International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.9, No.07 pp 587-595, 2016

Simulation analysis of hydrogen fuelled homogeneous charge compression ignition (HCCI) engine

Chaitanya Jakati, Aditya Patil, Amol Kulkarni and M. Mohamed Ibrahim*

Department of Automotive Engineering, School of Mechanical Engineering, Vellore Institute of Technology, VIT University, Vellore - 632014, Tamil Nadu, India.

Abstract : A single-zone zero dimensional model was developed to study the effect of intake charge temperature (ICT) and equivalence ratio on start of combustion (SOC) of homogeneous charge compression ignition engine, which used hydrogen as a fuel. Considering that when 99.99% of hydrogen is burned then it is said to be auto ignited the intake charge temperature range was chosen from 360-400K. For this range of temperature the equivalence ratio was varied from 0.1-1.0, and the results were plotted. It was observed from the results that there was no ignition at ICT of 361 K at equivalence ratio of 1 but the combustion initiated when the ICT was increased by 1K. It was seen from the results that as ICT increases, the combustion advances well before top dead centre (TDC) but the indicated mean effective pressure (IMEP) is reduced due to lesser utilization of heat from the fuel. The SOC combustion did not varied significantly at different equivalence ratios. Thus the SOC of combustion was more sensitive to the ICT as compared to the equivalence ratio. A single-zone model helps to predict this auto ignition point, although the estimated peak and mean effective pressures are over estimated by this model because of the assumptions of total homogeneity of the inducted charge.
Keywords: Homogeneous charge compression ignition (HCCI), single zone zero dimension, chemical kinetics, intake charge temperature, equivalence ratio, alternate fuels and emissions.

1. Introduction

It's been over a century since the birth of an internal combustion (IC) engine. Over these years it has undergone a lot of changes, from noisy inefficient machines to quiet and high power density prime movers. They have been catering the power requirements in various fields, but with stringent emission norms and decrease in availability of fossil fuel, the survival of conventional spark ignition (SI) and compression ignition (CI) engines is questionable by the end of 21^{st} century. This has led to various alternate combustion process adaptations with non-conventional fuels, one such approach is using hydrogen in homogeneous charge compression ignition (HCCI) mode of combustion.

The HCCI engine embodies benefits of both SI and CI engines. HCCI engines operate on well mixed charge which reduces the particulate matter (PM) emission. Also the auto ignition of air fuel mixture results in better efficiency, reducing throttling losses. White et al.[1] presented a comprehensive review of recent developments on hydrogen as a fuel in internal combustion engines where they found that these engines consume 15 to 20 percent less fuel. The use of hydrogen in HCCI engine neglects the carbon emission such as carbon monoxide (CO), carbon dioxide (CO_2) and soot formation. Unlike CI engines, HCCI engine uses low pressure fuel injection system which reduces the cost of an engine significantly[2].

The origin of this concept can be dated back to 1970's; it was then termed as Active thermo-atmosphere combustion (ATAC) by Onishi et al. At that time two-stroke engines faced problem of abnormal combustion at part throttle. HCCI (then called as ATAC) achieved stable combustion with lean mixtures at part throttle conditions. It was also found that there was significant reduction in fuel consumption, exhaust emissions and vibration of the two stroke gasoline fuelled engines[3].

HCCI in four stroke engine was studied by Thring[4] and permissible range for operating parameters was obtained for HCCI operation. It was found that with high EGR and higher intake charge temperatures the fuel economy of the HCCI mode was comparable with the same capacity CI engine. Effect of various operating parameters on performance of HCCI was earlier studied by Najt and Foster[5] on a single cylinder four stroke cycle. The study indicated that with increase in compression ratio the intake charge temperature required for the ignition reduced, but at the same time the energy release rates were more violent.

Though having many advantages, the use of HCCI was limited due to challenges like narrow operating range and high concentrations of CO and un-burnt hydrocarbon (UHC) emissions. These challenges are directly related to the kind of fuel used. Higher octane number gasoline fuels require more preheating of the charge, which lowers the volumetric efficiency and the power density. Whereas lower the octane number gasoline fuels lead to knocking, thus limiting the operating ranges. The diesel fuel shows a reverse trend, also it is difficult to form homogeneous mixture of the premixed charge due to less volatility of diesel. Due to difficulties involved in gasoline and diesel as a fuel for HCCI, a lot of research has been done on the other available alternate fuels like natural gas, biogas, ethanol, hydrogen etc.

Natural gas was considered as a favorable substitute due to its homogeneous mixture formation ability, good supply network and low cost. Effect of varying different parameters such as equivalence ratio, density, intake temperature on the auto ignition characteristics of natural gas was studied by Ando et.al[6].The effect of combustion efficiencies and operating conditions related to CO emissions as well as effect of fraction of n-butane on auto ignition of natural gas was investigated by Jun et al[7].The operating range of HCCI mode with CNG was still small as high intake pressure and temperature was required to auto ignite natural gas. Blended mixture of DME and natural gas widens the working range of HCCI[8]. Addition of DME to homogeneous mixture of methane and air also increases the HCCI operation range[9]. The challenge with DME blending is its cost of transport, storage and conditioning, which is nearly twice as that of diesel.

Hydrogen has been emerging as fuel for electricity generation as well as transportation facilities. HCCI faces a challenge of high CO and UHC emissions. This has been the reason for use of hydrogen as a fuel for HCCI, also the calorific value of hydrogen is much higher than the available fuels. Karim[10] has presented an overview of research done on SI engines considering hydrogen as a fuel. Hydrogen needs a relatively high intake charge temperature for auto-ignition though its ignition energy is low. Hence to use hydrogen in CI mode either high compression ratios or pre-heating is required.

This study focuses on use of single zone zero dimensional model for combustion process. The model over estimates the parameter because the effects of turbulence, charge motion are not considered and it assumes the charge distribution to be truly homogeneous. With lesser computational time, easier formulation it gives a fair estimate of the in-cylinder pressure data and combustion efficiency (η_{comb}) with relative air fuel ratio. The chemical reactions involved in the combustion process are solved using *Cantera*[11], an open source tool for chemical kinetics which is interfaced with MATLAB. The estimated parameters from this model can be utilized as input for experimental investigations.

2. Model description and methodology

The Model is formulated in MATLAB and chemical kinetics of the combustion process is determined using *Cantera*, an open source tool. The reaction mechanism used is GRI30 which consists of 53 species and 325 combustion reaction mechanism.

Single zone zero dimensional model is employed and the simulation is carried out for the period between intake valve closing (IVC) to exhaust valve opening (EVO). The model considers the combustion chamber as single zone, neglecting the activities happening at crevices and any turbulence in the chamber is not accounted into the simulation study. The details of chemical kinetics and thermodynamics in HCCI engine can be obtained using this model to forecast the start of combustion (SOC) with minimum computation time. To get the results closer to reality heat transfer model is included in the study.

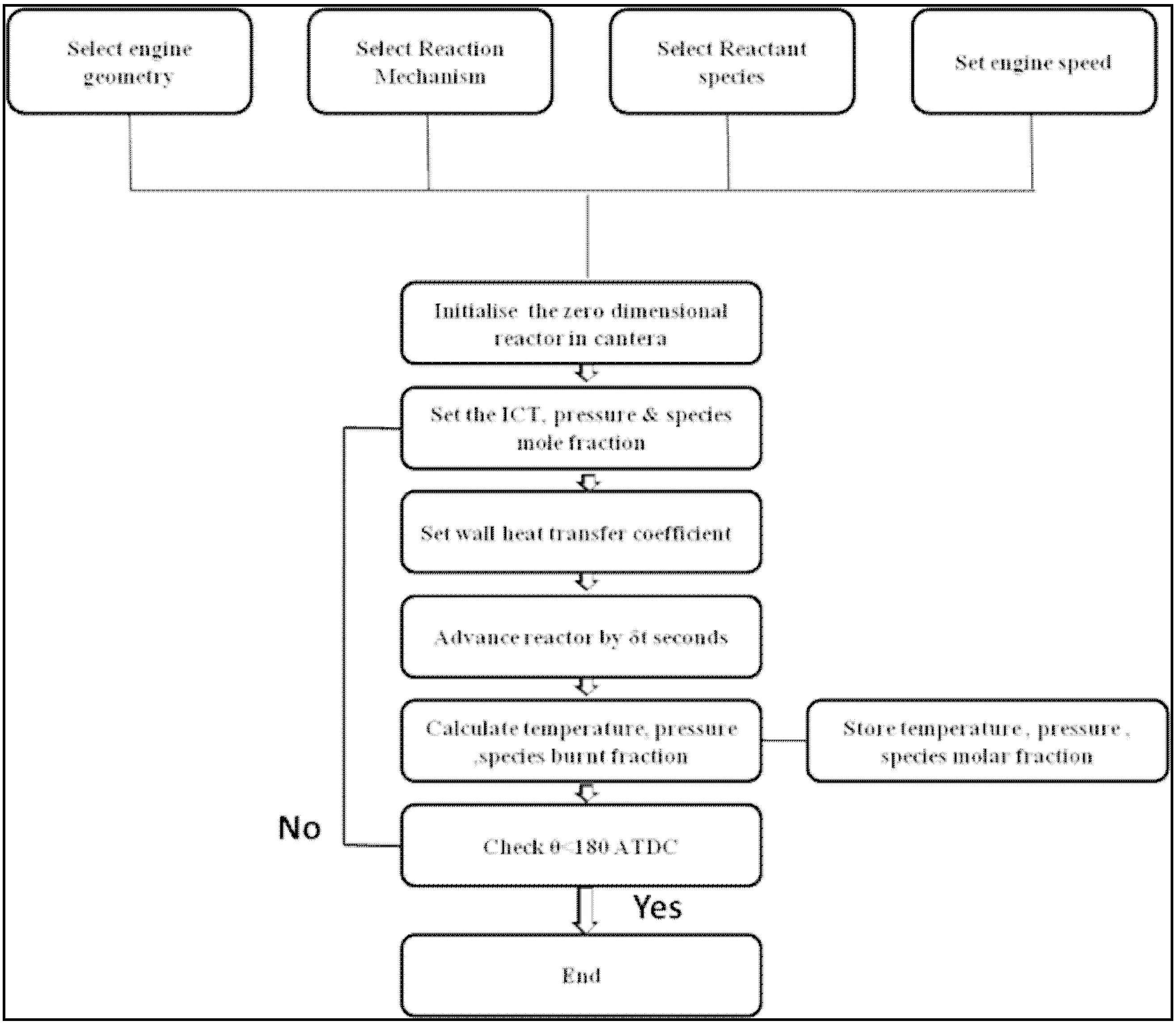

Fig. 1 Flow diagram of the in-house developed program for hydrogen fuelled HCCI operation

Figure 1 represents code created in Matlab in which engine geometry, reactant species, reaction mechanism and engine speed is fed to initialize the model for calculation of some the dependent variables. Then initial conditions for intake charge temperature, pressure and species mole fractions are set based on required equivalence ratio. With respect to initial conditions reference values for wall heat transfer coefficient is set and then the program loop is executed. It advances the engine by time step δt which is given by,

$$\delta t = \left(\frac{60}{N * i}\right)$$

N is engine rpm , i =10000 is number of time steps in the simulation study which advances the engine by 0.036° crank angle every time step hence capturing the start of combustion (SOC) precisely.

The mass conservation equation for single zone zero dimension model is given by

$$\frac{dm_i}{dt} = \frac{\omega_i M_i}{\rho} \quad i=1,2,3\ldots\ldots N_s$$

where m_i is the individual species mass fraction burnt, ω_i is species molar production rate, M_i is molar mass of i^{th} species and ρ is mixture density.

From first law of thermodynamics,

$$\frac{\rho V c_v dT}{dt} = -\frac{pdV}{dt} - \sum_{1}^{N_s} [(\omega]_i M_i u_i) + \dot{Q}_{ht}$$

c_v is the specific heat at constant volume, p is the pressure, T is the temperature, N_s is the total number of species present in the mixture and cylinder volume. V is the instantaneous velocity, calculated by using kinetic relationship of slider crank mechanism[12].

$$V(\theta) = V_c + \frac{\pi b^2 (l + a - a\cos\theta - \sqrt[2]{l^2 - ([a\sin\theta)]^2})}{4}$$

θ being instantaneous crank angle.

The convection heat transfer to cylinder walls $\dot{Q}_{ht}$ is given by

$$\dot{Q}_{ht} = hA(T - T_w)$$

T being instantaneous cylinder temperature at a given crank angle, A is the instantaneous cylinder area available for heat to transfer, T_w is the cylinder wall temperature and h is the heat transfer coefficient in this case Woschni heat transfer coefficient is used where h is given by

$$h = 3.26 b^{-0.2} P^{0.8} T^{-0.55} w^{0.8}$$

w is the average gas velocity given by the expression

$$w = c_1 s_p + \frac{c_2 V_d T_{ref} (P - P_{mo})}{P_{ref} V_{ref}}$$

$c_1 = 2.28, c_2 = 3.24e-3$ are constants where value of $c_2 = 0$ for compression, s_p mean piston speed, V_d cylinder displacement volume, T_{ref} ,$P_{ref} V_{ref}$ are temperature, pressure and volume at reference point , commonly at IVC , P is instantaneous cylinder pressure and P_{mo} is motoring pressure at same crank angle calculated using ideal gas law. The above equations are formulated in Matlab environment. The engine dimensions chosen for the simulation study are depicted in Table 1.

Table 1 Specifications of an engine used for simulation study[13]

Type of an engine	**Single cylinder, four-stroke, naturally aspirated CI engine**
Bore	80 mm
Stroke	110 mm
Connecting rod length	231 mm
Displacement volume	553 cc
Compression ratio	16
Wall temperature	400 K

3. Results and discussion

The results of simulation work present in this paper mainly concentrate on the use of hydrogen in the HCCI mode. In order to explore the effects of intake charge temperature and equivalence ratio on hydrogen fuelled HCCI engine, a single zone zero dimension model was used to predict the initial value of combustion controlling parameters. This section deals with minimum auto-ignition temperature to sustain the HCCI mode, the performance and combustion characteristics of hydrogen fuelled HCCI mode were evaluated and studied.

3.1. Combustion and performance characteristics of the hydrogen fuelled HCCI mode

As indicated in Fig. 2, combustion advances with increase in equivalence ratio with mixture getting rich and from the fact that increase in equivalence ratio in-cylinder gas temperature near top dead center (TDC) at end of compression stroke increases which triggers the ignition process for HCCI combustion. It was noticed that there is no combustion occurs at equivalence ratio of 0.2 for an ICT of 383 K. If we increase the value of ϕ to 0.3, then the combustion initiates and sustain for the same ICT. Further increase in equivalence ratio, the peak pressure increases and start of combustion (SOC) advances significantly. As the equivalence ratio increases, the compressibility of charge reduces which makes harder to compress. Hence the overall in-cylinder gas temperature increases with equivalence ratio as depicted later in Fig.6.

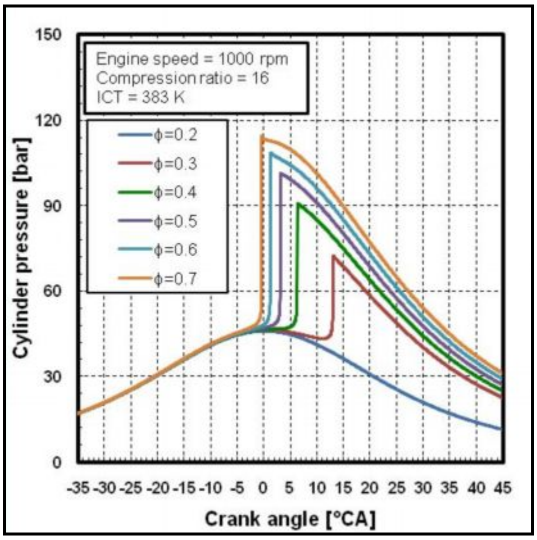

Fig. 2 Variation of cylinder pressure with respect to crank angle for a fixed intake charge temperature at different equivalence ratio

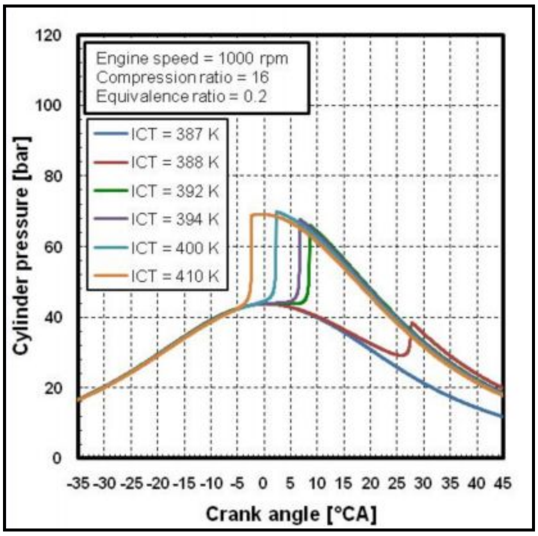

Fig. 3 Variation of cylinder pressure with respect to crank angle for a fixed equivalence ratio of 0.2 at different intake charge temperatures

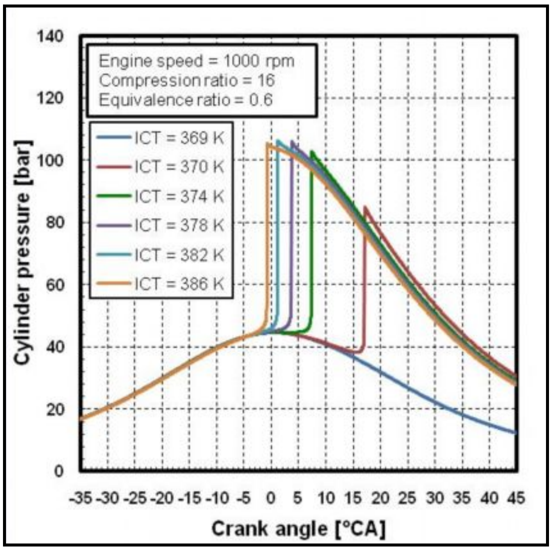

Fig. 4 Variation of cylinder pressure with respect to crank angle for a fixed equivalence ratio of 0.6 at different intake charge temperatures

Figure 3 indicates that an increase in intake charge temperature advances the combustion as the temperature during compression required for ignition is reached progressively early in the cycle with increase in intake charge temperature. For a constant equivalence ratio of 0.2, the charge auto-ignites at an ICT of 388 K. After which the HCCI combustion was stable for higher ICTs as well. But the combustion phasing was relatively too advanced for higher ICTs which leads to poor thermal efficiency because of the heat loss to the cylinder wall. As the equivalence ratio is increased, start of combustion gets advanced towards TDC as indicated in Fig.4.

The main parameters used to discuss the results are ICT and equivalence ratio (φ) as these parameters play important role in predicting the SOC as revealed from literature review. The minimum intake charge temperature (ICT) required for activating the combustion at different equivalence ratio is indicated in Fig. 5. The combustion is presumed to be activated by considering the burnt fraction of hydrogen at the point of exhaust valve opening, if 99.9% of hydrogen is burnt the combustion is said to be completed as assumed by J. Zheng and J.A. Caton [14] in their study.

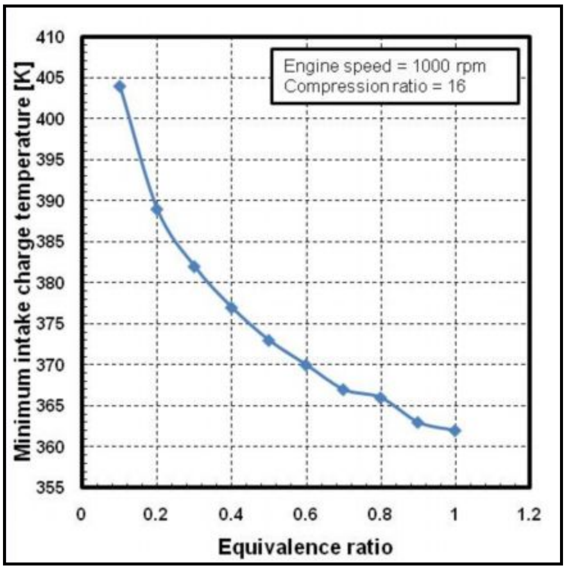

Fig. 5 Variation of minimum ICT with equivalence ratio

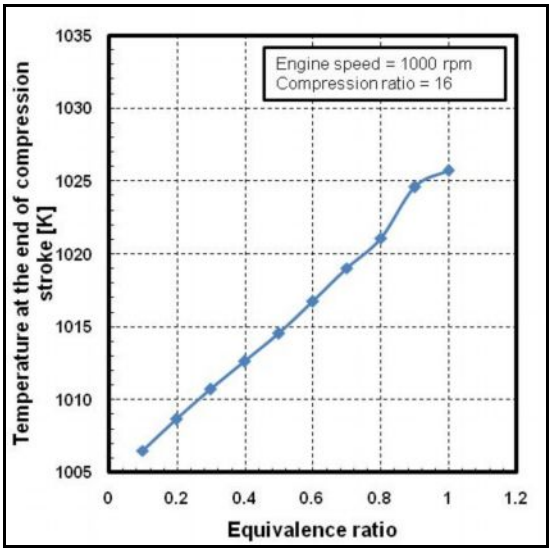

Fig.6 Variation of in-cylinder gas temperature at TDC with equivalence ratio for a constant ICT of 363 K

With increase in equivalence ratio (φ), ICT required to activate the combustion reduces. For mixture to auto ignite, temperature and composition plays a vital role. Temperature at the end of the compression stroke depends on the compression ratio of the engine and the specific heat ratio of the compressing charge. Figure 6 depicts the variation of temperature at end of compression at TDC for different equivalence ratio. The trend shows that as the equivalence ratio increases the temperature at the end of compression increases, which facilitates the auto ignition, hence ICT required to activate the auto ignition reduces with equivalence ratio.

Angle at which combustion starts i.e. start of combustion (SOC) angle is affected by equivalence ratio as stated earlier, when the mixture temperature reaches the optimum value required for auto ignition the charge sets off. The start of combustion is important parameter which decides the other performance, emission and combustion parameters of the engine such as thermal efficiency, mean effective pressure (MEP), torque and exhaust emission. Figure 7 shows variation of SOC with equivalence ratio. As the equivalence ratio increases the SOC advances towards TDC, also in later stages it passes TDC and moves before TDC.

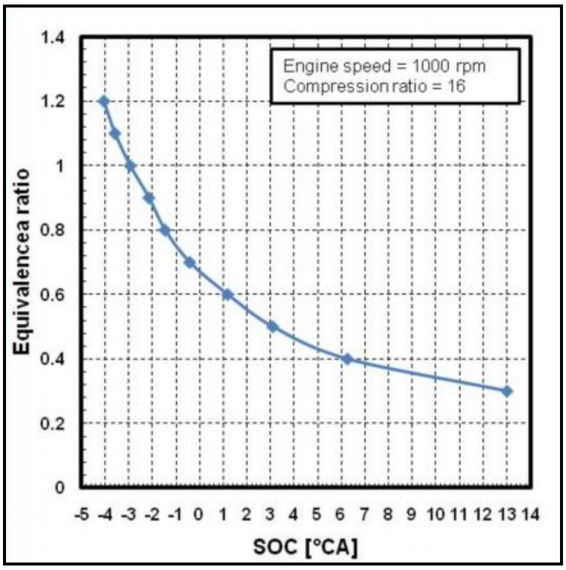

Fig. 7 Variation of equivalence ratio with start of combustion (SOC)

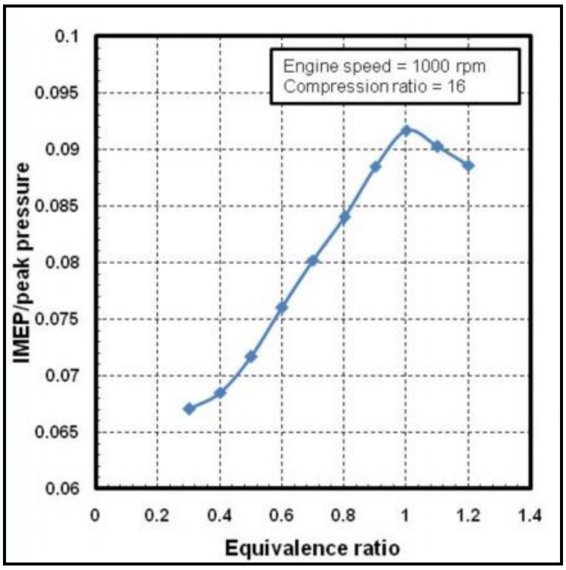

Fig.8 Variation of IMEP/peak pressure ratio with equivalence ratio for a constant ICT of 383K

As SOC advances it improves the performance by improving the IMEP (indicated mean effective pressure), also the peak cylinder pressure increases with SOC advance. As both mechanical compression as well as the pressure rise due to chemical energy release act together, it results in higher peak pressure which may cause structural damage to engine. Also if advance is relatively too high away from TDC it leads to thermal losses hence, reducing the heat utilization capability of the engine, and thus reducing the IMEP. To have more clarification on this, ratio of IMEP to peak pressure is taken to understand the gain in MEP with the cost of higher peak pressure. Figure 8 indicates the variation of the above ratio with equivalence ratio.

Gain in IMEP with cost of peak pressure increases initially with increase in equivalence ratio but as the mixture becomes too rich IMEP reduces and further follows the reducing trend.

It can be inferred that, with increase in ICT SOC advances and also the peak pressure increases. By changing the ICT by 1K the ignition is triggered also the SOC is too sensitive which can be seen from Fig. 9 as ICT increases from 362 K to 363 K SOC advances from 19ºaTDC to 13.3ºaTDC. With increase in ICT the combustion gets advanced as temperature required to ignite the mixture arrives early in the cycle, with advancing in combustion heat loss to cylinder walls increases hence reducing the heat utilization capacity of the engine resulting in reduced MEP which can be seen in the above Fig. 9.

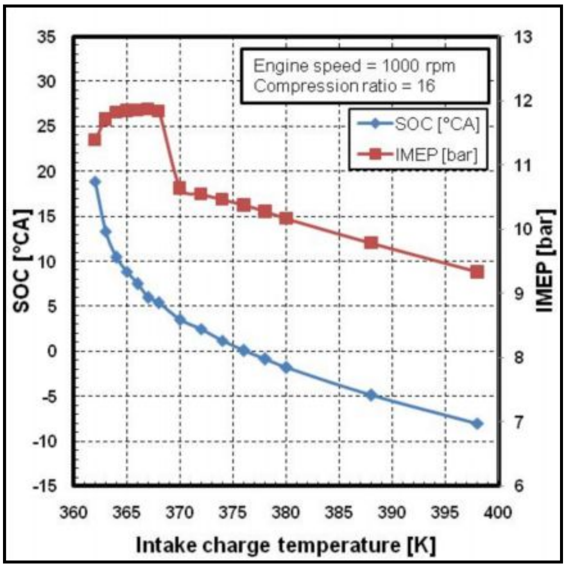

Fig. 9 Variation of start of combustion and IMEP with ICT for $\phi = 1$

The limit for increase ICT or equivalence ratio is limited by the rate of pressure rise which is limited by the mechanical design of the engine component for example at equivalence ratio of 0.2 with ICT of 408 K the rate of pressure rise (ROPR) is 12 bar/degCA at start of combustion for an engine speed of 1000 rpm which induces a force of 6.03 kN/degCA of force which acts on the piston surface it is transmitted to connecting rod which is straight and parallel to cylinder access as piston is closer to TDC this large force acting on the connecting rod might lead to buckling and damage to consequent structure.

4. Conclusions

In this study, a code for single zone zero dimensional model with heat transfer has been developed. The HCCI simulation using hydrogen as a fuel was evaluated by varying the intake charge temperature and equivalence ratio. Based on the simulation results, the following essential conclusions were drawn.

Intake charge temperature has relatively more effect on start of combustion than equivalence ratio, as change in ICT by 1-2 K initiates the combustion but similar level of sensitivity towards equivalence ratio is not observed.

The ICT cannot be increased after a certain value, as it leads to decrease in IMEP due to the thermal losses. It can be observed from results that as the temperature increases from 360K to 400K the IMEP drops below 10 bar.

Hence, it can be said that single zone model is an effective tool to predict the start of combustion (SOC) with minimum computation resources. HCCI engines are appropriate for application with narrow load limits. The estimated parameters from this model can be utilized as input for experimental study.

References

1. White CM, Steeper RR, Lutz AE. The hydrogen- fueled internal combustion engine: a technical review. Int J Hydrogen Energy 2006:31:1292–1305.
2. Aceves, S., Flowers, D., Martinez-Frias, J., Smith, J. et al. HCCI Combustion: Analysis and Experiments .SAE Technical Paper 2001-01-2077, 2001.
3. Onishi, S., Jo, S., Shoda, K., Jo, P. et al. Active Thermo-Atmosphere Combustion (ATAC) - A New Combustion Process for Internal Combustion Engines. SAE Technical Paper 790501, 1979.
4. Thring R. Homogeneous charge compression ignition (HCCI) engines. SAE Paper 8902068,1989.
5. Najt, P. and Foster, D. Compression-Ignited Homogeneous Charge Combustion.SAE Technical Paper 830264, 1983.
6. Ando T, IsobeY,Sunohara D, Daisho Y, Kusaka J. SAE Review 2003; 24:33- 40.
7. Jun, D., Ishii, K., and Iida, N. Combustion Analysis of Natural Gas in a Four Stroke HCCI Engine Using Experiment and Elementary Reactions Calculation. SAE Technical Paper 2003-01-1089, 2003.
8. Chen, Z., Konno, M., Oguma, M., and Yanai, T. Experimental Study of CI Natural-Gas/DME Homogeneous Charge Engine.SAE Technical Paper 2000-01-0329, 2000.
9. Fiveland, S. and Assanis, D.A Four-Stroke Homogeneous Charge Compression Ignition Engine Simulation for Combustion and Performance Studies.SAE Technical Paper 2000-01-0332, 2000.
10. Karim GA. Hydrogen as a spark ignition engine fuel. Int J Hydrogen Energy 2003:28:569–577.
11. Goodwin, D. G. An open-source, extensible software suite for CVD process simulation. In Proceedings of Chemical Vapor Deposition XVI and EUROCVD 14, (Eds M. Allendorf, F. Maury, and F. Teyssandier), 2003, ECS Proceedings Vol. 2003-08, pp. 155–162, 2003 (The Electrochemical Society). (The software Cantera, v. 1.5.4, is available from www.cantera.org.)
12. Heywood, J. B. Internal combustion engine fundamentals, 1988 (McGraw-Hill, New York)
13. M. Mohamed Ibrahim, A. Ramesh. Investigations on the effects of intake temperature and charge dilution in a hydrogen fueled HCCI engine**.** International Journal of Hydrogen Energy**,** Volume 39, Pages 14097–14108,2014.
14. Junnian Zheng, Jerald A. Caton . Use of a single-zone thermodynamic model with detailed chemistry to study a natural gas fueled homogeneous charge compression ignition engine. Int J Energy conversion and Management. Volume 53, pp. 298-304, 2012.

*****