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Mathematical Modelling Of Particulate Formation in Homogeneous Charge Compression Ignition (HCCI) Engine with NVO

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ABSTRACT

Homogeneous charge compression ignition (HCCI) combustion is now one of the most promising alternative combustion mode that is currently being used in new generations internal combustion engines. It combines the advantages of spark ignition (SI) method (homogeneous charges) and compression ignition (CI) method (increased efficiency). The HCCI combustion concept has the potential of ultra-low nitric oxide (NOx) and particulate matter (PM) emission in comparison to a conventional SI or CI engine. It is known that due to the health and environmental effects of particulate matter/soot and NOx emitted, the environmental legislation has become more stringent with particulate matter emission. Particulate matter from HCCI engine have more often been considered negligible, also the measurement of mass emission of PM (soot) from HCCI combustion systems, shows their negligible contribution to mass of PM. However recently, some studies conducted suggested that PM emission from HCCI cannot be neglected. This is especially for HCCI engines that uses exhaust gas recirculation (EGR), ethanol, and biodiesel. In many HCCI combustion using the NVO or positive valve overlap (PVO) concepts, a lot of EGR is used to control the combustion phasing. In this work a review is being carried out on the mathematical model of soot formation in NVO HCCI using a phenomenological model based on established concept of Argachoy and Pimenta was introduced to predict particulate mass (soot formation) output from direct injection (DI) HCCI combustion engine with negative valve overlap (NVO). Predicted results when compared show reasonable agreement and conformity in mass soot formation-crank angle trend except for a 20% error in maximum soot production occurring from 740deg crank angle. It was found that soot decreases as injection timing advances.

Keywords: ICE, NVO, HCCI, Soot Formation

INTRODUCTION

The arrival of the internal combustion engine (ICE) has made a remarkable development in human progress which has dramatically changed the world we live in today. Nicolaus Otto was one of the Engineers that made the ICE possible. It is a process that allows energy and mechanical power to be extracted from the combustion of air and fuel continuously by means of a piston, connecting rod and crankshaft in a cylinder.

The coming of ICE has lead to a great leap in terms of power creation over the coal and steam engines. Its smaller size, neater and diverse solutions has made this possible, despite the negative environmental impacts of these engines, they presently the dominating propulsion engines and other variety of applications. They play a significant role in modern society, from transportation of passengers, goods, electricity generation, construction, and to the production of food and raw materials. Today the ICE’s is now the most common form of prime mover in the world. It is regarded as a key enabler of globalization (Smil, 2007).

One particular fact about the ICE is the high power and energy content of their fuel makes them ideal for mobile applications. Although research and development of the ICE in the past years and currently have improved performance and efficiency, worldwide emission legislation and the reduction in fossil fuel have motivated ICE manufacturers to provide more advanced technologies producing cleaner exhaust and more efficient power. Alternative technologies such as fuel cells and electric vehicles that have been introduced in the market are very promising in the long-term future, nevertheless they are currently more expensive and less practical than hybrid and advanced engine strategies, and are expected to remain so in the near future.

Research and development of the ICE for applications in the automobile industries have over the years introduced various technologies. These technologies includes alternative fuels, combustion method, injection methods, materials, engine structure, and working cycles that have contributed to the achievement of lower emissions and fuel consumption yet maintaining or even improving output performance. One of such is the alternative combustion method known as the Homogenous Charge Compression Ignition (HCCI) which is a promising new combustion mode that combines the best features of spark ignition (SI) engines and compression ignition (CI) engines. Thus the HCCI engine could be seen as a hybrid between SI and CI engines.

The HCCI combustion is also known as Controlled Auto-Ignition (CAI) combustion when applied to SI engine or low temperature combustion (LTC), premixed-charge compression ignition (PCCI), etc. The combination of these two designs (SI and CI) offers a diesel-like high efficiency and at the same time, reduces NO_x and particulate matter emissions. In this technology the fuel is homogeneously mixed with air in the combustion chamber (similar to a regular SI engine). In this review work towards the mathematical modeling of particulate formation also known as soot is modeled with a two-step empirical soot model of Argachoy and Pimenta (2005), the mathematical model will be validated with results of simulations of Manimaram et al. (2013). The model will also be tested with different injection timing of the HCCI combustion, and then the soot produced will be compared to that of Argachoy and Pimenta.

HCCI Combustion mode

HCCI combustion is achieved by premixing air-fuel mixture, either in the manifold or by early direct injection as in SI engine to form homogeneous mixture, and thereby compressing the mixture until the temperature inside the combustion chamber reaches the auto ignition point and ignites, as in CI engine. The HCCI combustion combines the advantages of Spark Ignition engine (i.e. homogenous charge) and Compression Ignition engine (i.e. increased efficiency) with reduced emissions. However, unlike SI and CI engine where start of combustion is easily controlled by spark timing and fuel injection timing, there is no direct way to control the initiation of ignition, and as a result, it becomes difficult to control the process in order to extract maximum work from the engine cycle.

HCCI with negative valve overlap (NVO) enables the retention of a fraction of exhaust gas that can facilitate auto ignition and at the same time massively reduces raw NOx emission to a negligible level by the low combustion temperatures resulting from the dilution of the charge with EGR. However the utilization of EGR has the disadvantages of increasing PM especially the small size and UHC concentration that combines with the oil that find its way into the combustion chamber, thereby leady to engine wear. The PM and UHC concentrations increase at high engine load operation due to the addition of EGR that reduces oxygen concentration (Ramana et al.). Such increment in engine wear is due to the friction between PM contained in the inducted air in addition to the sulphuric acid accompanied with EGR that deteriorate the lubricating oil (Ramana et al.). Thus there is a need for modeling PM in HCCI with NVO so as to properly understand how the internal EGR (iEGR).

Soot formation and modeling is one of the least investigated and understood combustion areas especially in HCCI combustions and emissions. Particulate matter, or soot, is one of the major pollutants produced by diesel engines. The small nano size particles has been shown to be a health hazard. The small particles can penetrate deeply into lung tissues, and more stringent legislation only allows less and less soot to be emitted from diesel engines, engine manufacturers need to find ways to reduce the amount of soot produced by their engines. Not only do these particulate matter cause health hazard they also cause damages to the automobile engine and its effect of decreasing the overall engine performances. Hence, one robust way to investigate HCCI particulate formation is by using an appropriate soot model, this will facilitate the solution to reducing the particulate matter emissions. Although most of these soot models for HCCI particulate formation are computationally intensive and expensive. This calls for the reason for the Research to look into simpler models that are much flexible to use and computationally inexpensive like the two-step empirical soot model of Argachoy and Pimenta (2005).

This research is focusing on a simpler way of modeling of particulate mass output and history of the particulate formation in HCCI combustion with the two-step empirical soot model, with the following objectives to be achieved. The HCCI combustion mode to be modeled by the soot model is first selected. The formulation and computation of the spray model of the HCCI and the different sub-spray models will be carried out. The Computation of the net soot formations and oxidation component of HCCI combustion will be taken. Then testing and validating the mathematical model with valid results of Manimaram et al., (2013) will be carried out, with results compared and validated. The model performance will then be measured using different injection timings.

To achieve the above objectives, the following tasks will be performed. The models of the spray plume and the soot will be implemented in the Engineering Equation Solver (EES). The parametric simulation will be carried out in MS Excel. These parameters will include in-cylinder pressure, mass rate of injected fuel, injection velocity, bulk mean temperature, energy release rate, and the characteristics of injector nozzles.

This outcome of this research is expected to help in the concept stage of the advanced powertrain development, instead of more complex approach at the concept stage, a simpler method that can predict and control particulate matter formation from a HCCI NVO combustion especially during part load operation. Which is the regime these combustion modes are most suitable, due to misfire at low load and knocking combustion at high load. This method will facilitate the prediction of the mass and history of PM formation for improved control and reduction at early stage of design. As a result of this suitable sophisticated combustion control system for the HCCI engine, the engine could be hybridized efficiently into battery electric vehicle to reduce the particulate matter. Thus an Engineer From a practical point of view could use this particulate/soot formation/oxidation model to development of advanced combustion system with enhanced thermal efficiency to reduce soot formation and other emissions to meet future more stringent particulate emission standards at minimum cost. This soot formation/oxidation model can also be integrated into flame propagation dynamics simulation programs for better prediction of flame propagation and its effect on PM formations.

Over the last few years, there had been an exponential growth in the consumption of diesel and petrol fuel in the transportation sector. This has lead to a great deal of air pollution and environmental issues Such as the greenhouse effect, ozone layer depletion and weather disaster, which are all due to vehicle emissions. All these environmental impact of the fossil fuel based motor vehicles coupled with the limited availability, and unpredictable increase in fuel prices has motivated engineers, scientist, research institutes and automotive industry globally to seek an alternative form of technology such as the HCCI which is unlike the conventional modes of combustion in SI and the CI engines. The HCCI offers diesel-like high efficiency and at the same time low NO_X and particulate formation. Currently, researches are ongoing in the hybridization of the HCCI combustion mode and the battery electric, as well as on the challenges faced in HCCI combustion engine some of which are mixture homogeneity, combustion phasing, and limited operating range. It is therefore important also to look at the modeling of HCCI emissions such as particulate matter from one of its well-known highly researched valve strategies (NVO).

Fuel Emission Standards

Current Worldwide Emission Legislation

There are a number of emission standards enforced around the world this can be seen in (Delphi-Worldwide Emissions Standards, 2016/2017). There are four major types of pollutant legislation that is currently enforced around in the world today namely: European Standards (Euro, EC), America standards (EPA, CARB, CAAA), Japanese Standards and Brazilian Standards. How these standards are applied depends on the type of vehicle in question.

European Standards

The current standards applicable to Europe are the Euro standards (Regulation [EC] No. 715/2007 of the European Parliament and of the Council of 20 June 2007). There are a number of categories of Euro standards. They are denoted by the number Euro 1/2/3/4/5/6/ etc., with the higher number corresponding to the more rigorous and current standard.

American Standards

The US federal standards (United States Environmental Protection Agency-Clean Air Act) are what is currently enforced in America. Presently there are 3 sets of standards denoted by tier 1 and tier 2. Tier 2 is currently enforced for light duty road vehicles. It is mostly in vehicle categories, such categories denoted as bin 1 to bin 8. Different emission criteria are applied to each bin. The lower the bin number the more stringent the criteria and hence the cleaner the vehicle emission. Cars that have been newly registered fall into any one of the 8 bins as long as the vehicle manufacturer also meets a fleet average of bin 5.

Recently tier 3 has also been introduced. It was adopted in March 2014 and phase in 2017-2025. This regulation also tightens on sulfur limits for gasoline. It expresses both the Bins (Certification limits) and the fleet average standards using the sum of NMOG+NO_X emissions. The require emission durability is now increased to 150000miles or

15yrs. In California there are more stringent emissions criteria that must be satisfied. They were stipulated by the California Air Resources Board (CARB) (California Exhaust Emissions Standards and Test Procedures for 2001).

Japanese Standards

The current Japanese standards (Ministry of the Environment, Government of Japan, 1996) are the Post New Long Term [PNLT] and was enforced in October 2009. They supersede the New Long Term [NLT] standards which in turn supersede the New Short Term (NST) standards.

Brazilian Standards

The Brazilian standards (Federal Government of Brazil, 2009) comprises of a mix of the European and America standards. That is the FTP-75 is what is adopted, whereas the emissions are based on Euro standards. Brazil adopted a mix of different standards because the fuel they use contains high quantities of ethanol and they needed to alter their own standards. These 4 standards represent what is currently adopted throughout most of the world. Many countries adopt different levels of criteria that was earlier adopted some years ago by the original adopters of such standards which may have been laid off. These emissions standards can be compared with each other and similar emissions can be imposed.

Pollutants and Emissions from internal combustion engines

The emissions from internal combustion engines includes:

Carbon (IV) Oxide: it is also known as carbon dioxide, it is nontoxic and not regarded as a pollutant, however, measures are in place to reduce its emissions. Since as a greenhouse gas it has the effect of increasing the earth atmospheric temperature, and also land and sea temperature (UK Greenhouse Gas Statistics and Inventory Team, Science and Innovation group, 2013).

Carbon II oxide: this is produced due to rich fuel/air mixture combustion of carbon compounds in fossil fuels. The formation rate is controlled primarily by air-fuel ratio (Lambda λ). The process governing its formation can be controlled kinetically.

The formation process is represented by

$RH \rightarrow R \rightarrow RCO_2 \rightarrow RCHO \rightarrow RCO \rightarrow CO$, Where R means hydrocarbon radical Here the CO formed in the combustion process is then oxidized to CO_2 at a slower rate (Heywood, 1988). The CO concentrations in the exhaust are steadily increased in conditions of fuel-rich mixture and very little with leaner mixture conditions. CO is very dangerous to human health. During respiration it combines with the haemoglobin in the red blood cells hindering its ability to absorb oxygen. Thus, it causes respiratory problems and heart diseases, that eventually leads to death.

Nitrogen oxides (NO_x): are formed as a result of high temperature combustion in engine combustion chamber. The Nitric oxide (NO) and Nitrogen dioxide (NO_2) are usually grouped as NO_x emissions. Nitric oxide is the predominant of the oxides of Nitrogen produced inside the engine cylinder. These gases results in acid rain. Nitrogen dioxide is toxic and could lead to human respiratory diseases, while Nitrous oxide contributes directly to global warming. The mechanism of NO formation generally occurs in the combustion that is close to stoichiometric reaction.

Combustion and expansion process is being affected by the temperature and pressure distribution in the cylinder. NO emission peak at slightly leaner than stoichiometric air-fuel ratio. As the mixture gets leaned out, increase in oxygen concentration increases the gas temperature. However for richer mixtures, substantial NO decomposition occurs at the maximum in-cylinder pressure.

Fuel air-ratio, burned gas fraction and spark timing are the main parameters that affects the formation of NO_x. Hot residual gases has been used to bring NO_x emissions reduction to 90-95%, while advanced spark-timing have led to higher NO_x formation.

Unburnt hydrocarbon (UHC): these are volatile organic compound as a result of incomplete combustion of the hydrocarbon fuel. It ranges from 1000 to 3000ppm (Heywood, 1988) in the spark ignition combustion engine. It goes up rapidly when the air-fuel mixture becomes highly richer than when it is stoichiometric. For very lean mixture, HC emissions could rise rapidly by incomplete combustion or misfire. This usually happens higher in HCCI combustions than in SI combustion.

The following are several mechanisms that could contribute to HC emission, incomplete combustion, flame quenching at the combustion walls, absorption of fuel vapor into oil layers on the cylinder, the filling of unburnt mixture in the crevice volumes.

The SI engines are normally operated close to stoichiometric or slightly richer in order for smoother and reliable operation. However, when air-fuel ratio gets richer, UHC emission level increases rapidly. Lean mixtures could be used to produce lower UHC, provided the combustion quality does not deteriorates.

Particulate Matters (PM): these are small particles, formed by incomplete combustion of fuel and air mixture, this includes the burning of lubrication oil and the presence of impurities in the fuel. They are harmful and causes respiratory diseases and may be carcinogenic in nature, and mostly occur in greater quantity in diesel engines than in gasoline engines.

Overview of HCCI Technology

Emerging Combustion Mode

The two main combustion modes for internal combustion engines have been SI and CI engines which are commonly referred to as petrol (gasoline) and diesel engines respectively. In SI engine, the ignition is initiated by the spark plug, and in CI combustion engine, ignition occurs due to the compression of the air to a high pressure and temperature and fuel is injected into the charged mixture that lead to spontaneous ignition. The compression ratio, injection duration, injection pressure and timing of start of injection are used in controlling CI ignition. The combustion of an SI engine is characterized by propagation of a flame that emerges from the kernel of hot gases due to the spark flame, the CI combustion is more of a diffusion flame where the combustion occurs between the spray and the surrounding mixture. The negative environmental impact of these combustion engines has resulted in many governments imposing stringent conditions that stipulate the level of pollutants that may be emitted from vehicles. As a result of the increasing restrictions for these engines there is an urgent need to develop an alternative combustion system for the automotive industry.

The only alternative cost effective and feasible means of enhancing the efficiency and decreasing emissions of ICE is by modifying the combustion mode. The effective way this can be done is by introduction of homogeneous mixture of air and fuel in to the engine cylinder. According to (Heywood, 1988), this method of combustion can make use of variety of different fuels.. The HCCI has the following benefit,it is a fast combustion of lean mixture, high efficiency, lower peak temperature and reduced NOx emission.

Although the HCCI technology is considered a new developing technology it has been around for over 100years just like the spark ignition (SI) combustion in gasoline engine and compression ignition (CI) combustion in diesel engine. The first known patent was by Carl W. Weiss who invented a hot bulb 2-stroke engine in 1897 (Erlandsson 2002). In his engine kerosene was injected onto the surface of hot bulb. After which the mixture was then vaporized in a heated prechamber. The prepared air-fuel mixture is then transferred from the prechamber to the cylinder which is then auto-ignited inside the main chamber. Russian scientist Nikolai Semonov with his colleagues established the first theoretical and practical works on chemical-kinetics controlled combustion for diesel engine in the 1930’s (Zhao 2007). Later Semonov and Gassak (Shahbakhti et al., 2007) built the first HCCI/CAI engine that controls combustion by the use of active species which discharges from partially burned mixture in a separate prechamber. The investigation works of Onishi (Onishi et al. 1979) in 1970’s and Noguchi (Noguchi et al., 1979) in 1983 were the most recognized and first systematic early investigations to be done on HCCI/CAI engine. They studied the HCCI/CAI on a two stroke engine and this investigation works was then extended to a four stroke engine by Najit and Foster in the 1980’s (Najt and Foster, 1983). The terminology Homogeneous Charge Compression Ignition (HCCI) was introduced by Thring (Thring, 1989.) in the 1980’s in his research paper as he studied the external EGR and air-fuel ratio on HCCI. Since the 1990’s the HCCI technology have been of more interest by researcher and engineers all over the world (Aoyama et al., 1996; Ryan and Callahan, 1996) as a way of solving the higher fuel price and stringent emission norms in the US and Europe (European Federation for Transport and Environment, 2004).

HCCI technology has excellent fuel flexibility quality (Fiveland et al., 2001), it can be applied to a wide range of fuels with different octane numbers, ranging from biofuels (Arrafgle et al., 2009.), to hydrocarbon fuels (Yao et al., 2009.) and reforming fuels (Hosseini and Checkel, 2008.). HCCI engine exhibit similar properties over a wide range of size, this allowed the technology to be implemented on a larger HCCI engine-a 12 litre six cylinder engine proposed by Olsson et al., (2001) and on a mini HCCI engine-a 4.1 cc engine as described by Manente et al., (2007). Thus HCCI engine could be scaled to virtually any sizes of transportation engines a small motor cycle to a large ship engine or large stationary engine (U.S. Department of Energy, 2001). Also the features of the HCCI engine makes it virtually work with most of the fuels available. The HCCI engine is not only applicable to the automotive technologies but also in oil and gas production, power generation and pipeline pumping. Thus, HCCI technology has a wide application base. If the HCCI technology is fully enhanced and optimized and used on a day to day basis they are going to have a very large market. As a result of these factors there has been intense research in this area over the last few years.

Principle and Combustion Characteristics of the HCCI Engines

The HCCI combustion operation has the same mixture preparation process as the conventional SI combustion operation where air and fuel is premixed in the intake system or by direct injection in the cylinder. This premixed mixture is then compressed during the compression stroke and combustion is then initiated by auto-ignition just in a similar way as the conventional CI combustion operation. The auto-ignition is initiated by increasing the charge temperature at the beginning of the compression stroke above that of the conventional SI combustion. This is achieved by an intake heater or hot EGR. As a result, the intake charge is then heated which results in a higher gas temperature and a faster chemical reaction during the compression stroke. Thus a homogeneous combustion is initiated. The major heat release occurs at a temperature condition between 1050-1100K for gasoline and less than 800K for diesel. Also for many hydrocarbon components, low temperature oxidation reactions also occur. The heat release during such low temperature reaction is influenced by the chemical kinetics of the fuel, dilution strategy, and also temperature and pressure history that the mixture undergoes during the compression stroke.

The HCCI combustion is characterized by it's relatively fast and high peak heat release rate and shorter combustion duration rate than the conventional SI combustion. This can be seen from the investigation work done by Onishi et al. (1979) when he showed that the maximum heat release rate increased up to 30% over the conventional combustion. Also while that of Lada et al., (1997) showed that combustion duration can be shorter up to 30% by his use of a ceramic cylinder head rather than the conventional aluminium type. They also found that the lower heat transfer characteristic of the ceramic material enhances more advanced ignition and better combustion efficiency. The rapid combustion and high peak heat release rate faced in HCCI combustion due to simultaneous mixture combustion must be controlled in order to prevent engine damage and to control emission. This which can be done either by controlling the lean air-fuel mixture and (or) charge dilution.

HCCI Challenges and Proposed Solutions

HCCI combustion has been achieved by using many different methods over the last few decades. Much of the work performed in this area focused on achieving improved fuel economy and lower pollutant emissions, mainly particulate and NOx emissions. However, several obstacles exist which must be overcome for successful commercial application to occur, these include effective combustion control (timing)", limited power output" and homogenous mixture preparation". The most important of these is effective combustion control. This can be achieved by controlling the following parameters such as temperature, pressure and composition of the in-cylinder mixture generally through controlling a combination of these parameters (Zhao et al., 2007).

In SI engines, the start of combustion is depended on the externally-controlled spark timing, and the burn rate is limited by the flame propagation rate. While in CI engines, the start of combustion takes place after a short delay following the injection of fuel, and the burn rate depends on the externally-controlled fuel injection rate. But for the HCCI engine, the combustion of the pre-mixed charge starts spontaneously without any external control. Since there is no direct way to control the initiation of ignition therefore it is innately difficult to control the process in order to extract maximum work (i.e. maximum power output) from each cycle.

The start and rate of combustion are solely dependent on the thermo-chemical conditions inside the combustion chamber. It has been well established that such intrinsically controlled spontaneous combustion is dominated by chemical kinetics rather than thermodynamic effects.

This lack of external controls in HCCI combustion results in difficulties at low and high load operation. The low combustion temperature at low loads is insufficient to sustain a complete combustion of the air-fuel charge/mixture which results in increased emission of carbon monoxide and hydrocarbons. Misfire thus takes place, limiting the low load operating range of the engine. While at high loads, the rapid heat release causes the engine operation to be very noisy and unstable. This leads to Knocking and also deteriorating of the combustion efficiency as a result limiting the upper range of operation. Thus with Misfire at low load and knocking at high load, this will result in an impractically narrow HCCI operating envelope along the speed range.

There are two main ways in which combustion timing can be controlled, they are: (I) by controlling the temperature history and (II) by Changing mixture reactivity such as changing the fuel ratio (i.e. changing octane number of the fuel) like using two different fuel mixtures or additives to the fuel mixture. They could be furtherly grouped as in (Mahdi, 2009) below:

Controlling the temperature history
VVT and residual/exhaust gas trapping

by Exhaust gas trapping
by Modulating intake and exhaust flows
Combination of both Exhaust gas trapping and Modulating intake and exhaust flows
Variable Compression Ratio (VCR)
Variable EGR
Combustion Timing In-cylinder injection timing
Modulating intake temperature
Water injection
Variable coolant temperature
Changing mixture reactivity
Modulating 2 or more fuels
Fuel additives and reforming
Variable EGR

These are several combustion control strategies that have been suggested and studied in order to solve the control problem on combustion. NVO Valve Timing (Internal/exhaust gas recirculation (EGR)) and direct fuel injection are potential solutions, which will now be discussed in more detail in the next section.

Negative Valve Overlap Valve Timing

A negative valve overlap (NVO) is achieved with a variable valve train (VVT) or cam profile switching. Thus this helps in controlling the amount of trapped residuals or internal EGR (Jacob, 2009). This is the valve timing strategy utilized in this research. In NVO, the exhaust valve closing (EVC) is relatively early and the intake valve opening (IVO) is relatively late, which results in recompression of high amounts of trapped EGR. The exhaust gas could be used to influence combustion in two opposing ways- (i) using the hot EGR to increase the temperature of the mixture, thus advancing the combustion. Here normal ambient intake temperature could be used; (ii) or using the EGR as a diluent to retard combustion by lowering the concentration of the reactants and increasing combustion duration by absorbing thermal energy. In the investigation done by Kaahaaina (Jacob, 2009), he varied EVC timing and found that delaying it, EGR decreased and also phasing advanced. But in the investigation of Nitz (2008), he experienced the opposite for the engine that he used for his study. In his work, EGR increased and phasing advanced because temperature increased. This discrepancy could be said to have occurred due to the engines being operated in different regimes, where different effects of EGR dominated. But many studies have successfully used valve timing to control phasing (Jacob 2009).

Direct Injection

The timing of direct injection (DI) events is found to be effective in the control of HCCI combustion. DI enables the amount and timing of fuel injected to be varied and to allow for multiple injections per cycle. A promising injection strategy for engines with NVO is the injection of fuel during EVC and during IVO. This has been found to have an increasing effect on the lean limit and a reducing effect on the fuel consumption (Urushihara et al., 2003). It produces a nearly homogeneous mixture, which then results in an efficient, stable and fast combustion (Li et al., 2006). The early injection can also results in reduction in NO_X and uHC emissions for the same reason (Standing et al., 2005). Injecting during NVO can result in an increase in pumping losses as a result of drop in cylinder temperature and pressure as fuel evaporates (Leach et al., 2005). The opposite effect is observed when heat is given out during the NVO expansion (Standing et al., 2005).

During NVO, the fuel injected and EGR undergo recompression which results in heat release. This increases the temperature at IVC which advances combustion phasing. The heat released also helps in the vaporization of the remaining fuel that is injected during IVO. With the reactions that take place, the fuels ignitability is increased and the combustion phasing is advanced (Aroonsrisopon et al., 2007; Guohong et al., 2006; Waldman et al., 2007). This effect which is known as fuel reforming can expand the lean limit of combustion without increasing the NO_X emission (Urushihara et al., 2003). By advancing the injection, heat release is increased during NVO and the main combustion phasing is also advanced (Aroonsrisopon et al., 2007; Guohong et al., 2006; Waldman et al., 2007). This could also be as a result of an increase in fuel reforming (Aroonsrisopon et al., 2007; Guohong et al., 2006).

Also the amount of fuel being injected during NVO affects the NVO pressure. By injecting more fuel during NVO the peak NVO pressure is altered. This could be as a result of increased heat release. Also, a decrease can occur as a result of more fuel decreasing the specific heat capacity ratio and thus increasing the heat required to vaporize the fuel (Waldman et al., 2007). Increasing the fuel injected during NVO has been found to advance combustion phasing (Aroonsrisopon et al., 2007; Guohong et al., 2006; Waldman et al., 2007). It was seen that at higher loads the optimum quantity of fuel required to be injected during NVO decreases (Urushihara et al., 2003). This is because the EGR is hotter so less heat is required. This is due to the fact that since the EGR is hotter and thus less heat release during NVO is required to reach its ignition temperature during main combustion. It was found that under certain conditions, by increasing the total fuel injected there was a reduction in the heat release during NVO as less O_2 was available (Waldman et al., 2007).

DI can also enable partial fuel stratification by injecting some fuel closer to combustion top dead centre (TDC). This can be used in the reduction of rate of pressure increase at high power outputs whilst maintaining low NO_X emissions (Sjoberg and Dec, 2006).

Particulate Matter (PM)

Particulate matters are tiny solids and liquid particles, and are sometimes referred to as particulates, or fine particles and at times soot. They could be linked to human health issues. Environmental Protection Agency (EPA) defines particulate matter as any diesel exhaust substance that can be collected by filtering the diluted exhaust gas at ≤325 k (David, 1997). Particulate matter can be measured or computed and expressed mainly in two forms: "PM number" as used by Ojapah et al.,, (2014) and "PM mass" as used by Argachoy and Pimenta (2005). According to World Resource Institute et al., (Jun, 2010) has it that the size of particulates vary from several nanometers to several hundred microns. While soot which is one of the constituent of exhaust PM and although not clearly definable is comprised of solid carbon particles formed in the locally fuel-rich areas during combustion and as a result of incomplete combustion. Particulate is generally defined as the combination of solid, liquid and sometimes gas phase matter that is present in the engine exhaust. However, in most literature some of these terms are sometimes used interchangeably. In this research, in the interest of consistency, soot will be referred to, and used interchangeable with particulate matter. However, where the reference to the work of others is made, the terminology of the source has been adopted.

Diesel Particulate Matter (PM)

Engine exhaust comprises of different components, which includes mainly N_2, O_2, CO_2,CO, unburnt hydrocarbons, water vapor, and particulate matter (PM). Particulate matter, or soot, is one of the major pollutants emitted by diesel engines. It is commonly accepted that diesel PM is responsible for adverse health conditions, including carcinogenic ones. Diesel particulate matter which is a complex mixture is said to be composed of organic and inorganic or gas, liquid and solid phase materials (Johnson, 1992). The organic or hydrocarbon compounds include aldehydes, alkanes, alkenes and aromatic compounds while the inorganic compounds include sulfur, oxygen, carbon monoxide, elemental carbon and oxides of nitrogen (NO_2). The gas phase emission include $N0_x$ CO, and SO_2 while the solid phase emissions include small spherical carbon particles known as soot and the liquid phase emissions include organic or hydrocarbon component and sulfate. While some of the hydrocarbon may be found absorbed into the spherical carbon particle, some may be in the gas phase (Johnson, 1992).

In general diesel particulate matter is typically composed of two types of particles: (i) agglomerates of carbonaceous primary particles of soot (each 12-30nm in diameter) containing traces of metallic ash, with the agglomerated soot particles covered in condensed organic compounds and sulfate; (ii) nucleation mode particles (e.g. Alkynes from Acetylene [C_2H_2] upwards as well as PAH), condensed particles, and sulfate (Aaron, 2015). Lowenthal et al. (1994) did some measurements of heavy-duty diesel vehicle emissions. He found that PM comprise of 0.9% nitrate, 9.2% sulfate, 0.31% ammonium, 29.2% organic carbon and 53.4% elemental carbon. This is comparable to that of Kawatani et al. (1993). In his work he showed that soot component (or) elemental carbon is made up of 43% and 64% of total PM. In Tree and svensson (2007), the density of soot was reported to be 1.8-2.0 g/cm^3 range. While primary soot particle sizes ranges from 20-70nm.

Soot Formation

Soot which is most time known as particulate matter (PM) is formed in the fuel rich region (Turns, 2000) as a result of pyrolysis of the high temperature liquid fuel and the accumulation of oxygen depleted fuel vapor which results from not mixing properly (Crua, 2003). Many factors can influence the fuel to particulate matter conversions or species conversions (i.e. that are precursors to PM). They include the following: the availability of oxygen, residence time, temperature, pressure and the molecular structure of the fuel. The process of soot formation involves the conversion of small hydrocarbon molecules in the gas phase to solid particles that are mostly spherical. This is a complex process that may take only a few milliseconds behind shockwaves or tens of milliseconds in flames. In modeling the soot process in a diesel engine, the need to understand how the soot process actually take place during the course of combustion is essential. In simple steps soot process can be divided into soot formation and soot oxidation. A review of few literatures (Tree and Svensson, 2007; Richter and Howard, 2000; Dederichs, 2004) shows that soot formation

can be divided basically into: (i) pyrolysis, (ii) formation of precursors, (iii) soot particulate nucleation, (iv) particle condensation, (v) particle surface growth, (vi) particle coagulation, (vii) particle agglomeration, (viii) soot oxidation.
Pyrolysis

The process of fuel changing their molecular structure in the presence of high temperature without significant oxidation notwithstanding if oxygen species is present (Tree and Svensson, 2007). This process produces unsaturated hydrocarbon, polyacetylenes and aromatic compounds such as benzene and phenyl, and these molecules then grow into 2-dimensional poly-aromatic hydrocarbon (PAH) (Dederichs, 2004).

Formation of Precursors

In this stage larger PAH with molecular weight of 500-1000 amu are formed through the reactions of PAH-PAH and the addition of acetylenes onto PAH molecules (Richter and Howard, 2000). Then combination of these larger PAH molecules then form two dimensional PAH which will be the precursors for soot nucleation process.

Soot Nucleation (Inception)

Nucleation is said to be defined as the formation of particles from gas-phase reactants. Though soot particle inception/nucleation is not fully understood and is still under debate, a widely accepted explanation is that it is a process where the first particle arises from smaller fuel molecules after the fuel is oxidized and (or) pyrolysed. It occurs by the coalescence of moderately sized PAHs into stacked clusters. This is supported by the experimental evidence by Wang (Aaron, 2015). According to (Dederichs, 2004) it elaborates that it is when the two dimensional PAH merge into three-dimensional particle i.e. where mass is converted from molecular to particulate system. At this stage, the details of chemical reactions are still poorly understood. According to different investigation, particle inception takes place at a molecular mass between 500amu to 2000amu (Iliyana, 2007). PAH can be interpreted as solid particles rather than molecules when it is above these values. These first soot particles have C/H ratio of about 2 and are roughly spherical in shape. The observable solid particle size in flame is repeatedly in the range of 1.5-2.0nm (Aaron, 2015) and the temperature during particle inception varies from 1300-1600K, depending on the fuel.

Soot Particle Condensation

This stage is quite similar to the surface growth stage due to the fact that smaller molecules of two dimensional PAH condense on newly-formed three dimensional soot particles forming a larger soot particle. Here a chemical species from the gas phase sticks to the surface of the soot particles by Van der Waals force (Kraft, 2005) and not by chemical reaction.

Soot Particle Surface Growth

Particle surface growth is the addition of mass to the surface of the nucleated particles. It is the process whereby the bulk of solid phase material of soot is generated. It involves the addition of gas phase species to the surface of the particle. It also involves their incorporation onto the particulate phase. In surface growth the gas phase material is added through chemical reactions with active sites on the soot particle. Acetylene (C_2H_2) is generally accepted as the major growth species in hydrocarbon flames (Kennedy, 1997). This process generates majority of soot mass. It is estimated that 80% of the soot mass is added during surface growth (Aaron, 2015). Surface growth leads to an increase in the size of the particulate but not in the number (N) of the particulate matter.

Soot Particle Coagulation

As the name implies, coagulation is a process when two soot particles collide with one and coalesce to form one particulate. This is a physical process that reduces the number (N) of soot particle by forming a new soot particulate of increased size yet still maintaining the total soot mass. In the coagulation process two particles stick together and are glued together by a common outer shell generated by deposition similar to surface growth. Coagulation takes place only for relatively small particles characterized by high rates of growth ≤ 10nm in low pressure premixed systems (Iliyana, 2007).

Soot Particle Agglomeration/Aggregation

Soot particle agglomeration is a process that takes place at the late phase of soot formation. It involves the sticking of primary particles with one another to form clusters or chains. Here the structure of the individual primary particles known as spherules does not change. In the agglomerates there is a weak cohesive bonding between the particulates. Soot particle agglomeration is an extension of soot particle coagulation. In the early stage when the soot particles are still soft, collision of two soot particles may result in their combination into a single larger spherical particle, this process which is regarded as soot particle coagulation. While at a later stage when soot particles start to solidify before collision, the collision may cause these particles to form a cluster of soot which may not be spherical. But at a final stage, the soot particles may form a chain of discrete spherules which is likely due to electrostatic activity (Amann, 1982). Soot aggregate usually contain from 10 to 100 primary particles (Spherules).

Soot Particle Oxidation

Oxidation results in the conversion of carbon and hydrocarbons, forming gaseous CO and CO_2. Soot oxidation is a surface type of reaction and it may occur at any time during soot formation process. Thus it can occur from fuel pyrolysis to agglomeration process i.e. it is parallel to the surface growth soot formation processes. Potential soot oxidants includes O, O_2, OH and CO_2. Soot particle oxidation occurs when the temperature is above 1300 K (Tree, and Svensson, 2007). Oxidation is a two stage process. In the first stage, chemical attachment of the oxygen to the surface (absorption) occurs. In the second stage, desorption of the oxygen by the attach fuel component from the surface as a product is said to occur (Tree, and Svensson, 2007). In lean conditions, the oxidation of soot happens as a result of the attack by molecular oxygen, O_2 and OH radical. While in fuel-rich and stoichiometric conditions, OH is likely to dominate the soot oxidations process (Tree, and Svensson, 2007). Also according to Neoh et al. (Iliyana, 2007), the hydroxyl, OH radical is the most abundant oxidizing species under fuel-rich conditions. He stated that OH could suppress soot formation by oxidation destruction of precursors. Also Haynes and wagner (1981) made it clear that only about 10 to 20 % of all OH collision with soot are effective at gasifying the atom of carbon. OH radical is believed to be mainly responsible for the oxidation of soot particles. Also the presence of CO_2 has also been shown to reduce soot formation (Aaron, 2015).

The Effect of EGR on Particulate Formation and NO_X

Exhaust gas is recycled in order to modify charge composition and temperature control to reduce particulate emissions and NO_X emissions. Also EGR has a significant effect on the particle size distribution. Most of the particles in the EGR that re-enter the cylinder will be oxidized and transformed into CO_2 , yet some of the particles may survive and grow substantially. Such mechanism by which this happens has been investigated in an SI engine modified for single cylinder HCCI operation (David and Markus, 2014) with n-heptane fuel and an equivalence ratio of $\varphi=1.93$. It was investigated by extracting particle-laden in cylinder gases through snatched sampling, accumulated over a number of cycles in steady-state operation. This captured aggregate were analyzed by a Scanning Mobility Particle Sizer (SMPS) and a High-Resolution Transmission Electron Microscope (HRTEM). The distribution turns bimodal in a later stage of the cycle. This is due to the fact that there is inception, and since large aggregates is fund of collecting small particles. In the investigation it is seen that the first cycle starts without any soot present in the residual gases and within ten cycles the distribution has stabilized and the statistical noise has decreased substantially. It is also seen that there is consecutive growth of aggregates in each cycle. In fact aggregate larger than about 20 nm were recirculated for possibly several times before it was being emitted from the engine. In most diesel engines most of these large aggregates are oxidized but the surviving particles will act as sponge collecting other particles, fuel droplets remaining and engine oil. Such particles often lead to fouling of other engine components such as swirl flags that is found in modern diesel engines

Mathematical Modeling Methods

A method of simulating real-life situations with mathematical equations in order to forecast their future behavior is known as mathematical modeling. Mathematical modeling or briefly model is the process of setting up a model, solving it mathematically, and interpreting the result in physical or other terms. It is an important activity in science and engineering. It is a cheap, fast and efficient way in gaining insight into a working system. While a great deal of skills and resources is required to setup an experimental facility for HCCI combustion testing, it is possible to formulate a mathematical model showing similar outcome as that of an experiment as well as derive a set of relationships between various input parameter and output result with the knowledge gained from various previous experiments conducted on HCCI combustion. Such model can be further fine-tuned by validating it with respect to known experiment results or by conducting an experiment using exactly the same set of control parameters, as used in the simulation model. There are mainly two types of mathematical models that are used in describing the parameters occurring within the engine. They are mechanistic and phenomenological models. This two will be discussed in the details alongside their formulation of their mathematical model in the following section for the purpose of HCCI simulations.

Mechanistic Model

Mechanistic model is also known as Grey box model. They are developed using prior information about the system i.e. results of previous work conducted on a similar topic. These kind of models provide deeper understanding and more accurate prediction as compared to phenomenological models. Mechanistic model on HCCI combustion can be developed with the help of past researches already done on HCCI combustion engine by almost every academic institution, automobile manufacturers and consultants since the last 30years i.e. a glimpse of which is mentioned in the Literature Review section is quite sufficient.

Mechanistic model can be categorized as:

- Zero-dimensional model
- Quasi-dimensional model
- Multi-dimensional model

As one moves downwards from zero dimensional model to multi-dimensional models, the level of detail and closeness to real life physics increases along with intricacy and usage of these models. A trade-off always exist between the usability of the model and the ability to accurately predict the outcome.

The simplest and most suitable to model the effects of change of input parameters against heat release and pressure rise during HCCI combustion is the zero dimensional models. The zero dimensional models can be further classified depending upon the assumptions made with respect to division of zones inside the cylinder. Thus the zero dimensional can be classified as:

- Single zone models
- Two zone models
- Multi zone models

Phenomenological Model

Phenomenological model or Black box model is also known as empirical model. They are derived using experimental data only, using no prior information about the system, i.e. engine cylinder during HCCI combustion. Phenomenological models benefit by only focusing on those areas that are most closely related to the phenomenon of interest. It makes use of statistical principles to derive relationships among sensitive parameters affecting the final result. These kind of models involve setting up of an experiment where input parameters are controlled and output is measured. Here input parameters or experimental setup is altered and the corresponding effect on output result is studied. Graphs are plotted from results of experiment showing correlation between input parameters and measured results. These models are more general and applicable to many different kinds of problems. Though they could be of less predictive capability, but they may provide less insight into the problem or its possible solution. A typical example of Phenomenological model is the soot model.

Soot Model

Various model of soot formation and oxidation have been studied by automobile engineers. According to Kennedy, in his literature (Qingan, 2009) on soot modeling, soot models could be categorized into three groups: (i) empirical soot models; (ii) semi-empirical soot models and; (iii) detailed soot models.

The empirical soot model uses experimental data to predict trends in soot formations. These models are developed on the basis of experimentally derived phenomenological correlations of soot formations rates with combustion conditions. Such combustion conditions may be pressure, temperature and equivalence ratio. These models can be found in literature that is related to gas turbine and diesel engines that are computationally intensive to simulate. The empirical soot model is easy to understand and implement. It doesn’t require heavy computational load but has a limitation of not showing detailed insights into the soot formation processes.

The semi empirical soot models are models that solve rate equations for soot formation with the help of some input from experimental data. These model attempts to include some aspects of the physics and chemistry of the phenomenon. Thus, it is contrary to the empirical soot model which involves correlations of experimental data. A good example is the widely used two-equation soot model of Fairweather et al. (Qingan, 2009). Although this semi empirical soot model might not cover soot property details such as soot aggregates and polydispersity of soot particles. It also does not resolve the issue of detailed combustion chemistry.

Detailed soot models are models that seek to predict the concentration of all the species in a flame ranging from fuel to polyaromatic hydrocarbons to soot. It does this by solving the rate equations for elementary reactions that result to soot formation (Qingan, 2009). These models rely on empirical inputs for detailed soot information such as soot nucleation, growth, oxidation rates etc. and are limited intensively to specific conditions. That is they are limited to only conditions in which the rates were measured. Thus, they cannot easily be extended to different fuels or pressure conditions. These models are based on fundamental combustion chemistry and aerosol dynamics theory. They also seem to be more general than the simplified models. The detailed soot model can resolve soot issues such as aggregate structure, can provide particle size distribution, can model particle coagulation in the transition and continuum regimes. But they have the limitation of being difficult to implement. They are also too computationally intensive. Also owing to the fact that soot chemistry involves at least hundreds of species and thousands of reactions, it is practically impossible to use detailed modeling approaches which may be in conjunction with CFD. These might be so expensive. Therefore, simplified models which are less expensive and are much flexible to use are preferable.

We will now limit our scope of literature review on the two-step empirical soot model, a means of establishing semi empirical models thus leading to the area of study of this research.

Two-Step Empirical Soot Model

Two-step soot models has been used by many researchers (Ng, 2003; Kim and Sung, 2004; Wang et al., 2006). Hiroyasu's soot model (Hiroyasu and Nishida, 1989) was one of the first two-step soot formation model used. In the Hiroyasu's soot model, the soot formation process is considered having only two reaction steps: (i) the formation step, here the soot is linked directly to the fuel vapor molecules, and (ii) the oxidation step, which describes and links the destruction of soot particles to the attack of molecular oxygen (Tao et al., 2005). The net rate of change in soot mass is then given by the difference between the rates of formation and oxidation.

Patterson et al. (1994) investigated on the Hiroyasu's soot model and found out that it under-predicted the peak in-cylinder soot concentration. Patterson et al. then made use of the semi empirical formula proposed for the purpose of pyrolytic graphite oxidation by Nagle and Strickland-Constable (NSC) (Wan Mahmood, 2011). This he did by incorporating it into a new soot oxidation rate formula (Patterson et al., 1994).

Other model of the two-step soot models are Lee's model (Wan Mahmood, 2011) and Ladommatos et al. (Ladommatos et al., 2002). These two-step empirical models are simple in their form and are of reduced computational cost.

The 2-step empirical Soot model by Argachoy and Pimenta (2005)

The soot model used here is the one of Argachoy and Pimenta (2005). The model is of the so-called two-step empirical type of model as Bayer and Foster (2003), Seykens et al. (2009) Kazakov and Foster (1998). Which was first suggested by Hiroyasu and Kadota (1983).

The soot model of Argachoy and Pimenta is chosen because it describe soot formation in a burning diesel spray that follows the current conceptual view of diesel spray combustion as presented by Dec (1997). Besides this it shows certainly reasonable agreement as predicted values was close to measured values in his work that he carried out. One other reason is that the two step mechanism methods have not been extensively investigated on particulate matter from the HCCI.

Modelling Platform

Several modeling platforms have been developed to simulate internal combustion engine system. They include the following simulation packages:

- Ricardo Wave
- AVL fire
- G-power
- KIVA
- Lab View

Due to software cost, hardware requirement and training limitation, combined with the project time constraint of the research work to be undertaken, makes any of the above software packages difficult to use. Although the above simulation platforms are primarily based on computational fluid dynamics, however simple phenomenological models can be built and developed using any software packages/platforms that can offer computation ability to solve engineering problems like the Engineering Equation Solver (EES) and the Micosoft Excel is quite simple and much easier to use. In this modeling work, models of the spray plume and soot will be implemented in the Engineering Equation Solver (EES) while the parametric simulations will be carried out in MS Excel environment.

CONCLUSION AND RECOMMENDATIONS

In this work a two-step empirical soot model by Argachoy and Pimenta was used to model the net soot of formation (Particulate Matter) in a HCCI combustion engine.

The model predicts net soot production by relating soot formation and soot oxidation rates in characteristic regions of the burning fuel spray. The conditions required by the model include: in-cylinder pressure, injection velocity, mass rate of fuel injection, bulk mean temperature, energy release rate and the characteristics of injector nozzle. With this information the model predicts: general geometry of developed spray plume, mass history and mass of particulate matter in the combustion chamber. The models of the spray plume and the soot were implemented in the Engineering Equation Solver (EES) while the parametric simulations were carried out in MS Excel environment. The simulated results correctly reproduce practically observed trend of increased soot formation of the simulated results of Manimaram et al. (2013) as the crank angle degree advanced. However, the maximum soot yield occurs at masses slightly higher than that of Manimaram et al. (2013) by approximately 20% error at maximum soot production occurring from 740 degree crank angle. This which was due to the simple nature of the soot model applied, which does not take into account other important soot sub-process such as nucleation, condensation and coagulation. After the validation of the model, it was chosen to simulate soot production for different injection timings. This variable was chosen since it is one of the ways in which the ignition timings (combustion phase) and soot emissions of an HCCI engine can be controlled.

Due to the fact that the soot model is based on the fundamental phenomena important in soot formation, this model has considerable potential as a powerful tool to lend insight into the physical and chemical mechanisms that limits soot emissions in diesel engines.

RECOMMENDATIONS

The use of more chemical reactions is recommended to enhance the performances of the soot model.

The use of a complex chemistry solver is highly recommended to be used at the initial reaction point, to determine a detailed description of exhaust gasses that contribute to particulate emissions.

Incorporating the influence of turbulent mixing during spray break-up after the end of fuel injection is also recommended.

Evaporation and boiling mechanisms for fuel droplets should also be improved.

Since this model is considered as a simple soot model and it only resolves the two-step equation from overall soot formation process, it is necessary to perform the analysis with a more complex mathematical model that will consider multi-steps equation covering soot formation process like pyrolysis, formation of precursors, soot particulate nucleation, particle condensation, particle surface growth, particle coagulation, particle agglomeration.
Contribution to knowledge

This research work help exposes more on the fact that simple models like the two-step empirical soot model considered here can be used to predict soot emissions on modern engines like the HCCI engine especially with reasonable fidelity, thus reducing the time and cost of experimentations and avoiding much expensive sophisticated computations.

REFERENCES

[1]. Aaron, E. (2015) The influence of fuel molecular structure on particulate emission investigated with isotope tracing, Ph.D. Thesis, Mechanical Engineering Department.
[2]. Air Pollution Control Law Chapter III (1996), Ministry of the Environment, Government of Japan.
[3]. Aoyama, T. Hattori, Y. Mizuta, J. and Sato, Y. (1996) An Experimental Study on Premixed-Charge Compression Ignition Gasoline Engine". SAE Paper No. 1996-01-960081.
[4]. Argachoy, C. and Pimenta, A. P. (2005) Phenomenological Model of Particulate Matter Emission from Direct Injection Diesel Engines.
[5]. Aroonsrisopon, T., Nitz, D., Waldman, J., Foster, D. and Lida, M. (2007) A Computational Analysis of Direct Injection During the Negative Valve Overlap Period in an Iso-Octane Fueled HCCI Engine, SAE Paper No. 2007-01-0227.
[6]. Arrafgle, J. Tormos, B. Laopez, J. J. and Garcia A. (2009) Analysis of the Potential of Biodiesel as an Alternative Fuel for Current and Future HSDI Engines". SAE Paper No. 2009-01-0480, 2009.
[7]. Barbara, M. (2012) Investigation of Soot Processes In An Optical Diesel Engine, A thesis submitted for the degree of Doctor of Philosophy, School of Engineering and Design, Brunel University, United Kingdom.

[8]. Bayer, J., Foster D. E. (2003) "Zero-Dimensional Soot Modeling", SAE Paper 2003-01-1070.
[9]. Bradley, D., Hicks, R. A., Lawes, M., Sheppard, C. G. W., Woolley, R. (1998) "The Measurement of Laminar Burning Velocities and Markstein Numbers for Iso-octane-Air and Iso-octane-n-Heptane-Air Mixtures at Elevated Temperatures and Pressures in an Explosion Bomb", Combustion and Flame 115:126-144.
[10]. California Environmental Protection Agency Air Resources Board (CARB), 1999. California Exhaust Emissions Standards and Test Procedures for 2001 Through 2014 Model Criteria Pollutant Exhaust Emissions Standards and Test Procedures and 2009 Through 2016 Model Greenhouse Gas Exhaust Emission Standards and Test Procedures for Passenger Cars, Light-duty Trucks and Medium-duty Vehicles,
[11]. Crua, C., Kennaird, D.A. and Heikal, M.R. (2003) Laser-induced incandescence study of diesel soot formation in a rapid compression machine at elevated pressures. Combustion and Flame, 2003.
[12]. David, K. and Markus K. (2014) Particle Formation and Models in Internal Combustion Engines. Cambridge Centre for Computational Chemical Engineering ISSN 1473 – 4273.
[13]. David Y. C. (1997) Determination of particulate and unburned hydrocarbon emissions from diesel engines fueled with biodiesel, Retrospective Theses and Dissertations. Iowa. State University.
[14]. Dec, J. E. (1997) "A Conceptual Model of DI Diesel Combustion Based on Laser Sheet Imaging", SAE Paper 970873.
[15]. Dederichs, A.S. (2004) Flamelet Modelling of Soot Formation in Diffusion Flames, Department of Fire Safety Engineering, Lund Institute of Technology, Lund. p. 147.
[16]. Delphi, (2015/2016) Worldwide Emissions Standards: Passenger Cars and Light Duty Trucks.
[17]. Erlandsson, O. (2002) Early Swedish Hot-Bulb Engines - Efficiency and Performance Compared to Contemporary Gasoline and Diesel Engines. SAE Paper No. 2002-01-0115.
[18]. es-ICE user guide. (2011) version 4.16.001, CD-adapco.
[19]. European Federation for Transport and Environment. (2004) Waiting for Euro 5 and Euro 6 New Emission Standards for Passenger Cars, Vans and Lorries. http://www.t-e.nu/.
[20]. European Parliament. (2007) Regulation (EC) No 715/2007 of the European Parliament and of the Council of 20 June 2007. On Type Approval of Motor Vehicles with Respect to Emissions from Light Passenger and Commercial Vehicles (Euro 5 and Euro 6) and on Access to Vehicle Repair and Maintenance Information (Text with EEA Relevance), 2007.
[21]. Federal Government of Brazil. (2009) Resolution No 415 of 24 September 2009, Conama 415/2009.
[22]. Fiveland, S. B. Agama, R. Christensen, M. Johansson, B. Hiltner, J. Mauss, F. and D. N. Assanis, D. N. (2001) Experimental and Simulated Results Detailing the Sensitivity of Natural Gas HCCI Engines to Fuel Composition. SAE Paper No. 2001-01-3609.
[23]. Heywood, J. B. (1988) Internal Combustion Engine Fundamentals. McGraw Hill.
[24]. Haynes, B.S. and Wagner, H. Gg. (1981) Soot Formation. Prog. Energy Combust. Sci. 7(4): p. 229-273.
[25]. Hiroyasu, H., Kadota, T. and Arai, M. (1983) Development and Use of a Spray Combustion Modeling to Predict Diesel Engine Efficiency and Pollutant Emissions Combustion Modeling, Bulletin of the JSME, Vol. 26, No.214: p. 569-570
[26]. Hosseini, V. and Checkel, M. D. (2008) Reformer Gas Composition E®ect on HCCI Combustion of n-Heptane, Iso-Octane, and Natural Gas". SAE Paper No. 2008-01-0049.
[27]. Ibrahim, F., Wan Mahmood W. M. F., Abdullah1, S. and Abu, M. (2016) Numerical investigation of soot mass concentration in compression ignition diesel engine, Journal of Mechanical Engineering and Sciences (JMES) ISSN (Print): 2289-4659; e-ISSN: 2231-8380 Volume 10, Issue 3, pp. 2275-2287.
[28]. Iliyana I. N. (2007) Soot Formation Modeling during Hydrocarbon Pyrolysis and Oxidation behind Shock Waves, Ph. D Dissertation in Natural Sciences. Rupertus Carola University of Heidelberg, Germany.
[29]. Jacob R. Z. (2009) Fuel Effects on Homogeneous Charge Compression Ignition Combustion. University of Wisconsin Madison.
[30]. Jayashankara, B. and Ganesan, V. (2010) Effect of fuel injection timing and intake pressure on the performance of a DI diesel engine – A parametric study using CFD, Energy Conversion and Management, 51:1835–1848, 2010.
[31]. Johnson, J.H., Bagley, S.T., Gratz, L.D. and Leddy, D.G. (1992) A Review of Diesel Particulate Control Technology and Emissions Effects – 1992 Horning Memorial Award Lecture. SAE Papers, 1994(940233).
[32]. Jun Z. (2010) Particle Matter Emission Control and Related Issues for Diesel Engines. School of Mechanical Engineering, University of Birmingham.
[33]. Kawatani, T., Mori, K., Fukano, I., Sugawara, K. and Kayama, T. (1994) Technology for Meeting the 1994 USA Exhaust Emission Regulations on Heavy-Duty Diesel Engine. SAE Papers, 1993(932654).
[34]. Kazakov, A. and Foster, D. E. (1983) "Modeling of Soot Formation During DI Diesel Combustion Using a Multi-Step Phenomenological Model, SAE Paper 982463.
[35]. Kennedy, I.M. (1997) Models of Soot Formation and Oxidation. Prog. Energy Combust. Sci. 23(2): p. 95-132.

[36]. Kim, H. and Sung, N. (2004) Combustion and Emission Modeling for a Direct Injection Diesel Engine. SAE Papers, 2004(2004-01-0104).
[37]. Kraft, M. (2005) Modelling of particulate processes. KONA, 2005(23): p. 18-35.
[38]. Lada, N., Ichikura, T., Kase, K., Yoshiteru, E. (1997) 'Self-ignition and combustion stability in a methanol fuelled low heat rejection ceramic ATAC engine – analysis of cyclic variation and high wall temperatures and lean burn operation', JSAE paper 0389-4304/97.
[39]. Ladommatos, N., Song, H. and Zhao, H. (2002) Measurements and predictions of diesel soot oxidation rates. Proc Instn Mech Engrs Part D: J Automobile Engineering, 2002. 216: p. 677-689.
[40]. Leach, B., Zhao, H., Li, Y. and Ma, T. (2005). Control of CAI Combustion through Injection Timing in a GDI Engine with an Air-Assisted Injector, SAE Paper No. 2005-01-0134.
[41]. Li, Y., Zhao, H., Brouzos, N., Ma, T. and Leach, B. (2006). Effect of Injection Timing on Mixture and CAI Combustion in a GDI Engine with an Air-Assisted Injector, SAE Paper No. 2006-01-0206.
[42]. Lowenthal, D.H., Zielinska, B., Chow, J.C., Watson, J.G., Gautam, M. Ferguson, D.H., Neuroth G.R. and Stevens, K.D. (1994) Characterization of Heavy-Duty Diesel Vehicle Emissions. Atmospheric Environment.
[43]. Mahdi Shahbakhti. (2009) Modeling and Experimental Study of an HCCI Engine for Combustion Timing Control. University of Alberta.
[44]. Manimaran, R. Thundil Karuppa Raj, R. Senthil Kumar, K. (2013) Premixed Charge Compression Ignition in a Direct Injection Diesel Engine using Computational Fluid Dynamics, School of Mechanical and Building Sciences, Vellore Institute of Technology, VIT University, Tamilnadu-632014, India. WSEAS Transactions on Heat And Mass Transfer.
[45]. Manente, V. Tunest˚al, P. and Johansson, B. (2007) Mini High-Speed HCCI Engine Fueled with Ether: Load Range, Emission Characteristics and Optical Analysis. SAE Paper No. 2007-01-3606.
[46]. Naber, J. D., Siebers, D. L. (1996) "Effects of Gas Density and Vaporization on Penetration and Dispersion of Diesel Sprays", SAE Paper 960034.
[47]. Najt, P. M. and Foster, D. E. (1983) Compression-Ignited Homogeneous Charge Combustion. SAE Paper No. 830264.
[48]. Ng, H.K. (2003) The simulation of combustion in diesel engines using Kiva-3v on a PC Platform, School of Mechanical, Materials and Manufacturing Engineering, University of Nottingham, Nottingham.
[49]. Nitz, D. G. (2008) "Investigation into Expanding the Operating Range in a Gasoline Fueled Negative Valve Overlap HCCI Engine", M.S. Thesis, Mechanical Engineering Department, University of Wisconsin-Madison.
[50]. Noguchi, M. Tanaka, Y. Tanaka, T. and Takeuchi. Y. (1979) A Study on Gasoline Engine Combustion by Observation of Intermediate Reactive Products during Combustion". SAE Paper No. 790840.
[51]. Ojapah M. M. (2004) Experimental Studies of Performance and Emissions in a 2/4-Stroke Engine with Gasoline and Ethanol. School of Engineering and Design, Brunel University, London, United Kingdom.
[52]. Olsson, J. Tunest˚al, P. and Johansson, B. (2001) Closed-Loop Control of an HCCI Engine. SAE Paper No.2001-01-1031, 2001.
[53]. Onishi, S. Jo, S. H. Shoda, Jo, P. D. and Kato, S. (1979) Active Thermo-Atmosphere Combustion (ATAC) A New Combustion Process for Internal Combustion Engines". SAE Paper No. 790501.
[54]. Patterson, M.A., Kong, S.C., Hampson, G.J. and Reitz, R.D. (1994) Modeling the Effects of Fuel Injection Characteristics on Diesel Engine Soot and NOx Emissions. SAE Papers, 1994(940523).
[55]. Payri, F., Benajes, J. Margeo, X. and Gil A. (2004) CFD modeling of the in-cylinder flow in direct injection diesel engine. Computers & Fluids; 33:995–1021, 2004.
[56]. Peters, N. (2000) "Turbulent Combustion", Cambridge University Press.
[57]. Ramana, P. V. Maheswar, D. and Umameheswer Gowd, B. (2015) Review on Research and Development of HCCI Technology, International Journal of IT, Engineering and Applied Sciences Research (IJIEASR) ISSN: 2319-4413 Volume 4, No. 5.
[58]. Richter, H. and Howard, J. B. (2000) Formation of polycyclic aromatic hydrocarbons and their growth to soot--a review of chemical reaction pathways. Progress in Energy and Combustion Science, 2000. 26(4-6): p. 565-608.
[59]. Ryan, T. W. and Callahan, T. J. (1996) Homogeneous Charge Compression Ignition of Diesel Fuel". SAE Paper No. 961160.
[60]. Seykens, X.L.J. (2009) Development and validation of a phenomenological diesel engine combustion model, Eindhoven University of Technology.
[61]. Shahbakhti, M. Lupul, R. Audet, A. and Koch, C. R. (2007) Experimental Study of HCCI Cyclic Variations for Low-Octane PRF Fuel Blends ", Proceeding of Combustion Institute-Canadian Section (CICS) Spring Technical Conference, 6 pages, Ban®, Canada.
[62]. Sher, E. (1998) Pollutant Formation and Control, Handbook of Air Pollution from Internal Combustion Engines, Academic Press.

[63]. Siebers, D. L. (1999) "Scaling Liquid-Phase Fuel Penetration in Diesel Sprays Based on Mixing-Limited Vaporization", SAE Paper 1999-01-0528.
[64]. Siebers, D. L. and Higgins, B. (2001) "Flame Lift-Off on Direct-Injection Diesel Sprays Under Quiescent Conditions", SAE Paper 2001-01-0530.
[65]. Sj¨oberg, M., Dec, J. and Hwang, W. (2007). Thermodynamic and Chemical Effects of EGR and Its Constituents on HCCI Auto-ignition, SAE Paper No. 2007-01-0207.
[66]. Smil, V. (2007) "The Two Prime Movers of Globalization: History and Impact of Diesel Engines and Gas Turbines", Journal of Global History 2, pp 373-394.
[67]. Standing, R., Kalian, N., Ma, T., Zhao, H., Wirth, M. and Schamel, A. (2005). Effects of Injection Timing and Valve Timings on CAI Operation in a Multi-Cylinder DI Gasoline Engine, SAE Paper No. 2005-01-0132
[68]. Symonds, J. P., Reavell, K. S. J., Olfert, J. S,, Campbell, B. W. and Swift, S. J. (2007) Diesel soot mass calculation in real-time with a differential mobility spectrometer. Journal of Aerosol Science.
[69]. Tao, F., Srinivas, S., Reitz, R.D. and Foster, D.E. (2005) Comparison of Three Soot Models Applied to Multi-Dimensional Diesel Combustion Simulations, JSME International Journal, Series B, 48(4): p. 671-678
[70]. Thring, R. H. (1989) Homogeneous Charge Compression Ignition (HCCI) En-gines". SAE Paper No. 892068, 1989.
[71]. Tree, D.R. and Svensson, K.I. (2007) Soot processes in compression ignition engines. Progress in Energy and Combustion Science.
[72]. Turns, S.R. (2000) An Introduction to Combustion: Concepts and Applications. 2nd ed., McGraw-Hill, Singapore.
[73]. UK Greenhouse Gas Statistics and Inventory Team. (2013) Science and Innovation Group, DECC.
[74]. U.S. Department of Energy. (2001) Homogeneous Charge Compression Ignition Technology - A Report to the U.S. Congress, Technical report.
[75]. United States Environmental Protection Agency. (1990) Clean Air Act Title II Part A – Motor Vehicle Emission and Fuel Standards.
[76]. Urushihara, T., Hiraya, K., Kakuhao, A. and Itoh, T. (2003). Expansion of HCCI Operating Region by the Combination of Direct Fuel Injection, Negative Valve Overlap and Internal Fuel Reformation, SAE Paper No. 2003-01-0749.
[77]. Waldman, J., Nitz, D., Aroonsrisopon, T., Foster, D. and Iida, M. (2007). Experimental Investigation into the Effects of Direct Fuel Injection During the Negative Valve Overlap Period in a Gasoline Fueled HCCI Engine, SAE Paper No. 2007-01-0219.
[78]. Wan M. W. M. F. (2011) Computational studies of soot paths to cylinder wall layers of a direct injection diesel engine. PhD thesis, University of Nottingham.
[79]. Wang, R.C., Fang, T. and Lee, C.F. (2006) Comparisons of computed and measured results for a HSDI diesel engine operating under HCCI mode. SAE Papers, 2006(2006-01-1519).
[80]. Yao, M. Zheng, Z. and Liu, H. (2009) Progress and Recent Trends in Homogeneous Charge Compression Ignition (HCCI) Engines". Progress in Energy and Combustion Science, in press.
[81]. Zhang. (2009) Detailed Modeling of Soot Formation/Oxidation in Laminar Coflow Diffusion Flames. Ph. D Thesis in Mechanical and Industrial Engineering, University of Toronto.
[82]. Zhao, H. (2007) 'HCCI and CAI engines for the automotive industry', p. 12, Woodhead Publishing Limited, ISBN 978-1-84569-128-8.