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Dynamic Modeling of Combustion and Gas Exchange Processes for Controlled Auto-Ignition Engines

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Abstract

This paper is concerned with the development of a simple physical model of a gasoline engine cycle where the energy release is via Controlled Auto-Ignition. It uses simple thermodynamic concepts, and well-established gas exchange and heat transfer sub-models to predict the pressures and temperatures in the engine cycle. The combustion event itself is modelled in a semi-empirical fashion. The model is an important extension of existing single-zone models and it persists between multiple cycles, enabling the capture of the cycle-to-cycle exhaust gas coupling. The model was compared with data obtained at steady engine running conditions, and good agreement was found. Controlled Auto-Ignition was attained by diluting the mixture with exhaust gas trapped in the cylinder, as a result of an early Exhaust Valve Closing.

1. INTRODUCTION

Controlled Auto-Ignition (CAI), also known as Homogeneous Charge Compression Ignition (HCCI) has been receiving increased attention due to its potential to improve fuel economy and reduce emissions in gasoline internal combustion engines. The fuel economy results mainly from the fact that it can operate without throttling losses at part load. It is characterized by a flameless and fast combustion and, to avoid excessive rates of heat release, requires high levels of charge dilution. Ultra low Nitrogen Oxides (NOx) emissions result due to the low combustion temperatures and generally low CO emissions have been observed under lean CAI conditions, compared to SI [10]. There are several different strategies used to facilitate CAI combustion such as intake air heating, increased compression ratios and Exhaust Gas Recirculation [6]. All of these have the objective of creating, near firing TDC, conditions that will cause the mixture to spontaneously ignite.

Detailed computer models have been developed to simulate the chemistry and the gas exchange processes for CAI. These include multi-zone and stochastic models [11], [12]. Like any CAI model, their level of accuracy in predicting the combustion event is virtually entirely dependent on how well the chemistry can be modelled, and this is an area, especially for real fuels, of limited confidence. The large commercial packages for engine simulation have good simulations of the complex acoustic phenomena in the manifold systems which affect engine breathing, especially at high engine speeds, and for conventional IC engines have the benefit of being able to treat the burnt and unburnt mixture separately, but modeling heat transfer, for example is empirically based. As well as having the drawbacks indicated above, these complex models, of high order and long computational times are unsuitable for control design. Low-order control-oriented models that have been developed [2] yield reasonably accurate predictions of potential controlled variables such as cylinder pressure, work output and auto-ignition timing. They however lack detail in the gas exchange processes and they are single-cycle models.

The model described in this paper is a simple continuous-time, single-zone, physics-based model of the combustion chamber processes. It captures the effects of changes in valve timing, engine speed, fuel amount, and potentially intake air heating. It mainly consists of a simple chemistry equation, a single step reaction rate for predicting the onset of combustion, an energy balance equation and mass flow rate expressions for flows through orifices. Cylinder pressure, temperature, in-cylinder mass and species concentrations are computed every time step.

2. Model description

The model has been built in Matlab Simulink, which is a software widely used for real-time powertrain control in automotive research. The model consists of 5 mutually exclusive regions associated with the execution of different sets of equations. The region to be executed is determined based on whether any valves are open or combustion is taking place and the outputs of every region, which represent the same engine variable are fed to the same channel using carefully designed switches. The physical laws governing the in-cylinder dynamics in the different regions have significant similarities.

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Table 1. Model parameters

Parameter	Symbol	Value
Ex. disch. coef.	C_{De}	0.61
In. disch. coef.	C_{Di}	0.61
Wall Temperature	T_w	400 K
Ex. Man Pressure	P_e	$1.05 \cdot 10^5$ Pa
C atoms in fuel	n	8.26
H atoms in fuel	m	15.5
Fuel Lo. Heat. Val.	Q_{LHV}	44.0 MJ/kg
Comb. efficiency	n_f	0.95
Wiebe parameter	w_1	5.5
Wiebe parameter	w_2	2.4
Arrh. rate thres.	K_{th}	$1.357 \cdot 10^{-6}$
Arrh. rate param.	A	$7.2 \cdot 10^{12}\ (\frac{gmol}{cm^3})^{-0.8} s^{-1}$
Arrh. rate param.	E_a/R_u	20131 K
Arrh. rate param.	m_{ar}	0.25
Arrh. rate param.	n_{ar}	1.5

2.1. Mass flow rate equations

Variable valve actuation is currently the most attractive technology capable of providing sufficient thermal energy, by the means of residual gas, to trigger auto-ignition. The valve techniques employed for CAI can be divided into 2 main categories:

- The exhaust rebreathing strategy, where exhaust gas reenters the cylinder from one of the ports.
- The exhaust recompression strategy, where a significant fraction of the exhaust gas is trapped in the cylinder.

The valve profiles incorporated in the model are suitable for the exhaust gas recompression strategy. The exhaust valves close well before TDC, to trap exhaust gas and the inlet valves open well after TDC, to avoid significant backflow into the intake manifold. The absence of any valve overlap is called Negative Valve Overlap (NVO). It would be relatively easy, however, to replace the valve profiles with ones suitable for the exhaust gas rebreathing.

The mass flow rate into and out of the cylinder have been estimated using the flow rate expression for a steady, adiabatic and reversible flow, including a discharge coefficient C_D to represent the departure from ideality [7]. The generic form of the equation is

$$\frac{dm}{dt} = \frac{C_D A_R P_0}{(RT_0)^{\frac{1}{2}}} \left(\frac{P_T}{P_0}\right)^{\frac{1}{\gamma}} \left\{ \frac{2\gamma}{\gamma - 1} \left[1 - \left(\frac{P_T}{P_0}\right)^{\frac{(\gamma-1)}{\gamma}} \right] \right\}^{\frac{1}{2}} \tag{1}$$

if $[\frac{2}{\gamma+1}]^{\frac{\gamma}{\gamma-1}} \leq \frac{P_T}{P_0} \leq 1$, i.e. unchoked flow

$$\frac{dm}{dt} = \frac{C_D A_R P_0}{(RT_0)^{\frac{1}{2}}} \gamma^{\frac{1}{2}} \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} \tag{2}$$

if $\frac{P_T}{P_0} < [\frac{2}{\gamma+1}]^{\frac{\gamma}{\gamma-1}}$ i.e. choked flow where P_0 is the upstream stagnation pressure, T_0 is the upstream temperature, P_T is the downstream stagnation pressure, R the gas constant, γ is the specific heat capacity ratio and A_R is a valve reference area. The model allows for backflow, when the ratio $\frac{P_T}{P_0}$ is greater than 1. The pressures P_T and P_0 are interchanged and the difference in the thermodynamic properties of the flowing gas is taken into account. The reference area used in the model is the minimum valve area, calculated from the valve geometry [7]. The area is a function of the valve lift and the discharge coefficient is set constant. Manifold dynamics have not been included in the model, so intake and exhaust manifold pressures have been assumed to be constant.

2.2. Pressure and temperature calculations

The First Law of Thermodynamics applied to a control volume has been the key equation for estimating the rate of change of temperature. Neglecting kinetic and potential energy changes, this is

$$dQ - dW = dU + \sum dm_o h_o - \sum dm_i h_i \tag{3}$$

where Q is the heat transfer to the in-cylinder gas, W is the work done by the gas, U is the cylinder contents' internal energy, m denotes mass and h is the specific enthalpy. The subscripts "o" and "i" refer to the outgoing gas and the incoming air respectively. Using $dW = PdV$, $dU = mc_v dT$ and $Q = Q_{ch} - Q_{ht}$, where P is the cylinder pressure, V is the cylinder volume, T is the cylinder temperature, m is the in-cylinder mass, c_v is its specific heat capacity, Q_{ch} is the chemical energy released by the fuel, Q_{ht} is the heat transfer to the piston and walls, (3) becomes

$$\frac{dQ_{ch}}{dt} - \frac{dQ_{ht}}{dt} - \frac{PdV}{dt} = mc_v \frac{dT}{dt} + (h_o - c_v T)\frac{dm_o}{dt} + (c_v T - h_i)\frac{dm_i}{dt} \tag{4}$$

which is the general form of the equation used in all regions of the model. $\frac{dQ_{ch}}{dt}$ has a meaning only during combustion. Neglecting crevice effects, the second and third terms on the RHS of (4) become zero when all valves are shut. With the NVO strategy, the second and third terms on the RHS of (4) are zero during the intake and exhaust stroke respectively. The cylinder contents were assumed to behave as perfect gases in the temperature and pressure

ranges of CAI operation and the ideal gas law was used. The chamber volume V can be trivially calculated from the crank position and the engine geometry [7].

2.3. Prediction of Start of Combustion

The ignition timing in CAI is almost solely determined by the chemical kinetics in the cylinder. Even low-order chemistry mechanisms may include up to 100 species and 500 reactions [11]. The computational times required for detailed chemical-kinetics models are long. Given that the detailed chemistry for real fuels is unknown, simple semi-empirical techniques are used extensively. The simplest possible prediction of CAI combustion initiation is to assume that it occurs at a certain temperature level, since the exponential effect of temperature in the reaction rate is dominant.

Here, we use a slightly more complex model, where the temperature/time history, fuel and air effects are modelled [3]. Combustion is triggered when the Integral of an Arrhenius-type expression exceeds a constant threshold K_{th}. It occurs at the time $t = t_{soc}$, the time of Start Of Combustion, when

$$A \int_{t_{ivc}}^{t} Texp\left(-\frac{E_a}{R_u T}\right) [C_n H_m]^{m_{ar}} [O_2]^{n_{ar}} dt = K_{th} \qquad (5)$$

where t_{ivc} is the time of Inlet Valve Closing (IVC), $\frac{E_a}{R_u}$ is the fuel activation temperature. The constants m_{ar}, n_{ar} and $\frac{E_a}{R_u}$ for pure hydrocarbons are tabulated in [8]. The values for iso-octane were chosen. An estimate for K_{th} was found using a least squares approach from CAI data with different fuel rates and speeds.

2.4. Heat release and heat loss models

The heat release rate $\frac{dQ_{ch}}{dt}$ during combustion was modelled using the simple equation

$$\frac{dQ_{ch}}{dt} = M_f Q_{LHV} n_f \frac{dx_b}{dt} \qquad (6)$$

where M_f is the fuel mass in the cylinder before the start of combustion, Q_{LHV} is the lower heating value of the fuel, n_f is the combustion efficiency and x_b is the mass fraction burnt profile. Values for Q_{LHV} are tabulated both for practical fuels and for pure hydrocarbons [7]. The combustion efficiency has been set to 0.95, the lowest value suggested for SI engines [7], as the crevice effects, which similarly affect the rate of change of temperature, have been neglected. The mass fraction burnt profile, x_b, was modelled as a function of the crank angle θ, by the widely used Wiebe function

$$x_b = 1 - \exp\left[-w_1 \left(\frac{\theta - \theta_0}{\Delta\theta}\right)^{w_2+1}\right] \qquad (7)$$

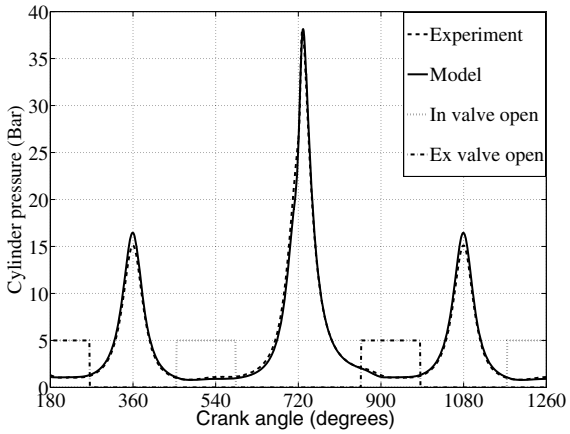

Figure 1. Comparison of modelled cylinder pressure with real averaged cylinder pressure at 2000RPM, 2.6 Bar BMEP.

where θ_0 is the angle of start of combustion and $\Delta\theta$ is the combustion duration. w_1 and w_2 are adjustable parameters which have been set by matching the modelled profile with the profile obtained from heat release analysis on real data. The parameters were estimated based on a single comparison making use of the Rassweiler Withrow method [7]. The heat transfer to the cylinder walls and the piston crown surface is assumed to be purely by convection given by

$$\frac{dQ_{ht}}{dt} = h_c A (T - T_w) \qquad (8)$$

where A is the surface area, varying with the piston position, T_w is the wall temperature and h_c is the heat convection coefficient given by the Woschni model [4].

2.5. Combustion chemistry

Only main combustion products and reactants have been included in this calculation. If intermediate products were to be included, the model would become slow and inappropriate for the purposes it was designed for. Further, it has been demonstrated that the cylinder pressure and ignition timing are captured reasonably well with chemistry of low level of complexity [1]. The chemistry equation used for lean combustion is

$$k_1 C_n H_m + k_2 O_2 + k_3 N_2 + k_4 CO_2 + k_5 H_2O \rightarrow k_3 N_2 + [k_2 - k_1(n + \frac{m}{4})]O_2 + (k_4 + nk_1)CO_2 + (k_5 + \frac{m}{2}k_1)H_2O \qquad (9)$$

where each coefficient on the LHS of the reaction is the number of mols of the corresponding compound at Inlet

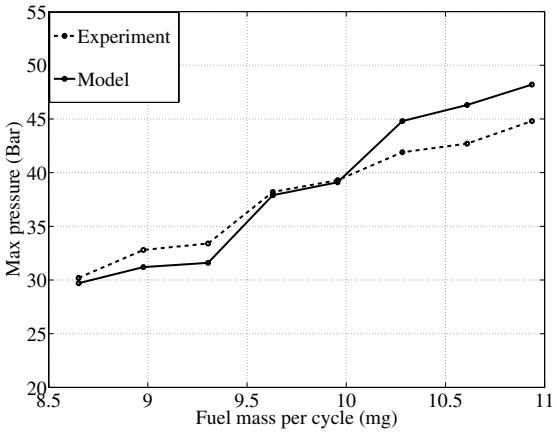

Figure 2. Maximum cylinder pressure comparison with different fuel amounts in steady state CAI.

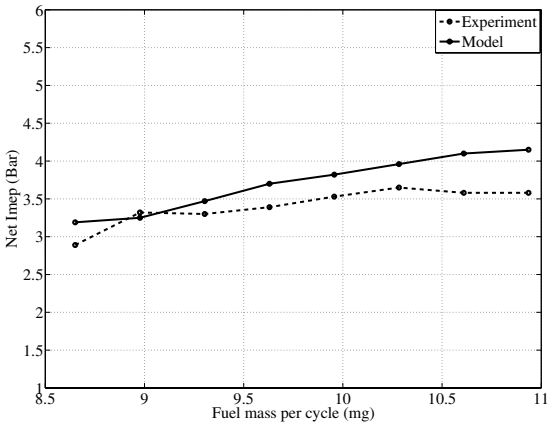

Figure 3. Net IMEP comparison with different fuel amounts in steady state CAI.

Valve Closing (IVC) and each coefficient on the RHS is the number of mols at the end of combustion. The chemistry equation is more general than equations widely used for lean combustion [7]. It allows dynamic calculation of cylinder species' concentrations due to AFR and RGF changes during transient operation. An equation for a rich combustion is also incorporated in the model and is activated if $\frac{k_2}{k_1} < n + \frac{m}{4}$. Even though lean combustion has been the target in steady state CAI operation, the inclusion of rich combustion in the model is important for transient operation.

2.6. Gas properties

Cylinder contents' specific heat capacities , c_p and c_v, their ratio γ and their difference R are used in different parts of the model. Each of the above is calculated as the weighted average of the individual species ones, based on their molar fractions. Their temperature dependence was taken into account using look-up tables built from JANAF data [9].

3. Experimental set-up

A Ford 2.0L I4 16 valve engine coupled to a dynamometer via a pneumatic actuator has been used to parameterize and validate the model. The engine speed is controlled by the hardware dynamometer controller and a torque output reading is given by the dyno load cell. The engine was run with gasoline of 95 Research Octane Number. Variable Cam Timing was controlled in a feedback configuration remotely. 4 Kistler 6123 piezoelectric transducers in combination with AVL charge amplifiers facilitated individual cylinder pressure monitoring and recording. An optical encoder provided a pulse every degree of crank revolution, triggering ADC cards for high-frequency data recording. A Horiba Universal Exhaust Gas Oxygen (UEGO) sensor attached to the exhaust tailpipe has been used to track the AFR. Thermocouples attached to the intake and exhaust ports provided temperature readings. Precise measurement of the fuel flow rate was obtained from a coriolis flow meter.

Table 2. Engine settings at the CAI operating point about which model validation was performed.

Parameter	Value	Units
Speed	2000	RPM
Throttle opening	100	%
Ex. Val. Closing angle	275	deg
In. Val. Opening angle	455	deg
Start Of Injection	390	deg
Spark angle	680	deg
Fuel rate	2.34	kgh^{-1}

4. Model validation

The model was calibrated at a single CAI operating point and all the parameters except combustion duration were left unchanged for model comparison with experimental data. The combustion duration was found from thermodynamic analysis of pressure signals and is input to the model. A quantity used to represent the engine work output is the Net Indicated Mean Effective Pressure (Net IMEP),

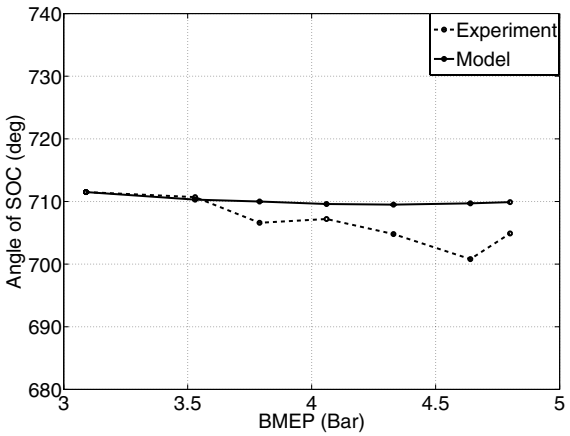

Figure 4. Comparison of angle of Start Of Combustion at different loads in steady state CAI, Speed=2000 RPM.

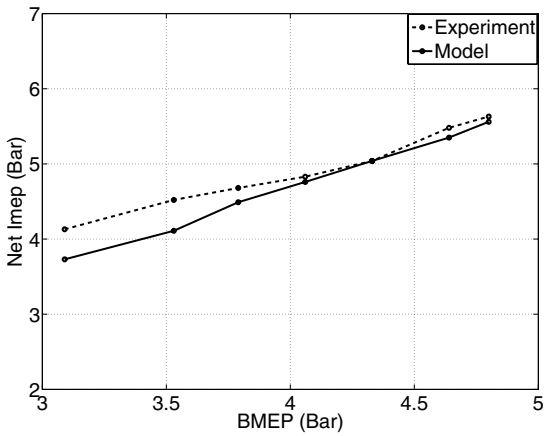

Figure 5. Net IMEP comparison at different loads in steady state CAI, Speed=2000 RPM.

which is independent of the engine size. It is defined as,

$$(IMEP)_{net} = \frac{\oint PdV}{V_d} \tag{10}$$

over the entire cycle, where V_d is the displaced volume. The useful work delivered can be characterised via the Brake Mean Effective Pressure (BMEP), defined as

$$BMEP = \frac{2\pi n_r T_r}{V_d} \tag{11}$$

where T_r is the engine torque and n_r is the number of strokes per revolution. The angle of Start Of Combustion (SOC), θ_0, is represented by the crank angle at which 1% of the fuel has been burnt. The model was validated by comparing the average cylinder pressure, the Net IMEP over 80 cycles of steady state CAI operation to the outputs of the model when the transients due to the initial conditions died away. The engine was run at the nominal operating point of 2000RPM, 2.6 Bar BMEP, with the engine settings shown on Table 2. Fig. 1 shows a pressure trace comparison at these conditions. The model shows slightly higher pressure in the NVO, which might be because of the simplifying assumption of a constant exhaust manifold pressure for all operating conditions. Note that the kink in the real pressure trace indicating the start of combustion has been smoothed by the averaging.

The fuel amount was varied while the rest of the settings were unchanged. The range was limited by knocking combustion at high fuel rates and misfiring due to very low exhaust gas temperatures at low fuel rates. Reasonably good agreement in the maximum cylinder pressure has been observed (Fig. 2) as well as the Net IMEP (Fig. 3).

In another set of validation experiments, the experimental and modelled Net IMEP and θ_0 were compared as the load was varied at 2000 RPM, in steady state operation (Figs. 4, 5). An increase in the load is achieved by increasing the fuel rate. For stable CAI, this change has to be accompanied by retarding the exhaust valve closing angle (EVC) and essentially reducing the amount of exhaust gas trapped. The Inlet Valve Opening angle was set symmetric to EVC, about TDC. The rest of the engine settings are as in Table 2. The model's angle of SOC shows reasonably good agreement with experimental data but without strictly following the real trend. Increasing BMEP is achieved by increasing fuel rate and reducing Residual Gas Fraction. These are two competing effects for the gas temperature when valves are shut, which is the critical parameter in driving the Arrhenius integral beyond the pre-set threshold. Some imprecision in the temperature calculation, most probably due to the heat transfer model, causes this slight deviation.

5. Model functions

The main model outputs are the cylinder pressure and temperature, the in-cylinder mass and the species concentrations. Variables that are widely used in automotive research, to characterise the engine's operating point, such as the AFR, the RGF and the Net Imep, can be derived from the above. Furthermore, there is access to all the parameters in the combustion and gas exchange processes.

Fig. 6 presents the CO_2 molar fraction variation in similar conditions. The small dip in the NVO is due to the fuel injection and the two peaks in the intake stroke are due to the simplifying assumption that air flows both during for-

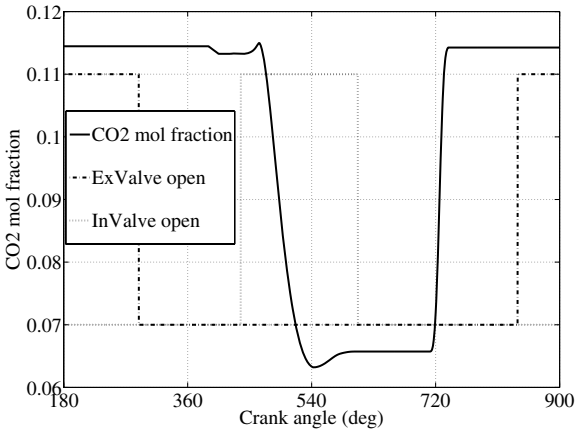

Figure 6. CO_2 mol fraction in steady state.

ward and reverse flow. The RGF level, by mass, can be estimated to be 57.4% using,

$$RGF = \frac{(\tilde{\chi}_{CO_2})_{Com}}{(\tilde{\chi}_{CO_2})_{NVO}} \tag{12}$$

where $(\tilde{\chi}_{CO_2})_{Com}$ and $(\tilde{\chi}_{CO_2})_{NVO}$ are the CO_2 mol fractions during compression and NVO respectively.

6. Conclusions

A non-linear low-order model of variable valve actuated CAI combustion has been built and validated in steady state. Potential controlled variables, such as the work output and the combustion phasing show reasonably good agreement with experimental values. The inclusion of the gas exchange processes in the core of the model allows it to run continuously by switching between the different regimes of the cycle. It is based on the in-cylinder dynamics and assumes constant manifold pressures. Other main simplifying assumptions are: Constant mol fractions of gas constituents during the gas exchange processes, heat transfer to the cylinder walls only by convection, no account for the fuel heat of vaporization, only main combustion products and reactants present in the cylinder.

Even though all the main processes have been modelled at a basic level compared to the complexity involved in them in reality, the right trends have been observed. The model can give a useful insight on how the processes and model parameters affect the engine performance variables and it has the potential to serve as a model for control, if its structure is simplified slightly. On the other hand, it is versatile and flexible. If the level of accuracy is to be increased, adding terms in the existing equations is straightforward. Engine geometry, valve geometry and profiles can easily change and intake air heating investigations are possible.

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