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Sensitivity Analysis of Combustion Timing and Duration of Homogeneous Charge Compression Ignition (HCCI) Engines

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Abstract— **The goal of this paper is to investigate which factors have a more dominant effect and should be included in a control oriented model that predicts the start of combustion and combustion duration of a Homogeneous Charge Compression Ignition (HCCI) engine. Qualitative and quantitative information on the individual effects of fuel and exhaust gas recirculation (EGR) on the HCCI combustion is provided. Using sensitivity analysis around several operating points obtained from an experimental gasoline HCCI engine, we find that temperature is the dominant factor in determining start of combustion. In determining combustion duration, temperature is not necessarily the dominant effect compared to composition. The influences from the fuel and oxygen compositions, however, either tend to cancel each other or are very limited at all the operating conditions we investigated. Therefore, a model without the composition terms should be adequate for model-based regulation of the combustion timing in an HCCI engine.**

I. Introduction

The basis of HCCI engines is their fast and flameless combustion after an autoignition process of a homogeneous mixture. The main advantages of HCCI engines include [1]: (i) their high fuel efficiency resulting from high compression ratio and rapid heat release and (ii) low NOx and low particulate matter (PM) emissions due to low cylinder peak temperature (below 1700 K).

The autoignition of HCCI combustion, however, cannot be actuated directly. The autoignition timing of HCCI combustion is determined by the cylinder charge conditions, rather than the spark timing or the fuel injection timing that are used to initiate combustion in spark ignition (SI) and compression ignition (CI) engines, respectively [2]. Indeed, controlled autoignition requires regulation of the charge properties, namely, temperature, pressure, and composition at the Intake Valve Closing (IVC) as demonstrated by many experimental results [3], [4]. To regulate the HCCI combustion phasing, such as the crank angle where 50% of fuel is burned (CA_{50}) as in [5], [6], correct models for the start of combustion timing (SOC) and the combustion duration ($\Delta\theta$) are necessary.

In this paper we use sensitivity analysis to identify which factors have a more dominant effect on and should be included in the start of combustion (SOC) and combustion duration ($\Delta\theta$) models. Existing single-zone models for autoignition combustion timing and duration of isooctane are checked for their ability to predict gasoline ignition. Sensitivity analysis is conducted around the operating points obtained from single-cylinder gasoline engine experimental data with different fuel and exhaust gas recirculation (EGR) in [7]. Our results corroborate results of a simulation study based on an engine model with detailed chemical kinetics calibrated with a four-stroke single-cylinder engine fueled with isooctane [8].

In Sec. II the mechanism of combustion initiation is explained by the generation of radicals from a chain reaction. In Sec. III and IV, we summarize two models for SOC [7], [9]. The model in Sec. III depends only on temperature and is calibrated and validated with experimental data from a single-cylinder gasoline engine. The model in Sec. IV is a parameterized Arrhenius integral containing the concentration effect for isooctane [9] and its ability to predict gasoline ignition is examined. In Sec. V we analyze the sensitivity of the model in [9] to determine which parameters are the most important for initializing autoignition. The effect of temperature and composition on the ignition timing through changes in the hot dilution amount in the cylinder is studied. We find that temperature has the dominant impact around various operating points with different fuel and EGR. In Sec. VI, several models for combustion duration are considered. The prediction ability of these models is evaluated using experimental data. Finally, the sensitivity of the combustion duration model with respect to different parameters is analyzed. We find that combustion duration depends equally on temperature and on composition but that the effects of the fuel and oxygen compositions during EGR changes are canceled. Therefore, the combustion duration model in [7] without the composition terms is found, again, adequate for predicting the experimental data.

The fact that temperature (not composition) is the dominant mechanism for controlling the combustion timing and duration, has a direct implication in system stability and controller design. Specifically, the residual gas trapped in the cylinder of an HCCI engine constitutes an internal thermal feedback loop, which affects the stability of the temperature dynamics as analyzed in [10]. An intelligent control design accounting for the temperature dynamics is necessary to stabilize the HCCI engine under certain conditions such as during large load changes.

II. Chain Reaction for Combustion Initiation

The combustion process is itself a chain reaction, the initiation of which is characterized by a substantial concentration of radicals from stable species [11]. Radicals are

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molecules with an unpaired electron such as O, OH, N, CH_3. Therefore, a flammable mixture of fuel F and O_2 reacts and generates the radicals $R\bullet$: $F+O_2 \rightarrow R\bullet+\cdots$, for example, $CH_4+O_2 \rightarrow CH_3+HO_2$. The production rate of the radicals $R\bullet$ is then represented in the Arrenius form:

$$\frac{d[R\bullet]}{dt} = \kappa p_c(t)^n exp(-\frac{E_a}{RT_c(t)})[F](t)^a[O_2](t)^b \qquad (1)$$

where T_c and p_c are cylinder temperature and pressure, respectively, κ is the pre-exponential factor, E_a is the activation energy for the reaction generating the radicals and n, a and b indicate the reaction's sensitivity to pressure and concentration of fuel and oxygen respectively. At the intake valve closing (IVC) of an internal combustion engine, the radicals are negligible $[R\bullet](t_{ivc}) = 0$. Integration of (1) from t_{ivc} until the combustion is initiated t_{soc} corresponds to a critical value of the concentration of radicals $[R\bullet]_c$.

$$[R\bullet]_c = \int_{t_{ivc}}^{t_{soc}} \kappa p_c(t)^n exp(-\frac{E_a}{RT_c(t)})[F](t)^a[O_2](t)^b dt \ . \qquad (2)$$

Therefore, the combustion timing of an autoignition process can be described as an integral that sums up the reaction rate of radicals until the concentration of radicals reaches a critical value [12]. The initiation of combustion can be defined as the time when 1% of the fuel is burned t_{CA01} similar to the ignition delay in SI engines [13]. Since only 1% of the fuel is burned during the process, the chemical concentration $[F]$ and $[O_2]$ can be considered constant throughout the interval t_{ivc} to t_{soc} and equal to the concentrations at IVC. Furthermore, the factor κ is assumed to be independent of pressure and temperature since the largest contribution to the integral is made near the high pressure and high temperature when autoignition occurs [12]. Based on all of the assumptions above, the Arrhenius integral (3) used to predict the start of combustion (SOC) should depend on the mixture composition (fuel and air) at IVC as indicated by many other researchers [9], [14].

$$AR = \int_{t_{ivc}}^{t_{soc}} \beta\left([F](IVC),[O_2](IVC)\right) p_c(t)^n exp(-\frac{E_a}{RT_c(t)})dt \ . \qquad (3)$$

III. Ignition Model Based on Temperature

Using the principle in (3), it is shown in [7] that the combustion timing is captured without accounting for concentration in the Arrhenius integral. A single constant A in (4) was sufficient to match all the experimental data collected at different fueling levels and different EGR levels. The model in [7] is denoted with the subscript "DJR" using the initials of the first author:

$$\begin{aligned} &AR_{DJR}(\theta_{soc}) = 1 \quad \text{where} \quad AR_{DJR}(\theta) = \textstyle\int_{\theta_{ivc}}^{\theta} RR_{DJR}(\vartheta)d\vartheta \\ &\text{and} \qquad\qquad RR_{DJR}(\vartheta) = Ap_c^n(\vartheta)exp(-\frac{E_a}{RT_c(\vartheta)}) \end{aligned} \qquad (4)$$

Note that assuming a small variation in engine speed during the period $IVC \rightarrow SOC$, we change the integration argument from the time domain (t) to the crankangle domain (ϑ). Employing the volumetric ratio $v_{ivc}(\vartheta) = V_c(\vartheta_{ivc})/V_c(\vartheta)$ with $V_c(\vartheta)$ the cylinder volume at crankangle ϑ, and after assuming a polytropic compression from IVC to SOC, we represent the Arrhenius integrand as a function of the pressure p_{ivc} [kg/cm^2] and temperature T_{ivc} [K] at IVC,

$$RR_{DJR}(\vartheta) = Ap_{ivc}^n v_{ivc}^{n_c n}(\vartheta)exp(-\frac{E_a v_{ivc}^{1-n_c}(\vartheta)}{RT_{ivc}}) \qquad (5)$$

with $A = 0.4167$, $E_a = 1831930$ J/kg, $n = 1.367$, $n_c = 1.3$ and $R = 296.25$ is the gas constant [J/kg/K]. The parameters are determined using a standard nonlinear optimization routine (constr.m from Matlab) that minimizes the error between θ_{soc}, modeled through (4)-(5), and the experimentally determined CA01 for fueling sweep and internal EGR rate sweep experiments in a single-cylinder gasoline HCCI engine [7]. In the experiment setup the intake and exhaust manifold pressures are adjusted for unthrottled operation. The intake flow is heated to 90^{o}C, which can be typically achieved in the vehicle by a heat exchanger between the intake and exhaust gas. The dilution of the experimental gasoline engine is controlled by an actuator called rebreathing lift (rbl), which is a second opening of the exhaust valve during the intake stroke, as shown in Fig. 1.

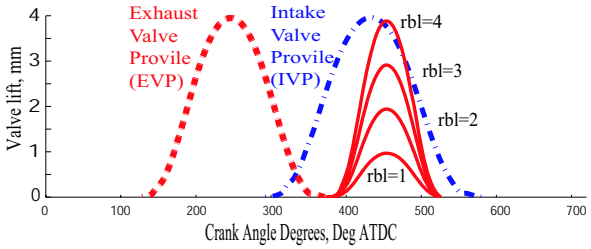

Fig. 1. Exhaust, intake and rebreathing valve profiles

Two sets of data from this experimental gasoline engine are used in this paper: Test A and Test B [7]. In Test A, both fuel and rbl vary. Specifically, rbl is decreased when fuel increases. In Test B, rbl varies while the amount of fuel is fixed. The data for 1% fuel burned are shown in Fig. 2 with square symbols, and the θ_{soc} based on (4)-(5) of the DJR model are shown with x's. The good agreement between the DJR model and the data indicates that composition could be ignored without degrading the prediction of SOC. The same conclusion is reached by Najt *et al.* [4] and [15].

Before concluding that temperature is the dominant factor for SOC we shall verify that the sensitivity of SOC to composition is small even for models that include composition in their predictive equations.

IV. Ignition Model for Isooctane

To explore further which variables dominate the autoignition process we analyze the sensitivity of a parameterized Arrhenius integral for isooctane derived from the ignition delay formula in [9]. The HCCI ignition timing of isooctane (i-C_8H_{18}) mixtures is of particular interest because isooctane

is one of the primary reference fuels that determine octane numbers and knocking tendencies of gasoline mixtures under spark ignition operating conditions. Moreover, the chemical kinetics of engine knock are very similar to the kinetics of ignition under HCCI conditions [12]. Furthermore, experiments have shown that isooctane behaves very much like gasoline except that isooctane requires a slightly higher temperature to ignite [16]. Trendwise, isooctane closely resembles gasoline.

In [9] the ignition delay time from the end of compression to the start of combustion is estimated from the pressure time history generated by a rapid-compression facility (RCF) with isooctane, oxygen, nitrogen and argon mixtures. The inverse of the ignition delay time is the integrand of the Arrhenius integral [12], which is denoted here with the subscript "XHe" using the first author's name in [9]:

$$AR_{XHe} = \int_{\theta_{ivc}}^{\theta_{soc}} \frac{1}{\tau_{XHe} N} \frac{60}{360} d\vartheta$$
$$= \int_{\theta_{ivc}}^{\theta_{soc}} 1282.1 \left(\frac{\chi_{O_2}}{\chi_{C_8H_{18}}}\right)_s^{0.77} p_c^{1.05} \chi_{C_8H_{18}}^{0.77} \chi_{O_2}^{0.64} exp\left(\frac{-33700}{R(1.09T_c)}\right) d\vartheta \quad (6)$$

where τ_{XHe} is the ignition delay time [sec] identified in [9]; N is the engine speed: 1000 rpm; p_c is pressure [atm]; T_c is temperature [K]; $R = 1.99$ is the gas constant [cal/mol/K]; $\chi_{C_8H_{18}}$ and χ_{O_2} are the fuel and oxygen mole concentrations in percent [%] respectively; and Φ_c is the equivalence ratio ($\Phi_c = \frac{\chi_{C_8H_{18}}}{\chi_{O_2}} / \left(\frac{\chi_{C_8H_{18}}}{\chi_{O_2}}\right)_s$), where the subscript s represents stoichiometric condition. The pressure and temperature histories during compression are calculated using a polytropic compression from IVC to SOC, $p_c = p_{ivc} v_{ivc}^{n_c}$ and $T_c = T_{ivc} v_{ivc}^{n_c - 1}$ with coefficient $n_c = 1.3$. Note that the constant 1.09 multiplying to T_c in (6) is a correction from the original model in [9] that accounts for the difference between isooctane and gasoline based on the experimental evidence in [16].

For the mole fractions $\chi_{C_8H_{18}}$ and χ_{O_2}, consider first the global reaction of the combustion of isooctane:

$$C_8H_{18} + 12.5\lambda(O_2 + 3.773N_2) \rightarrow$$
$$8CO_2 + 9H_2O + 12.5(\lambda - 1)O_2 + 47.16\lambda N_2 \quad (7)$$

where λ is the relative air to fuel ratio which is a measure of the relative amounts of oxidizer, air and fuel, C_8H_{18} in the fresh charge inducted through the intake. The mixing of the fresh charge and reinducted product during the induction process for lean or stoichiometric isooctane HCCI can then be represented as:

$$C_8H_{18} + 12.5\lambda(O_2 + 3.773N_2)$$
$$+\alpha\{8CO_2 + 9H_2O + 12.5(\lambda - 1)O_2 + 47.16\lambda N_2\} \rightarrow$$
$$C_8H_{18} + 12.5(\alpha\lambda - \alpha + \lambda)O_2$$
$$+47.16\lambda(\alpha + 1)N_2 + 8\alpha CO_2 + 9\alpha H_2O \quad (8)$$

where $\alpha \equiv N_{egr}/N_{frsh}$ is the ratio of the moles of reinducted product N_{egr} to the moles of inducted fresh charge N_{frsh}, similar to [5]. Thus the mole percent of the fuel C_8H_{18} and oxygen O_2 can be computed:

$$\chi_{C_8H_{18}} = \frac{N_{C_8H_{18}}}{N_{total}} = \frac{1}{60\alpha\lambda + 4.5\alpha + 60\lambda + 1} \cdot 100\% \quad (9)$$

$$\chi_{O_2} = \frac{N_{O_2}}{N_{total}} = \frac{12.5(\alpha\lambda - \alpha + \lambda)}{60\alpha\lambda + 4.5\alpha + 60\lambda + 1} \cdot 100\% \quad (10)$$

and the in-cylinder equivalence ratio can be expressed as

$$\Phi_c = \frac{\chi_{C_8H_{18}}}{\chi_{O_2}} / \left(\frac{\chi_{C_8H_{18}}}{\chi_{O_2}}\right)_s = \frac{1}{\alpha\lambda - \alpha + \lambda} \ . \quad (11)$$

With the information above, we can compute $\chi_{C_8H_{18}}$, χ_{O_2} and Φ_c using λ and α from the experimental data and check the applicability of the isooctane ignition model for gasoline ignition. Figure 2 shows a comparison of the data and the SOC predicted by the DJR [7] and XHe [9] models. Both models overpredict SOC at low fuel and hight rbl operating points in Test A and similarly underpredict SOC at low rbl values in Test B. However, the DJR model introduces a small prediction error, even after attempts to reparameterize the concentration exponents in the XHe [9] model.

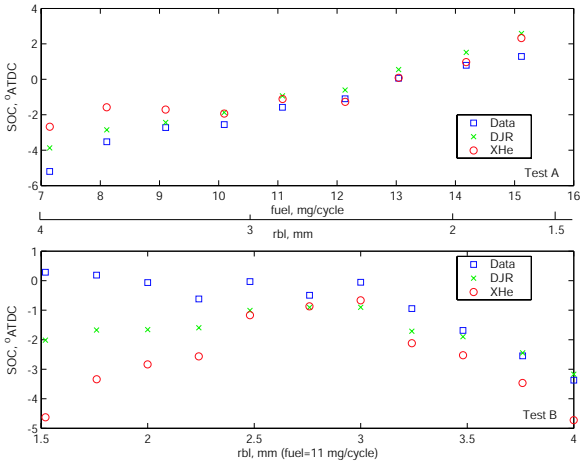

Fig. 2. Start of combustion: Test A and Test B versus DJR model and XHe model.

The computed $\chi_{C_8H_{18}}$, χ_{O_2} and T_{ivc} can then be used for sensitivity analysis of (6) in the next section.

V. Sensitivity Analysis

The sensitivity of the Arrhenius integral in (6) with respect to parameter X (p_{ivc}, T_{ivc}, $\chi_{C_8H_{18}}$, χ_{O_2}, compression ratio CR and θ_{ivc}) is

$$S_X = \frac{X}{AR_{XHe}} \left(\frac{\partial AR_{XHe}}{\partial X}\right) \cdot 100\% \ . \quad (12)$$

The sensitivity calculation provides local information and depends on the operating conditions. The sensitivity of the Arrehenius integral in (6) is calculated at operating points used in Test A and B, and the results are summarized in TABLE I. As can be seen, temperature (T_{ivc}) is obviously a more dominant factor than composition in determining the combustion timing. Note also that p_{ivc} is an important variable. In fact, p_{ivc} is as important as the fuel and oxygen

concentration, indicating the importance of the manifold filling dynamics and flow patterns for the autoignition timing, which was originally highlighted in [7]. Compression ratio CR and IVC timing θ_{ivc} also have a strong influence on the ignition timing, indicating the possibility of using IVC timing as an actuator for ignition timing control as proposed in [17].

TABLE I

THE SENSITIVITY OF THE ARRHENIUS INTEGRAL (AR_{XHe}) WITH RESPECT TO p_{ivc}, T_{ivc}, $\chi_{C_8H_{18}}$, χ_{O_2}, COMPRESSION RATIO CR AND θ_{ivc}.

	$S_{p_{ivc}}$	$S_{T_{ivc}}$	$S_{\chi_{C_8H_{18}}}$	$S_{\chi_{O_2}}$	S_{CR}	$S_{\theta_{ivc}}$
Test A	105%	1590% to 1680%	77%	64%	531% to 593%	-715% to -685%
Test B	105%	1614% to 1637%	77%	64%	538% to 566%	-701% to -694%

We further investigate if the experimental data correspond to conditions that can possibly disguise the importance of concentration. Specifically, one needs to check if the experimental data was collected at conditions where the oxygen and fuel concentration are dependent, with the one concentration increasing and the other decreasing by an amount necessary to cancel their joint contribution. A close evaluation of the two sets of data reveals that both $\chi_{C_8H_{18}}$ and χ_{O_2} decrease when rbl increases, because λ (air to fuel ratio in the intake) is kept fixed (see (9) and (10)). Thus, the effect of the fuel and oxygen concentration cannot cancel each other when (6) is applied to the two sets of data. We conclude that the sensitivity in TABLE I is not an artifact of special operating points in our small set of experiments.

VI. LAMINAR BURNING VELOCITY FOR COMBUSTION DURATION

After the initiation of the chain reaction substantial radicals are formed from stable species as described in Sec. II. The radicals start to react with the fuel and two types of reaction can occur: chain propagating and chain branching [11]. Chain propagating reactions produce the same number of but different radicals: $F + R\bullet \rightarrow R\bullet + F^*$, for example, $CH_4 + OH \rightarrow CH_3 + H_2O$, where F^* is an excited state of F or some new species (H_2O in this example). In chain branching reactions, more radicals are produced than destroyed: $F + R\bullet \rightarrow \gamma R\bullet + F^* \quad (\gamma > 1)$, for example, $CH_4 + O \rightarrow CH_3 + OH$. Finally, the reaction terminates as the radicals are destroyed by gas reactions or by collisions with surface (wall).

The whole process from the initiation to termination of the reaction is defined as the combustion duration. The combustion duration $\Delta\theta$ is defined as the period from 1% to 99% fuel burned and is correlated with the laminar burning velocity S_l in [13]:

$$\Delta\theta \sim (S_l)^{-2/3} \ . \tag{13}$$

The formula for laminar burning velocity S_l is derived in [18] by the following procedure: (i) using collision theory to find the number of collisions when a particle diffuses at a distance and (ii) applying a series of Arrenius reaction rate to the chain propagating and chain branching process to estimate the probability of when the chain branching reactions occur after a collision:

$$\begin{aligned} & S_l = k_0 T_u \left[\frac{1}{T_m} [F]^a [O_2]^b exp\left(\frac{-E_c}{R_u T_m} \right) \right]^{1/2} \\ \text{where} \quad & T_m = T_u + e\Delta T \ . \end{aligned} \tag{14}$$

The parameter E_c is the activation energy of the global reaction representing the combustion process and R_u is the universal gas constant. T_u is the temperature of the unburned mixture and T_m is the mean flame temperature. The parameter ΔT denotes the adiabatic temperature rise due to combustion. The parameter e represents an averaging parameter of the released thermal energy during combustion. The exponents a and b are the reaction order with respect to fuel and oxygen. For all hydrocarbons that have been examined by Tabaczynski *et al.* [19], $a + b = 1$. Taking isooctane (C_8H_{18}) for example, we have $a = -0.71$ and $b = 1.71$. By substituting (14) into (13) and replacing T_u, $[F]$ and $[O_2]$ with T_{soc}, $\chi_{C_8H_{18}}$ and χ_{O_2} respectively, the formula for the combustion duration becomes

$$\begin{aligned} & \Delta\theta_{Taba} = k T_{soc}^{-2/3} T_m^{1/3} \chi_{C_8H_{18}}^{0.23} \chi_{O_2}^{-0.57} exp\left(\frac{E_c}{3R_u T_m} \right) \\ \text{where} \quad & T_m = T_{soc} + e\Delta T \end{aligned} \tag{15}$$

with $k = 5$ and $e = 0.74$. Therefore, ideally the combustion duration should be a function of the charge composition. In [7] the assumption was made that the charge composition does not affect the combustion (autoignition timing, burn duration, combustion efficiency, etc). Specifically, [7] neglects $\chi_{C_8H_{18}}^{0.23}$ and $\chi_{O_2}^{-0.57}$ in (15) and defines the combustion duration $\Delta\theta_{DJR}$, following [20] as:

$$\begin{aligned} & \Delta\theta_{DJR} = k(\theta_{soc}) T_{soc}^{-2/3} T_m^{1/3} exp\left(\frac{E_c}{3R_u T_m} \right) \\ \text{where} \quad & T_m = T_{soc} + e(\theta_{soc})\Delta T \\ \text{and} \quad & \Delta T = \frac{Q_{LHV} W_f \tau}{c_v m_c} \ . \end{aligned} \tag{16}$$

The combinations of independently optimized values of k and e to the data of Test A and B resulted in a single relation (17) for which the value for e is uniquely determined by the value for k:

$$\begin{aligned} & e = a_0 + a_1 k \\ \text{where} \quad & k(\theta_{soc}) = b_0 + b_1 \theta_{soc} + b_2 \theta_{soc}^2 \end{aligned} \tag{17}$$

with $a_0 = 1.0327$, $a_1 = -5.4544$, $b_0 = 0.1621$, $b1 = 0.0055$ and $b2 = 0.0017$. The parabolic relation of k on θ_{soc} revealed by the data is justified by the fact that there should be an optimum θ_{soc}^*. As a result, the parameter e that represents efficiency should drop for retarded or advanced values from the optimum θ_{soc}^*.

The combustion duration $\Delta\theta_{Taba}$ calculated using (15) predicts a monotonic trend and cannot match all the data of Test A when both fuel and rbl change, as shown in Fig. 3. On the other hand, the reasonable match in the steady state validation of $\Delta\theta_{DJR}$ shown in Fig. 3 suggests that the omissions in our model are probably of secondary

importance, at least under the conditions of Test A and Test B. The impact from the air-to-fuel ratio (AFR) can be omitted if we are able to design a controller for tight regulation of AFR. The amount of the inducted fresh air, however, could not be controlled by us and might have had a strong influence on the combustion duration.

Therefore, to further evaluate the composition effect, we first modify the Tabaczynski model in (15) by making e a function of θsoc to match the data, as shown in Fig. 4.

$$\Delta\theta_{TabaNew} = k_1 T_{soc}^{-2/3} T_m^{1/3} \chi_{C_8H_{18}}^{0.23} \chi_{O_2}^{-0.57} exp\left(\frac{E_c}{3R_u T_m}\right)$$
$$\text{where} \quad T_m = T_{soc} + e(\theta_{soc})\Delta T$$
$$\text{and} \quad e = c_0 + c_1\theta_{soc} + c_2\theta_{soc}^2 \tag{18}$$

with $k_1 = 0.9909$, $c_0 = 0.1728$, $c_1 = -0.0447$ and $c_2 = -0.0105$. The parameter e again captures the apparent fuel efficiency that lumps (i) combustion efficiency and (ii) heat losses through the walls. We then eliminate the composition term $\chi_{C_8H_{18}}^{0.23}\chi_{O_2}^{-0.57}$ in (18) and obtain

$$\Delta\theta_{NoComp} = k_2 T_{soc}^{-2/3} T_m^{1/3} exp\left(\frac{E_c}{3R_u T_m}\right)$$
$$\text{where} \quad T_m = T_{soc} + e(\theta_{soc})\Delta T$$
$$\text{and} \quad e = d_0 + d_1\theta_{soc} + d_2\theta_{soc}^2 \tag{19}$$

where $k_2 = 0.2494$, $d_0 = 0.2173$, $d_1 = -0.0503$ and $d_2 = -0.0114$ are tuned using the data. As can be seen in Fig. 4, with or without the composition terms the results are quite close, indicating that the effect of the composition term $\chi_{C_8H_{18}}^{0.23}\chi_{O_2}^{-0.57}$ is not needed under Test A and Test B conditions.

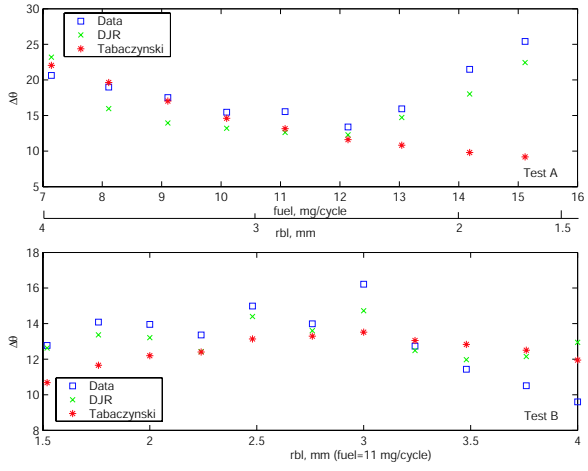

Fig. 3. Combustion duration: Test A and Test B versus DJR model and Tabaczynski model.

Despite the fact that neither of the data sets we considered points to the necessity of composition, one needs to explore if the two tests are such that the effect of the two variables cancel each other. Both $\chi_{C_8H_{18}}$ and χ_{O_2} drop as the amount of residual increases (α increases). The effect of $\chi_{C_8H_{18}}$ and χ_{O_2} on combustion duration, however, cancel each other due to the opposite sign of the exponents. Thus, the data sets A and B do not provide conclusive evidence for neglecting composition from combustion duration.

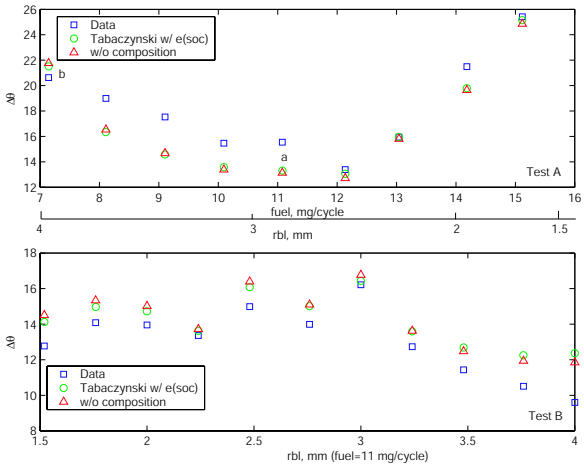

Fig. 4. Combustion duration: Test A and Test B versus the new Tabaczynski model and the model without composition terms.

The sensitivity of the new Tabaczynski model in (18) at different operating points in the tests is shown in TABLE II. Test A.a corresponds to operating point a ($fuel = 11mg/cycle$) and Test A.b corresponds to operating point b ($fuel = 7mg/cycle$) in Fig. 4. The sensitivity to θ_{soc} varies considerably at different operating points in Test A mainly due to the parabolic function $e(\theta_{soc})$. For instance, the sensitivity to θ_{soc} at point **a** is much smaller than that at point **b** since point **a** corresponds to the peak of the parabolic curve $e(\theta_{soc})$. Note that $\chi_{C_8H_{18}}$ affects the combustion duration in (18) in two conflicting ways: One from $\chi_{C_8H_{18}}^{0.23}$ and the other from ΔT, where the fuel heating energy is distributed to the whole cylinder mass. The negative sign of the sensitivity on T_{soc} suggests that higher temperature shortens the duration. As can be seen from the table, temperature is not the dominant effect compared to the compositions.

TABLE II

THE SENSITIVITY OF THE COMBUSTION DURATION WITH RESPECT TO θ_{soc}, T_{soc}, $\chi_{C_8H_{18}}$, AND χ_{O_2}.

	$S_{\theta_{soc}}$	$S_{T_{soc}}$	$S_{\chi_{C_8H_{18}}}$	$S_{\chi_{O_2}}$
Test A.a	-0.67%	-67%	15%	-57%
Test A.b	163%	-70%	-35%	-57%
Test B	-1.18% to 4.15%	-67%	6% to 16%	-57%

Since composition cannot be assumed negligible based on Test A and Test B, we proceed to investigate whether the composition terms become significant when only fuel changes. This evaluation is important because fuel steps correspond to load changes in vehicle application. During fuel step changes $\chi_{C_8H_{18}}$ and χ_{O_2} change in opposite directions. With the opposite sign in the exponent, the composition terms will not cancel each other. The change in χ_{O_2} during fuel steps, however, is negligible since we are running lean. On the other hand, $\chi_{C_8H_{18}}$ affects the combustion duration by changing $\chi_{C_8H_{18}}^{0.23}$ and ΔT in (18). The fuel step responses of the model with the DJR model in (16) and the new Tabaczynski model in (18) are shown in Fig. 5. Both models are able to capture the transient trends of CA_{50} and exhaust

runner temperature. Therefore, the composition terms are not necessary to capture the performance variable CA_{50} during fuel steps. The injected fuel amount mainly affects combustion duration through the temperature rise ΔT resulting from the heat release process.

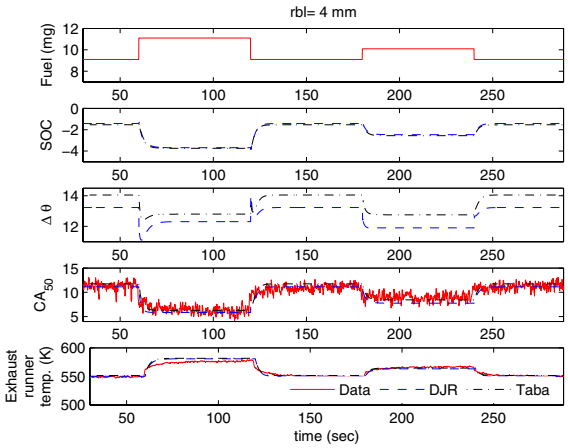

Fig. 5. Fuel step response validation: DJR model versus the new Tabaczynski model.

VII. Conclusion

In this sensitivity study the charge heating effect and dilution effect on the ignition timing and combustion duration in HCCI engines are explored. Note that the parameters for the formulas are picked for isooctane whereas the data are collected from an gasoline engine. Therefore, it is the trend rather than the exact values that one should look at. We find that the start of combustion (SOC) timing depends much more on temperature than on composition. This result agrees with the conclusion in [8]. There might be, however, conditions when composition changes more than temperature does, such as when there is high heat loss in the cylinder and cylinder temperature does not change much despite increased dilution (hot exhaust gasses) [21]. It is not clear at this point if such extreme heat transfer conditions will benefit an automotive engine application. Thus, we propose that the composition effects be eliminated from a control-oriented model for ignition timing.

Moreover, we find that the combustion duration depends equally on temperature and on compositions. The dilution effect does result in longer combustion duration as suggested in [8], but the overall effect is found to be very limited at the operating conditions we studied. Specifically, the effects from the fuel and oxygen composition tend to cancel each other when rbl is changed. The composition effect is also negligible when fuel is changed, as shown in Fig. 5. The explicit dependency of the combustion duration $\Delta\theta$ on the start of combustion (SOC), on the other hand, is necessary to capture the combustion efficiency and heat transfer in the conditions of these tests.

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