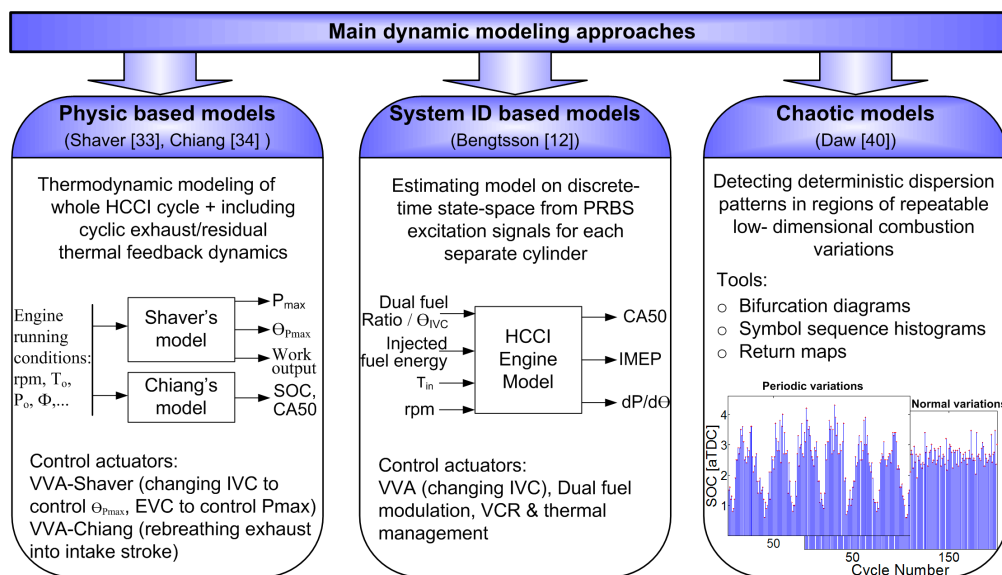


Figure 1: Main modeling approaches to predict HCCI cycle-to-cycle combustion timing for control applications.

The second category of models are used for cycle-to-cycle control of HCCI combustion to manage the transition between different load-speed regions and mode transition between HCCI operation and SI or Compression Ignition (CI) operation. These models can be based on the category-I (steady-state) models but incorporate the cyclic transition dynamics from one cycle to the next cycle. The three main approaches in the literature for the category-II (transient) models are illustrated in Figure 1. The first group are the physic-based models [33, 34, 35, 36] which are mainly thermodynamic models that include exhaust/residual thermal feedback dynamics from one cycle to the next cycle.

The physic-based models in category-II are developed based on the category-I models and they can predict HCCI ignition timing, the engine output work and the peak pressure. The second group are the estimated discrete-time state-space models [12, 37, 38] obtained from applying system identification methods for different load ranges. In these works, Pseudo-Random Binary Sequence (PRBS) excitation signals using both VVA and DFM are used to find the Multi-Input Multi-Output (MIMO) models to predict ignition timing and Indicated Mean Effective Pressure (IMEP). Inputs for these models include the injected fuel energy, dual fuel ratio / valve timing and charge properties. The third group are chaotic models [39, 40] that are based on the recognition of the deterministic dynamics of cyclic oscillations. Results of these models show that consecutive heat release values can be approximated by a sequence of non-linear patterns in a low-dimensional dynamic map.

A new dynamic physics-based control-oriented model is developed in this study to capture the key dynamics for HCCI combustion in transient fueling operation. The model predicts cycle-to-cycle combustion phasing for an HCCI engine without requiring large computation time and doesn't require inputs that are difficult to measure real-time on an engine. A mean-value model of HCCI combustion from our previous work [41, 42] is extended to a full-cycle simulation model that considers the dynamics of cycle-to-cycle thermal coupling and transient fueling dynamics. Among different ignition timing parameters, the most reliable for feedback control of HCCI combustion is CA50, the crank angle for 50% of the fuel mass fraction burnt [43, 44]. CA50 is chosen as the main output of the model and simulated CA50 is experimentally validated with transient fueling tests where n-Heptane and iso-Octane fuels are modulated to provide fuels at different octane numbers and different equivalence ratios.

In this paper, the following two sections describe the structure of the HCCI combustion model and the fuel transport model. The governing equations of these two main models are introduced and the methodology to parameterize them is discussed. Next, the experimental setup to collect steady-state and transient data is explained. Then, the model is experimentally validated with transient tests. Finally, conclusions and future work are outlined.

HCCI MODEL

The auto-ignition mechanism for the saturated compounds including paraffins such as n-Heptane and iso-Octane exhibits a two-stage ignition attributed to chain branching reactions via alkoxyperoxide dissociation [3, 45]. The two combustion stages as shown for n-heptane in Figure 2 involve Low Temperature Reactions (LTR) for cool flame (1^{st} stage) and High Temperature Reactions (HTR) for the main (2^{nd} stage) combustion. LTR can be easily distinguished from HTR for the fuels in this study since the fuels are low PRF blends (PRF0 - PRF40) and a high percentage of n-Heptane exists in each fuel. In this work, start of the LTR or cool flame combustion is denoted as SOC-CF and it is defined as the crank angle where the net Heat Release Rate (HRR) is 10% of the peak of the HRR for LTR region [2]. The start of the main (2^{nd} stage) combustion, denoted here as SOC, is defined as being the point at which the third derivative of the pressure trace with respect to the crank angle (θ) in CAD (Crank Angle Degree) exceeds a heuristically determined limit (dp3Lim) [46, 47]:

$$\left. \frac{d^3 P}{d\theta^3} \right|_{ign} = 0.25 \frac{\text{bar}}{\text{CAD}^3} \quad (1)$$

The dp3Lim value is determined from the available experimental data in this study and must be determined for each specific engine. CA50 is defined as the crank angle where 50% of the mass fraction of fuel is burnt and the crank angle for the End of Combustion (θ_{eoc}) is described as the crank angle where 99% of the fuel mass is burned (CA99). Definitions of ignition timing are shown in Figure 2 for a sample point using Rassweiler method [48] to calculate fuel mass fraction burnt from the experimental pressure trace data. In Figure 2 θ_d indicates the combustion duration which is the crank angle between SOC and θ_{eoc} .

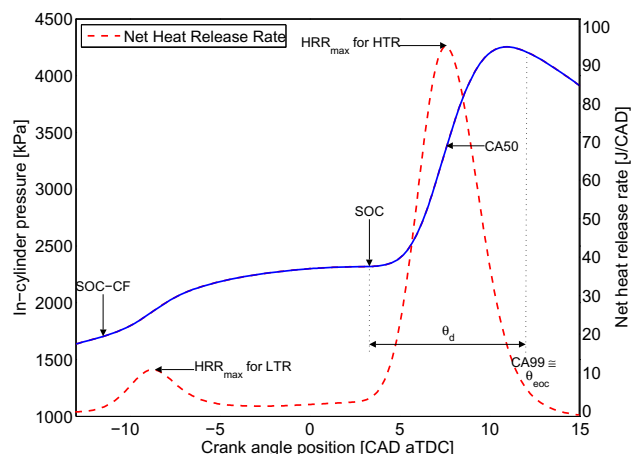


Figure 2: Ignition timing definitions - using in-cylinder pressure trace and net heat release rate for PRF0, N= 810 rpm, $\Phi=0.5$, EGR= 0%, $T_m=82^\circ\text{C}$, $P_m=101\text{ kPa}$.

The models used to simulate an HCCI cycle are explained in this section and are broken down into a sequence of valve events: intake stroke, compression stroke, combustion, expansion stroke, and exhaust stroke.

INTAKE STROKE (IVO → IVC)

IVC temperature & pressure correlation

The intake temperature and intake pressure are usually measured in the intake manifold in the production engines but the mixture condition at Intake Valve Closing (IVC) moment is more important as it predominantly determines the HCCI ignition timing [41]. Two simple semi-empirical correlations are used for the intake process to estimate the pressure and temperature of the mixture at IVC from the measured values of the intake manifold. IVC pressure is predicted using a correlation from a previous study [41] that is parameterized using the steady-state experimental data collected for this study:

$$P_{ivc} = \frac{N^{0.027} \Phi^{0.046}}{T_m^{0.005}} P_m \quad (2)$$

where, N is the engine speed in rpm, and P_m and T_m are the gas pressure and temperature in the intake manifold in kiloPascals (kPa) and in Celsius (°C) respectively and Φ is the equivalence ratio. Conditions of the experimental data to parameterize correlation (2) are detailed later in the *Experimental Engine Setup*. Half of the steady-state experimental data is used to parameterize the correlation and the other half is used to validate the correlation. An error analysis on the steady-state experimental data to validate the correlation (2) indicates an average error of 2.1 kPa and a standard deviation error of 1.8 kPa.

The temperature of air-fuel mixture at IVC (T_{ivc}) is predicted using the following correlation [49]:

$$T_{ivc} = (A T_m^2 + B T_m + C) \frac{\Phi^D \cdot N^E}{(1 + EGR)^F} \quad (3)$$

where A , B , C , D , E and F are the parameters of the correlation that need to be determined. In order to find these parameters, a detailed HCCI Thermo-Kinetic Model (TKM) [47] for arbitrary blends of PRF mixture of n-Heptane and iso-Octane is run to obtain the values of T_{ivc} . The model is run for the same experimental points used to parameterize correlation (2). Table 1 indicates the values of the estimated parameters using simulation results from the TKM. The T_{ivc} correlation is found to be octane number dependent as shown in Table 1. HCCI Correlation (3) is cross-validated using the same data points used to test correlation (2) with the half of the data that is not used to parameterize the correlation. The results of an error analysis indicate 2.2 °C and 1.9 °C for the average error and the standard deviation error respectively.

Results from [50] indicates a relation between the variation in volumetric efficiency and charge heating/cooling

¹PRF number is defined as the volume percentage of iso-Octane in fuel mixture of n-Heptane and iso-Octane.

Table 1: Parameters (par.) for the T_{ivc} correlation

Par.	PRF0 ¹	PRF10	PRF20	PRF40
A	-0.0073	-0.0017	-0.0017	-0.0007
B	1.4829	0.4073	0.5533	0.3470
C	110.3672	101.2723	113.4466	112.3506
D	-0.1488	-0.0431	-0.1164	-0.0051
E	-0.0850	-0.0162	-0.0426	-0.0175
F	0.0092	0.0024	0.0002	0.0012

effect due to the heat transfer and fuel vaporization during the induction process. Thus another approach to find T_{ivc} can be by extending the semi-empirical model from [50] which uses the variation in volumetric efficiency to predict the mixture temperature at BTC.

Residual gas model (initial value)

The composition of the residual gas is considered to be a combination of combustion products for a complete, lean combustion that consists of H_2O , CO_2 , N_2 and O_2 gases. Residual gas fraction (X_r) is defined as:

$$X_r = \frac{m_r}{m_t} \quad ; \quad m_t = m_a + m_{egr} + m_f + m_r \quad (4)$$

where, m presents the mass and indexes of a , egr , f , r and t respectively stand for air, EGR, fuel, residual gas and total when the intake valves are closed. A model [51] is used to get an starting value for the X_r :

$$X_r = \sqrt{\frac{1}{C}} \frac{\pi \sqrt{2}}{360} \frac{r_c - 1}{r_c} \frac{OF}{N} \sqrt{\frac{R T_m |P_{exh} - P_m|}{P_{exh}}} \left(\frac{P_{exh}}{P_m} \right)^{\frac{k+1}{2k}} + \frac{1}{C} \frac{r_c - 1}{r_c} \Phi \frac{V_{ivo}}{V_{dis}} \left(\frac{P_{exh}}{P_m} \right)^{\frac{1}{k}} \quad (5)$$

where, r_c indicates the compression ratio; P_{exh} is the exhaust pressure; R is the gas constant, and k is the ratio of specific heats. V_{ivo} is the cylinder volume at IVO moment and V_{dis} is the displacement volume. OF is the valve overlap factor that is calculated by using geometry and timing of both intake and exhaust valves. The parameter C is calculated as:

$$C = \left[1 + \frac{LHV}{c_v T_m \left(\frac{m_t}{m_f} \right) r_c^{k-1}} \right]^{\frac{1}{k}} \quad (6)$$

where, LHV represents the lower heating value of the fuel and c_v is the constant-volume specific heat capacity of the in-cylinder gas at the IVC moment. The value of X_r obtained from equation (5) is used as the starting value to initialize the HCCI model to solve the thermodynamic equations. The value of X_r is then determined at the end of the simulation cycle based on the amount of mass retained inside the cylinder at the moment of Exhaust Valve Closing (EVC). Then an iterative process is performed with the new X_r until it converges to the X_r obtained at the end of the cycle.

LHV for an arbitrary blend of PRF fuels ($\%V_n + \%V_{iso}$; iso for iso-Octane, n for n-Heptane) is evaluated by:

$$LHV = \frac{\%V_n \rho_n LHV_n + \%V_{iso} \rho_{iso} LHV_{iso}}{\%V_n \rho_n + \%V_{iso} \rho_{iso}} \quad (7)$$

where, $\%V$ is the volume percentage and ρ is the density of the fuel.

Mixing temperature equation

Mixing of the fresh charge with the residual gas from the previous cycles affects the mixture temperature at IVC, but the T_{ivc} values obtained from equation (3) don't consider this effect. A modified temperature for IVC moment ($T_{ivc,mod}$) is calculated to account for the mixing process. In-cylinder gases are considered as ideal gases and assuming energy is conserved in the mixing process of the residual gas and fresh charge yields:

$$T_{ivc,mod}(i) = (1 - X_r) \left(\frac{c_{v,ch}}{c_{v,t}} \right) T_{ivc}(i) + X_r \left(\frac{c_{v,r}}{c_{v,t}} \right) T_r(i - 1) \quad (8)$$

where, i is the cycle number index and subscripts r , ch and t represent the residual gas, the charge (air+fuel+EGR), and the total in-cylinder gas at IVC respectively. The NASA polynomials database [52] is used to determine the c_v properties of different gas components in equation (8).

Dilution fraction equation

Residual gas from previous cycles influences the mixture conditions at IVC not only in terms of the temperature, but also in terms of the dilution level. A parameter is defined as the mixture dilution fraction (X_d)

$$X_d = EGR + \frac{X_r}{1 - X_r} \quad (9)$$

that accounts for the dilution caused by (external) EGR contained in the fresh charge and the dilution caused by the residual gases (internal EGR): since both influence the combustion timing and the fuel burn rate.

COMPRESSION STROKE (IVC $\rightarrow$ SOC)

Isentropic compression

Compression of the unburned mixture prior to combustion can be approximated accurately by an adiabatic isentropic process using a polytropic relation ($PV^k = \text{constant}$) [53]. Here, blow by is ignored and a polytropic relation is used to calculate the temperature and pressure of the in-cylinder mixture at the Start of Combustion (SOC) using the available data at IVC:

$$T_{soc} = T_{ivc,mod} \cdot \left(\frac{V_{ivc}}{V_{soc}} \right)^{k_c - 1} \quad (10)$$

$$P_{soc} = P_{ivc} \cdot \left(\frac{V_{ivc}}{V_{soc}} \right)^{k_c} \quad (11)$$

where, V is the cylinder volume and k_c is the average polytropic exponent for the compression process. The constant k_c can be determined by finding a best polytropic relation between the temperature or pressure at IVC and SOC by simulations from the TKM [47]. Using the results from [30] for different PRF blends at different fueling rates $k_c = 1.32$ is chosen.

SOC model

A Modified Knock-Integral Model (MKIM) [30] is used to predict SOC:

$$\int_{\theta_{ivc}}^{\theta_{soc}} \frac{\Phi^B}{A \exp \left(\frac{C (P_{ivc} v_c^{k_c})^D}{T_{ivc,mod} v_c^{k_c - 1}} \right) N} d\theta = 1.0 \quad (12)$$

where, θ is the engine crank angle, B , C , and D are constant parameters. The value of the expression being integrated increases as the point of SOC is approached. A and v_c are determined by:

$$v_c(\theta) = \frac{V_{ivc}}{V(\theta)}, \quad A = E_1 X_d + E_2 \quad (13)$$

where, E_1 and E_2 are constant parameters and the cylinder volume, $V(\theta)$, is calculated at any crank angle using slider crank mechanism [53]. Parameters E_1 , E_2 , B , C , and D need to be determined to be able to use the MKIM to predict SOC. Similar to [30], simulation results from a virtual engine at a range of operating conditions are required to parameterize the MKIM. To do this the TKM [47] is calibrated for the Ricardo engine described in Table 2. Calibration of the TKM is done by using only 1% of the steady-state experimental points used in this study.

Table 2: Configuration of Ricardo single-cylinder engine

Parameters	Values
Combustion Chamber	Pent-roof design
Bore $\times$ Stroke [mm]	80 $\times$ 88.9
Compression Ratio	10
Displacement [L]	0.447
Number of Valves	4
IVO, IVC ² [aBDC]	-175°, 55°
EVO, EVC [aBDC]	-70°, -175°

In Table 3, 10880 simulated operating conditions are used to explore the engine variable parameter space. Results of running TKM for 10880 simulations lead to 6554 combustion with complete ignition from which late ignited³

²Valve opening/closing point is defined at the valve lift of 0.15 mm. [53]

³TKM simulations in which the second stage of HCCI combustion occurs at the crank angle higher than 15 degrees after Top Dead Center (TDC).