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Predicting Start of Combustion Using a Modified Knock Integral Method for an HCCI Engine

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ABSTRACT

Homogeneous Charge Compression Ignition (HCCI) is a promising combustion concept for internal combustion engines to reduce emissions and fuel consumption. Unlike spark ignition and diesel engines in which ignition is controlled by spark and spray injection timing respectively, HCCI combustion auto-ignites given the correct mixture conditions which makes HCCI ignition difficult to control. It is thus critical to understand the characteristics of HCCI ignition timing in order to find suitable strategies for ignition control.
This paper presents a modified model of ignition timing which is based on the Knock-Integral Method. Since this model doesn't require instantaneous in-cylinder parameters, it is suitable for control application on HCCI combustion. The model is tested using both simulation results of a Thermo-Kinetic Model and experimental data. With seven model parameters, the ignition timing of over 250 HCCI points at different conditions for four different Primary Reference Fuels (PRF) is predicted to within an average error of less than 1.5 degrees of crank angle.
This model is computationally efficient and could be implemented in the engine control unit of an HCCI engine to calculate the required inputs that are needed to get the desired ignition timing.

INTRODUCTION

For HCCI combustion to take place at the appropriate crank angle, the correct cylinder charge is needed at the beginning of combustion. If the combustion event occurs too early, the hot combustion gases must be compressed, decreasing the thermal efficiency of the engine, increasing the NO_x emissions, and potentially leading to knock. If the combustion event occurs too late, not all of the fuel will react decreasing the thermodynamic efficiency of the engine and increasing the unburned hydrocarbon and carbon monoxide emissions [1, 2]. To account for variations in the combustion chamber while still accurately controlling HCCI combustion timing, feedback from the combustion chamber is needed [3]. In-cylinder pressure measurement with sufficient bandwidth is one possible feedback signal although it is expensive to implement. Simulation models can provide insight into the important parameters and inputs that affect ignition timing. They also can be used as a tool to evaluate the performance of different control strategies for ignition timing in HCCI engines.

Different types of models 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 ([4, 5]) and multi-zone models ([6, 7]), to simple control-oriented models [8, 9]. For real-time control a compromise between the computation speed and accuracy in a model is required. Ignition control of HCCI combustion is grouped into the following five categories of models. The simplest model defines a temperature threshold to find the start of ignition [10]. This model fails to capture combustion phasing at different operating conditions. This is due to the dependance of the initiation of the combustion reaction on not only the temperature, but also on the concentration of species present in the cylinder [10]. The Shell model [11] is another model used in [9] to predict HCCI ignition timing. The results from the Shell model show an accurate estimation of the HCCI ignition timing for the temperature and engine speed sweep, but less accurate results when changing the load. In [8, 9, 12, 13], models based on two-step Arrhenius-type reaction rate [14] are used. Here the integration of the Arrhenius global reaction rate for the fuel is tracked until it reaches a threshold value defined from experimental data. This model type is accurate, but depends on having instantaneous fuel and oxygen concentrations as well as in-cylinder gas temperature which is

impractical for on-board ignition timing control. The knock-integral model [15] is a fourth category in 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 [3, 16, 17]. Although this model produces accurate results, again there is a need for some parameters which are difficult and expensive to measure. This limits using this model for real-time control. To make more accurate models, a fifth category of models has been defined. This includes the model presented in [18] where the effects of residual gas and air fuel ratio (AFR) have been added to the knock-integral model and also another model [17] in which a pressure term has been added to the knock-integral model to benefit from the physics of Arrhenius reaction rate based models.

Despite a plurality of different HCCI ignition models, improved control-oriented models which work with easily measurable inputs and which include variable working conditions are still needed. The model proposed in this paper addresses some of the compromises of existing models. In particular it is designed to be a control-oriented model which also works for different conditions including variable load, air temperature, engine speed, AFR, and EGR (Exhaust gas recirculation)[1]. Instantaneous in-cylinder gas temperature, pressure or the concentrations of fuel and oxygen are not required, instead measured EGR, AFR and gas temperature and pressure at the moment of intake valve closing (IVC) are required.

In this paper, the first section explains the methodology used to modify the original knock integral model. Then, our existing HCCI combustion Thermo-Kinetic Model (TKM) [19] is used as a virtual engine to produce the required data for parameters estimation of the model. Next, the proposed model is applied on HCCI combustion and the performance of the model is validated for 250 HCCI TKM simulations/experiments at different engine conditions. Finally, conclusions are reached.

MODEL DESCRIPTION

In this section, the original Knock Integral Model and its application to HCCI combustion are explained and then the model is further developed into a Modified Knock Integral Model.

KNOCK INTEGRAL MODEL (KIM) Auto-ignition in spark ignition (SI) engines has been investigated for decades [15, 20]. The initial interest was motivated by the phenomenon of engine knock due to the premature autoignition of the fuel and air mixture prior to the spark. A method to predict the conditions under which knock would occur for various fuels was needed. Livengood and Wu [15] developed the first correlation to predict the autoignition of a homogeneous mixture, it was later termed the Knock-Integral Method (KIM) [21]. The basis of the correlation stems from the ignition delay of various fuels using a rapid compression testing machine. The resulting empirical relationship in the general form is:

$$\tau = Ae^{(b/T)p^n} \tag{1}$$

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, and A, b, and n are empirical constants. The constants are the model parameters which are determined for each engine.

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:

$$\frac{(x)}{(x)_c} = \int_{\theta_o=0}^{\theta=\theta_e} \frac{1}{\omega\tau}\, d\theta = \int_{\theta_o=0}^{\theta=\theta_e} \frac{1}{A\omega e^{(b/T)p^n}}\, d\theta = 1.0 \tag{2}$$

where θ_e is 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 revolutions per minute (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 intake valve timing(IVC) where no appreciable reaction has begun ($\theta_o = \theta_{IVC}$). The selection of θ_o is not critical since the value of the equation being integrated is small before either a significant reaction or large compression has occurred. The value of the expression being integrated $(1/(\omega\tau))$ increases as the point of autoignition is approached as shown in Figure 1.

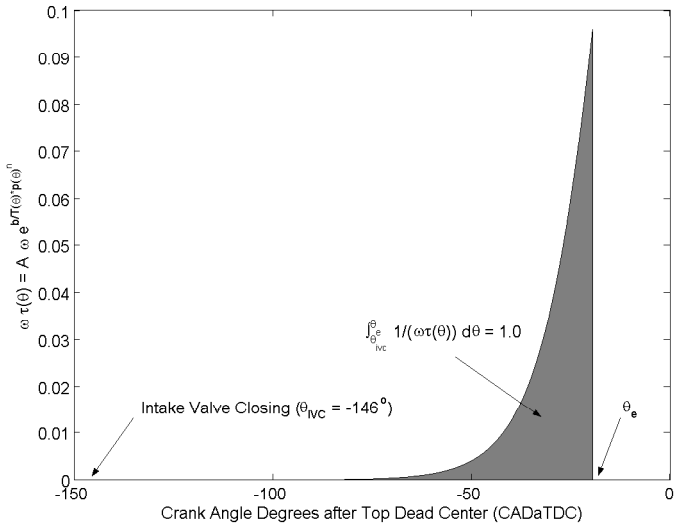

Figure 1: Graphical integration of $1/(\omega\tau)$ from the intake valve closing to the start of combustion. In this example, the start of combustion is defined as the crank angle where 1% of the fuel has burned.

[1] Most of the control-oriented HCCI ignition models don't incorporate AFR and EGR effects; therefore, those model don't work well when EGR and AFR are changed.

Equation (2) is for an engine operating at a constant AFR with no exhaust gas recirculation (EGR). To adapt this correlation to an HCCI engine with varying AFR rates and EGR typical of HCCI operation, these factors have to be accounted for.

To test the performance of the KIM, the engine simulations[2] are used to determine the model parameters. Then the start of combustion (SOC) is predicted for these same simulations to show if the correlation can capture the relationship between the changing engine operating conditions and the start of combustion. Two different SOCs are defined. In the first approach, SOC is defined as the crank angle as 1% of the mass fraction fuel burns, while in the second approach SOC is defined as a threshold of the third derivative of pressure with respect to crank angle degrees (CAD) [22]:

$$\left.\frac{d^3P}{d\theta^3}\right|_{ign} = 0.05\frac{\mathrm{kPa}}{\mathrm{CAD}^3} \tag{3}$$

The KIM did a good job predicting the start of combustion, for both definitions. For both 1% mass burned and the pressure derivative limit definitions of SOC and for both n-heptane and iso-octane fuels, the average error of the ignition prediction was less than $1.0\ CAD$.

Figures 2 and 3 are two samples of simulation results showing the ability of the KIM to predict the SOC for the two fuels. The resulting parameters are also shown.

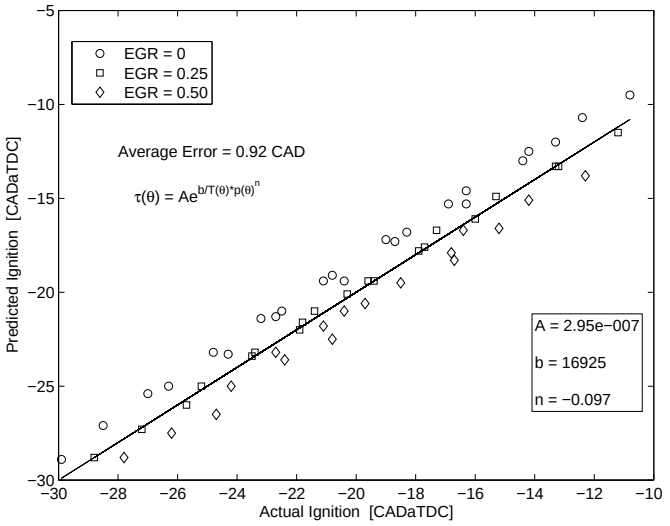

Figure 2: Predicted SOC based on 1% mass burned, using the KIM with iso-octane as fuel. The line represents where the prediction is the same as the actual SOC.

[2]The engine simulations are explained in details in *Model Setup* section of the paper.

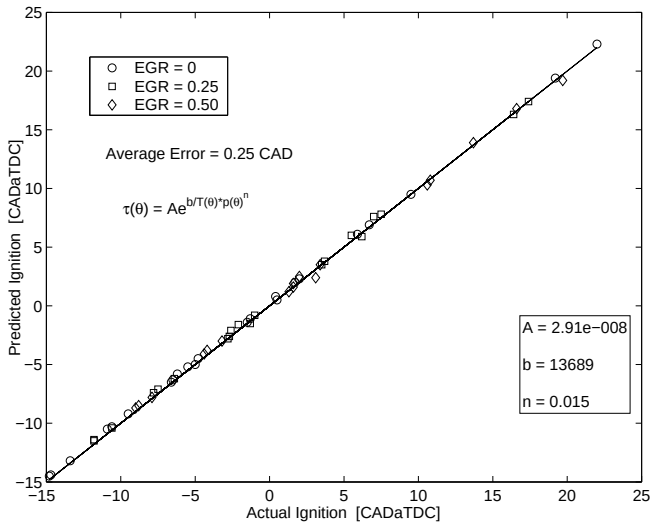

Figure 3: Predicted SOC based on the pressure derivative limit, using the KIM with iso-octane as fuel. The line represents where the prediction is the same as the actual SOC.

MODIFIED KNOCK-INTEGRAL MODEL (MKIM) Although the KIM does a good job predicting ignition, it is impractical for a real engine operation. Engine conditions, such as temperature, pressure and mass fraction burned, must be available during compression (here every $0.1\ CAD$). In the TKM simulations this is possible, but on a real engine, it is not.

The KIM developed for SI engines is only applicable over a range of specific temperatures for a particular pressure [15]. However in HCCI engines this restriction may not be important due to typically lower peak cylinder temperatures than in traditional SI engines [23]. In the simulations done here, no evidence is found of the KIM giving erroneous predictions (due to cylinder temperatures being outside of the acceptable range of the correlation).

Polytropic Compression To avoid the requirement of crank angle measurements of temperature and pressure during the engine compression, the SOC can be predicted using the KIM if the temperature and pressure rise in the cylinder is assumed to occur as a polytropic process [8]. This assumption neglects any pre-ignition heating resulting from reactions that occur before the SOC. Thus, the start of combustion is defined as 1% of mass fraction burned since only a small amount of heat release has occurred.

The compression of the gases in an engine from IVC to SOC can be predicted by a polytropic process [24]. To consider a polytropic process ($PV^\gamma = constant$), the ratio of specific heat capacity (γ) for the gases in the cylinder of an engine is needed. As the mixture and concentrations of species in the cylinder of the engine change, γ varies too. Two methods to obtain γ for the gases in the cylinder of an engine at θ_{IVC} are given. Knowing the initial pres-

sure, temperature and species concentrations, the ratio of specific heat capacity can be found analytically using NASA polynomials [19]. This method requires significant computation and data for species concentrations and temperatures in the cylinder. The other method is to obtain the temperature or pressure at IVC and SOC of multiple simulations and use a best fit method to find the ratio of specific heat capacity. The resulting equations to calculate the temperature and pressure at the SOC become:

$$T_{SOC} = T_{IVC}\ v_{SOC}^{n_c-1} \tag{4}$$

$$P_{SOC} = P_{IVC}\ v_{SOC}^{n_c} \tag{5}$$

$$where\ \ v_{SOC} = \frac{V_{IVC}}{V_{SOC}}$$

where the constant n_c does not represent the actual specific heat capacity, but rather the average of all the simulations are determined by a numeric best fit. The volume of the cylinder can be calculated at any crank angle from engine geometry.

To predict the SOC with only the initial temperature and pressure, equations (4) and (5) are substituted into the KIM (2). The resulting integral becomes:

$$\int_{\theta_{IVC}}^{\theta_{SOC}} \frac{1}{\tau}\ d\theta = \int_{\theta_{IVC}}^{\theta_{SOC}} \frac{1}{A\omega\ exp\left(\frac{b(P_{IVC}v_c^{n_c})^n}{T_{IVC}\ v_c^{n_c-1}}\right)}\ d\theta = 1.0 \tag{6}$$

$$where\ \ v_c = v_c(\theta) = \frac{V(\theta_{IVC})}{V(\theta)}$$

Simulation results based on the Modified Knock Integral Model (MKIM) equation (6) show that the modified correlation does not predict the SOC as accurately as the original KIM. This is not surprising since in the MKIM only one value of each pressure and temperature (at IVC) is used, while the KIM uses the whole time sequence of pressure and temperature from the IVC to SOC. However the equivalence ratio and EGR rate also effect the SOC [19]. These two parameters are incorporated into a further improved MKIM.

Fuel and Oxygen Concentrations The concentrations of the fuel (C_iH_j) and oxygen (O_2) are indicative of the equivalence ratio and EGR rate [9, 10]. A crank angle measurement of these concentrations is required for the MKIM which is possible in the TKM simulations but not practical in the real engine. Thus an approach similar to that used to describe the polytropic process is developed to predict the concentrations during compression.

To predict the concentrations, it is assumed that the mass of the fuel and oxygen remains constant until the SOC. The change of concentration is proportionally related to the change in volume. The concentration, defined as mass divided by volume [$\mathrm{kg/cm^3}$], of species N at any crank angle after the intake valve closes (θ_{IVC}) and before the SOC (θ_{SOC}) is:

$$[N](\theta) = [N](\theta_{IVC})\left(\frac{V(\theta_{IVC})}{V(\theta)}\right) = [N]_{IVC}\, v_c \tag{7}$$

Using this relationship in MKIM equation (6), the new MKIM is:

$$\int_{\theta_{IVC}}^{\theta_{SOC}} \frac{1}{A\omega\ exp\left(\frac{b(P_{IVC}v_c^{n_c})^n}{T_{IVC}\ v_c^{n_c-1}}\right)} ([C_iH_j]_{IVC}\, v_c)^x \times ([O_2]_{IVC}\, v_c)^y\ d\theta = 1.0 \tag{8}$$

where $A,\ b,\ n,\ x$ and y are the constant parameters. These parameters are found using a modified optimization algorithm. The unknowns i and j are dependent on the chemical properties of the fuel. The increased complexity of MKIM in equation (8) increases the computational time to determine the parameters. Once the parameters are determined, equation (8) can be simply integrated to predict the SOC for different initial conditions.

The TKM simulations for n-heptane and iso-octane are used to parameterize and evaluate equation (8). The results are not presented and showed a good ability to predict the SOC for both fuels with only the initial temperature, pressure, and concentrations of the fuel and oxygen as inputs. This is not surprising since the model parameters are derived from the same data as the validation

Equivalence Ratio In most engine applications, the initial concentrations of the fuel and oxygen are not available. Although it is possible to determine these parameters using an exhaust gas analyzer and oxygen sensors, an exhaust analyzer is not present on production engines. Representing the initial concentrations of fuel and oxygen as the parameters that are easy to measure, but still describe the amount of fuel and air in the engine is more practical.

The equivalence ratio (ϕ) is a good indication of both the amount of fuel and air available in the engine charge and it can also be measured on an operating engine without difficulty using a broadband oxygen sensor. Therefore, an equivalence ratio (ϕ) term replaces the species concentrations in the MKIM. The equivalence ratio is represented in the MKIM equation (8) as follows:

$$\int_{\theta_{IVC}}^{\theta_{SOC}} \frac{1}{A\omega\ exp\left(\frac{b(P_{IVC}v_c^{n_c})^n}{T_{IVC}\ v_c^{n_c-1}}\right)}\ \phi^x\ d\theta = 1.0 \tag{9}$$

where, A, b, n, x are the model parameters.

MODEL SETUP

To parameterize the MKIM, three steps are required. First, simulation / experimental data covering a diverse range of the engine operation is collected. This data is divided into two groups: Estimation Data and Validation Data; with the estimation data used to parameterize the data and the validation data used to check the model on a different set of data. Second, polytropic parameter (n_c) is determined using a best-fit methodology over compression part of simulation data. Third, an optimization is used to find the best values for the parameters of the MKIM. These three steps will be detailed below.

THERMOKINETIC MODEL SIMULATIONS For accurate parameter estimation, the MKIM requires the data of the engine at different working conditions. Since there was a limited number of experimental data over a limited engine range, TKM simulations are used to parameterize the MKIM.

The TKM used is a single zone thermo-kinetic model developed by Kirchen [19] to describe the in-cylinder thermo-kinetic state of an HCCI engine from intake valve closing 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 primary reference fuel blends (i.e. blends of iso-octane and n-heptane). The chemical kinetic mechanism is composed of several sub-mechanisms. The ignition, large molecule decomposition, high temperature sub-mechanisms are taken from Zheng et al. [25], with fuel specific rate constants from Li et al [26]. The mechanism from Zheng et al [25] is modified to include a more comprehensive hydrogen/oxygen sub-mechanism from Marinov et al [27]. The interaction between the two reference fuels is described using the reaction presented by Tanaka et al [28]. The resulting model which couples together the thermodynamic model with the chemical kinetic mechanism was validated with HCCI experimental engine data [29] at different conditions with maximum error of 1 CAD in predicting the SOC.

Here, each parameter is varied independently and simulated with the TKM engine to determine the effects of these engine parameters on the ignition timing. In particular, the engine speed, initial mixture temperature and pressure, EGR percentage[3], and equivalence ratio are varied over the ranges outlined in Table 1. The parameter ranges given in Table 1 are chosen to represent typical HCCI operation. Table 1 also lists the engine geometry which matches the engine configuration used in TKM validation. [19]

TKM simulations for the complete parameter variation of Table 1 for two primary reference fuels (PRF) n-heptane $(ON = 0)$ and iso-octane $(ON = 100)$ are performed. From the resulting 1621 simulations, complete combustion occurred in 176 simulations including 92 simulations with n-heptane and 84 simulations with iso-octane. The MKIM is only valid for a complete combustion thus only these 176 simulations are used for both parametrization, and validation of the MKIM ignition correlation.

[3]EGR(%) is defined as the percent of the total intake mixture which is recycled. [21]

Table 1: Parameter variations carried out using the TKM.

Engine Speed	1000, 2000, 3000 rpm
Initial Temperature	300, 310,..., 440, 450 ^oK
EGR(%)	0%, 0.25%, 0.5%
Equivalence Ratio	0.5, 0.7, 0.9
Initial Pressure	50, 100 kPa
Fuel	n-heptane, iso-octane
Compression Ratio	12:1
Cylinder Bore	8.3 cm
Piston Stroke	11.4 cm
Intake Valve Closing	-146 CAD aTDC
Exhaust Valve Opening	130 CAD aTDC
Wall temperature	390K

FINDING THE POLYTROPIC PARAMETER Using the engine parameter variations for n-heptane and iso-octane, 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. Figures 4 and 5 show the resulting constant n_c and the predicted temperature at the SOC as a function of the actual temperature at the SOC.

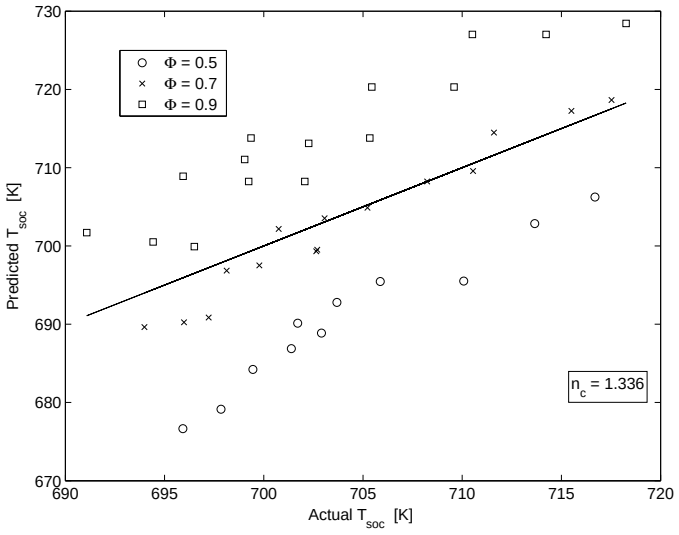

Figure 4: Optimum value of n_c, defined in (4), for simulations using **n-heptane** as fuel at 3 equivalence ratios. The line represents where the prediction is the same as the actual T_{SOC}.

From Figures 4 and 5, it can be concluded that the equivalence ratio (ϕ) has an effect on the temperature required

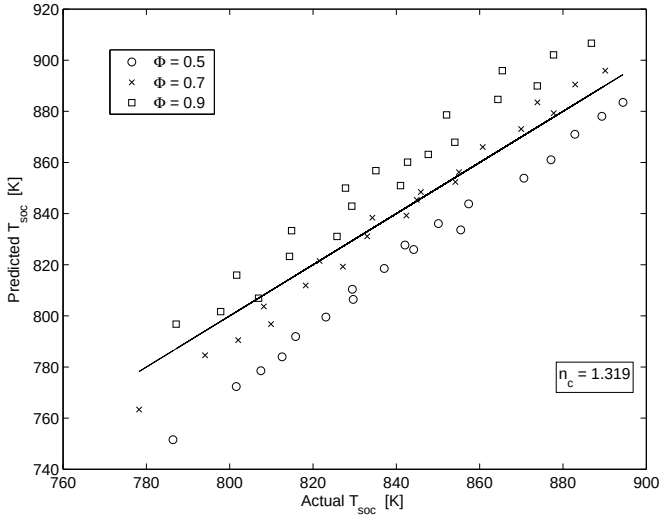

Figure 5: Optimum value of n_c, defined in (4), for simulations using **iso-octane** as fuel at 3 equivalence ratios. The line represents where the prediction is the same as the actual T_{SOC}.

for the SOC with both fuels and since the MKIM is using a constant n_c for each of these two fuels, it overpredicts T_{SOC} for high equivalence ratios and underpredicts T_{SOC} for low equivalence ratios. An additional analysis was done using NASA polynomials [19] to determine the magnitude of the effect of the equivalence ratio on the calculated constant n_c. It was found that in the simulations using equivalence ratios of 0.5, 0.7 and 0.9 and EGR rates of 0%, 0.25% and 0.50%, the value of n_c only differed by 0.021. The values of n_c found for the simulations involving n-heptane and iso-octane also agree with the calculated specific heat capacity ratios using analytical techniques. The n-heptane simulation results in Figure 4 show more scatter of the data compared to the iso-octane simulation results in Figure 5. Furthermore, the temperatures at the SOC are higher for iso-octane compared to n-heptane. This result agrees with other investigations of the pre-ignition chemistry leading up to combustion in HCCI engines [30], [23]. Studies in chemical kinetics of HCCI combustion have found that the ignition is controlled by the decomposition of hydrogen peroxide (H_2O_2). High octane fuels do not release much heat before the hydrogen peroxide decomposition, while low octane fuels generate substantial heat producing reactions at temperatures below the range that this decomposition occurs.

OPTIMIZING THE MKIM PARAMETERS In order to fit the parameters of the MKIM equation (9) the error of the integration should be minimized, 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 [31]. The integration is carried out numerically with the rectangular method with a step size of $0.1\ CAD$. The program then uses the pre-determined optimized parameters and computes the predicted ignition point by integrating (9) until it equals 1.0. The resulting crank angle is taken as the predicted angle of ignition.

RESULTS & DISCUSSION

Using 176 TKM simulations, the parameters of the MKIM were determined. Figure 6 shows the excellent ability of equation (9) in predicting the SOC for n-heptane and that in this case the SOC is not affected substantially by EGR.

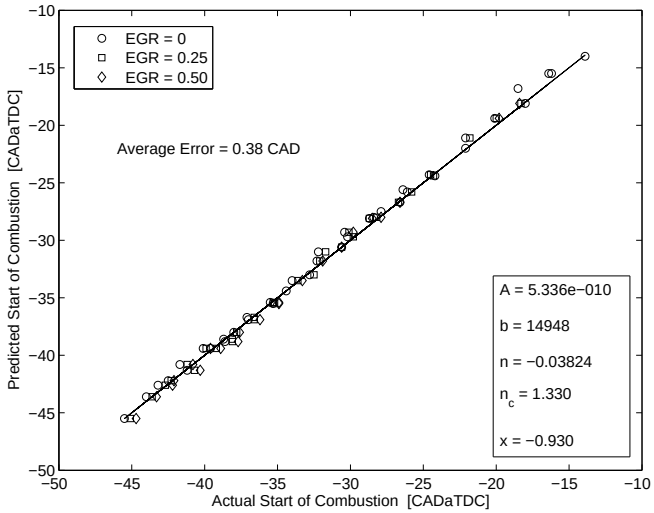

Figure 6: Predicted SOC for **n-heptane** simulations at various engine conditions using the MKIM (9). The line represents where the prediction is the same as the actual SOC.

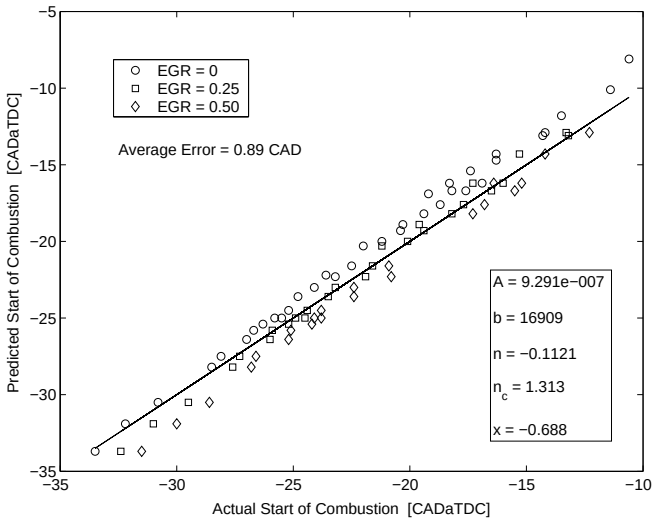

Figure 7: Predicted SOC for **iso-octane** simulations at various engine conditions using the MKIM (9). The line represents where the prediction is the same as the actual SOC.

However, for the iso-octane case the amount of EGR changes the ability of the correlation to accurately predict the SOC as shown in Figure 7. To determine the relationship that EGR has on the SOC, the parameter A was determined for different rates of EGR while keeping the other parameters (b, n, and x) constant. It is found that

the parameter A is linearly dependent on the rate of EGR for iso-octane. This was generalized for all fuels resulting in a further improved MKIM:

$$\int_{\theta_{IVC}}^{\theta_{SOC}} \frac{\phi^x}{A\omega\ exp\left(\frac{b(P_{IVC}v_c^{n_c})^n}{T_{IVC}v_c^{n_c-1}}\right)}\ d\theta = 1.0 \qquad (10)$$

$$where \quad A = C_1 EGR + C_2$$

Here, C_1 and C_2 are constant parameters.

The performance of equation (10) is shown in Figures 8 and 9. The new correlation does an excellent job predicting the SOC in the presence of EGR. Comparing Figure 8 with Figure 6 and Figure 9 with Figure 7, it can be seen that the average error in predicting the SOC for iso-octane was substantially reduced from 0.89 CAD to 0.44 CAD, while for n-heptane it was reduced slightly from 0.38 CAD to 0.35 CAD. Clearly n-heptane improved less because it did not have a strong dependence on EGR . This is also evident by comparing parameter A in Figures 8 and 9 where the slope of A (parameter C_1) for n-heptane is smaller than that of iso-octane.

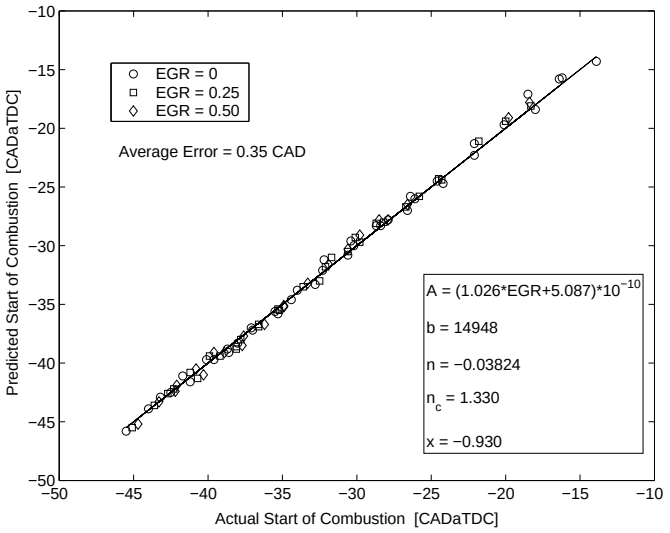

Figure 8: Predicted SOC for **n-heptane** at various engine conditions using the MKIM (10). The line represents where the prediction is the same as the actual SOC.

The values of parameters $A,\ b,\ n,\ n_c$, and x in equation (10) determined for the two fuels are shown in Figures 8 and 9. By examining these parameters it can be seen that for both fuels (iso-octane and n-heptane) 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 [9].

The values of parameter x from equation (10) in Figures 8 and 9 also indicate that equivalence ratio is more effective on the SOC of n-heptane than that of iso-octane. Therefore, with the same amount of change

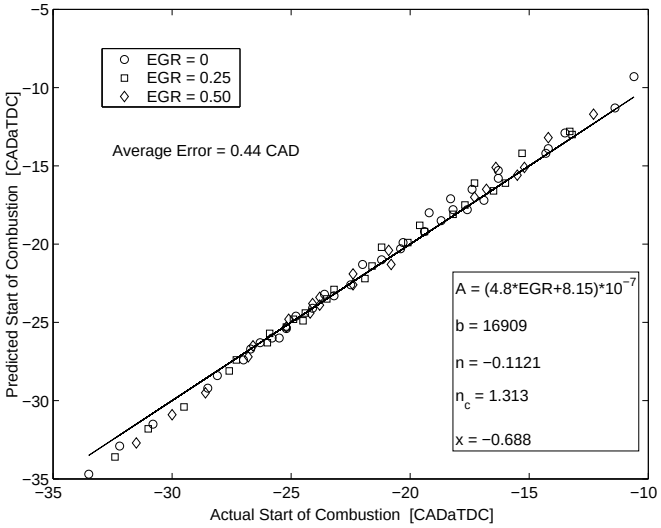

Figure 9: Predicted SOC for **iso-octane** at various engine conditions using MKIM (10). The line represents where the prediction is the same as the actual SOC.

in ϕ, the SOC of n-heptane changes more. Furthermore, by comparing the values of parameter n in Figures 8 and 9, it is evident that the contribution of initial pressure to the SOC is higher in iso-octane than that of n-heptane. Therefore, boosting the intake pressure in an HCCI iso-octane fueled engine advances the SOC more, comparing with an HCCI engine burning n-heptane.

The 176 points in Figures 8 and 9 cover a diverse range of engine speed, initial temperature, initial pressure, EGR rate and equivalence ratio. The results presented in Figures 8 and 9 extends previous works [8, 9, 10, 17, 18] on control-oriented modeling of HCCI ignition timing by accurately predicting SOC over a range of engine speed, initial temperature, initial pressure, EGR rate and equivalence ratio. However, the model still needs to be cross validated with experimental data which is the subject of the next section.

EXPERIMENTAL VALIDATION The correlation is validated with the experimental data from HCCI experiments [2, 29]. Note, the TKM was calibrated for this exact engine. The available experimental data includes 77 different HCCI operating points at a diverse range of equivalence ratio (0.7-1) and EGR (0%-30%) with two different fuels (PRF20 and PRF40)[4]. Experiments were done in W.O.T (Wide Open Throttle) condition with the ambient pressure of 90 kPa at engine speed of 700 rpm with the intake air heated to 88^oC.

The TKM is rerun for the conditions listed in Table 1 for the two new fuel mixtures. Next, the results of TKM simulations are used to determine the MKIM parameters of equation (10). Since the start of the combustion from experimental data is based on a 10% mass fraction burned

[4]Primary reference fuels with octane number of 20 (PRF20) and 40 (PRF40).

(MFB) of fuel, this definition is also used in TKM simulations. The predicted SOC from equation (10) (parameterized by TKM model) is compared to the experimental data for PRF20 and PRF40 respectively in Figures 10 and 11.

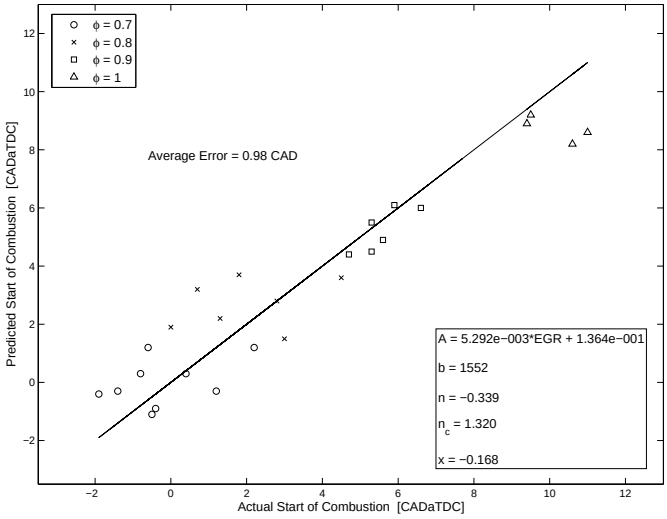

Figure 10: Comparison between predicted and experimental SOC for **PRF40** at various engine conditions using the MKIM (10). The line represents where the prediction is the same as the actual SOC.

The average error for 22 operating points for PRF40 fuel in Figure 10 is 0.98 CAD and the maximum error is 2.5 CAD. For the 50 operating points with PRF20 fuel, these errors are 1.34 CAD for average error and 2.7 CAD for maximum error as shown in Figure 11. The agreement between the SOC of MKIM and experiment is quite good considering that MKIM was parameterized using the TKM simulation and then validated with experimental data.

By comparing Figures 10 and 11 with Figures 8 and 9,

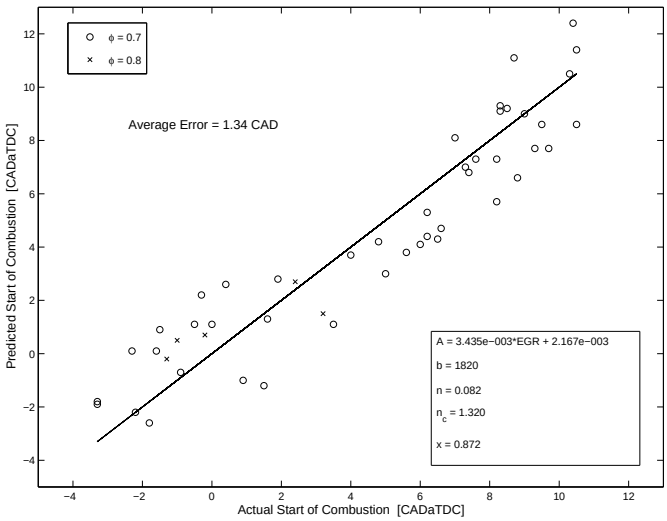

Figure 11: Comparison between predicted and experimental SOC for **PRF20** at various engine conditions using the MKIM (10). The line represents where the prediction is the same as the actual SOC.

it can be seen that there is a higher error between MKIM and experimental data than MKIM and TKM simulations. This is attributed to three major causes. Firstly, parameters of the MKIM in Figures 10 and 11 are estimated using TKM simulations. As expected the TKM does not exactly represent the real engine. One possible way to avoid this is to have more extensive measurement data from the engine. If there was enough experimental data for estimating the parameters of the MKIM, the existing error in experimental validation should decrease. Secondly, the definition of the SOC from 1% MFB of fuel in Figures 8 and 9 was changed to 10% MFB of fuel in Figures 10 and 11 (Due to difficulties in getting accurate 1% MFB with experimental data). Thus for the case of 10% MFB, the pre-ignition heating by the reactions that occur before the SOC violates the polytropic assumption used in the MKIM. Thirdly, PRF20 and PRF40 in Figures 10 and 11 are blends of iso-octane and n-heptane; therefore, they have a more complicated kinetic mechanism than each component separately. This could make it more difficult to predict SOC.

CONCLUSIONS

A Modified Knock Integral Model (MKIM) for HCCI combustion has been developed and validated using simulation and experiment results. The parameters of the MKIM are identified with a minimization method using simulation/experimental data for a specific engine. Once these parameters have been identified, the MKIM needs only EGR rate, equivalence ratio and temperature and pressure at intake valve closing to predict ignition timing.

The MKIM is able to predict ignition timing for the experimental HCCI engine with an average error of less than 1.5 CAD and maximum error of 2-3 CAD. This error level seems acceptable for a control-oriented model like the MKIM since the MKIM could be augmented with additional information from, for example, a knock sensor or Ion sensor in the ECU. Therefore, the MKIM seems promising for HCCI engine control and could be used to schedule engine variables such as intake temperature (heater), EGR levels, and fuel type (two fuel system) in order to obtain the desired ignition timing.

FUTURE WORK

Although the start of combustion is successfully predicted by the correlation presented in this paper, there are many other issues to be investigated. Since the MKIM was validated with the experimental data in a fairly narrow region of HCCI operation, a validation with more comprehensive experimental data is still needed to accomplish a complete cross-validation of the MKIM. Furthermore to make the MKIM more practical for the ECU, use of intake manifold pressure and temperature data instead of those values at IVC is needed. Finally, adapting the MKIM for any PRF would allow ignition timing to be predicted as PRF is changed.

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ABBREVIATIONS

AFR: Air Fuel Ratio
CAD: Crank Angle Degree
CFD: Computational Fluid Dynamics
ECU: Engine Control Unit
EGR: Exhaust Gas Recirculation
HCCI: Homogeneous Charge Compression Ignition
IVC: Intake Valve Closing
KIM: Knock Integral Model
MFB: Mass Fraction Burned
MKIM: Modified Knock Integral Model
NASA: National Aeronautics & Space Administration
PRF: Primary Reference Fuels
SI: Spark Ignition
SOC: Start of Combustion
TKM: Thermo-Kinetic Model