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# HCCI COMBUSTION: MATHEMATICAL MODELLING APPROACH USING VISUAL BASIC FOR APPLICATIONS

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## ABSTRACT

In recent times, alternative combustion technology such as Homogenous Charge Compression Ignition (HCCI) has been studied and results have been positive. HCCI combustion has the potential to reduce fuel consumption and NOx emissions pertaining to the most stringent of legislation of both present and future. HCCI technology is attractive as there is no need for major modifications to the existing structure of IC engines and with significantly low NOx emissions, after treatment systems are not required. However, it is difficult to control the process and achieve constancy every cycle. Therefore, globally experts are studying HCCI combustion in depth to understand the associated idiosyncrasies. Through advent of modern computers, it has become possible to simulate HCCI combustion by creating a mathematical model that can solve complex equations within minutes. This paper details mathematical modelling approach to model HCCI combustion using Visual Basic for Applications (VBA), along with insight on different types of modelling techniques and submodels required to construct the simulation model.

**KEYWORDS:** HCCI, Auto Ignition, Mathematical Modelling, Mechanistic Model, Visual Basic for Applications (VBA)

## INTRODUCTION

The current scenario of fossil fuel shortage, increase in prices and environmental problems due to vehicle emissions, has motivated engineers, scientists, technical education institutes and companies globally, to come up with an alternative technology to the conventional form of burning the fuel and extracting energy out of it. Several approaches have been adapted to solve this problem such as:

**Alternative Fuel:** Use of fuel having better properties than gasoline or diesel in terms of self ignition temperature, volatility and calorific value

**Alternative Combustion Method:** A combustion method that is more efficient than conventional methods in terms of work output and emissions.

**Alternative Materials:** Materials that can sustain higher forces, and therefore high pressure and temperature can be used inside the cylinder so as to extract more work

**Alternative Engine Structure:** Radically change the engine structure so as to reduce number of moving parts and hence, reduce frictional loss

**Alternative Working Cycle:** Explore the use of alternative working cycle to Otto or Diesel cycle that can provide more work output.

For the purpose of this paper, an alternative combustion method namely, Homogeneous Charge Compression Ignition (HCCI), is studied with the purpose of creating a simulation model.

## HCCI

HCCI combustion is achieved by premixing the air-fuel mixture, either in the manifold or by early direct injection, as in Spark Ignition (SI) engine, and compressing the mixture until the temperature inside the combustion chamber reaches the auto ignition point and ignites, as in Compression Ignition (CI) engine. It is also known by following terms –

- Controlled Auto Ignition
- Active Thermo Atmosphere Combustion
- Controlled Auto Ignition (CAI)
- Active Thermo Atmosphere Combustion (ATAC)
- Premixed Charge Compression Ignition (PCCI)
- Homogenous Charge Diesel Combustion (HCDC)
- Premixed Lean Diesel Combustion (PREDIC)
- Compression Ignited Homogenous Charge (CIHC)

HCCI engine combines the advantages of Spark Ignition engine (Homogenous Charge) and Compression Ignition engine (increased efficiency) with reduced emissions. However, unlike SI and CI engine where start of combustion is controlled by spark timing and fuel injection timing respectively, there is no direct way to control the initiation of ignition, and as a result, it becomes innately difficult to control the process in order to extract maximum work from each cycle.

According to various researches done on HCCI engine, combustion happens simultaneously within the cylinder as opposed to flame front phenomenon in conventional SI or CI engine. Hence the combustion duration is comparatively lower resulting in lower peak temperature. Therefore, harmful NOx emissions, which are temperature driven, are reduced considerably. This has motivated scientists and engineers throughout the globe to undertake research on HCCI combustion for better understanding and thereby exploring possibilities for commercial application. The following section highlights some of the research findings pertaining to HCCI.

## LITERATURE REVIEW

Autoignition has been investigated from the start of automobile mass production era, albeit not as a process but to understand fuel properties such as autoignition temperature. Only more recently, autoignition process has been studied with the purpose of extracting positive work from the engine.

Onishi et al. in 1979 examined the possibility of running a two stroke engine on autoignition mode for their research. They concluded that there was little cycle by cycle variation with respect to peak combustion pressure and that the reaction happened spontaneously at several points within the cylinder. The importance of radicals was also studied and it was shown that their concentration was higher and had longer life than in an SI engine.

They also suggested maintaining uniform quantity of mixture and the air to fuel ratio from cycle to cycle in order to attain HCCI. They obtained adequate combustion over a wide range of air to fuel ratios and concluded that HCCI reduces both exhaust emissions and fuel consumption for the entire range.

In 1983, Najt et al. studied in detail what parameters affect HCCI combustion using a single cylinder four stroke cycle engine with a pancake combustion chamber and a shrouded intake valve. They concluded that this autoignition phenomenon was not knocking but an even energy release process that can be controlled by manipulating temperature and mixture strength. They independently controlled inlet temperature and used EGR, simultaneously using different fuels for their experiments and following conclusions were drawn:

- Chemical species in the EGR gases did not affect the Heat Release Rate (HRR), as a result EGR was used to modulate initial temperature of air fuel mixture so as to facilitate autoignition.
- The combustion process was sensitive to delivery ratio through changes in the concentrations of air and fuel in the fresh charge, i.e. at high delivery ratios the energy release became unstable.
- It was easy to ignite fuels having lower octane numbers

Thring, in 1989, used a single cylinder four stroke internal combustion engine to examine the feasibility of HCCI combustion. He performed several experiments with intake temperature as high as 425 $^{o}$C, equivalence ratios ranging from 0.33 to 1.3 and EGR rates up to 33 %, using both diesel and gasoline to map the satisfactory operating regions. He observed that EGR was required in order to raise the intake temperature while there was low cyclic variability and fuel economy results were comparable with diesel engine. He concluded that there were three unsatisfactory regions, dictated by mixture strength, i.e. equivalence ratio –

- Mixture was too rich resulting in misfiring or knocking, labelled as ‘misfire region’ and ‘knock region’
- Mixture was too lean resulting in low power production, labelled as ‘power limited region’

Lei Shi et al. investigated the effect of internal and external EGR on emissions and performance of four stroke HCCI engine running on diesel fuel. They observed that by injecting fuel before Top Dead Centre (TDC) of exhaust stroke, and employing negative valve overlap (NVO), the homogeneous mixture, when burned achieves low NOx and smoke emissions. It was also noticed that internal EGR benefited in the formation of homogeneous mixture, further reducing smoke emissions, however, high load limit of HCCI was affected negatively. Whereas cooled external EGR delayed the start of combustion, thereby helping to avoid knocking, this in turn expanded the high load limit of HCCI engine. Due to no fuel rich regions in the cylinder, smoke emissions were on lower side as compared to a conventional diesel engine.

Osbourne et al. conducted a study on evaluating HCCI combustion mode for future gasoline power trains, with prime objective being to develop a greater understanding of in-cylinder processes. Based on experimental results they developed a 1D simulation model using Ricardo Wave software a CFD based 3D model to perform computations. As per their observation, there was 99% reduction in NOx emissions and an 8% reduction in ISFC compared with the baseline direct injection gasoline engine condition for a standard key point. Also, HC emissions for HCCI operation were comparable to other conventional gasoline engine modes of operation. Finally, they suggest the concept of two-stroke/four stroke switching HCCI engine, made possible by using camless, electro mechanical variable valve actuation.

## HCCI MATHEMATICAL MODELLING

Mathematical modelling is a cheaper, faster and efficient way to gain an insight into the working of a system. It requires great deal of skills and resources to setup an experimental facility for HCCI combustion testing. However, with knowledge gained from various experiments conducted on HCCI combustion, it is possible to formulate a mathematical model and derive a set of relationships between various input parameters and output results. This model can further be fine tuned by validating against known experiment results or by conducting an experiment using exactly similar set of control parameters, as used in simulation model. The following section provides details on formulation of a mathematical model for the purpose of simulation of HCCI combustion.

## MODELLING APPROACH

There are mainly two types of mathematical models that are used to describe the physical phenomena occurring within the engine cylinder:

### Phenomenological Model (Black Box Model)

A phenomenological model or an empirical model is derived using experimental data only, using no prior information about the system, i.e. engine cylinder during HCCI combustion. Statistical principles are used to derive relationships among sensitive parameters affecting the final result. For such models, an experiment is set up where input parameters are controlled and output is measured. Input parameters or experimental setup is altered to study the corresponding effect on output result. From results of experiment, graphs are charted showing correlation between input parameters and measured results. Phenomenological models are more general and applicable to many different kinds of problems. However, they provide less insight into the problem or its possible solution and less predictive capability.

### Mechanistic Model (Grey Box Model)

A mechanistic model is developed using prior information about the system, i.e. results of previous work conducted on similar topic. They provide deeper understanding and more accurate prediction as compared to phenomenological models.

Globally, research on HCCI combustion engine has been undertaken by almost every academic institution, automobile manufacturers, and consultants since last 3 decades. Also, from the detailed research done by the author, the information gathered so far on HCCI combustion, a glimpse of which is mentioned in Literature Review section, is sufficient to develop a mechanistic model on HCCI combustion.

The various mechanistic engine combustion models that have been developed so far can by categorised as per below:

- Zero dimensional models
- Quasi-dimensional models
- Multi-dimensional models

The level of detail and closeness to the real life physics increase as one moves from zero dimensional models to multi-dimensional models, along with the intricacy of models and using these models. There is always a trade-off between the usability of the model and the ability to accurately predict the outcome.

Zero dimensional models are the simplest and most suitable to model the effects of change of input parameters on heat release rate and pressure rise rate during HCCI combustion. Depending upon the assumptions made with respect to division of zones inside the cylinder, zero dimensional models can be further classified into –

**Single Zone:** The entire cylinder is considered as a single zone and calculations are done by applying first law of thermodynamics. The combustible fluid mixture in the engine is assumed to be a thermodynamic system that undergoes the process of energy exchange with the surroundings.

**Two Zones:** The cylinder is divided into two zones, a burned and an unburned zone. These zones are two different thermodynamic systems with energy and mass exchange between them and common surrounding, i.e. the cylinder wall.

**Multi Zones:** Multi zone models are used to evaluate energy and mass interactions through several zones, thus providing more accurate results, albeit with increasing level of complexity.

For HCCI combustion modelling, two zones model is used to simulate the unburned and burned zones.

## MODELLING PLATFORM

Several packages have been developed to simulate the internal combustion engine system. Most notable simulation packages, currently used in automotive research are:

- Ricardo Wave
- Lotus Engine Simulation
- AVL fire
- GT-Power
- KIVA
- MATLAB Simulink
- LabVIEW

However, software costs, hardware requirements and training limitations, combined with project time constraint of the research work undertaken by the author, renders any of the above software packages difficult to use. While above simulation platforms are primarily based on computation fluid dynamics, simple mechanistic models, can be built and developed using any software package offering computation ability to solve engineering problems, program event based automation and a graphic tool to visualize outcome, such as Visual Basic for Applications (VBA) with Excel spreadsheet.

## SIMULATION STRUCTURE

The simulation structure is prepared based on several assumptions related to thermodynamic principles, which are listed below:

- The gases present in burned and unburned zones are ideal gases with different properties
- No heat transfer between unburned and burned zone
- Instantaneous pressure in both the zones is the same because flame is a deflagration combustion wave

- The characteristic gas constants within both zones do not vary much with pressure and temperature; in case of any variance, they can be modelled using thermodynamic relationships of gas constants with temperature and pressure
- Since enthalpy connected with injected fuel is insignificant, it is ignored
- The work required to transfer fluid from unburned zone to burned zone is negligible
- Average instantaneous heat transfer rates are assumed to estimate heat transfer to the cylinder wall
- Crevice losses are ignored

## SUBMODELS

Several submodels have been used or developed to describe all relevant incylinder processes and are vital for the main model to work. The submodels used for the HCCI combustion modeling are as per below -

**Cylinder Geometry**: Cylinder geometry includes bore diameter, stroke, compression ratio and connecting rod length. These attributes determine the basic structure to the simulation model.

**Piston Motion:** This submodel is also known as crank-slider model. The instantaneous position of the piston in the cylinder is evaluated from this submodel. From the instantaneous position of the pistion, the instantaneous volume of the combustion chamber is also determined, as a function of crank angle.

**Air and Fuel Properties:** For the purpose of simulation, air fuel mixture is assumed to have same properties as air. Properties of air such as gas constant for air, ratio of specific heat capacities for air, and fuel properties such as Lower heating value of the fuel and stoichiometric air to fuel ratio are required to calculate pressure and temperature difference as piston moves inside the cylinder.

**Engine Cycle:** HCCI combustion works on Otto cycle as compression (heat addition) and expansion (heat release) happens at constant volume. Therefore, the changing chemical state of the air fuel mixture and changing thermodynamic state of the cylinder are depicted using Otto cycle equations. Based on previous knowledge of Otto cycle, certain points like peak pressure and start of combustion are fixed, in terms of crank angle degrees. To maintain cycle to cycle consistency, EGR percentage would be varied using various degrees of negative valve overlap. Mass flows through open valves will be calculated by one dimensional compressible flow equations for flow through a restriction of filling and emptying models.

**Heat Release Rate:** The heat release rate is the amount of heat released from the chemical reaction with respect to crank angle degree. Pressure and corresponding values of temperature are calculated for unit increment in crank angle degrees. Heat release rate with respect to crank angle degree is calculated using the difference in instantaneous temperature and temperature at fixed points in the engine cycle. The heat release rate calculated is the gross value and when divided by the specific content of the fuel, combustion reaction rate is obtained.

**Heat Transfer:** Heat transfer occurs through conduction, convection and radiation from hot burned gases to piston head, inlet and exhaust valves, cylinder walls, cylinder liners and coolant. For physical testing, water is circulated through the cooling channels as engine runs on the test rig. The difference between inlet temperature and outlet temperature is used to calculate heat transfer, i.e. heat energy dissipated and could not be used to extract work.

**Valve Motion:** This submodel describes the effect of valve motion on the final output of the combustion model. For the purpose of HCCI combustion modelling, internal EGR is used using Negative Valve Overlap (NVO). To vary the percentage of EGR, the duration of NVO is varied and practically this is possible via variable valve technologies.

An effective variable valvetrain enables the engine to breathe smoothly to increase the volumetric efficiency, while allowing the engine to operate on lean mode at low load conditions.

## CONCLUSIONS

The current paper presents an approach to mathematically model HCCI combustion using visual basic for applications. In the current scenario of the need to increase the power output and reduce fuel consumption and emissions, at the same time, HCCI combustion offers the best alternative to conventional combustion concepts used in gasoline and diesel engine. There is no need to radically change the engine design for HCCI combustion to work, and as per major experimental work conducted so far, NOx emissions are reduced by 90 % to 95 % when operating in HCCI mode.

However, it is a challenge to increase the load capacity and globally research is undertaken to understand in cylinder processes in detail so as to enable HCCI to work outside the laboratory, in a vehicle. Through mathematically modelling, HCCI combustion can be simulated and tested for sensitivity with respect to various parameters. Various types of mathematical models have been presented and a two zone zero dimensional mechanistic model is found to be a good compromise between accuracy, computational speed and level of detail. Various submodels that are used to construct the simulation model have also been explained. The final model is constructed on Microsoft Excel 2007 and control automation is achieved through visual basic for applications programming. The simulation results will be presented in a different paper.

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