A combustion phasing control-oriented model applied to an RCCI engine

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Abstract: Low temperature combustions such as Reactivity Controlled Compression Ignition (RCCI) have been shown to be a promising way to reduce pollutants at the exhaust, i.e. NO_x and soot emissions, and increase the thermal efficiency of future engines. However, such concepts are subject to substantial control sensitivity, e.g. combustion phasing, due to their lack of direct actuation for controlling the ignition of the mixture. This work investigates a control-oriented model based on physical equations aimed to predict the start of combustion and the crank angle of 50% fuel burnt (CA50). The model was developed for predicting the ignition using a modified knock integral model and a linear equation was used to estimate the burn duration between the start of combustion and the combustion phasing. The calibration and the validation of the model were performed using experimental data from a heavy-duty engine showing good results under transient operation.

Keywords: Reactivity controlled compression ignition, control-oriented model, modified knock integral model.

1. INTRODUCTION

Among the Low Temperature Combustion (LTC) concepts aimed to reduce NO_x and soot emissions, such as Homogeneous Charge Compression Ignition (HCCI) or Premixed Charge Compression Ignition (PCCI), the Reactivity Controlled Compression Ignition (RCCI) combustion has demonstrated a great potential (Kokjohn et al., 2011; Reitz, 2013; Molina et al., 2015). This strategy consists in a combustion of a blend mixture composed by a low reactivity (e.g., gasoline) and a high reactivity (e.g., diesel) fuel (Benajes et al., 2014). In contrast to conventional diesel and spark ignited combustion engines, premixed compression ignition modes lack of ignition control (Yao et al., 2009). In this sense, RCCI also proved a better ability respect to the heat release rate and the combustion phasing control thanks to its dual-fuel reactivity operation (Wissink et al., 2012; Benajes et al., 2015). However, the combustion process being sensitive to several factors such as intake temperature, recirculated gases amount, etc., it is usually assumed that a closed-loop control using incylinder pressure feedback is necessary (Carlucci et al., 2014).

Efficient control of such combustion concept is of great importance for getting the full benefits of it. In this regard, two main controller categories can be found. The first of them consists in experimentally tuned controllers based on Proportional-Integral-Derivative (PID) actions such as those presented in Olsson et al. (2001), Hanson and Reitz (2013) and Arora and Shahbakhti (2017). The other approach relies on control-oriented models (COM). Such method consists in identifying the physical process of the combustion while ensuring a fast computation time making it suitable for real-time control applications (Ravi et al., 2010; Bidarvatan et al., 2014).

Up to now, only a few control-oriented models in RCCI combustion have been investigated (Bekdemir et al., 2015; Khodadadi Sadabadi et al., 2016; Nithin et al., 2017) and an application to a model-based controller was proposed by Khodadadi Sadabadi and Shahbakhti (2016). In Bekdemir et al. (2015), the authors firstly suggested a multi-zone approach model in a natural gas-diesel RCCI heavy duty engine to describe the auto-ignition process and to predict the in-cylinder pressure trace. After has been validated, the model was used to develop a realtime, map-based, control which was then implemented into a closed-loop controller relying on Proportional-Integral (PI) actions on the gas and the diesel injected quantities but also on the diesel injection timing. More recently, Nithin et al. (2017) proposed a COM to predict the combustion phasing (refered as the crank angle of 50% fuel burnt, CA50) during steady-state and transient operations. The physics-based model includes a Start Of Combustion (SOC) prediction using a Modified Knock Integral Model (MKIM), derived from the original correlation proposed by Livengood and Wu (1955) to predict knock in spark ignition engines, and a Wiebe function was used to describe the combustion process. The COM was experimentally validated showing an average error of 1.7 CAD in the prediction of the CA50. The model was then used as a virtual RCCI engine to design a PI controller aimed to track the desired combustion phasing. Similar modeling approaches can be found in literature for HCCI engines (Swan et al., 2006; Shahbakhti and Koch, 2010).

Other methods have been employed to characterize the ignition process of HCCI engines such as the Arrhenius-

Table 1. Engine specifications

Manufacturer/model	Volvo/D8K320
Number of cylinders	6
Bore x Stroke	$110~\mathrm{mm} \ge 135~\mathrm{mm}$
Crank length	67.5 mm
Total displacement	$7700 \ {\rm cm}^3$
Compression ratio (nominal)	17:1
Compression ratio (RCCI configuration)	12.5:1

like models used in Shaver et al. (2004) and Mayhew et al. (2009). On the contrary to the aforementionned KIM models, those models were dependant on the in-cylinder oxygen and fuel concentration, although some works have been developed removing such variables (Chiang and Stefanopoulou, 2006; Widd et al., 2008). Auto-ignition models need to be calibrated using experimental data or experimentally validated more complex engine model in order to make the reaction rate correspond to the experimental SOC.

This paper presents a control-oriented model based on physical equations to describe the RCCI combustion in an engine. In particular, the objective of the model is to predict the CA50 in a cycle-to-cycle basis. While the majority of the Arrhenius like functions have been applied to single fuel highly premixed combustion engines, this study presents a model developed to assess the dual-fuel strategy of the RCCI combustion. Especially, a modified knock integral model which takes into account the fuel blending ratio of both fuels is used to describe the ignition process of the in-cylinder mixture. Indeed, in such combustion mode, the SOC has been identified to be sensitive to the global reactivity of the mixture and the in-cylinder oxygen concentration (Kokjohn et al., 2009; Desantes et al., 2014). The model was then designed to encompass such effect and the gasoline fraction is used as a key parameter for the mixture reactivity estimation and the air dilution by the exhaust gas recirculation (EGR) is implemented in the model through an estimation of the oxygen concentration at the intake. Finally, an estimation of the CA50 is obtained as a function of the estimated SOC and a linear equation aimed to represent the duration between SOC and CA50 based on a statistical analysis on the main control variables affecting such duration. The model is then calibrated using a set of experimental data and validated in a load transient test.

2. EXPERIMENTAL SETUP

In this study the COM was developed and validated using experimental data coming from a six cylinder heavy-duty diesel engine modified to be operated in RCCI combustion, i.e. each cylinder was equipped with a port fuel injector. In order to extend the operating range and increase the efficiency of the RCCI concept, the pistons were modified, leading into a lower compression ratio (Benajes et al., 2016). The engine specifications are listed in Table 1.

In addition to the conventional available sensors (e.g., air mass flow, intake pressure and temperature), each cylinder was equipped with an in-cylinder pressure Kistler 6125C sensor. Furthermore, an Horiba Mexa-One gas analyzer was used to measure the oxygen and the CO_2

concentration at the exhaust and an additional sensor was used to measure the CO_2 concentration at the intake. The EGR rate was then calculated using (1):

$$EGR = \frac{[CO_2]_{int} - [CO_2]_{atm}}{[CO_2]_{exh} - [CO_2]_{atm}}$$
(1)

where $[CO_2]_{atm}$ is the atmospheric concentration of CO_2 , that is 0.04%.

The fuels used to run the engine were commercial gasoline as port-fuel injected (PFI) and diesel as direct injected (DI). With the aim of developing the model described in the following section, such fuels were considered as isooctane and n-heptane for gasoline and diesel respectively.

The control of the injection was performed using a realtime National Instruments controller (PXIe-8135) and an embedded Field Programmable Gate Array (FPGA) chassis with dedicated modules (NI-9155) while the acquisition of the signals was carried out by a 16 analog channels acquisition card (PXIe-6358).

The in-cylinder pressure *pegging* was done by using the intake manifold pressure near the intake BDC. Then, a Butterworth low-pass filter, tuned at 3 kHz for removing high frequency components associated to the in-cylinder pressure resonance, was applied.

3. MODEL DESCRIPTION

In this section the control-oriented model developed for describing the RCCI combustion is explained. This model aims to predict the start of combustion of the in-cylinder mixture and the CA50 using physical equations based on measurable operating conditions variables. The COM is divided into three parts including the estimation of the in-cylinder conditions at Intake Valve Closure (IVC), the compression from IVC to SOC and the combustion process until the CA50.

$3.1 \ IVC \ conditions$

The in-cylinder charge conditions at the IVC are of great importance in the combustion timing of RCCI engines (Wu et al., 2014). In this model some simplifications are made, that is, the residual gases from previous cycle are not considered since the valve overlap in the engine was assumed to be sufficient to clean the in-cylinder end gases. Also, the in-cylinder pressure at IVC was considered to be equal to the intake manifold pressure. Considering those assumptions, the in-cylinder temperature at IVC can be then approximated using the ideal gas law (2):

$$T_{ivc} = \frac{P_{ivc} \cdot V_{ivc}}{m_{cyl} \cdot R} \tag{2}$$

with R the ideal gas constant equal to 287 J/kg.K and V_{ivc} the volume at IVC obtained from geometrical equations.

The in-cylinder trapped mass m_{cyl} was estimated using a volumetric efficiency map calibrated from experimental data and calculated using (3):

$$m_{cyl} = \frac{\eta_v \, P_{int} \, V_{dis}}{R \, T_{int}} \tag{3}$$

where η_v is the volumetric efficiency and V_{dis} is the cylinder displacement.

3.2 Compression (from IVC to SOC)

The compression of the in-cylinder composition was assumed to follow a polytropic form $(PV^k = constant)$. It was then possible to estimate the instantaneous in-cylinder pressure P and temperature T, see (4):

$$P(\theta) = P_{ivc} \cdot \left(\frac{V_{ivc}}{V(\theta)}\right)^k \tag{4}$$

$$T(\theta) = T_{ivc} \cdot \left(\frac{V_{ivc}}{V(\theta)}\right)^{k-1}$$
(5)

where k denotes a constant polytropic coefficient, V is the volume and ivc stands for the value at the intake valve closing.

For the SOC estimation, a modified knock integral model was used. This integral model increases as the moment of auto-ignition is approached and the SOC is considered where this expression reaches the unit (6):

$$\int_{\theta_{ivc}}^{\theta_{soc}} \frac{1}{A N \exp\left(\frac{b}{T(\theta)} P(\theta)^n\right)} \, d\theta = 1.0 \tag{6}$$

where A, b and n are constants which need to be calibrated, N is the engine speed, and T and P are the instantaneous in-cylinder temperature and pressure respectively.

The constant b can be associated to the activation energy Ea of the fuel, being b = Ea/R. However, in this work the model needs to be adapted to an RCCI combustion taking into consideration the effect of both fuels, that is the mixture reactivity. As proposed by Khodadadi Sadabadi et al. (2016), the activation energy of a fuel was considered as a function of its cetane number CN (7).

$$Ea = c_1/(CN + c_2) \tag{7}$$

Thus, it was possible to approximate the activation energy of the mixture considering a global cetane number CN_{mix} estimated from the proportion of each fuel and their respective CN (8):

$$CN_{mix} = GF \cdot CN_{pfi} + (1 - GF) \cdot CN_{di} \tag{8}$$

where GF is the gasoline fraction defined by the ratio of the gasoline mass m_{pfi} to the total injected mass m_{fuel} , $GF = m_{pfi}/m_{fuel}$.

Another parameter which drives the combustion timing is the available concentration of oxygen in the cylinder which mainly depends on the EGR rate. Thus, in order to take into account its effect, the oxygen concentration at the intake $[O_2]_{int}$ was included in the MKIM and was calculated as presented in (9) where $[O_2]_{atm} = 21\%$.

$$[O_2]_{int} = [O_2]_{atm} \cdot (1 - EGR) + [O_2]_{exh} \cdot EGR \qquad (9)$$

The constant A from the MKIM in (6) can be associated to the EGR rate in order to take into account the effect of a change in the oxygen concentration at the intake. In this work, according to the calibration data used and the intake oxygen levels studied, this was modeled by including such concentration in the calibration of the constant A through a linear equation. The final modified knock integral model used in this work is then (10):

$$\int_{\theta_{ivc}}^{\theta_{soc}} \frac{1}{A N \exp\left(\frac{c_1}{(CN_{mix}+c_2)R T(\theta)} P(\theta)^n\right)} d\theta = 1.0 \quad (10)$$

where $A = c_3 + c_4([O_2]_{atm} - [O_2]_{int})$

3.3 Combustion (from SOC to CA50)

In such combustion models, the prediction of the CA50 is usually obtained using a burn duration model coupled with a Wiebe function (Shahbakhti and Koch, 2007; Khodadadi Sadabadi et al., 2016). In this study the burn duration value was considered only from the SOC to the CA50 itself. Indeed, after have been processed, the tests used for the calibration of the model shown that this value was almost constant within a range of \pm 1.2 Crank Angle Degree (CAD) compared to the mean value (see Fig. 2). After a statistical analysis, an algebraic linear model considering the relevant variables affecting θ_d was investigated and is proposed in (11):

$$\theta_d = CA50 - SOC = b_0 + b_1 T_{soc} + b_2 \phi \tag{11}$$

where b_0 , b_1 and b_2 are constants to be calibrated, T_{soc} is calculated using the instantaneous polytropic temperature T at θ_{soc} and ϕ is the global equivalence ratio obtained from (12):

$$\phi = \left(\frac{1 + EGR}{m_{cyl}}\right) \left(\frac{m_{pfi}}{FAR_{st,pfi}} + \frac{m_{di}}{FAR_{st,di}}\right)$$
(12)

where FAR_{st} refers to the fuel-air ratio at stoichiometric conditions for each fuel.

For obtaining (11), a multiple variables regression model was investigated using a set of eventual affecting parameters such as the gasoline fraction, the temperature at SOC, the equivalence ratio, the intake pressure (Khodadadi Sadabadi and Shahbakhti, 2016) and it was found that T_{soc} and ϕ were able to represent the major part of the training data leading into a coefficient of determination R^2 of 0.71. It is important to note that such value of R^2 was also affected by the cycle-to-cycle dispersion of such combustion mode as presented in Fig. 2 and thus the results and trend obtained were considered as acceptable.

The CA50 estimation was thus found using (11) and the SOC value of the corresponding cycle.



Table 2. Operating conditions for model calibration



4. MODEL CALIBRATION AND VALIDATION

4.1 Calibration

In order to calibrate the constants used in this model, a set of experimental tests has been used. The operating conditions consisted in a constant engine speed at different EGR rates and a sweep in the intake pressure and the incylinder reactivity (see Table 2).

To estimate the experimental variables such as SOC and CA50, the Apparent Heat Release Rate (AHRR) presented in (13) was used:

$$AHRR(\theta) = \frac{k}{k-1} \cdot P(\theta) \cdot dV(\theta) + \frac{1}{k-1} \cdot V(\theta) \cdot dP(\theta)$$
(13)

with θ the crank position, k a constant polytropic coefficient, P the in-cylinder pressure and V the instantaneous chamber volume.

Low temperature combustions such as RCCI are usually characterized by a heat release rate where two different zones can be easily identified, i.e. a Low Temperature and a High Temperature Heat Release (LTHR and HTHR respectively). In this work the SOC used as a reference to calibrate the MKIM was considered as the SOC of the HTHR, see Fig. 1.

The calibration of the constants b and n in (6) were done using a test with no EGR and a constant fuel mixture reactivity performing intake pressure sweep. Then, an optimization calibration was done in order to decrease the root mean squared error between the value at θ_{soc} , obtained from experimental data, of the integral part of (6) and the desired value, being the unit. The same principle was then applied to a test at constant intake pressure with no EGR and a change in the reactivity of the mixture in order to calibrate the constants from (7). Finally the EGR effect was calibrated at a constant intake pressure and mixture reactivity with two levels of EGR rate.



Fig. 2. Experimental and estimated θ_d from model calibration

Table 3. Calibration constants values



Fig. 3. SOC and CA50 estimation from the COM against experimental values from tests used for calibration

Fig. 2 presents the nearly constant θ_d and its estimation as explained in the previous section. Note that (11) was calibrated for the chosen experimental tests at a specific engine speed where such value appeared to be almost constant. For a proper calibration of the θ_d estimation, a sweep in engine speed and a higher sweep of the intake temperature and EGR rate would need to be performed.

Table 3 presents the calibration constants obtained for this model while Fig. 3 shows the results obtained for SOC and CA50 estimation of several cycles coming from the different operating conditions listed in Table 2. The respective errors distribution are shown in Fig. 4.

The results obtained from the model show a good agreement with the experimental data leading into a mean absolute error of 0.39 CAD and 0.36 CAD for the SOC and the CA50 estimation respectively. The different dispersions obtained could be explained by: the calibration constants which cannot be perfectly fitted for all the operating conditions, the modeling assumptions, but also by the injector



Fig. 4. SOC and CA50 error distribution from the results presented in Fig. 3

model. Indeed, the injectors are controlled in terms of injection duration (energyzing time) and not in mass. Thus, the accuracy of the injector model allowing to convert the desired mass into the proper injection duration is of great importance. Nevertheless, the obtained results were considered good enough to apply the model to transient operation.

4.2 Transient operation validation

The model was applied to an experimental test where a step in load, being the Indicated Mean Effective Pressure (IMEP), was performed at the same engine speed than the tests used for calibration, that is 1200 rpm. The goal was to verify the ability of the model to predict the CA50 under transient operation using the available inputs and model calibration constants detailed in previous section. In this test a step in the total injected mass and gasoline fraction is performed while the EGR valves and the Variable Geometry Turbocharger (VGT) positions were fixed. Fig. 5 presents the results obtained in the CA50 estimation using the control-oriented model developed in this work.

The COM shows a good prediction of the CA50 at low load while some bias can be observed at the highest IMEP value during the first 100 cycles. This could be explained by the injector model inaccuracies as previously explained, leading into some bias in the real injected fuel mass estimation when performing the load transient. Furthermore, as shown in (11), the model chosen for the CA50 estimation depends directly on ϕ and thus a bias in the injected fuel mass estimation would create an additional error (see (12)). Finally, the lack of real-time measurement of the oxygen concentration at the intake and the simple model used for the EGR effect on the SOC prediction can also explain the estimation penalty. Despite the difference obtained during the first cycles after the load transient step, the estimated CA50 shows a good agreement with the experimental CA50 value even when the latter was decreasing due to the dynamics of the air



Fig. 5. Control-oriented model performance in a load transient test

path and thus the intake pressure. The average error for the complete transient operation resulted in a ± 0.43 CAD.

5. SUMMARY AND CONCLUSIONS

In this work a control-oriented model has been proposed for an RCCI combustion. The model aimed to predict the SOC and the CA50 using available sensors and variables. The SOC estimation has been performed using a modified knock integral model where the effect of the mixture reactivity and the available O_2 concentration were included in order to apply the KIM to a dual-fuel combustion with air dilution by recirculation of exhaust gases. The CA50 estimation has been calibrated using a reduced burn duration estimation which corresponded to the crank degrees between SOC and the CA50 itself. Such estimation has been set as a simple linear function of relevant contributing variables. The model was calibrated using experimental data coming from a heavy-duty engine modified to operate in RCCI at constant engine speed under different intake pressure, EGR rate and mixture reactivities. The model has shown encouraging results in the estimation of the SOC and the CA50 within a mean absolute error of 0.39 and 0.36 CAD respectively for the selected experimental tests. The COM has been finally tested in transient operation where an IMEP step was performed. The model has exhibited good results in the CA50 estimation with an average error of ± 0.43 CAD which was considered as acceptable for the purposes of this work. Indeed, such model aims at being integrated as a feedforward information in a closed-loop control application in a future work where the injection settings will be cycle-to-cycle corrected to overcome an eventual bias in the CA50 result. Nevertheless, despite the results obtained in this work, a deeper analysis of the RCCI combustion modeling under a wider range of operating conditions must be performed to adapt the model. Furthermore, the start of injection of the late diesel injection could lead into some stratification of the in-cylinder charge when delaying its value and could thus lead into some additional errors. Thus, a model able to encompass such effect must be investigated.

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