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Mechanistic Modelling Approach to HCCI Combustion

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Abstract: ***Homogeneous Charge Compression Ignition (HCCI) has become a promising alternative combustion method over conventional methods of Spark ignition (SI) or Compression Ignition (CI). HCCI combines the advantages of SI method (homogeneous charge) and CI method (compression ignition). It has also been proven by every researcher that there is almost 95 per cent reduction in NOx emissions with HCCI combustion, and other emissions such as CO2 and HC are comparable to SI engine, which can be reduced using after treatment systems. However, it presents a challenge with respect to controlling sensitive parameters that have profound effect on the outcome. As with SI and CI engine, there is no definitive start of combustion event, which can be controlled independently. In HCCI combustion, air fuel mixture is ignited spontaneously throughout the cylinder and this event is governed by chemical kinematics. Therefore, it is important to understand the inherent chemical reaction process and its effect on pressure and temperature within the cylinder. Through mechanistic modelling, the combustion process can be simulated and the relationships between input and output quantities can be examined. For this research paper, a zero dimensional single zone model has been created to model the effects of EGR % on Heat Release Rate (HRR).***

Keywords: HCCI, Mechanistic Modelling, HRR, EGR, Autoignition, MBF, Wiebe Function

1. Introduction

With increasing awareness and understanding of the impact of vehicle exhaust emissions on environment, combined with the shortage of fossil fuels and increasing cost has provided an impetus to experts to radically improve the current combustion methods used to extract energy from fuel. Majority of engines can be classified into SI or CI, based on fuel used, combustion method, working cycle and chemical kinematics. In SI engine, the air fuel mixture is mixed prior to injecting into the port or directly into the cylinder in case of GDI engines, whereas in CI engine, only fuel is injected into the cylinder. Moreover, as the name suggests, fresh charge in SI engine is ignited with the help of a spark at precise time in every cycle. In CI engine, the air is compressed, which raises the temperature inside the cylinder to the point at which the fuel, when injected will auto ignite. However, in real life, there is a delay in ignition from the point of injection to the point of ignition. The common phenomenon between SI and CI engine is the concept of flame front that is initiated where reactant mixture is rich and travels towards unburned mixture.

It has been observed that in HCCI combustion, there is no prominent flame front and reactant mixture gets ignited spontaneously [2]. Therefore, the burn duration in HCCI mode is less than SI or CI combustion. As a result, the peak temperature reached during the combustion period is less than SI or CI engine resulting in reduction of emission molecules, driven solely by temperature, i.e. NOx.

HCCI is basically autoignition of homogeneous reactant, albeit in a controlled way. The major challenge in HCCI engine is to control this autoignition process in a way that constancy is achieved from cycle to cycle, and behaves steadily during transient stage, i.e. when engine speed is reduced or increased. Due to inherent design of the internal combustion engine, it operates at its highest efficient point at full load. At part load, the efficiency gets reduced due to increase in pumping work. Several new technologies such as variable valve technology, EGR, stratification have enabled to the engine to run lean and therefore use less fuel. However, if the mixture becomes too lean misfire will happen, and also catalytic converters are designed to program at full efficiency only near equivalence ratio equal to 1.

As seen from the above discussion, internal combustion engine is a very complex system and there is always a trade-off among several desirable outcomes. It is important to understand how every parameter affects the final outcome, as well as each other. Normally experiments are setup in a way that one unique parameter is focused upon and modulated to study its effect whilst keeping values of other parameters as constant. However, in real life it is difficult and expensive to prepare such experiments, setup of which is again not flexible so as to do quick changeover for evaluation of other parameters. Hence, mechanistic modelling is used to model the physical and chemical process as close to reality as possible, by using simulation tools and powerful processors. Simulation tools allow scientists and engineers to create a model, which in turn enables them to gain an insight into the chemical and physical kinematics. This research paper documents the mechanistic modelling approach vis-à-vis HCCI combustion by presenting inter-dependencies of various parameters, based on principles of thermodynamics and conservation of energy.

2. Modelling Approach

As mentioned earlier, internal combustion engine is a very complex system, and therefore it is fairly difficult to create a combustion model that is simple yet complete. The modelling approach has been to first create a simple model based on first principles, and then gradually add various submodels into the mix, thereby increasing the accuracy. Through previous researches conducted in HCCI, it is known that heat addition in HCCI occurs at constant volume [1]. Therefore, the HCCI combustion cycle can be modelled on Otto cycle.

3. Starting Parameters

The starting parameters are the basic values needed to create a simulation structure. In order to maintain simplicity, the simulation structure is first made in Microsoft Excel spreadsheet. Following table shows initial parameters, along with their values in SI units –

Table 1: Engine Geometry Details

Engine Geometry (single cylinder)					
Displaced volume	Vd	250149.315	mm3	0.000250149	m3
Bore	b	70	mm	0.070	m
Stroke	s	65	mm	0.065	m
Compression Ratio	Rc	9	m3/m3		
Clearance Volume	Vc	27794.36834	mm3	2.77944E-05	m3
Connecting rod length	l	150	mm	0.15	m
Engine Speed	N	1500	rpm		
No of cylinders	n	1			
No of power stroke per cycle	sp	1			

The engine geometry parameters define the physical size of the system to be modelled. Values of bore and stroke are assumed based on standard production engines. Compression ratio is assumed to be as per Otto cycle, which can be further modulated to study the effects of compression ratio on final outcome. Displaced volume is the total volume that can be filled by air fuel mixture. It is calculated from bore and stroke as per below –

$$Vd = \frac{\pi b^2 s}{4} \qquad \text{Eq.1}$$

Clearance volume is the instantaneous volume in the cylinder when piston is at Top Dead Centre (TDC). Combustion process happens within clearance volume after which due to rapid increase in temperature and pressure, piston is pushed downward, i.e. mechanical work done by the system.

Table 2: Constants (Ideal Gs)

Constants (Ideal Gas)					
Gas constant	Ra	0.2871	kJ/Kg K	287.1	J/Kg K
Ratio of specific heat capacities	Y	1.40			
Specific heat at constant pressure	Cp	1.005	KJ/Kg K	1005	J/Kg K
Specific heat at constant volume	Cv	0.718	KJ/Kg K	718	J/Kg K
Ambient Pressure	Pa	100	kPa	100,000	Pa
Ambient Temperature	Ta	27	deg C	300	K

The above table shows values of constants that are frequently used in the calculation. The ambient, i.e. atmospheric temperature and pressure are assumed to be 1 bar and 300 K. For the purpose of simplicity the fresh charge of air and fuel mixture is assumed to be having same properties as ideal gas. Hence, gas constant and specific heat at constant pressure and constant volume of reactant is same as air. The ratio of specific heat capacities (γ) is a dimensionless quantity, known as the isentropic expansion factor.

$$\gamma = \frac{Cp}{Cv} \qquad \text{Eq. 2}$$

Table 3: Air & Fuel Properties

Air & Fuel Properties					
Lower heating value of fuel	Q_{LHV}	44000	kJ/Kg	44,000,000	J/Kg
Stoichiometric air to fuel ratio	AFRs	14.7	Kg/Kg		
Equivalence Ratio	ϕ	1			
Self ignition temperature	Tsig	285	deg C	558	K
mass of reactant	mr	0.000290432	Kg		
mass of ar	ma	0.000270675	Kg		
mass of fuel	mf	1.97573E-05	Kg		

The lower heating value of fuel is an indication of the energy stored in the fuel, which is extracted by combusting the fuel air mixture under high pressure. Every fuel has a characteristic stoichiometric air to fuel ratio (AFR), i.e. number of moles of air required to enable combustion to happen under standard temperature and pressure (STP) conditions for 1 mole of fuel. For practical purposes, the ratio is taken in terms of mass (Kg/Kg). Equivalence ratio (ϖ) is the ratio of Actual AFR to stoichiometric AFR. In real life, equivalence ratio is always more than 1 so as to ensure complete combustion of fuel [1]. Self ignition temperature is the temperature at which fuel gets ignited without any external spark. At self ignition temperature, the kinetic energy of molecules is high enough to collide with molecules of air and initiate combustion. Mass of reactant, i.e. fresh charge inside the cylinder is calculated from standard gas equation –

$$PV = mRT \qquad \text{Eq. 3}$$

By rearranging terms in Eq. 3, expression for mass is obtained as per below -

$$m = \frac{PV}{RT} \qquad \text{Eq. 4}$$

Values of pressure and temperature are taken at ambient point, as mentioned in Table 2.
From AFR, mass of air and mass of fuel present in the cylinder at the time of Inlet Valve Closing (IVC) are evaluated.

4. Combustion Cycle

As mentioned earlier, in HCCI heat addition occurs at constant volume, and therefore for HCCI combustion the ideal cycle would be Otto cycle. For Otto cycles following assumptions are made:

- The engine operates in a closed loop
- The working fluid is air
- The air behaves as an ideal gas
- All processes are reversible
- The combustion process can be replaced by an external heat source
- The exhaust process can be replaced by a heat rejection process

4.1. Properties at the state points in the cycle

4.1.1. State

Taking the starting point for the cycle as the start of the compression process then from the inlet conditions:

$$p_1 = p_{in}$$

$$T_1 = T_{in}$$

Assuming that the gas behaves as an ideal gas:

$$v_1 = \frac{RT_1}{p_1} \quad \text{Eq. 5}$$

The mass in the cylinder is given by:

$$m = \frac{V_1}{v_1} \quad \text{Eq. 6}$$

4.1.2. State 2

From the definition of the compression ratio

$$r = \frac{v_1}{v_2} = \frac{V_1}{V_2} \quad \text{Eq. 7}$$

$$v_2 = \frac{v_1}{r}$$

Since the process from 1 to 2 is an isentropic (reversible and adiabatic) compression process then:

$$p_2 v_2^{\gamma} = p_1 v_1^{\gamma} \quad \text{Eq. 8}$$

$$p_2 = p_1 \left(\frac{v_1}{v_2}\right)^{\gamma} = p_1 r^{\gamma}$$

Thus the temperature can be found:

$$p_2 v_2^{\gamma} = p_1 v_1^{\gamma} \quad \text{Eq. 9}$$

$$\left(\frac{RT_2}{v_2}\right) v_2^{\gamma} = \left(\frac{RT_1}{v_1}\right) v_1^{\gamma}$$

$$T_2 = T_1 \left(\frac{v_1}{v_2}\right)^{\gamma-1} = T_1 r^{\gamma-1}$$

4.1.3. State 3

The process from 2 to 3 is a constant volume heat addition process, thus:

$$v_3 = v_2 = \frac{v_1}{r}$$

Applying the first law and noting that no work is done during this process:

$$q_{23} - w_{23} = (u_3 - u_2)$$

$$q_{23} = c_v (T_3 - T_2) \quad \text{Eq. 10}$$

$$T_3 = T_2 + \frac{q_{23}}{c_v} = T_1 r^{\gamma-1} + \frac{q_{23}}{c_v}$$

Then assuming that the gas behaves as an ideal gas:

$$p_3 = \frac{RT_3}{v_3} = \frac{rRT_3}{v_1} = r\frac{p_1 RT_3}{RT_1} = p_1 \left(r^{\gamma} + \frac{r q_{23}}{c_v T_1}\right) \quad \text{Eq. 11}$$

4.1.4. State 4

At state 4 the piston has returned to its initial position thus:

$$v_4 = v_1$$

The process from 3 to 4 is an isentropic (reversible and adiabatic) expansion process thus:

$$p_4 v_4^{\gamma} = p_3 v_3^{\gamma}$$

$$p_4 = p_3 \left(\frac{v_3}{v_4}\right)^{\gamma} = p_3 \left(\frac{1}{r}\right)^{\gamma} = p_3 r^{-\gamma} = p_1 \left(1 + \frac{r^{1-\gamma} q_{23}}{c_v T_1}\right) \quad \text{Eq. 12}$$

Thus the temperature can be found:

$$p_4 v_4^{\gamma} = p_3 v_3^{\gamma}$$

$$\left(\frac{RT_4}{v_4}\right) v_4^{\gamma} = \left(\frac{RT_3}{v_3}\right) v_3^{\gamma} \quad \text{Eq. 13}$$

$$T_4 = T_3 \left(\frac{v_3}{v_4}\right)^{\gamma-1} = T_3 r^{1-\gamma} = T_1 + \frac{r^{1-\gamma} q_{23}}{c_v}$$

5. Fixed Cycle Points

In HCCI combustion, there is no direct way to initiate combustion; hence it is important to establish the controlling parameter that can be explicitly monitored and a closed loop control system can be designed around the controlling parameter. Now, for an internal combustion engine, it is desirable to have peak pressure after Top Dead Centre (ATDC) to avoid waste of energy in pushing against the direction of piston travel. As per previous research, peak pressure normally happens between 10 CAD to 30 CAD ATDC [1]. Therefore, the crank angle degree (CAD) at which peak pressure is achieved is first fixed to be within the above mentioned range. Therefore, every cycle input parameters have to be modulated in order to maintain cycle to cycle consistency with respect to peak pressure, and as a result mean effective pressure (mep), torque and power values are also consistent.

Also, peak pressure is obtained when combustion process is 90 % over [2], therefore the peak pressure point and 90 % combustion completion CAD should be within 5 to 10 CAD of each other. The burn duration is the time of combustion reaction, i.e. from start of combustion (SOC) to end of combustion (EOC). To model burn duration, Wiebe Function is used –

$$MFB(\theta) = 1 - \exp\left[-a\left(\frac{\theta - \theta_0}{\Delta\theta}\right)^{m+1}\right] \quad \text{Eq. 14}$$

[3]

MFB (θ) = Mass Fraction Burned at corresponding CAD (θ)
θ = corresponding CAD
θ_0 = CAD corresponding to SOC
$\Delta\theta$ = CAD corresponding to burn duration
m = constant (typical value = 3)
a = constant (typical value = 5)

The values of MFB will be within the range from 0 to 1. A sample of Wiebe Function curve is shown below –

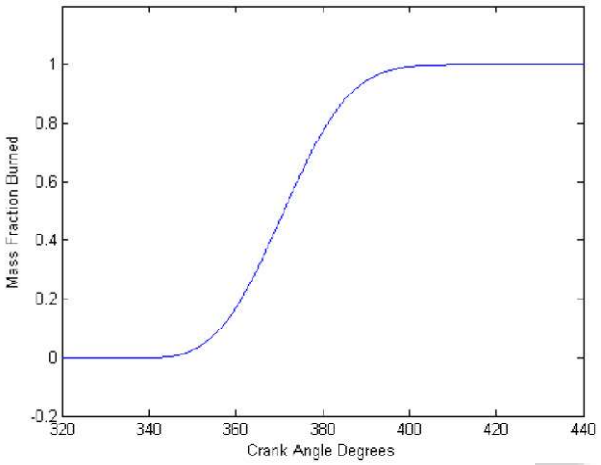

Figure 1: Sample Wiebe Function Curve [3]

6. Inter Dependencies

While modelling any form of combustion it is important to note how different parameters are affecting each other. For example, during combustion phase in internal combustion engine, temperature increases due to progress of chemical reaction. As chemical reaction progress, fuel energy is released in the form of heat, due to which temperature increases rapidly. As a result, chemical reaction rate increases. Thus, temperature and chemical reaction rate are interdependent parameters. Similarly with increase in temperature, pressure also increases, which in turn contributes to increase in temperature.

For HCCI combustion to happen in a production engine, the most suitable technique is to use EGR with negative valve overlap (NVO) [4]. EGR makes the overall mixture more dilute and raises the temperature of reactant mixture. Due to this, the specific heat of mixture at the time of IVC is higher than SI or CI combustion. Now to achieve SOC point in every cycle within $\pm$ 5 CAD of fixed SOC point, temperature of mixture, i.e. fresh charge + EGR at IVC has to be monitored. By varying EGR %, temperature at IVC can be maintained within a set tolerance. Again by varying NVO duration, EGR % can be increased or decreased depending on previous cycle. It would be difficult to enable such control on a physical engine using conventional variable valve technology (VVT) of cam changing or cam phasing [5]. This calls for electromechanical control of valves opening and closing, which can be modelled on a simulation platform to further enhance the practicality of such system.

7. Conclusion

HCCI combustion is a promising alternative to conventional SI and CI combustion as there is significant reduction of NOx emissions and increased power output. However, as in SI or CI combustion, there is no direct event to initiate combustion because reactant mixture spontaneously ignites when sufficient temperature and pressure conditions are reached. Therefore, several parameters have to be monitored together to make HCCI combustion work in a physical engine with consistent output cycle by cycle. This requires deeper analysis of chemical and physical kinematics. Through mechanistic modelling it is possible to further understand the correlation between various parameters and output.

8. Scope For Further Research

There is an upper limit in terms of engine speed for HCCI combustion, after which detonation starts occurring, which is harmful for the engine. The major factor contributing to detonation is the temperature and pressure inside the cylinder, i.e. if HRR exceeds certain value, the flame speed will travel faster than the speed of sound and result in generation of shock wave. To prevent this generation of shock wave, practical HCCI engines have a limit of around 4000 rpm. There are several ways to approach the solution to this problem, wherein lies scope for further research. One way is to model pressure rise rate (PRR) in terms of HRR and establish relationship between HRR and PRR at various mixture strengths and engine speeds. The other way is to study the process of deflagration to detonation and try to model the reverse process. Also, flame velocity, i.e. laminar and turbulent can further be studied to understand their effects on physical and chemical process.

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