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Modeling of HCCI Engine Combustion for Control Analysis

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Abstract— **Operation of homogeneous charge compression ignition (HCCI) engines are very sensitive to timing variations in the combustion of the air-fuel charge mixture and require precise control of the ignition instant to run properly. It is therefore essential to understand the characteristics of timing variations under various operating conditions in order to find suitable control strategies. This paper presents a first step towards the construction of an HCCI engine model aimed at studies on timing control strategies. The goal is to (qualitatively) reproduce the timing effects that may be observed on a real engine. The proposed model includes a lumped chemical kinetic model for hydrocarbon fuels to predict autoignition. Single-cycle simulations are compared with experimental results from a real engine to validate the model. Comparisons are also made with a model based on the knock-integral.**

I. INTRODUCTION

In homogeneous charge compression ignition (HCCI) engines the ignition timing is defined by the autoignition properties of the air-fuel mixture in use. Small variations in the cylinder environment may greatly influence the ignition timing. In order to control engine operation it is therefore necessary to have good models and substantial understanding of the ignition and combustion process. This work aims at describing the major thermodynamic and chemical interactions in the course of an engine stroke and their influence on ignition timing. The goal is to construct a simulation model that (qualitatively) reproduces HCCI engine operation for the purpose of synthesizing, analyzing, and evaluating various ignition timing control strategies. Common strategies for timing control includes varying the inlet temperature and fuel composition, or to employ variable valve timing. Previous work on control of HCCI engine timing is presented in, e.g., [1], [2], [3], [4], [5]. The present work is a feasibility study on requirements and choice of complexity level for a suitable model, and is to be regarded as a first step towards a complete model. The proposed model structure consists of a zero-dimensional cylinder model, combined with a reduced chemical kinetic model to describe the ignition process. Experiments on a real engine with dual fuels and inlet air temperature control have been conducted to collect information on the phenomena to reproduce and to compare to simulated results. The experimental setup is described in Section II, followed by the model description in Section III. Section IV presents experimental and simulated results, which are discussed in Section V. Finally, conclusions are stated in Section VI.

TABLE I
ENGINE SPECIFICATIONS.

Operated cylinders	6
Displaced Volume	2000 cm^3
Bore	131 mm
Stroke	150 mm
Connecting Rod Length	260 mm
Number of Valves	4
Compression Ratio	18.5:1
Fuel Supply	port fuel injection

II. EXPERIMENTAL SETUP

A. Research Engine

Experiments were performed on a six cylinder converted diesel engine. The experimental setup (Fig. 1 and Table I) consisted of a heavy duty Volvo diesel engine, with a displaced volume of 12 l. The engine was converted to port fuel injection with dual fuels. The engine was equipped with 14 mm cylinder pressure transducers on all cylinders and a Variable Geometry Turbo (VGT) which made it possible to adjust the boost pressure. It also had an intercooler and an inlet air heater for controlling inlet air temperatures. The used dual fuels were ethanol and a fifty-fifty mixture of n-heptane and ethanol. The use of a mixture instead of pure n-heptane was to improve precision of the control. The dual fuels give Research Octane Number (RON) ratings from 53 up to 106.

B. Data Acquisition

The data acqusition system ran on a standard PC with GNU/Linux operating system, resulting in a flexible platform with good soft real-time properties. All data coming from various sensors around the engine were collected in the main control program (Fig. II). These data included various temperatures and pressures collected via a data logger sampling at low sampling rate, various temperatures and cylinder pressures collected via a Microstar DAP sampling at fast sampling rate, and exhaust emissions data from the emission system sampling at low sampling rate. The cylinder pressure data acquisition was controlled by an encoder connected to the crank shaft of the engine. A sample was taken at every encoder pulse, i.e., every 0.2 crank angle degree. The cylinder pressure data was sampled by a Microstar 5400A/627 data acquisition processor. As soon as one cylinder passed exhaust valve opening, pressure

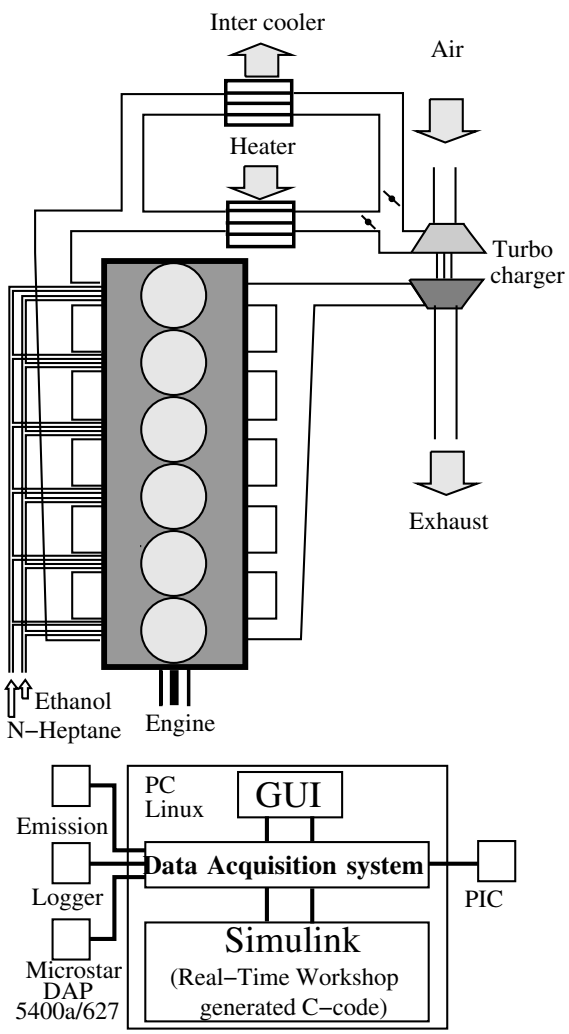

Fig. 1. Experimental set-up consisting of a 6-cylinder, 12 l, heavy duty Volvo diesel engine, with a data acqusition system.

data were transferred from the AD card to the control program. When new pressure data was available in the data acqusition system, a simplified rate of heat release calculation based on pressure, [6], was performed and thereafter combustion timing was calculated. The two fuels have different autoignition temperatures, a property that was used to change the combustion timing. The experimental set-up also allow for closed-loop control with controllers implemented using Simulink and converted to C-code using the automatic code generation tool of Real Time Workshop. However, in this paper all experiments were carried out in open-loop.

C. Experiments

In the experiments, the volume ratio, R_f, of the dual fuels ethanol and n-heptane, fuel energy per cycle, Q_{in}, inlet air temperature, T_{in}, and the engine speed, w, were changed according to Table II. By changing the injected fuel energy per cycle the load is changed and $Q_{in} = 1000$ J corresponds to a FuelMEP of 5 bar and $Q_{in} = 1500$ J corresponds to a FuelMEP of 7.5 bar. Only low load experiments in open loop were performed, when the engine temperature was at steady state. At each operating point, data of 500 cycles were collected. Mean value of these 500 cycles was thereafter used in comparison with the result from the model.

TABLE II
EXPERIMENTAL CONDITIONS

T_{in} [°C]	100–115	100	100	100
$w[rpm]$	1200	1000–1500	1200	1200
$Q_{in}[J]$	1400	1400	1000–1500	1400
R_f [vol%]	0.93	0.93	0.93	0.892–1.0

III. MODEL

HCCI combustion is often achieved without a complete homogeneous mixture, but from a control-oriented point of view it is a reasonable approximation that the mixture is homogeneous and simultaneous ignition of the mixture occur. Hence, it is reasonable to use a zero-dimensional (single-zone) cylinder model. Several alternative approaches are possible for modeling the instant of autoignition for fuels. To reproduce the effects relevant for ignition-timing control it is required that the autoignition model captures the effects on ignition delay (induction time) of varying species concentrations, temperature trace, and fuel quality. Large models, e.g. [7] (PRF fuels, 857 species, 3,606 reactions, CHEMKIN/LLNL), have been used to model complete combustion. In addition to ignition prediction, such models are also aimed at describing intermediate species and end product composition. Reduced chemical kinetics models, e.g. [8] (PRF fuels, 32 species, 55 reactions, CHEMKIN), have also been proposed, where reactions with little influence on the combustion has been identified and removed. For simulation of multi-cycle scenarios it is necessary to keep the model complexity low in order to arrive at reasonable simulation times. An attractive and widespread alternative is to use the Shell model [9], which is a lumped chemical kinetics model using only five representative species in eight generic reactions. This model is aimed at prediction of autoignition rather than describing the complete combustion process. Compression ignition delay may also be described by empirical correlations, such as the *knock integral* condition $\int_{t=0}^{t_i} \frac{dt}{\tau} = 1$, where t_i is the instant of ignition and τ is the estimated ignition time (ignition delay) at the instantaneous pressure and temperature conditions at time t, often described by Arrhenius type expressions [10]. A drawback is that dependence on species concentrations is normally not regarded. An integral condition with concentration dependence was used in [11], [5] in a similar study for propane fuel, where also autoignition models based on very simple reaction mechanisms were evaluated. A final alternative is to use empirical look-up tables. This gives very little physical insight, and require

substantial efforts to calibrate. In this work, the Shell model was chosen to describe the process of autoignition. A static model is then used to describe the major part of the actual combustion and corresponding heat release. The result from the Shell model is compared with result from an integrated Arrhenius rate threshold model.

A. Cylinder Model

The cylinder gas dynamics are described by the first law with volume-pressure work

$$\delta Q_{HR} = (1 + \frac{c_v}{R})pdV + \frac{c_v}{R}Vdp + \delta Q_{HT}$$

where p is the cylinder pressure, V the volume, R_u the universal gas constant, $c_v = c_p - R_u$ the specific heat capacity, and n the molar substance amount contained in the cylinder. The time derivatives of Q_{HR} and Q_{HT} denote rates of heat released by the combustion process and heat flowing from the wall.

B. Gas Properties

The gas is described as a mixture of dry air and fuel, and the combustion products nitrogen, carbondioxide and water. Specific heat for each species i is described by NASA polynomial approximations of JANAF data

$$c_{p,i}(T) = \frac{R_u}{M_i}\sum_{j=1}^{5} a_{i,j}T^{j-3}$$

where M_i is the molar mass of species i and T is the cylinder temperature. The mixture specific heat is then

$$c_p(T) = \frac{1}{n}\sum_i n_i M_i c_{p,i}(T)$$

where n_i is the mole of species i.

C. Shell Autoignition Model

The Shell autoignition model for hydrocarbon fuels [9], C_aH_b, is based on a general eight step chain-branching reaction scheme with lumped species: The hydrocarbon fuel RH, radicals $\bar{R}$, intermediate species Q, and the chain branching agent B.

$$RH + O_2 \xrightarrow{k_q} 2\bar{R} \quad \text{(initiation)}$$
$$\bar{R} \xrightarrow{k_p} \bar{R} + \text{products and heat} \quad \text{(propagation cycle)}$$
$$\bar{R} \xrightarrow{f_1 k_p} \bar{R} + B \quad \text{(propagation forming } B\text{)}$$
$$\bar{R} + Q \xrightarrow{f_2 k_p} \bar{R} + B \quad \text{(propagation forming } B\text{)}$$
$$\bar{R} \xrightarrow{f_3 k_p} \text{out} \quad \text{(linear termination)}$$
$$\bar{R} \xrightarrow{f_4 k_p} \bar{R} + Q \quad \text{(propagation forming } Q\text{)}$$
$$2\bar{R} \xrightarrow{k_t} \text{out} \quad \text{(quadratic termination)}$$
$$B \xrightarrow{k_b} 2\bar{R} \quad \text{(degenerate branching)}$$

Autoignition is described by integrating the time variations of species concentrations from the beginning of the compression stroke.

$$\frac{d[\bar{R}]}{dt} = 2\left\{k_q[RH][O_2] + k_b[B] - k_t[\bar{R}]^2\right\} - f_3 k_p[\bar{R}]$$
$$\frac{d[B]}{dt} = f_1 k_p[\bar{R}] + f_2 k_p[Q][\bar{R}] - k_b[B]$$
$$\frac{d[Q]}{dt} = f_4 k_p[\bar{R}] - f_2 k_p[Q][\bar{R}]$$
$$\frac{d[O_2]}{dt} = -g k_p[\bar{R}]$$

The species $\bar{R}$, Q, and B are not considered in thermodynamic computations for the gas mixture. The stoichiometry is approximated by assuming a constant CO/CO_2 ratio, γ, for the complete combustion process, with oxygen consumption $g = 2[a(1-\gamma)+b/4]/b$ mole per cycle. The heat release from combustion is given by

$$\frac{dQ_{HR}}{dt} = k_p q V[\bar{R}]$$

where q is the exothermicity per cycle for the regarded fuel. The propagation rate coefficient is described as

$$k_p^{-1} = \frac{1}{k_{p,1}[O_2]} + \frac{1}{k_{p,2}} + \frac{1}{k_{p,1}[RH]}$$

To capture dependence of induction periods on fuel and air concentrations the terms f_1, f_3, and f_4 are expressed as

$$f_i = f_i^{\circ}[O_2]^{x_i}[RH]^{y_i}$$

Rate coefficients and rate parameters k_i and f_i° are then described by Arrhenius rate coefficients

$$k_i = A_i \exp\left[\frac{E_i}{R_u T}\right], \quad f_i^{\circ} = A_i \exp\left[\frac{E_i}{R_u T}\right]$$

Calibrated parameters for a number of fuels, including a set of Primary Reference Fuels (PRF), are found in the literature [9]. PRFx is a mixture of n-heptane and iso-octane, where the octane number x is defined as the volume percentage of iso-octane. Parameters for PRF90 was used in the simulations. Autoignition was defined as the crank angle where the explosive phase of combustion starts.

D. Integrated Arrhenius Rate Threshold

The Arrhenius form can be used to determine the rate coefficient describing a single-step reaction between two molecules [12]. The single-step rate integral condition is based on the knock integral with

$$K_{th} = \int_{\theta_{\text{IVC}}}^{\theta} 1/\tau \; d\theta/w$$
$$1/\tau = A\exp(E_a/(R_u T))[\text{Fuel}]^a[O_2]^b$$

where θ is the crank angle and θ_{IVC} is the cank angle of the inlet valve closure. The integral condition describes a generalized reaction of fuel and oxygen and this is an extreme simplification of the large number of reactions that

TABLE III

SIMULATION CONDITIONS

T_{in} [°C]	100–115	100	100	100
$w[rpm]$	1200	1000–1500	1200	1200
$Q_{in}[J]$	1400	1400	1000–1500	1400

take place during combustion. The empirical parameters A, E_a, a, b and K_{th} are determined from experiments. Values for n-heptane and iso-octane from [12] was used in the comparison below. Autoignition was defined as the crank angle where integral condition has reached the threshold K_{th}.

E. Combustion

When autoignition is detected by the Shell model or the Integrated Arrhenius Rate Threshold, the completion of combustion is described by a Vibe function [13].

$$x_b(\theta) = 1 - \exp\left[-a(\frac{\theta - \theta_0}{\Delta\theta})^{m+1}\right]$$

where x_b denotes the mass fraction burnt, θ is the crank angle, θ_0 start of combustion, $\Delta\theta$ is the total duration, and a and m adjustable parameters that fix the shape of the curve. The heat release is computed from the rate of x_b and the higher heating value of the fuel.

F. Heat Transfer

Heat is transfered by convection and radiation between in-cylinder gases and cylinder head, valves, cylinder walls, and piston during the engine cycle. In this case the radiation is neglected. This problem is very complex, but a standard solution is to use a Newton's law for external heat transfer

$$\frac{dQ_W}{dt} = h_c A_W (T - T_W)$$

where Q_W is the heat transfer by conduction, A_W is the wall area, T_W is the wall temperature, and the heat-transfer coefficient, h_c, is given by the Nusselt-Reynold's relation by Woschni [14].

$$h_c = 3.26 B^{-0.2} p^{0.8} T^{-0.55} (2.28 S_p)^{0.8}$$

where S_p is the mean piston speed and B is the bore.

G. Simulations

The described models were implemented and simulated in Matlab™ for single engine cycles with given initial gas mixtures and states. Cylinder specifications were set according to Table I and simulation conditions according to Table III.

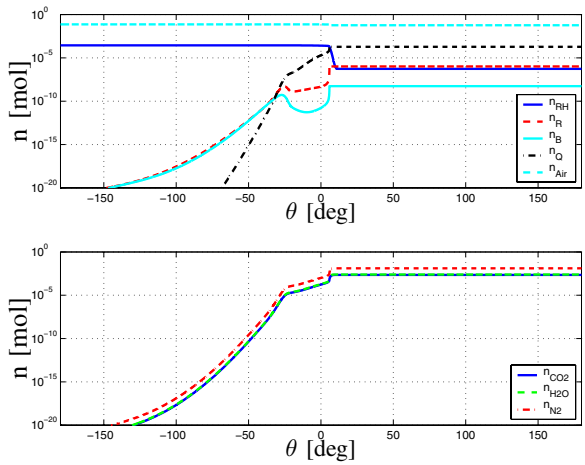

Fig. 4. Concentrations of gas species from Shell model ignition dynamics for nominal conditions, $T_{in} = 373$ K, $Q_{in} = 1400$ J, $w = 1200$ rpm for PRF90 fuel.

IV. RESULTS

Experiments were carried out to investigate the influence on ignition timing from inlet temperature, engine speed, fuel energy, and fuel ratio. There are several alternatives how to calculate the combustion timing and in this paper the combustion timing is calculated as the crank angle where 50% of the energy has been release, α_{50}, [6]. The timing effects on α_{50} were studied by varying the corresponding variables from a nominal operating condition of $T_{in} = 373$ K, $Q_{in} = 1400$ J, $w = 1200$ rpm, and $R_f = 0.93$ vol% as described in Table II. The acquired pressure, reconstructed temperature traces, and reconstructed heat release [15] for the nominal condition are shown in Fig. 2.

Fig. 3 shows pressure trace, temperature trace, and heat release for a simulation of a nominal operating point of $T_{in} = 373$ K, $Q_{in} = 1400$ J, $w = 1200$ rpm for PRF90 fuel. The dynamics of the ignition model is illustrated by the species concentrations in Fig. 4. Note that the concentrations of $\bar{R}$, Q, and B are frozen as the Shell model is switched for the Vibe combustion model. As earlier described the autoignition was defined as the crank angle where the explosive phase of the combustion phase and it can be observed that approximately 10% of the fuel has been burned at this crank angle. This is some few percentage above what was measured burned fuel in the experiment at the point where the ignition started. Timing effects on α_{50} from variations of inlet temperature, fuel energy and engine speed according to Tables II and III are summarized in Fig. 5. It can be noted that the Shell model gives quite accurate estimation of the timing for the temperature and the engine speed sweep. The model is slightly less accurate when changing the load, but still gives the correct trend.

Results from simulations using the integrated Arrhenius model are also shown in Figure 5. This method gives good results for load variations. The results for speed variations are less accurate at higher speeds. However, the model fails

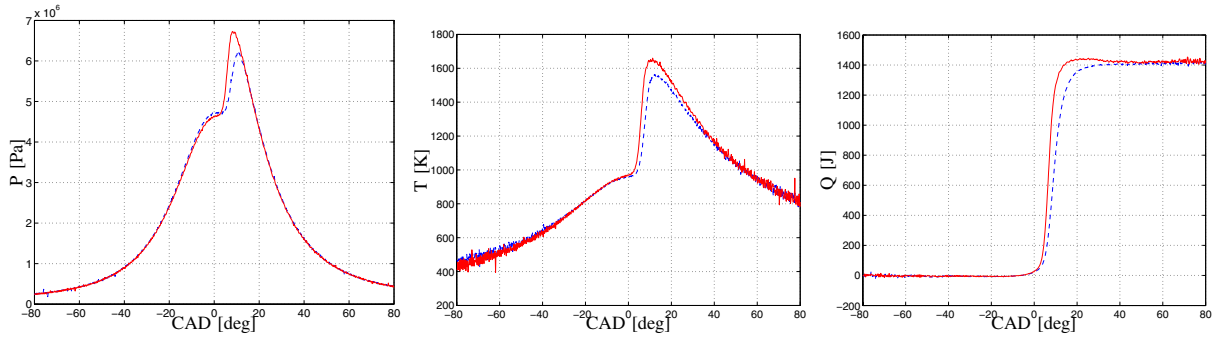

Fig. 2. Pressure trace (left), temperature trace (middle), and heat release (right) from experiment at $T_{in} = 373$ K, $Q_{in} = 1400$ J, $w = 1200$ rpm (*solid*) and $w = 1500$ rpm (*dashed*).

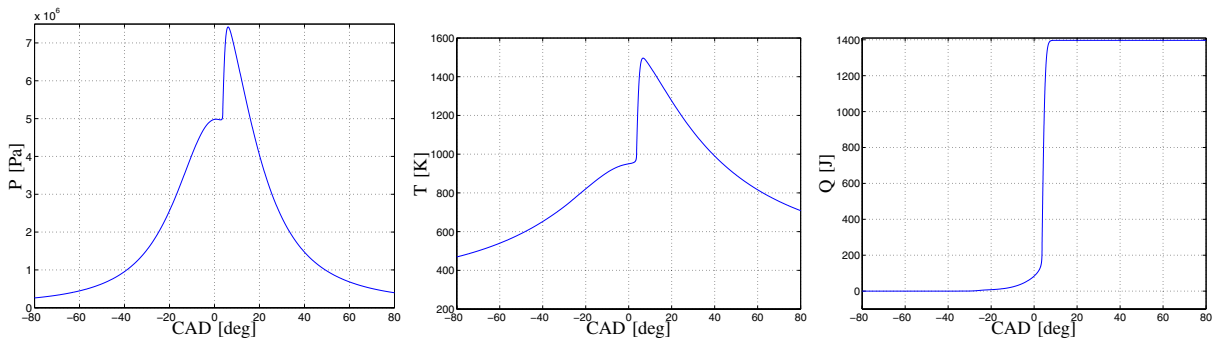

Fig. 3. Pressure trace (left), temperature trace (middle), and heat release (right) of simulation at nominal conditions, $T_{in} = 373$ K, $Q_{in} = 1400$ J, $w = 1200$ rpm for PRF90 fuel.

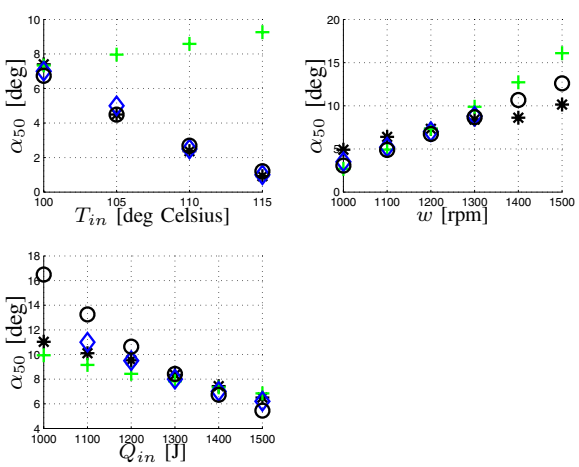

Fig. 5. Effects on ignition timing of variations from nominal conditions, $T_{in} = 373$ K, $Q_{in} = 1400$ J, $w = 1200$ rpm. The experimental results are marked as '*', the Shell model results with 'o', the Arrhenius Rate Integral results with '+', and the Planet mechanism with '◇'.

at variations of the inlet temperature.

In order to compare the ignition prediction accuracy of these low complexity models with more refined ones, results from homogeneous calculations using detailed chemical kinetics are included in Figure 5. Here, detailed chemistry for an ethanol/n-heptane mixture was obtained through the Planet mechanism for PRF fuels. For more details on the physical and chemical modeling, see references [16], [17]. From Figure 5 it can be observed that the Shell model gives similar result of prediction of α_{50} as the Planet mechanism for inlet temperature variations. This observation is also true for the speed variations. But in the case of load variation the Planet mechanism gives significant better result.

V. DISCUSSION

The results indicate that the proposed model may be used for studies on feedback strategies for ignition control. Qualitative timing behavior is correctly reproduced at variations in inlet temperature, engine speed, and load.

The simulation model was only crudely calibrated. Further work will address calibration issues, and the quantitative results are then expected to improve. The Shell-model parameters of [9] are from experiments on a rapid compression machine. Preliminary attempts with manual tuning of the parameters have shown to yield better agreement with the ignition process in a heavy-duty engine.

The proposed model performed better than the integrated Arrhenius model in the comparisons. It should be noted that the results were obtained with nominal PRF90 parameters from the literature. The latter model has an advantage of having few parameters and engine specific calibration is likely to be easier. As in [12] the integral expression can

also include explicit temperature dependence, which also was included in [5]. It may then be possible to improve the results for temperature variations. The Shell model gave in the prediction of α_{50} almost similar behavior as the detailed chemistry Planet mechanism, indicating that low complexity models can be used on feedback strategies for ignition control.

Presently, the model contains single-cylinder behavior for single-cycle simulations. It is of interest to study transient effects over multiple cycles. This requires the inclusion of gas-exchange models, wall heat dynamics, etc.

The Shell autoignition model is only applicable for single-component fuels. Therefore, no simulation results are presented to show the timing effects of varying the fuel ratio. A possible extension of the model is to include multi-component fuels. Parameters for a number of PRF fuels are available in the literature. These may be used to describe fuel quality variations, with restrictions to a limited set of fuel ratios. However, ignition control using dual fuels is a less practical approach, as it requires new infrastructure and the consumer need to refuel to fuels. The current trend is to instead use variable valve timing, for which the proposed model is straightforwardly applicable in its current form.

The experiments were performed in open-loop at low load conditions. The applicability of a model calibrated from low load experiments at high load conditions need to be further investigated. For high load experiments it is necessary to apply closed-loop control of ignition timing.

VI. CONCLUSIONS

The presented results indicates that a fairly simple autoignition model may be used to predict timing behaviour of HCCI engines at low load. It is therefore reasonable to extend this model to multi-cycle simulations including effects of heat dynamics and gas exchange.

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