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Control Oriented Modeling of Combustion Phasing for an HCCI Engine

Mahdi Shahbakhti and Charles Robert Koch

Abstract— **A promising method for reducing emissions and fuel consumption of internal combustion engines is the Homogeneous Charge Compression Ignition (HCCI) engine. Control of ignition timing must be realized before the potential benefits of HCCI combustion can be implemented in production engines. A model suitable for real time implementation is developed and this model is able to predict ignition timing with an average error of less than 2 crank angle degrees. A modified knock-integral model (MKIM), with correlations for gas exchange process and fuel heat release, is used to predict HCCI combustion timing (CA50, crank angle where 50% of the fuel mass is burnt). The MKIM model is parameterized using a thermokinetic simulation model. Experimental data from a single cylinder engine at several HCCI operation conditions and three fuel blends is used to validate the model.**

I. INTRODUCTION

In an HCCI engine, premixed air and fuel are compressed until the charge autoignites. This results in homogeneous combustion with fast heat release that can significantly reduce NOx and particulate emissions, while achieving high thermal efficiency. In an HCCI engine the charge composition at intake valve closing is the predominant factor affecting combustion timing. The control of ignition timing is critical in order to make HCCI practical for production engines [1]. Despite the extensive work done on control-oriented modeling of HCCI ignition timing, improved models that work with easily measurable inputs and which include variable engine working conditions are still needed.

Several model types have been used to simulate the ignition timing of HCCI engines. They differ in the complexity and required input data. These models range from multi-dimensional CFD models ([2], [3]) and multi-zone models ([4], [5]), to simple control-oriented models [6], [7].

For real-time control, a compromise between the computation time and the accuracy of the model is required. Low-order control oriented models can predict HCCI ignition timing with a reasonable accuracy while having short computational time [8]. Several approaches to control oriented modeling of HCCI combustion have been investigated. In the simplest approach, HCCI ignition timing is measured as a function of engine variables that affect HCCI combustion [9] but this requires a large number of experiments. A temperature threshold to find the start of combustion [10] is another simple modeling method but may fail to capture combustion phasing at different operating conditions. The

Shell model [11] is used in [6] to predict HCCI ignition timing with an accurate estimation of the HCCI ignition timing for temperature and engine speed variations, but with less accurate results when changing the load. In [6], [8], [12], models based on Arrhenius-type reaction rate [13] are used. This model type is accurate, but requires instantaneous fuel and oxygen concentrations and in-cylinder gas temperature which are impractical to measure. To remove the need for in-cylinder composition data, some researchers [14], [15] omit the mixture composition term from the Arrhenius reaction rate and assume that the composition term in Arrhenius reaction rate is of secondary importance compared to other terms. Their results seem accurate in the studied HCCI range, but still need to be validated over a wide range of HCCI operation. The knock-integral model [16] is another category of control-oriented modeling of HCCI combustion timing. This model is based on an exponential correlation which includes the elements of in-cylinder gas pressure and temperature to predict the auto-ignition of a homogeneous mixture [17], [18], [19]. Although this model produces accurate results, again there are some variables that are difficult and expensive to measure, limiting the real-time control application of this model.

To improve existing models, another category of models has been developed [19], [20], [21] and [22]. The model proposed in this paper is designed to be a control-oriented model which also works for different engine conditions including variable load, air temperature, engine speed, air fuel ratio (AFR), and EGR (Exhaust Gas Recirculated). Instantaneous in-cylinder gas temperature, pressure and concentrations of fuel and oxygen are not required, instead measured AFR, EGR and intake gas temperature and pressure are required. This model extends our previous work [22] because the inputs are easier to measure (the intake temperature and pressure) and CA50 is predicted.

In this paper, section II explains the model developed to predict HCCI combustion timing. Section III shows the methodology used to parameterize the model and section IV explains the experimental setup and conditions of the HCCI test points. Finally, the proposed model is experimentally validated and conclusions are reached.

II. MODEL DESCRIPTION

A. IVC temperature & pressure correlation

HCCI combustion is mainly affected by the properties of air fuel mixture at Intake Valve Closing (IVC). To predict the start of combustion (SOC) our offline HCCI simulation requires temperature and pressure of the air fuel mixture at IVC. Since temperature and pressure of the air fuel mixture

are easily measured in the intake manifold, correlations are used to predict pressure and temperature of the mixture at IVC from the measured values of the intake manifold. Two correlations for P_{ivc} and T_{ivc} are detailed below.

The following correlation is found to fit well on the available experimental data:

$$P_{ivc} = \frac{N^{0.038} \, \Phi^{0.020}}{T_{man}^{0.022}} P_{man} \qquad (1)$$

where, N is presented in rpm and P_{man} in kiloPascals (kPa) and T_{man} in Celsius (C). Using the correlation (1) over available experimental data, the average error and error standard deviation are 1.33 kPa and 0.97 kPa respectively and the maximum relative error is less than 4%.

Since it is difficult to experimentally measure the mixture temperature at IVC, the values of T_{ivc}, are obtained from Thermo-Kinetic Model simulation (TKM[1]) which is run for all the experimental HCCI points used in this study. Simulated T_{ivc} values that match experimental SOC are chosen as the correct T_{ivc}. By plotting the change of T_{ivc} with respect to T_{man}, it was noticed that after a specific intake temperature (i.e. $T_{man} = 110^oC$), T_{ivc} decreases with an increase in T_{man}, while the reverse trend is seen for the cases with T_{man} lower than 110^oC. This comes from a change in the direction of heat transfer between the in-cylinder mixture and cylinder walls, where a constant wall temperature is assumed in the TKM for all the available HCCI experiments.

The following correlation was found based on the available experimental data:

$$T_{ivc} = (a \, . \, T_{man} + b) \frac{\Phi^c \, . \, N^d}{(1 + EGR)^e} \qquad (2)$$

where a, b, c, d, and e are the parameters of the correlation that should be determined and Φ represents equivalence ratio of the air-fuel mixture. The correlation suggests a linear relation between gas temperature at IVC and the intake manifold temperature. The sign of a changes from positive to negative from the cases with $T_{man} < 110^0C$ to the cases with $T_{man} \geq 110^0C$. This implies to the change of heat transfer direction after a certain thermal condition. The correlation also suggests that T_{ivc} is increased with an increase in engine speed. This can be caused by a combination effects of pressure rise in cylinder gas and the less available time for heat transfer. Furthermore, for the zone of $T_{man} < 110^0C$, T_{ivc} is decreases with an increase in EGR, while it increases with an increase in equivalence ratio. This trend is reversed when $T_{man} \geq 110^0C$. This is because of the influence of EGR and Φ on the heat transfer, while the direction of heat transfer is controlled by the temperature difference between the in-cylinder gas temperature and cylinder wall temperature. Increasing EGR

[1]The details of the TKM is explained later in section III.

leads to an increase in the specific heat capacity of the mixture which reduces the rate of heat transfer.

Using the correlation (2) for the available experimental data, the maximum average error and maximum error standard deviation are 3.1^oC and 2.9^oC respectively.

B. SOC Model

The original Knock Integral Model (KIM) for predicting SOC of HCCI engine is introduced and then modified in this section.

1) Knock Integral Model (KIM): Kinetics of HCCI combustion are very similar to the chemical kinetics of knock in SI (Spark Ignition) engines [15]. Knock in SI engines has been investigated for decades [16], [23]. Livengood and Wu [16] developed a correlation to predict the autoignition of a homogeneous mixture, it was later termed the Knock-Integral Model (KIM) [24]. Livengood and Wu proposed that there is a functional relationship between the concentration ratio, $(x)/(x)_c$, of the significant species in the reaction and the relative time, t/τ. The critical concentration ratio, $(x)_c$, is the concentration of the species at the end of the reaction being studied. Using the crank angle instead of time, the ignition correlation of Livengood and Wu becomes:

$$\frac{(x)}{(x)_c} = \int_{\theta_o=0}^{\theta=\theta_e} \frac{1}{\omega\tau} \, d\theta = \int_{\theta_o=0}^{\theta=\theta_e} \frac{1}{A\omega e^{(b/T)}p^n} \, d\theta = 1.0 \quad (3)$$

where τ is the ignition delay, T is the mixture temperature as a function of time, p is the mixture pressure as a function of time. A, b, and n are empirical constants which are determined for each engine. θ_e represents the crank angle that autoignition or knock occurs and θ_o is the initial crank angle that the integration begins. The engine speed (ω) is represented in rpm, the pressure in kiloPascals (kPa), and the temperature in Kelvin (K). The value of θ_o is selected to be the crank angle of IVC timing where no appreciable reaction has begun ($\theta_o = \theta_{IVC}$). The value of the expression being integrated increases as the point of autoignition is approached as shown in Figure 1.
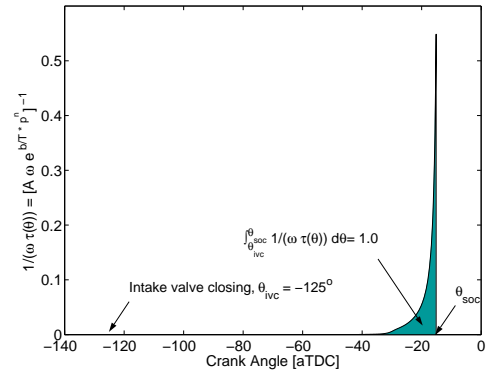

Fig. 1. Graphical integration of $1/(\omega\tau)$ from the IVC to the SOC.

In this study, experimental 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 [25]:

$$\left.\frac{d^3 P}{d\theta^3}\right|_{ign} = 0.0125 \frac{\text{kPa}}{\text{CAD}^3} \qquad (4)$$

2) Modified Knock-Integral Model (MKIM): Although the KIM can predict HCCI ignition, it is impractical for a real engine operation. Engine conditions, such as temperature, pressure and mass fraction burned must be continuously available during compression. In simulations this is possible but on an engine it is not practical. Furthermore, the KIM is restricted to engine operation at a constant AFR without EGR. To adapt KIM to an HCCI engine which has varying AFR rates and EGR these factors need to be included by the following three modifications:

- To avoid the requirement of crank angle measurements of temperature and pressure during the engine compression, the temperature and pressure rise in the cylinder is assumed to occur as a polytropic process [14]. This assumption neglects any pre-ignition heating resulting from reactions that occur before the SOC.
- The SOC changes when the concentrations of the fuel and oxygen are varied [1], [26]. A crank angle measurement of these concentrations is available in the TKM simulation and can be used in a modified KIM to account for the AFR changes but this information is not available in the real engine. The concentrations of the fuel and oxygen are indicative of the equivalence ratio [6], [10]. The equivalence ratio is a good indication of both the amount of fuel and air concentrations in the engine charge and it can be easily measured on an operating engine using a broadband oxygen sensor. Therefore, an equivalence ratio term is added to the KIM to account for the changes in AFR of the mixture.
- For some fuels such as iso-octane the amount of EGR seems to affect SOC. To generalize the correlation for these fuels, one term is added to account for the changes in EGR levels.

The resulting MKIM is [22]:

$$\int_{\theta_{IVC}}^{\theta_{SOC}} \frac{\Phi^x}{A\omega \, exp\left(\frac{b(P_{IVC} v_c^{n_c})^n}{T_{IVC} v_c^{n_c-1}}\right)} \, d\theta = 1.0 \qquad (5)$$

$$v_c(\theta) = \frac{V(\theta_{IVC})}{V(\theta)}, \; A = C_1 EGR + C_2$$

where, C_1, C_2, b, n, n_c, and x are constant parameters. The constant n_c represents the average specific heat capacity ratio of all the simulations determined by a numeric best fit. The cylinder volume, $V(\theta)$, is calculated at any crank angle from engine geometry.

3) Combustion Phasing (CA50): Combustion duration of an HCCI engine can differ considerably with the same SOC. The crank angle where 50% of fuel mass has burned, denoted here as CA50, is the best indication of HCCI combustion

phasing [27]. CA50 seems to be a robust indication of HCCI combustion timing, since a small error of combustion phasing results in a small error of the phasing in CAD as the slope of energy release is very steep. CA50 is useful for feedback control of HCCI combustion [27].

A modified Wiebe function to predict fuel Mass Fraction Burned (MFB) is used to calculate CA50:

$$x_b(\theta) = 1 - exp\left(-a\left[\frac{\theta - \theta_s}{\theta_d}\right]^n\right) \qquad (6)$$

$$\theta_d = CD(1 + EGR)^x \Phi^y$$

where, θ_s and θ_d are SOC crank angle and combustion duration (here 0.5 is 50%) in CAD respectively. θ_s, EGR and Φ are the three required inputs. Values of θ_s come from the MKIM and parameters a, n, CD, x, and y are determined by applying an estimation code on the experimental data. As seen in the correlation, combustion duration varies with a change in Φ and EGR level which is consistent with the observations in [1], [26] and [27].

III. MODEL SETUP

To parameterize and validate the MKIM model requires three steps that are detailed below.

A. Thermokinetic Model Simulations

For accurate parameter estimation, the MKIM requires data from the engine at many different working conditions. TKM simulation is used as a virtual engine to provide the required data to parameterize the MKIM. The TKM is a single zone thermo-kinetic model [28] which describes the in-cylinder thermo-kinetic state of an HCCI engine from IVC to exhaust valve opening. The chemical kinetic mechanism, consisting of 58 species and 102 reactions, is used to describe the ignition and combustion of arbitrary blends of a Primary Reference Fuel (PRF) mixture of N-heptane and Iso-octane.

The resulting model which couples together the thermodynamic model with the chemical kinetic mechanism was validated with HCCI experimental data from [29]. The model is calibrated for the single-cylinder engine described in Table I. To calibrate the TKM for the new engine, less than 10% of the experimental points, that later will be used to validate the MKIM, are used. The TKM predicts SOC for the single-cylinder engine with a maximum error of 1 CAD over the different conditions.

TABLE I

CONFIGURATIONS OF THE RICARDO SINGLE-CYLINDER ENGINE

Parameters	Values
Bore $\times$ Stroke [mm]	80 $\times$ 88.9
Compression Ratio	10
Displacement [L]	0.447
Number of Valves	4
IVC [aBDC]	55°
EVO [aBDC]	−70°

The engine speed, initial mixture temperature and pressure, EGR percentage, and equivalence ratio are varied over the ranges outlined in Table II and a TKM simulation is performed. The parameter ranges given in Table II are chosen to represent typical HCCI operation of the Ricardo single-cylinder engine.

TABLE II

PARAMETER VARIATIONS CARRIED OUT USING THE TKM

Engine Speed	800, 1000 rpm
Initial Temperature	80, 85,..., 155, 160 ^oC
EGR(%)	0, 10, 20, 30
Equivalence Ratio	0.5, 0.6, 0.7, 0.8
Initial Pressure	95, 100, 105, 110, 115 kPa
Fuel	PRF0, PRF10, PRF20
Wall temperature	390 $^\circ K$

From the resulting 8160 simulations, complete combustion occurred in 5131 simulations. Since near to TDC firing conditions are of practical interest, late ignited[2] TKM simulations are excluded. This results in 4727 TKM simulations which are used to estimate the MKIM parameters.

B. Finding the Polytropic Parameter

Using the engine parameter variations for the applied PRF fuels, the values of n_c can be determined by fitting a best polytropic relation between the temperature or pressure at IVC and SOC of the simulations. The value of $n_c = 1.32$ is chosen using the simulation results of [22].

C. Optimizing the MKIM Parameters

The parameters of the MKIM equation (5) are fit to minimize the error of the integration, where the target value is 1.0. The numerical minimization is performed using the built-in Matlab function $fminsearch$, which uses the Nelder-Mead simplex minimization method [30].

IV. EXPERIMENTAL SETUP

A single cylinder Ricardo Hydra Mark III engine with a Rover K7 head is used to run the HCCI experiments – see Table III. Port fuel injection is used and is timed to ensure closed intake valves. The fresh intake air entering the engine is heated by the electric air heater positioned upstream of the throttle body. Exhaust gases are recirculated (EGR) using an insulated return line from the exhaust to the intake manifold directly after the throttle body. Intake temperature is measured with a K-type thermocouple to include EGR heating effects. The cylinder pressure is measured with a Kistler ThermoCOMP (model 6043A60) piezoelectric pressure sensor that is flush mounted in the cylinder. For each experimental point, pressure traces from 100 consecutive engine cycles are recorded with 0.1 CAD resolution.

[2]TKM simulations in which the second stage of HCCI combustion happens at the crank angle higher than 15 degrees after TDC.

TABLE III

ENGINE'S OPERATING CONDITIONS FOR HCCI VALIDATION

Engine Speed	800, 1000 rpm
Manifold Temperature	60 - 140 ^oC
EGR(%)	0 - 28.5
Equivalence Ratio	0.43 - 0.95
Manifold Pressure	90.5 - 96.3 kPa
Fuel	PRF0, PRF10, PRF20
Coolant Temperature	70 - 80 ^oC
Oil Temperature	70 - 80 ^oC

V. RESULTS & DISCUSSION

Using 4727 TKM simulations, the parameters of the MKIM are determined. The estimation process is done in two stages. In the first stage, parameters b, n, x, and A are determined by applying the estimation code on the all the TKM simulation results. Then, the parameter A is determined for each group of TKM simulations with the same EGR level, keeping the values of b, n, and x constant from the first stage. Figure 2 indicates the predicted SOC for PRF20 TKM simulations with and without the EGR term. As seen in the figure, both average error and error standard deviation are substantially reduced when EGR level is considered in the MKIM. In addition, Figure 2 shows the accuracy of the MKIM predictions deteriorates for late ignitions. This is because the pre-ignition heating by the reactions that occur during the large time span before late ignitions violates the polytropic assumption used in the MKIM. For 709 points in the Figure 2, the average error and error standard deviation are 1.68 CAD and 1.41 CAD respectively. The range of average error and error standard deviation for all TKM simulations are 1.62-2.25 CAD and 1.38-1.79 CAD respectively.

Sample values of parameters A, b, n, n_c, and x in equation (5) determined for the PRF blends are shown in Figure 2. The order and sign of these parameters are the same for all TKM simulations. By examining these parameters it can be seen that for the three PRF blends the SOC advances by increasing the initial temperature and initial pressure, while it retards with an increase in the engine speed. This trend has been also observed in [6]. Furthermore for all three PRF blends studied, SOC happens sooner when equivalence ratio is increased, while SOC is delayed when EGR level is increased (at constant temperature) similar to [1].

The 4727 points, partly shown in Figure 2, cover a substantial range of initial temperature, equivalence ratio, EGR, initial pressure, and engine speed extending previous work [14], [6], [10], [19], [21] on control-oriented modeling of HCCI ignition timing. However, the model still needs to be cross validated with experimental data which is the subject of the next section.

A. Experimental Validation

The MKIM has been parameterized by the TKM simulation. The real test of the MKIM model is how well it works with the experimental data from HCCI experiments
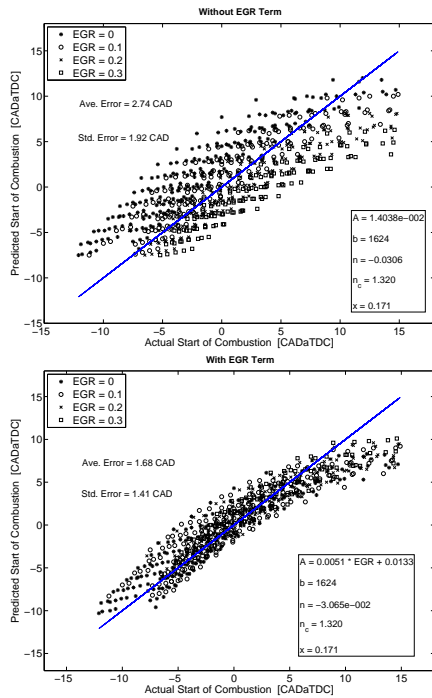
Fig. 2. Predicted SOC for PRF20 TKM simulations at various engine conditions at 800 rpm using the MKIM. The line represents where the prediction is the same as the actual SOC.
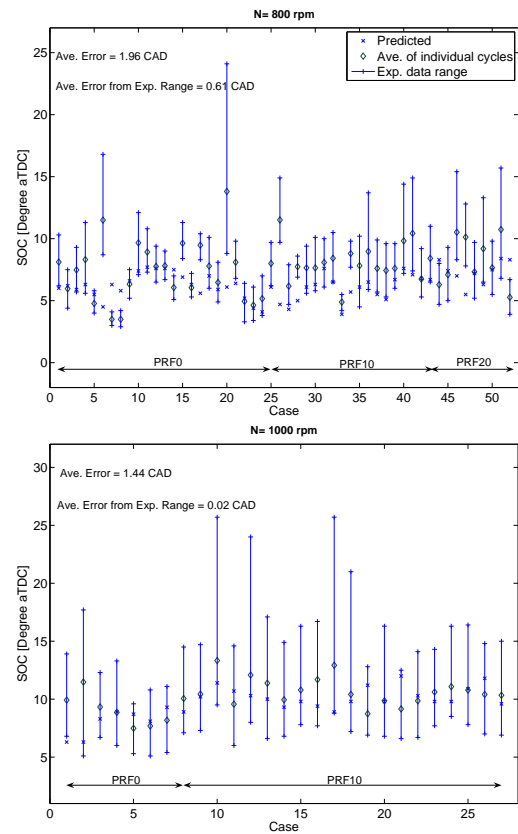

Fig. 3. Comparison between predicted and experimental SOC for three PRF blends at various engine conditions, using the MKIM with IVC correlations.

described in section IV. In Figure 3 the MKIM predicted SOC values are compared to the corresponding experimental points for three different fuels at different conditions. Since the experimental data consists of 100 measured cycles the range of SOC variation is also shown for each HCCI experiment. Figure 3 shows good agreement between the MKIM prediction and the measured experimental SOC. The total average error for 79 operating points in Figure 3 is 1.76 CAD, while the total average error[3] from the range of experimentally calculated SOCs is 0.39 CAD.

Experimental HCCI data has cyclic variations in SOC due to the normal variations in equivalence ratio and dilution rate [31] or mixture inhomogeneity [32]. Furthermore, a late combustion in one cycle can be correlated with an early combustion in the next cycle, and vice versa [31] which leads to a large range of HCCI cyclic variation. Examining Figure 3, it can be seen that the cases with high cyclic variations produce a large percentage of the error between the MKIM prediction and the measurement. It is important to note that the MKIM model does not model cyclic variations of HCCI combustion.

To parameterize the modified Wiebe Function (6) half of the experimental data is used, while the next half is used to validate the correlation. Figure 4 shows the estimation and validation results. A positive sign of x and a negative sign of y in the figure imply that the combustion duration increases with an increase in EGR or with a decreases in Φ. This trend has been also observed in [1]. Average error of

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[3]To calculate this term, no error is considered when predicted SOCs are within the range of SOCs of individual cycles for each experimental point.

predicted CA50 is 1.84 CAD and the average error from the experimental range is 0.6 CAD. The two plots in the bottom of Figure 4 compare the predicted MFB curve with those of experiments from all individual cycles. They show that the model can predict not only CA50, but also the shape of MFB curve. The agreement between the predicted and experimental CA50 is good considering that MKIM was parameterized using the TKM simulations and then validated with experimental data.

VI. CONCLUSIONS

A Modified Knock Integral Model (MKIM) was extended with semi-empirical correlations for gas exchange process and fuel energy release to predict HCCI combustion timing (CA50). The resulting model doesn't require instantaneous in-cylinder parameters but only intake manifold temperature and pressure, EGR rate, and equivalence ratio to predict CA50. The model was tested for a large number of TKM simulations (4727 points) and HCCI experiments (79 points). The MKIM model is able to predict combustion phasing for the experimental HCCI engine with an average error of less than 2 CAD. This error level seems an acceptable compromise between accuracy and computational load. The MKIM seems promising for HCCI engine control and could be used to schedule engine variables such as intake temperature (heater), intake pressure (super/turbo charger), EGR level (electronic valve), and fuel type (fuel modulating system).
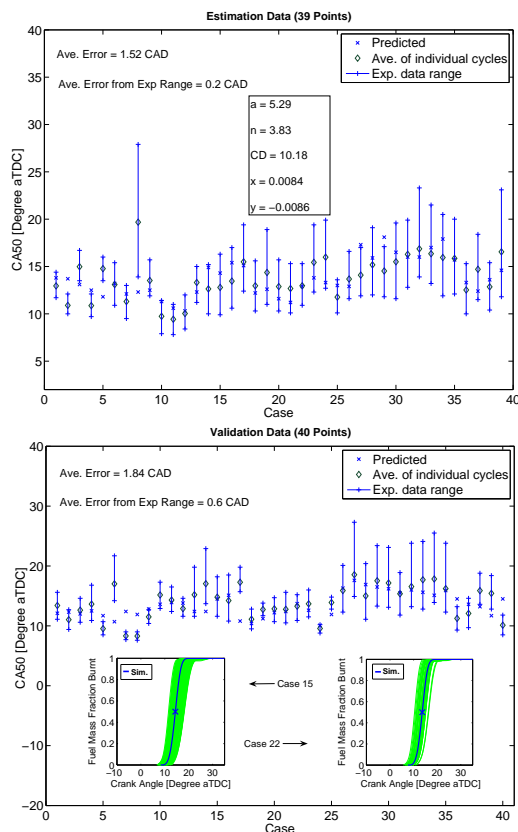
Fig. 4. Comparison between predicted and experimental CA50 for three PRF blends at various engine conditions.

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