THERMO-KINETIC COMBUSTION MODELING OF AN HCCI ENGINE TO ANALYZE IGNITION TIMING FOR CONTROL APPLICATIONS

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ABSTRACT

Ignition timing in Homogeneous Charge Compression Ignition (HCCI) engines is dominated by thermo-kinetic reactions that are dependant on the charge properties. A single zone thermodynamic model, coupled to a kinetic mechanism, is developed to predict the ignition timing of Primary Reference Fuels (PRFs) in an HCCI engine. The model, consisting of 120 chemical reactions and 58 species, is validated against the experimental data from a single cylinder engine for various operating conditions. The model is able to predict the effects of different charge parameters on the HCCI ignition timing. This model is used to perform a sensitivity analysis of HCCI ignition timing to the variations of engine charge properties in order to examine the relative importance of different charge properties for control applications. The sensitivity analysis is done for these main charge variables: initial temperature, initial pressure, Exhaust Gas Recirculation (EGR) rate, equivalence ratio, and octane number. The simulation results show that the sensitivity of HCCI ignition timing is dependant on the crank angle position of the Start of Combustion (SOC). The highest sensitivity of HCCI ignition timing is always seen to the variation of the charge temperature.

INTRODUCTION

HCCI is a fast heat release mode of combustion based on the auto-ignition of a homogeneous mixture by compression. An HCCI engine can be thought of as a hybrid of SI (Spark Ignition) engine and CI (Compression Ignition) engine. As in an SI engine, fuel is homogenously premixed with air, but the fuel auto-ignites from compression heating, as in a CI (diesel) engine. The HCCI principle incorporates the advantages of both the SI and the diesel engine principles. The mixture is homogeneous and combustion temperature is low, which minimizes the Particulate Matter (PM) and NOx emissions. The mixture is compression ignited using high compression ratios, without throttling losses and with shorter combustion duration, which leads to high efficiency. The combination of both high efficiency and low emission of soot and NOx has made the HCCI engine a promising alternative to traditional engines [1].

Control of ignition timing is the most challenging problem in HCCI engines [2]. To predict and control ignition timing in HCCI engines, combustion simulation models are useful to understand the effect of modifying the properties of the engine charge on ignition timing. The HCCI combustion model serves as a qualitative tool for ignition timing sensitivity analysis for different variables of an HCCI engine and for simulating parameter variations needed for development of a control-oriented HCCI model. There are a wide range of HCCI combustion models in the literature that are mainly different in the level of complexity and the level of details in the applied kinetic mechanism. There are four main categories of Thermo-Kinetic Models (TKM) for modeling of HCCI combustion: 1) Zero dimensional TKMs [3]; 2) Multi-zone TKMs [4]; 3) Sequential CFD based multi-zone TKMs [5]; 4) Coupled CFD-kinetic TKMs [6]. Each type of these models is intended for a different purpose. Single zone TKMs, with low computational requirements, are useful tools for predicting SOC [3, 5] and performance studies [7], but single zone TKMs lack the accuracy for predicting combustion peak pressure and combustion duration. Multi-zone TKMs address this problem by accurately predicting combustion peak pressure and combustion duration, but they don't seem accurate for predicting HC and CO emissions. Predictions of HC and CO can be improved by sequentially coupling multi-zone TKMs with a CFD code to determine temperature and mass distribution at the beginning of the engine closed cycle. Furthermore, more accurate prediction of emissions can be obtained by using coupled CFD-kinetic TKMs, but require extensive computation.

In this study, the main target is modeling HCCI combustion to analyze ignition timing (SOC) for eventual control of SOC. To do this, a single zone HCCI combustion model from our previous work [3] is extended using a modified Woschni heat transfer correlation adopted for HCCI engines. The resulting model is calibrated for a single cylinder engine and then validated against ignition timing from cylinder pressure data taken from the experimental engine for four different PRF[1] fuels over a range of equivalence ratios, intake temperatures, intake pressures, EGR rates, and engine speeds. Then a sensitivity analysis of SOC to variations in the properties of the engine charge is performed by using the developed TKM. This analysis helps to compare the relative importance of different charge properties which will be useful in future control of SOC.

MODEL DESCRIPTION

A single zone TKM is developed to describe the in-cylinder thermo-kinetic state of an HCCI engine from (Intake Valve Closing) IVC to exhaust valve opening. The energy balance and modeling, kinetic mechanism and solution methodology of the developed model are detailed below.

Energy Balance

The combustion chamber of an HCCI engine is considered as a single thermodynamic zone with the assumption of a uniform thermodynamic state within the zone. It is assumed that all species in the zone can be treated as ideal gases and blow-by is negligible and mass of in-cylinder mixture is constant. Evaporation of fuel in the intake port and combustion chamber is also neglected and it is assumed that the entire mixture is in the gas phase. Furthermore, an average temperature of combustion chamber walls is used to consider the convective heat transfer between the zone and its surroundings. The first law analysis of the system is used to determine the variation of the thermodynamic state of the mixture with time. The details of the model can be found in [3].

The heat transfer to the cylinder walls is modeled using the Modified Woschni heat transfer correlation that is adopted for HCCI engines [8]:

$$h(t) = \alpha_{scaling} \times L(t)^{-0.2} \times P(t)^{0.8} \times T(t)^{-0.73} \times \omega(t)^{0.8} \tag{1}$$
$$\omega(t) = C_1 S_p + \frac{C_2}{6} \frac{V_d T_r}{P_r V_r}(P - P_{mot})$$

where, L is the instantaneous cylinder height, P and T are the gas temperature and pressure, ω is the local gas velocity, S_p is the average piston speed, T_r, P_r and V_r are temperature, pressure and volume at the IVC moment, V_d is the displacement volume and P and P_{mot} are instantaneous pressure and the corresponding motoring pressure at the same firing condition. C_1 and C_2 are constant values and $\alpha_{scaling}$ is the scaling factor for different engine geometries.

The developed TKM requires the mixture temperature at IVC (T_{ivc}). But experimentally measuring the T_{ivc} is difficult and using the gas temperature in the intake manifold (T_{man}) as T_{ivc} yields erroneous SOC from the TKM. Thus the following semi-empirical correlation is used to predict T_{ivc} from the manifold values [9]:

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

where a, b, c, d, e and f are the parameters of the correlation that are determined from comparing experimental and TKM simulated pressure traces, Φ represents equivalence ratio of the air-fuel mixture and EGR is the percentage of the total intake mixture which is recycled.

Kinetic Mechanism

The chemical kinetic mechanism consists of 58 species and 102 reactions for describing the combustion of arbitrary PRF blends. The chemical kinetic mechanism is composed of several sub-mechanisms. The ignition, large molecule decomposition, high temperature sub-mechanisms are from Zheng et al. [10], with fuel specific rate constants from Li et al [11]. The interaction between the two reference fuels is described using the reaction presented by Tanaka et al [12].

[1] PRF number is defined as the volume percentage of iso-octane in fuel mixture of N-heptane and iso-octane.

Solution Methodology

The mathematical model results in a set of stiff ordinary differential equations that are integrated with the ode15 solver in Matlab. The tolerances for this multi-step numerical solver was determined heuristically to provide a compromise between calculation speed and solution convergence.

MODEL VALIDATION

The developed thermokinetic model is validated based on its ability to predict SOC for a single cylinder experimental engine running in the HCCI mode.

Engine Setup

A single cylinder Ricardo Hydra Mark III engine with a Rover K7 head is used to carry out HCCI experiments. Configuration of the engine and experimental setup of the engine are detailed in [13]. Fuel is injected into the intake port and is timed to ensure injection on closed intake valves. The charge entering the engine is heated by the electric air heater positioned upstream of the throttle body and the intake manifold pressure is increased using a supercharger driven by an electric motor. The cylinder pressure is measured with a Kistler ThermoCOMP (model 6043A60) piezoelectric pressure sensor that is flush mounted in the cylinder. Pressure traces from 200 consecutive engine cycles with 0.1 CAD (Crank Angle Degree) resolution are recorded for each experimental operating point.

SOC Definition

In order to compare the simulation and experiment, SOC for both the experimental and simulated engine cycles is defined as being the point at which the third derivative of the pressure trace with respect to the crank angle (θ) in CAD exceeds a heuristically determined limit [14]:

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

Results

For the Ricardo engine experimental conditions given in Table 2, the TKM model is tested. Four different PRF fuels are used to validate the ability of the TKM model to predict ignition timing for different octane numbers. In order to cover the operating region of the Ricardo engine, each of the 14 points in Table 2 corresponds to the conditions close to the limits for which HCCI operation with reasonable cyclic variations is possible at the PRF blend used. The mixture pressure at IVC, P_{ivc}, is taken from the experimental pressure trace. Figure 1 shows a typical simulated pressure trace in comparison with experimental pressure traces from 200 consecutive engine cycles for the test point #14 in Table 2.

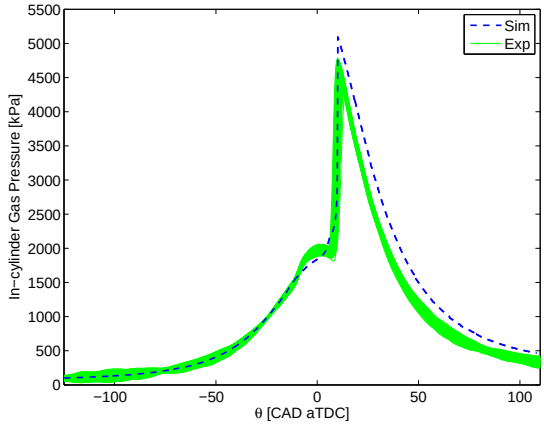

Figure 1: Comparing simulated and experimental pressure traces for test point #14 in Table 2.

As expected simulation in Figure 1 has a higher peak pressure than those of experimental traces. This is inherent to the single zone approximation used in the model [5] where it is assumed that the entire mixture is uniform in temperature, pressure and composition and it ignites and combusts concurrently.

Table 2, a comparison of experimental and simulated ignition timings for four PRF blends, indicates that the TKM model is capable of predicting the ignition timing for different PRF blends over a range of equivalence ratios, intake temperatures, intake pressures, EGR rates, and engine speeds. Comparing SOC from the TKM with average values

from 200 cycles for different operating points, the TKM predicts SOC for the Ricardo engine with an average error of less than 0.8 CAD.

Table 1: Comparison of HCCI experimental and simulated SOC. (Values on the top of the vectors are the average values from all individual cycles.)

Test No.	Fuel [PRF]	N [rpm]	Φ	EGR [%]	T_{man} [^oC]	P_{ivc} [kPa]	SOC [CAD aTDC]	
							Experiment	Simulation
1	0	800	0.49	0	140	107	2.3 $\xrightarrow{3.7}$ 5.2	4.4
2	0	800	0.72	17	80	107	2.9 $\xrightarrow{3.8}$ 4.8	4.9
3	0	1000	0.58	9	100	110	5.1 $\xrightarrow{7.7}$ 12.4	6.2
4	0	1000	0.67	18	100	112	3.8 $\xrightarrow{6.5}$ 10.5	5
5	10	800	0.57	0	60	109	2.5 $\xrightarrow{5.5}$ 8.4	6.4
6	10	800	0.66	15	90	107	5.1 $\xrightarrow{8.1}$ 12.6	8.3
7	10	1000	0.52	0	110	109	4.6 $\xrightarrow{6.6}$ 10	8
8	10	1000	0.68	16	100	110	6.5 $\xrightarrow{11.4}$ 23.2	10.8
9	20	800	0.53	0	90	106	4.2 $\xrightarrow{6.9}$ 11.1	6
10	20	800	0.38	0	120	125	5.6 $\xrightarrow{6.8}$ 8	6.9
11	20	1000	0.42	0	129	128	4.6 $\xrightarrow{6.2}$ 7.6	6.4
12	20	1000	0.75	11	100	111	5.7 $\xrightarrow{6.7}$ 7.9	7.1
13	40	810	0.45	0	110	147	-0.1 $\xrightarrow{0.8}$ 1.7	1.5
14	40	810	0.72	0	90	101	4.8 $\xrightarrow{5.9}$ 7.1	6.8

Table 2: Comparison of HCCI experimental and simulated SOC. (Values on the top of the vectors are the average values from all individual cycles.)

Test No.	Fuel [PRF]	N [rpm]	Φ	EGR [%]	T_{man} [^oC]	P_{ivc} [kPa]	SOC [CAD aTDC]	
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SENSITIVITY ANALYSIS

The developed TKM is used to perform a sensitivity analysis of SOC to initial temperature, initial pressure, EGR rate, equivalence ratio, and Octane Number (ON). This analysis can be applied to analyze ignition timing for control applications. In particular, the sensitivity analysis can be used for three different purposes. First, it helps to evaluate the relative importance of different charge properties for HCCI control-oriented modeling where a compromise among accuracy, computational time, and number of necessary measurements is required. Second, the sensitivity analysis can be used to choose an effective actuator to control ignition timing for different operating regions of an HCCI engine. Third, the sensitivity analysis is useful to determine the minimum and maximum possible incremental change of ignition timing for different actuators when defining control targets for an HCCI engine.

Table 3 indicates the base points chosen for the sensitivity analysis. These base points are selected to represent the conditions in the middle of the operating region for the two ranges of PRF blends the Ricardo engine could be run. A range of equivalence ratio is used to examine the sensitivity analysis for different SOC positions.

Table 3: Base line points used for the sensitivity analysis

No.	PRF	N [rpm]	T_{ivc} $[^oC]$	P_{ivc} [kPa]	Φ	EGR [%]
1	0	800	110	110	0.46, 0.57, 0.75	10
2	40	800	130	130	0.38, 0.58, 0.75	10

Table 4 quantifies the sensitivity or slope of SOC with the change in the charge properties. Results are shown for three different positions of SOC. Early ignitions ($\cong$ 4 CAD bTDC) are achieved with the richest Φ limit of Table 3 and late ignitions ($\cong$ 10 CAD aTDC) are obtained with the leanest Φ limit of Table 3 for both PRF0 and PRF40 cases. Examining the sign of values in Table 4 shows that SOC advances with an increase in IVC temperature, equivalence ratio and IVC pressure, but SOC retards with an increase in EGR rate and octane number. Minimum and maximum possible changes of SOC on a real engine are bounded with actuators' limitations. Knowing the resolution of the engine's actuators in combination with the information from Table 4, minimum and maximum possible changes of SOC on the Ricardo engine can be determined. For instance, the resolutions of the supercharger and EGR valve in the Ricardo engine for changing intake pressure and EGR rate are 1 kPa and 4% respectively. Thus from Table 4 for PRF40 in TDC firing conditions, increasing the intake pressure causes SOC to change only 0.15 CAD (advance), but a minimum change of SOC with increasing EGR rate is 2.75 CAD (retard).

Table 4: Rate of the change of SOC with the change in the charge properties for the base points of Table 3 . (bTDC: before Top Dead Center; aTDC: after Top Dead Center)

Fuel	PRF0			PRF40		
SOC Position	bTDC	TDC	aTDC	bTDC	TDC	aTDC
$\Delta SOC/\Delta T_{ivc}$ $[CAD/^oK]$	-0.425	-0.6	-1.05	-0.5	-0.5	-0.9
$\Delta SOC/\Delta Phi$ $[CAD/0.01Phi]$	-0.1	-1.17	-1.2	0.025	-1.15	-1.4
$\Delta SOC/\Delta EGR$ $[CAD/\%EGR]$	0.175	1.02	0.575	0.2	0.6875	0.45
$\Delta SOC/\Delta P_{ivc}$ $[CAD/kPa]$	-0.2	-0.15	-0.5	-0.2	-0.15	-0.35
$\Delta SOC/\Delta ON$ $[CAD/1ON]$	0.8	0.75	1.35	0.225	0.175	0.3

To examine the relative importance of different charge properties on SOC, a normalized sensitivity function ($S_x = |\frac{\partial SOC}{\partial X}| \times \frac{X_b}{SOC_b} \times 100$) is used, where X is the variable and index b denotes for the base point. Sensitivity analysis is performed around the operating points in Table 3 and each variable (X) is separately changed in a small range around the base points. The variation range of X is determined based on the minimum possible change of a variable on the Ricardo engine. As using the base values of EGR and ON when they are zero gives a false sensitivity interpretation, their maximum possible values for the Ricardo engine are used for X_b. Figure 2 shows the simulation results.

Figure 2: Normalized sensitivity results for SOC using TKM simulations and base points of Table 3.

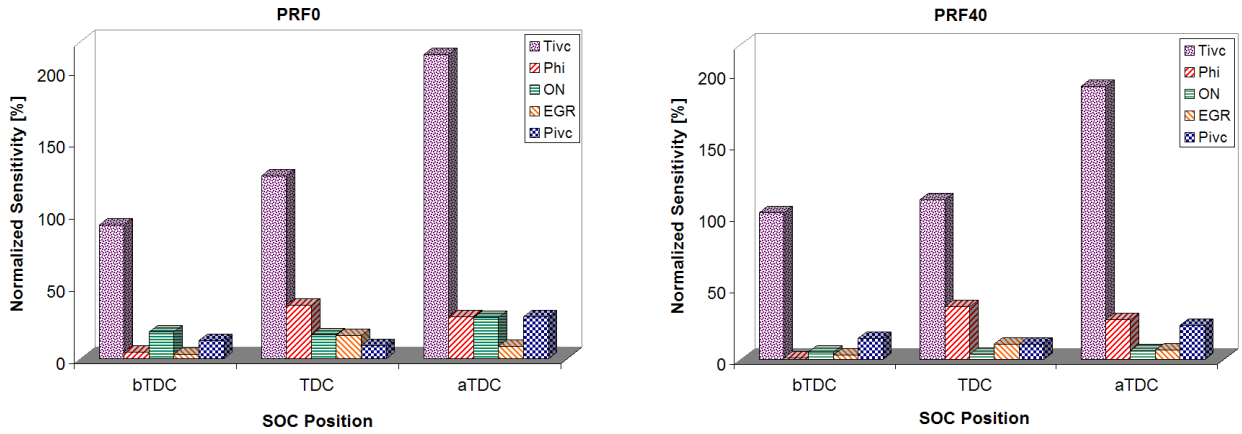

Figure 2 shows that the sensitivity of SOC to the variations of charge properties is dependant on the position of SOC with less sensitivity being observed for early ignitions. SOC shows the most sensitivity to the variations of the intake charge temperature, regardless of SOC position. The influence of equivalence ratio is pronounced for combustion happening around TDC and also late combustion, but less pronounced for early combustion. For both PRF0 and PRF40, a similar trend of change in sensitivity with respect to SOC position is seen for all charge properties except for the octane number of the charge. PRF40 shows less sensitivity to the changes in the octane number compared to that of PRF0.

CONCLUSIONS

A one zone thermokinetic model using a chemical kinetic mechanism for primary reference fuels is extended and validated against the experimental data from a single cylinder engine. The developed model can predict SOC for the studied engine running in HCCI mode with an average error of less than 0.8 CAD over a range of equivalence ratios, intake temperatures, intake pressures, EGR rates, PRF blends, and engine speeds. Sensitivity analysis using the experimentally validated simulation model indicates that SOC shows a different order of sensitivity to the variation of charge properties when the position of SOC varies. While SOC is the most sensitive to the charge temperature variations and Φ variations for the combustion occurs around TDC or a late combustion, SOC shows a small sensitivity to Φ for an early combustion. In addition, more sensitivity is observed in SOC to the variation of octane number when an HCCI engine runs with a PRF blend at a low octane number.

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References

[1] H. Zhao. *"Homogeneous Charge Compression Ignition (HCCI) and Controlled Auto Ignition (CAI) Engines for the Automotive Industry"*. Woodhead Publishing Limited, Brunel University UK, 2007.

[2] X. Lü, W. Chen, Y. Hou, and Huang Z. "Study on the Ignition, Combustion and Emissions of HCCI Combustion Engines Fueled With Primary Reference Fuels". SAE Paper No. 2005-01-0155, 2005.

[3] P. Kirchen, M. Shahbakhti, and C. R. Koch. "A Skeletal Kinetic Mechanism for PRF Combustion in HCCI Engines". *Journal of Combustion Science and Technology*, Accepted and to appear, 2007.

[4] P. Kongsereeparp, M. D. Checkel, and B. Kashani. "A Stand-alone Multi-Zone Model for Combustion in HCCI Engines". *ASME Internal Combustion Engine Division 2005 Fall Technical Conference*, ICEF2005-1241, 2005.

[5] S. M. Aceves, D. L. Flowers, C. K. Westbrook, J. R. Smith, W. Pitz, R. Dibble, M. Christensen, and B. Johansson. "A Multi-Zone Model for Prediction of HCCI Combustion and Emissions". SAE Paper No. 2000-01-0327, 2000.

[6] S. C. Kong and R. D. Reitz. "Numerical Study of Premixed HCCI Engine Combustion and its Sensitivity to Computational Mesh and Model Uncertainties". *Combustion Theory and Modeling*, pages 417–433, 2003.

[7] S. B. Fiveland and D. N. Assanis. "A Four-Stroke Homogeneous Charge Compression Ignition Engine Simulation for Combustion and Performance Studies". *SAE Paper No. 2000-01-0332*, 2000.

[8] J. Chang, O. Guralp, Z. Filipi, D. Assanis, T. Kuo, and Najt. "New Heat Transfer Correlation for an HCCI Engine Derived From Measurements of Instantaneous Surface Heat Flux". SAE Paper No. 2004-01-2996, 2004.

[9] M. Shahbakhti, R. Lupul, and C. R. Koch. "Sensitivity Analysis & Modeling of HCCI Auto-Ignition Timing". *The Fifth IFAC Symposium on Advances in Automotive Control*. Manuscript submitted in Jan. 2007.

[10] J. Zheng and et al. "A Skeletal Chemical Kinetic Model for the HCCI Combustion Process". SAE2002-01-0423.

[11] H. Li, D. L. Miller, and N. P. Cernansky. "Development of a Reduced Chemical Kinetic Model for Prediction of Preignition Reactivity and Autoignition of Primary Reference Fuels". SAE Paper No. 960498, 1996.

[12] S. Tanaka, F. Ayala, and J. C. Keck. "A Reduced chemical kinetic model for HCCI combustion of primary reference fuels in a rapid compression machine". *Combustion and Flame*, 133:467–481, 2003.

[13] M. Shahbakhti, R. Lupul, and C. R. Koch. "Cyclic Variations of Ignition Timing in an HCCI Engine". *Proceeding of ASME/IEEE Joint Rail Conference & Internal Combustion Engine Spring Technical Conference*, 2007.

[14] M. D. Checkel and J. D. Dale. "Computerized Knock Detection From Engine Pressure Records". SAE Paper No. 860028, 1986.