Towards control of HCCI combustion by ozone addition: a mathematical approach to estimate combustion parameters

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Abstract: The effect of ozone addition on combustion of Homogeneous Charge Compression Ignition (HCCI) engine was examined to define a 0D physical model of combustion and proposed a predictive static model of combustion parameters. All parameters of the physical model were identified using a single-cylinder fueled with iso-octane running at constant engine speed (1500 rpm) and equivalence ratio (ϕ = 0.3) but various EGR rate and ozone rate. Experimental data are used to validate the physical model. The results show that the 0D one zone model yields good results to capture combustion parameters like in-cylinder pressure maximum (Pmax), the corresponding angle (CADpmax) and the crank angle degree when 50% of the fuel had burned (CA50). All these parameter are strongly dependent on ozone addition and EGR rate. Then, mathematical equations are presented to describe the static relation between combustion parameters and both EGR rate and ozone addition.

Keywords: HCCI, 0D model, EGR and ozone addition effect, combustion parameters (Pmax, CADpmax, CA50), HCCI control, mathematical equation.

1. INTRODUCTION

Due to the continual increased in fossil fuel consumption and the current interest in halting global warming, the automotive industry have the task to developed new engine with high efficiency. Among the proposed solutions, the Homogeneous Charge Compression Ignition (HCCI) offers best compromise. Combustion of HCCI engine offers gains in efficiency over traditional combustion concepts, and its characterized by a very low level of Nitric Oxide (NOx) and Particulate Matter (PM) emissions (Yao et al. 2009). Another advantage of HCCI engine is that it enables the use of a large range of fuels and additives. However, the challenge is to control the stability of the combustion over the full range of engine operating points and during transition between two operating point.

Combustion of HCCI engine process is strongly dependent to thermal, chemical and physical effects. So, many research have been done in order to control cycle-to-cycle variations of the combustion through varying initial temperature of the mixture (Lü et al. 2005; Cinar et al. 2015), wall temperature (Komninos et al. 2015), intake pressure (Olsson et al. 2001), Variable Compression Ratio (VCR) (Christensen et al. 1999), Variable Valve Timing (VVT) (Gregory M Shaver et al. 2006; Prasad et al. 2013) but a fast response actuator is needed and implementing these controls are complex and need changing the engine architecture.

Chemical effects are actually the best and efficient way to control this combustion using equivalence ratio, residual or rate of Exhaust Gas Recirculation (EGR) or incorporated additives in the mixture. As shown in (Jung et al. 2015), the slow response of the EGR actuator doesn’t allows the control of cycle-to-cycle variations and these can lead to three possibilities in the operating point behaviour: combustion, misfire or knock. The solution to compensate cycle-to-cycle variations is to combined dilution using EGR valve (slow response) and adding a proportion of additives in the mixture (fast response). Recently, the effect of ozone addition is investigated experimentally (Foucher et al. 2013; Pinazzi et al. 2015) and it shown the use of a small mass flow of ozone, a strong oxidizer species, can improve the combustion and forward the phasing of combustion. A flow of air is used to produce the ozone concentration through an ozone generator. This generator is working on principle of a dielectric barrier discharge. During transitions between two operating points, the ozone addition can act like a chemical actuator to compensate cycle-to-cycle variation and improve the combustion over full range of operating points.

Before try to control cycle-to-cycle combustion phasing a model that give good estimation and prediction of the combustion phasing using position of the EGR valve and ozone mass flow must be developed. Two main techniques are used in the context of combustion of HCCI engine modelisation: thermo-kinetic models and control-oriented models. Thermo-kinetic models depends on thermodynamical and chemical states within combustion chamber, such as the zero-dimensional Thermo-Kinetic Models (0D-TKM) of Fiveland et al. 2000 and multi-zone models (Neshat et al. 2014). The accuracy of the multi-zone models to predict in-cylinder pressure and emissions levels depends on the initial imposed zones, decomposition of combustion chamber and interaction between zones.

Control-oriented models depend on ignition timing correlations, such as the steady-state models of Rausen et al. 2005 or Nikzadfar et al. 2015. Control-oriented model can be based also on simplified physical equation (Shahbakhti et al. 2006).
2010) and system identification approach to find the model parameter (Gregory M. Shaver et al. 2006; Bidarvatan et al. 2014).

The objective of the present study is to find an empirical equation that allows prediction of the combustion parameters using two inputs: ozone concentration and EGR rate. This static model has the advantage of running at real time. The paper is arranged as follows. Firstly, the 0D physical model is presented. It is based on Probability Density Function (PDF) and detailed chemistry approach to take into account temperature fluctuation within combustion chamber, ozone addition impact and the variation of species concentrations. Then, accuracy of the developed model will be demonstrated using comparison of in-cylinder and combustion parameters between simulated and experimental data. Finally, based on the extrapolation of results given by the 0D physical model a steady-state empirical equation will be found and evaluated.

2. Modelling approach

2.1 Model description

The present model focuses on the temperature fluctuations that have major role in HCCI combustion process. 0D modelling of a spatial phenomenon, in particular thermal stratification, is a real challenge; a solution is to use a statistical approach through a Probability Density Function (PDF). The combustion chamber is considered as one-zone model as shown in Figure 1. During compression, combustion and expansion, a thermal boundary layer will be created between hotter gases in the core of chamber and gases near wall due to heat losses through wall. The main physical phenomena are described via sub-model. The species law conservation is used to follow the evolution of the mass of every species presented in the detailed kinetic scheme. To evaluate the thermodynamic states (temperature, pressure) of the system, the first law of conservation of energy is used. And finally, to describe the turbulence phenomena during cycle, a 0D K-k model is used.

Figure 1: thermodynamic model of combustion chamber

2.2 General conservation equations

The first law of conservation of energy is applied to the closed one-zone thermodynamic model, with assumption that the pressure in the combustion chamber is spatially uniform and only function of time. It is assumed also the working of fluid is ideal gas. The energy balance indicates the fluid within control volume exchanges heat with the wall and delivers work to the piston:

\[ \frac{dv}{dt} = \frac{dw}{dt} + \frac{dQw}{dt}, \tag{1} \]

where \( \frac{dv}{dt} \) is the variation of the internal energy, \( \frac{dw}{dt} \) is work delivered to the piston and \( \frac{dQw}{dt} \) is the thermal heat losses.

The heat transfer to the cylinder walls is mainly due to convective heat transfer in HCCI engines. The radiation heat transfer in HCCI engines is negligible because of low soot and low temperature combustion (Ogink et al. 2004). So, the wall heat transfer is evaluated using well-known Woshni heat transfer correlation (Woschni et al. 1967), then, the convective heat transfer from mixture to combustion chamber wall can be calculated using:

\[ \frac{dQw}{dt} = q_w = h_w(T_w - T). \tag{2} \]

Finally, equation (2) can be combining with (1) and rearranged in order to evaluate the rate of change of the in-cylinder mixture temperature:

\[ \frac{dT}{dt} = -\frac{\sum_k y_k \Delta H_k}{c_p} \frac{d\bar{y}_k}{dt} + \frac{v d\bar{y}_k}{mc_p} \frac{dQw}{dt}. \tag{3} \]

Species mass fraction will be calculated based on convective-diffusion equations with assumption that total mass is constant. So, the individual species are produced or destroyed according to (4):

\[ \frac{dv_k}{dt} = v \bar{\omega}_k W_k, \tag{4} \]

where \( \bar{\omega}_k W_k \) are respectively the mean molar production rate and molecular weight of \( k \)th species, \( V \) is the instantaneous volume of the combustion chamber and \( V = V/m \) specific volume.

One of combustion models objective is to determine the mean of the production rate generated by the chemical reactions. The production rate depends on thermal stratification in combustion chamber. 0D modelling of a spatial phenomenon, in particular thermal stratification, is a real challenge; a solution is to use a statistical approach through a Probability Density Function (PDF). This approach consists to presume the temperature shape in the combustion chamber that evolves function of time. Then, the mean production/destruction rate of \( k \)th species is linked to the local production/destruction rate through the PDF:

\[ \bar{\omega}_k = \int_0^1 \bar{p}(\theta^*) \bar{\omega}_k d\theta^*, \tag{5} \]

with \( \bar{p}(\theta^*) \) : the probability density function and \( \theta^* \) the local normalized temperature.

CHEMKIN II tool package was selected to evaluate the local production/destruction rate of the \( k \)th species that is obtained from the kinetic theory. The detailed kinetic scheme used in this study is the PRF oxidation scheme issue from literature (Curran et al. 1998; Curran et al. 2002) and coupled with ozone sub-scheme used by the Halter et al. 2011 that is validated with methane/air/ozone flame velocity data for
equivalence ratios from 1 to 1.3, pressure equal to 1 Bar and temperature equal to 300 Kelvin. The resulting detailed scheme involved 1037 species and 4255 reactions, most of them being reversible.

2.3 In-cylinder thermal stratification: presumed Probability Density Function (PDF) approach

The presumed probability density function (PDF) is a statistical approach handled, in this study, to evaluate the auto-ignition during the cycle.

The presumed PDF should be numerically easy to implement and compute, should change the shape dependent on local conditions. The beta-PDF is chosen and written as follow:

$$
\tilde{p}(\theta^*) = \theta^{a+1}(1 - \theta^*)^{b-1} \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)^2} \quad (6)
$$

where:

- \(a = \theta^* \left( \frac{\theta^* - \theta^0}{\theta^0} \right) - 1 \),
- \(b = \frac{\theta^0}{\theta^0} - a \).

The normalized temperature is defined as follow:

$$
\theta^* = \frac{T - T_\text{ad}}{T_\text{ad} - T_\text{w}} \quad (7)
$$

where \(T\) is the mean temperature, \(T_\text{ad}\) is the adiatic combustion temperature and \(T_\text{w}\) is wall temperature.

Mean temperature \(T\), temperature variance \(\nu_T\), and the normalization temperature \(\theta^*\) conditions will make possible to completely determine the shape of the PDF at each calculation point. So, solving the equations for the mean value (obtained through the energy conservation law) and the variance is sufficient via PDF, to determine any statistical quantity whose local and instantaneous value is only a function of temperature, in particularly the production rate of any species.

The temperature variance should be determined from the enthalpy variance value, using the following equation:

$$
\nu_h = C_2^h(T)\nu_T \quad (8)
$$

It is indeed to develop an enthalpy variance equation in order to find the temperature variance. The enthalpy variance definition demonstrates that it depends on local enthalpy and following mean. So, it is necessary to have an equation for each component. The detailed approach which leads to the enthalpy variance will be shown in the later paragraph.

2.4 Enthalpy variance model

The purpose of this section is to propose a model for the variance equation in the global HCCI engine combustion chamber. The local enthalpy variance for homogeneous mixture is written as follow:

$$
\frac{\partial \nu_h}{\partial t} + \frac{\partial \nu_h u_i}{\partial x_i} = 2\left( \frac{\partial h}{\partial x_i} \right)^2 \frac{\mu_e}{\rho} - C_{dl} \nu_h u_i \frac{\varepsilon}{k} \quad (9)
$$

Where \(\mu_e\) and \(Pr_e\) are respectively turbulent viscosity and Turbulent Prandtl number. The coefficient \(C_0\) is the ratio of the turbulent integral scale to the thermal time scale. An analytical solution was developed (Donzis et al. 2005) to reproduce the behavior of \(C_0\) as a function of the turbulent Reynolds number \(Re_e\).

The first term on the left corresponds to production term of enthalpy variance while the second term corresponds to dissipation terms.

The production term is needed to be closed. This term is mainly dependent on heat transfer on the wall. Therefore, using the volume integral for the local enthalpy variance, the production term can be approximated as follow:

$$
\int \int_{V} \left( 2 \left( \frac{\partial h}{\partial x_i} \right)^2 \frac{\mu_e}{\rho} \right) dV \approx \int_{0}^{H} \int_{0}^{2\pi} \int_{R_{\delta}}^{R} \left[ 2 \left( \frac{\partial h}{\partial x_i} \right)^2 \frac{\mu_e}{\rho} \right] dV, \quad (10)
$$

where \(\delta\) is the boundary layer thickness.

A temperature profile formulation in the boundary layer is the key to solve the integration. Using Fourier law and benefit from quasi-steady assumption in the boundary layer (Monpean et al. 1994), the production term is closed. Finally, the differential equation of the enthalpy variance takes form:

$$
\frac{d\nu_h}{dt} = 2\pi \nu_h \left( \frac{C_{0h} \nu_h}{\lambda} \right)^2 \ln \left( \frac{R}{R_{\delta}} \right) - C_{dl} \nu_h \frac{\varepsilon}{k} \quad (11)
$$

The boundary layer thickness appears in the production term, and the ratio of viscous dissipation and turbulent kinetic energy appears in the dissipation term. According to (Fiveland et al. 2001) the boundary layer thickness is obtained first by writing the energy equation in terms of enthalpy and one-dimensional model, as follows:

$$
\frac{dC_p}{dt} = \left( \frac{g}{C_p} \right) \left[ \frac{\partial C_p}{\partial t} \right] + \frac{\partial \nu_h}{\partial t} \frac{\partial C_p}{\partial \nu_h} + \frac{\partial \nu_{h}^{2}}{\partial t} \frac{\partial C_p}{\partial \nu_{h}^{2}} + \frac{\partial \nu_{h}}{\partial t} \frac{\partial C_p}{\partial \nu_{h}} + \frac{\partial C_p}{\partial \nu_{h}} \frac{\partial \nu_{h}}{\partial t}.
$$

Concerning the turbulence model, it is based on zero-dimensional energy cascade applied during the compression and the expansion cycle (Agarwal et al. 1998):

$$
\frac{d\kappa}{dt} = -2\nu_t C_p \frac{K}{L^2} v_t.
$$

$$
\frac{dK}{dt} = -2\nu_t C_p \frac{K}{L^2} + 2 \left( \frac{K}{3} \right) \frac{\nu_t}{\varepsilon} - \frac{\varepsilon}{L},
$$

where \(v_t\) is the turbulent viscosity (universal); \(C_p\) is an adjustable constant fixed to 1 in this study and \(L\) is the representative geometric length scale.

3. EXPERIMENTAL VALIDATION

3.1 Experimental set-up

Experimental data was obtained from PSA DW10 engine modified to HCCI mono cylinder mode for research studies. The engine speed was 1500 rpm and the fuel-air equivalence ratio 0.3. Ozone was generated by an ANSEROS COM-AD-01 ozone generator. The experimental results showed that the ozone can improve the combustion of each operated point and move forward their phasing. The reader is referred to
(Pinazzi et al. 2015) for more details about experimental setup and experimental data. The basic engine specifications for current study are shown in Table 1. The fuel used was isooctane.

Table 1: Engine characteristics

| Engine type          | PSA DW10 |
|----------------------|----------|
| Displacement volume (cm³) | 499      |
| Bore (cm)            | 8.5      |
| Stroke (cm)          | 8.8      |
| Rod length (cm)      | 14.5     |
| Compression ratio    | 16:1     |

3.2 Comparison with experiment

Experimental results were obtained by varying the EGR rate and concentration of ozone in each experiment. The fuel used is isooctane.

Figure 2, 3, 4, and 5 show the in-cylinder pressure curve versus crank angle degree of the examined cases for both experimentally and numerically result for different ozone concentrations seeded in the intake of HCCI engine and EGR rate for air fuel ratio equal to 0.3. The shaded areas correspond to the lower and upper limits of variations over the 100 cycles recorded; the black curve corresponds to the simulated result. The number into the rectangle corresponds to the ozone concentration (in ppm) seeded in the intake of HCCI engine. The EGR is employed to dilute the mixture and is composed by only nitrogen. In fact, in real engine, the EGR fluid can be accompanied with an active thermal component, as CO and HC that have an effect on the phasing of the combustion. Therefore, to study the effect of ozone on HCCI combustion, it is necessary to use an inert composition of EGR. The simulated results show a good agreement with experimental data for each experiment.

Figure 2 and figure 3 show the in-cylinder curve for air-fuel equivalence ratio equal to 0.3 and EGR rate equal to 5% and 10% respectively with different concentration of ozone. As shown, the ozone seeded can improve the combustion and move forward the phasing of the combustion.

In the other hand, as shown in figure 2 and 3, the maximum in-cylinder pressure tends to decrease while adding an exceed of 5% of EGR rate without ozone and the crank-angle corresponding to in-cylinder maximum move little bit.

Figure 2: In-Cylinder pressure as function of crank angle degree and ozone concentration; \( \phi=0.3 \) and EGR=5%

Figure 3: In-Cylinder pressure as function of crank angle degree and ozone concentration; \( \phi=0.3 \) and EGR=10%

Figure 4: In-Cylinder pressure as function of crank angle degree and ozone concentration; \( \phi=0.3 \) and EGR=15%

Figure 5: In-Cylinder pressure as function of crank angle degree and ozone concentration; \( \phi=0.3 \) and EGR=20%

The in-cylinder maximum (74 bars) in figure 3 is higher than in-cylinder maximum (70 bars) in figure 4 without ozone seeded. But, adding 1 ppm of ozone with EGR rate equal to 15%, the in-cylinder pressure reaches same value (74 bars) of 10% of EGR and without ozone.

The in-cylinder maximum (70 bars) in figure 3 is higher than in-cylinder maximum (65 bars) in figure 4 without ozone seeded. But, adding 1 ppm of ozone with EGR rate equal to 20%, the in-cylinder pressure reaches same value (70 bars) of 15% of EGR and without ozone. Turning to corresponding angle of in-cylinder maximum, this angle moves backward while adding an exceed of 5% of EGR rate; in figure 4, it is
equal to 5.4 CAD, in figure 5, it is equal to 6.4 CAD; but adding 1 ppm for 20% EGR rate, the corresponding angle of in-cylinder maximum move forward about 2 CAD to reach same value (5 CAD) of 15% EGR rate and without ozone. As consequently, the ozone seeded raises the in-cylinder pressure and EGR rate decreases it. Also, the ozone seeded move forward the phasing of combustion and EGR rate move it backward.

In the other hand, the in-cylinder pressure curve can figure out the HCCI combustion processes. In figure 2, The pressure slope rises directly when combustion occurs, even without ozone addition; it seems to be knock combustion. So, the ozone addition seems to be useless in this case. By rising EGR rate by 5% to 10% and without ozone, as shown in figure 3, the pressure slope seems to be acceptable and combustion occurs in good conditions. Same tendency is shown in figure 4. The ozone addition is necessary to compensate the decreases of in-cylinder pressure in case of exceed of EGR rate. Figure 5 shows the cycle variability of combustion with 20% of EGR rate and without ozone; it seems to be a bad condition for combustion that is near misfire area. In this case, the ozone addition compensates the cycle variability and improves combustion. As consequently, the ozone addition is an important additive to the HCCI combustion in case of exceed of EGR rate in an operated point also, it can stabilize and contribute to reach set point. Finally, the ozone addition can be considered a chemical actuator to control the HCCI combustion.

Then, a comparison between experimentally and simulated combustion parameters is made in order to investigate the accuracy of the developed model to predict the combustion parameters. This comparison is done for equivalence air-fuel ratio equal to 0.3 and EGR rate equal to 20% with different ozone concentration. The error bars correspond to the lower and upper limits of variations over the 100 cycles recorded. The round points correspond to the simulated results.

Figure 6 shows a comparison between in-cylinder pressure maximum experiments and simulated. The absolute error is lower than 1 bar. The in-cylinder pressure maximum tends to increase while ozone concentration increases. Figure 7 shows a comparison between crank angle degrees correspond to in-cylinder pressure maximum experiments and simulated. The absolute error is lower than 2 CAD. The crank angle degrees correspond to in-cylinder pressure maximum tends to decrease while ozone concentration increases. Figure 7 shows a comparison between crank angle degrees correspond to 10% of the fuel had burned (CA10) experiments and simulated. The absolute error is lower than 2 CAD. The CA10 tends to decrease while ozone concentration increases. Figure 8 shows a comparison between crank angle degrees correspond to 50% of the fuel had burned (CA50) experiments and simulated. The absolute error is lower than 1 CAD. The CA50 tends to decrease while ozone concentration increases. Figure 9 shows a comparison between crank angle degrees correspond to 90% of the fuel had burned (CA90) experiments and simulated. The absolute error is lower than 1 CAD. The CA90 tends to decrease while ozone concentration increases.

4. STEADY-STATE IDENTIFICATION

The purpose of this section is to find mathematical equations that relate the static value of combustion parameters \( P_{\text{max}}, \) \( \text{CAD}_{\text{max}} \) and CA90 to ozone concentration and EGR rate. Based on simulated data gives by the 0D physical model obtain below and using curve fitting tool of MATLAB identification Toolbox, the equation that linked \( P_{\text{max}} \) to EGR rate and ozone concentration can be written as follow:

\[
P_{\text{max}} = 76.52 - 0.359[O_3]^2 + 2.684 [O_3]
\]
\[-4.394EGR_{rate} - 0.209[O_3]EGR_{rate}\]  \hspace{1cm} (13)

Figure 11 show good results for the equation of P\(_{\text{max}}\) function of ozone concentration and EGR rate. As shown in figure 12, the difference between the simulated data and the predicted value are less than 2 Bars. The coefficient of determination, R\(^2\), measures how successful the fit in explaining the variation of data. The R\(^2\) is equal to 0.9616. Noted that the value of adjusted R\(^2\) closer to 1 indicate a better fitting. Root Mean Square Error (RMSE) is obtained by squaring the residual, then averaging the square root. The RMSE is equal to 0.313. As shown in the below section, the ozone addition tends to increase the P\(_{\text{max}}\) and EGR rate tends to decrease it. According to equation (13), the impact of ozone concentration to the P\(_{\text{max}}\) is higher than the EGR rate but the interaction between ozone concentration and EGR rate exists. The equation of CAD\(_{\text{pmax}}\) is:

\[
\text{CADpmax} = 3.003 - 1.35[O_3] + 0.6239EGR_{rate} + 0.3867[O_3]^2 - 0.0672[O_3]EGR_{rate} + 0.181EGR_{rate}^2 \hspace{1cm} (14)
\]

As shown in figure 14, the residuals are less than 0.5 CAD. The R\(^2\) is equal to 0.9402. The adjusted R\(^2\) is equal to 0.313. As shown in the below section, the ozone addition tends to move forward the CAD\(_{\text{pmax}}\) and EGR rate tends to move backward it, also figure 13 shows same tendency. According to equation (14), the impact of EGR rate to the CAD\(_{\text{pmax}}\) is higher than the EGR rate but the interaction between ozone concentration and EGR rate exists.

The equation of CA\(_{50}\) is:

\[
\text{CA}_{50} = -1.175 - 0.90[O_3] + 1.11EGR_{rate} + 1.092[O_3]^2 - 1.47[O_3]EGR_{rate} + 0.61EGR_{rate}^2 - 0.82[O_3]^3 + 0.066[O_3]^2EGR_{rate} - 0.55[O_3]EGR_{rate}^2 + 0.34EGR_{rate}^3 - 0.077[O_3]^4 + 1.208[O_3]^3EGR_{rate} - 0.9998[O_3]^2EGR_{rate}^2 + 0.321[O_3]EGR_{rate}^3 \hspace{1cm} (15)
\]

As shown in figure 15, the residuals are less than 0.05CAD. The R\(^2\) is equal to 0.9999. The adjusted R\(^2\) is equal to 0.9984. The RMSE is equal to 0.0831. As shown in the below section, the ozone addition tends to move forward the CA\(_{50}\) and EGR rate tends to move backward it, also figure 13 shows same tendency. According to equation (15), the impact of ozone concentration to the CAD\(_{\text{pmax}}\) is higher than the EGR rate but the interaction between ozone concentration and EGR rate exists.

4. CONCLUSIONS

In this work, a comparison of in-cylinder pressure curve between simulated and experimentally result is done through 0D one zone HCCI combustion model. This comparison is
made for air fuel ratio equal to 0.3 with different EGR rate and ozone concentration. Then, a comparison between experimentally and simulated combustion parameters is done. The simulated results show a good agreement with experimental data for in-cylinder pressure and combustion parameters. Finally, mathematical equations for combustion parameters are found through simulated combustion parameters. Future work will be dedicated to use the developed model to predict combustion parameters over wide range of operating point, and then find a mathematical equation. This static model of combustion parameters could be used to develop a real time gain-scheduling control laws in order to control HCCI combustion by ozone addition.

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