POTENTIAL OPTION FOR COMPUTATIONAL FLUID DYNAMIC (CFD) SCHEME IN BIODIESEL STUDIES: A REVIEW

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ABSTRACT

Biodiesel fuel represents a unique opportunity in the current global energy scenario owing to its sustainability, renewability and potential to be universally accessible. Experimental and analytical works have established a mismatch between fuel chemistry and current diesel engine design. This, to some extent, accounts for observed challenges in performance and emissions from engines running on biodiesel. Computational schemes have played an increasingly important role in defining the scope of these challenges. Computational models’ reliability has improved over time in predicting engine performance and emissions. Identifying a combustion strategy that works best for biodiesel is a research imperative. This review presents some of the strategies that have the potential to enhance biodiesel’s advantages and mitigate the observed challenges.

Keywords: Biodiesel, Fuel chemistry, Performance, Emission, Model, Novel engine.

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1. INTRODUCTION

On the global energy scene, the challenge of increasing demand, accelerating depletion rate of fossil fuel, and negative environmental impact of unregulated use of conventional energy sources makes advocacy for renewable energy source (RES) an imperative. On the demand side, based on British petroleum estimates, global energy consumption is estimated to be 9.7 Gtoe with a significant proportion consumed in North America. This region’s demand is projected to grow at 1.5 % from 2002 to 2030. The Asia Pacific region will grow at 3.9 % within the same period and global energy demand is expected to be peak at 16. 487 Gtoe by the year 2030 [1]. The observed trend in demand growth shows that developing and
underdeveloped regions have higher scope for demand growth than developed regions such as North America and Europe, therefore demand strain will only get more challenging. On the supply side, finite fossil fuels (petroleum, natural gas and coal) account for 80% of global energy consumption. Nuclear energy as at 2009 accounted for about 13%, with renewable energy consumption filling the remaining gap [2]. Petroleum derived energy sources have a checkered history, with 63% of global oil reserves occurring in the Middle East. Given its finite nature, peak oil is projected to occur between 2015 and 2030 [1]. The highly localized nature of oil finds comes with significant geopolitical risk and this has often precipitated conflict, price fluctuations and supply uncertainty. The existential threat posed by any potential accident ensuing from the use of nuclear energy has heighten public resistance to its proliferation. After Chernobyl and Fukushima, a phasing out policy regarding nuclear energy has been adopted in Japan and Germany [3]. This is an indication that in the energy spectrum, supply from fossil and nuclear sources are constrained going forward. Added to these points are the issues of environmental sustainability. Griffin [4] and many others have stated that increasing use of petroleum fuel will intensify global warming caused by carbon dioxide (CO2) emissions not to mention the other countless health risks posed by the unregulated emission of oxides of nitrogen (NOx), soot, carbon monoxide (CO), unburnt hydrocarbon (UHC) and aldehydes [5]. Against these backgrounds, renewable energy sources have been identified as the only energy sources that meet the sustainability criteria. It is evident that a significant percentage of energy is consumed in the transportation sector and since the internal combustion (IC) engine is a key component, the renewable energy source options available in that sector will play a vital role in the drive toward sustainability. Biodiesel has been identified as a viable option in this regard.

Biodiesel is composed of fatty acid methyl esters (FAME) produced from vegetable oil or animal fat through a trans-esterification process. This is achieved using alcohol in the presence of an alkaline catalyst. Besides being carbon neutral, the use of biodiesel in internal combustion engines has been reported to result in the reduction of CO, UHC, particulate matter (PM) and soot precursor emissions [6]. Its primary challenge has been a marginal drop in engine power [7, 8], increases in oxides of nitrogen (NOx) emission at high combustion temperature [9, 10], poor reactivity leading to higher emission of CO and UHC at start-up, and low load conditions due to poor flow properties at low temperatures. These advantages and challenges have triggered intense research efforts aimed at finding combustion strategies that can harness the potential of biodiesel and mitigate the challenges obstructing its wider application.

Given the size of the parameters, properties and system features that need to be controlled, monitored and evaluated in combustion studies, direct physical experimentation is often unhelpful. The most efficient means to conduct combustion studies, in terms of cost and research time, is through numerical methods. This can be accompanied by well-targeted experiments to obtain data for validation purposes. This approach requires a careful selection of study parameters that closely approximate the physical reality being investigated. Combustion is a multi-phase, multi-state and thermally intense process with significant levels of thermal and charge stratification. As a result of these, surrogate chemical kinetic mechanisms that closely represent the chemical properties and processes of the charge to compute the chemistry need to be selected. The physics of flow process and thermal exchange also guides the selection of the model that will compute the flow and thermal behaviour of the charge.

A computational approach to research on the internal combustion engine (ICE) and engine development has had a long and successful history. Progressive applications of models with increasingly higher fidelity alongside state-of-the-art engine diagnostic tools have resulted in
the full resolution of most important processes in fuel combustion in ICE, making it possible to predict engine performance and emissions with increasing levels of accuracy, and to develop novel combustion strategies that improve performance and mitigate or eliminate undesirable emissions. The convergence of biodiesel potential with the capability of computational fluid dynamics (CFD) is improving the chances of a perfect ‘green ICE’. A perfect green ICE would be where a carbon neutral fuel source produces zero UHC, CO, NOX and PM with a higher cycle efficiency. Computational studies in ICE often involve the use of chemical kinetic mechanisms, appropriate flow models with multi-scale (spatial and temporal resolution) and multi-phase capability, coupled with the use of specific experimental data obtained with appropriate engine diagnostic tools for validation purposes of any given combustion strategy.

2. NUMERICAL TECHNIQUES AND ENGINE DIAGNOSTICS

The application of numerical techniques ranges from simple general processes with approximation using zero dimensions (0D) to fully resolved 3D or 4D (space and time) CFD simulations. The former is more cost effective in terms of CPU runtime and hardware. However, significant errors are associated with the former in comparative terms. Length and time scale in ICE plays an important role in model fidelity. Length scale in ICE ranges from angstroms (10^{-10} m, atomic/molecular process), to several nanometres (10^{-9} m, soot precursor) to micrometers (10^{-6} m, spray droplets), to a fraction of millimetre (10^{-3} m, smallest aerodynamic flow scales), to centimetre (10^{-2} m, cylinder diameter). Time scales range from picoseconds (10^{-12} s), to nanoseconds (10^{-9} s), to microseconds (10^{-6} s), to milliseconds (10^{-3} s) and through to seconds (s) [11], as illustrated in Figure 1.

The range of simulation approaches applicable to combustion systems include: quantum mechanics (QM) which describe intra-atomic processes for a small number of atoms; molecular dynamics (MD); the kinetic Monte Carlo (KMC) method which describes intermolecular activities for a population of molecules; and continuum mechanics that describe chemical and physical activities at the macro-scale.

Continuum mechanics have currently three identifiable categories based on their range for resolved spatial and temporal scales. They consist of: direct numerical simulation (DNS) where the continuum-mechanics governing equations are solved directly and all relevant continuum scales are resolved; large eddy simulation (LES), where spatially filtered forms of the governing equations are solved and the dynamics of large scales are captured explicitly
while the effects of small scales must be modeled; and finally Raynold-averaged Navier-Stokes (RANS) where the probabilistic averaged forms of the governing equations are solved and the effects of any fluctuation about the average must be modelled. Figure 1 shows the time and length scale for the various simulation approaches.

An example of a typical DNS fully resolved simulation of a turbulent, premixed, methane-air, slot Bunsen flame with chemical model consisting of just 12 reactive species had a computational domain decomposed of 200 million cells. The simulation itself was performed by 7000 processors on a CrayXT3 machine [11]. This basically underscores the challenges associated with the use of high-resolution techniques such as QM, MD and KMC. Currently, only RANS and to some extent, LES are practicable for ICE studies, given the current computing resources available. These computations are done in zero dimension (0D), one dimension (1D) and 3D.

2.1. Application of Numerical Simulation

As a result of advances in computing power, numerical simulation has assumed an important position in theoretical studies of combustion processes in internal combustion engines, particularly for biodiesel powered engines. Five categories of application are currently in use and are discussed below.

2.1.1. Zero-Dimensional Single-Zone Model with Detailed Chemistry

A zero-dimensional single-zone model with detailed chemistry is the simplest model in engine simulation. In this approach, the engine is modelled using the first law of thermodynamics by resolving the work absorbed/produced by the piston and the heat exchange between charge (not in all cases), but not the mass blow-by. In this model, the thermodynamic (pressure, temperature, composition) and transport (viscosity and conductivity) properties are considered homogenous. Since temperature and charge stratification are not considered, this model tends to overestimate the heat release rate, pressure rise and maximum combustion pressure. The model also experiences difficulties in describing the formation of UHC and CO [12] because of the assumed charge homogeneity, particularly in HCCI engines. Apart from these limitations, this model can be used to effectively estimate ignition timing and the formation of NOX emissions. This is because both events are linked to the highest temperature region which is therefore also linked to the mean gas temperature. This model can be used as an effective tool in comparing the closeness or accuracy of a reduced chemical kinetic to that of a detailed chemical kinetic [11]. The ability of this model to assess the relative importance of a chemical reaction is an important advantage because it helps to fast-track the process of developing new reduced mechanisms for use in biodiesel studies [13]. In addition, this model strategy can be adopted to study the combustion chemistry of not only neat biodiesel but also various blends of biodiesel/diesel, biodiesel alcohol/diesel etc. and their effect on ignition timing, fuel emissions of NOX and behaviours in HCCI control strategy since these represent the future of combustion research on biodiesel [14].

Brakora and Reitz [15] conducted a zero-dimensional single-zone model study using the SENKIN code of the CHEMKIN package where the zone was considered adiabatic for study purposes in order to investigate the formation of NOX from biodiesel and diesel fired HCCI engines. The diesel surrogate was n-heptane and a mixture of 2/3 n-heptane and 1/2 methyl butanoate was used as the biodiesel surrogate. This proportion was found to yield a better C:H:O approximation of the biodiesel ratio for real biodiesel than either the neat methyl butanoate or methyl decanoate. For the biodiesel, the chemical reaction mechanism consisted
of 56 species and 169 reactions [16]. The NOX formation mechanism was included by [16] via 7 species and 19 reactions as developed by Yoshikawa and Reitz [17].

It was observed that ignition timing played an important role in the formation of NOX. With similar energy release and the same ignition timing, the two surrogates produced approximately the same (separated by only 20 k) peak combustion temperature and a similar yield of NOX emission at the exhaust valve opening (EVO). It was difficult to establish a connection between the oxygen content of the fuel to the produced NOX emissions. NOX in the biodiesel was 26 % higher than in the diesel surrogate. However, the peak temperature was about 13 k lower for the biodiesel. This indicates that fuel bound oxygen could play a role in NOX formation under limited O2 concentrations. In the same study, it was observed that under the same energy content ignition timing and total N:O ratio for the two fuels, diesel yielded higher NOX emission. This implies that having the same amount of oxygen in the air as opposed to only that in the fuel-bound oxygen increases NOX emission because of the alteration of the heat capacity of the mixture which gives rise to higher flame temperature for the diesel surrogate.

2.1.2. Multi-Zone with Detailed Chemistry: Quasi-Dimensional

One way to deal with the problems associated with the use of a single zone model is to deploy a multi-zone model. In this model the combustion chamber is divided into several regions or zones with each zone possessing uniform thermodynamic properties. The acceptable number of zones is determined by a sensitivity analysis where the minimum number is defined as the number beyond which the simulation results tend to converge. Each zone is initialized by different initial parameters. Mass and heat transfer between the zones can be assumed. Normally, crevices and boundary layers (low temperature zones) are included to obtain good resolution of UHC and CO production for HCCI combustion. A number of works on multi-zone have been published often with differences between them being based on any of the following: the number of zones, the type of zone (e.g. adiabatic core zones, boundary layers, crevices and mass exchange zones) and the types of interaction between the zones (pressure-volume work, heat transfer, mass exchange). They are described as quasi-dimensional because they represent crevices, core zones and boundary layers.

Fiveland and Assanis [14] developed a comprehensive quasi-dimensional model to predict performance and emissions particularly under turbo-charge conditions. It is a full cycle simulation code with an adiabatic core, a predictive boundary layer model and crevice region. The unburned thermal boundary layer is driven by compressible energy considerations and hence is of varying thickness and is resolved at multiple geometries along the piston line interface. Given the thermal gradient between the adiabatic core and the boundary layer, there is an enthalpy flux and turbulent interaction between them. The adiabatic core is a perfectly stirred reactor with turbulent mixing and interacts with the piston via work transfer. The model gave a good result for UHC but the CO results were not satisfactory due to lack of detailed thermal resolution at the near wall regime (See Figure 2).
2.1.3. Detailed Chemistry with One-Dimensional Engine Cycle

The limitation of the zero-dimensional and the quasi-dimensional model described above is that these models only capture engine processes at the start of intake valve closure (IVC) and the end of EVO. This means that initial parameters have to be specified at IVC. This is often riddled with difficulties because average mixture temperature, equivalent ratio and residual gas fraction (RGF) are difficult to determine. To overcome these challenges, the aforementioned models are combined with engine cycle stimulation codes which can compute the parameters at IVC. These one-dimensional codes predict engine parameters from air intake to exhaust pipe. Given that the computation includes a complete engine cycle, the gas exchange processes can be modeled.

Ogink [18] produced a SENKIN-BOOST single-zone model which predicted auto-ignition timing and heat release rate for a HCCI gasoline engine. Variable valve timing (VVT) impact on gas exchange processes in HCCI engines was studied by Milovanovic et al. [19]. Gasoline was used in both the experimental and simulation studies. The simulation was executed with the Aurora detailed chemical kinetic code from CHEMKIN III with the ID fluid dynamic Lotus engine simulation (LES) code. This model was extended to include the SENKIN-BOOST multi-zone detailed chemical kinetic [20] to accurately predict fuel consumption, emission and indicated mean effective pressure (IMEP) for various ranges of experimental conditions.

2.1.4. 3D CFD with Detailed Chemistry

Multi-dimensional fluid dynamics with detailed chemistry has the best potential to predict more accurately engine activities when the complete geometry of the combustion chamber is fully resolved and detail kinetic chemistry is employed to evaluate chemical events. The computational resources for such procedures are significant and depend on CFD mesh resolution and the size of the chemical kinetic mechanism.

Agarwal and Assanis [21] performed a simulation of natural gas ignition consisting of detailed chemical kinetic mechanisms of 22 species and 104 reactions using the multi-dimensional CFD reacting flow code KIVA-3V. The purpose was to explore auto-ignition of natural gas injected into a quiescent chamber in CI-like conditions. The complete kinetic was executed up to the ignition point. Kong et al. [22] used a similar approach up to ignition point, but for post-ignition a reaction rate with chemical kinetic and turbulent mixing was
incorporated. The turbulent time scale was the time for eddy break-up, while the kinetic time scale was the time needed for a species to reach the equilibrium state under perfect-mixing conditions. Kong et al.’s [22] numerical scheme also studied the effect of turbulence on premixed iso-octane HCCI engine using a numerical scheme. Their model used the KIVA code modifiers and CHEMKIN as the chemistry solver. HCCI was found to be impacted by turbulence with its main effect being wall heat transfer. The result gave a hint that it is better to incorporate detailed chemistry in CFD codes for HCCI evaluation to better understand the effect of turbulence on wall heat transfer. In addition, it was observed that ID onset of ignition is highly sensitive to initial conditions, hence a higher level of accuracy at initial state is essential for good prediction, further underscoring the importance of detailed chemistry and complete resolution of flow conditions. Tominaga et al. [23] evaluated the effect of inhomogeneous distribution of exhaust gas recirculation (EGR) within the combustion chamber using multi-dimensional CFD with detailed chemistry for natural gas. The result showed that when EGR is densely located in low temperature zones (near walls and crevices), its effect on combustion is reduced compared to when its distribution is homogenous. But when EGR is density packed in high temperature zones (near the cylinder centre) its effect is more pronounced and it tends to moderate combustion as opposed to when it is uniformly distributed.

3. ENGINE DIAGNOSTICS
Optical diagnostics have evolved as an effective means by which in-cylinder processes can be effectively observed, after having been discovered in 1979 [24, 25]. This approach possesses the capability to deliver comprehensive as well as detailed information on flow pattern, species and temperature distribution with high spatial and temporal resolution in a combustion chamber. Its non-intrusive in-situ techniques which enable non-interference in flow or combustion processes are valuable features that make it an essential tool in validation of combustion modeling results [25].

3.1. Diagnostic for In-Cylinder Charge / Air Mixing
Optical diagnostics are frequently used to evaluate the in-homogeneity in fuel distribution and temperature in the pre-mixture in HCCI and their effects on auto-ignition and combustion processes.

Richter et al. [26] used planner laser induced fluorescence (PLIF) in HCCI to evaluate distribution of fuel and OH in the combustion chamber. The author achieved homogeneity of mixture by using two different premixing procedures. The first was the standard port injection and the second was the use of a 20 L preheated mixing tank. The PLIF confirmed that fuel preparation affects the fuel/air homogeneity and inhomogeneity had a modest effect on spatial variation of the combustion process. Lida et al. [27, 28] used a framing camera with an optically accessible engine to build a 2D images of the chemiluminescence of the engine charge. Di-methyl ether (DME) was the test fuel. Various optical diagnostics have been deployed to observed in-cylinder mixture formation and many have suggested (as a result of these observation) practical ways such as stratified charge compression ignition (SCCI), premixed charge compression ignition (PCCI), and low temperature combustion (LTC) as a means of increasing the high load limits for HCCI.

3.2. Optical Diagnostic for Combustion Process

3.2.1. Chemiluminescence and Spectral Analysis
Glassman [29] stated that chemiluminiscence normally starts at low temperatures because of the relaxation of excited combustion radicals in their base. This normally indicates the start of exothermic reaction (fuel oxidation and heat release) for diesel fuel, which involves two aspects. Chemiluminiscence and soot luminosity. Chemiluminiscence in diesel originates from the visible and near ultraviolet band due to OH, CH, CH\textsubscript{2}O and C\textsubscript{2} radicals [30]. Even though this occurs after the start of ignition (SOI), it often comes with weak signals. An intensified charge coupled device (ICCD) camera is normally deployed to observe these early non-luminous flames. It has been observed that although chemiluminiscence exists for the entire length of the combustion process, it is effectively drawn-out by the much stronger radiation from soot luminosity. It has been further stated that soot signal is not a good marker for tracking the flame front because it only represents rich-burn (\(\phi > 1\)) areas. The same problem is encountered when spectral analysis is adopted. But these two methods can be used for low soot regime combustion strategies like SI and HCCI. And, significantly, biodiesel combustion diagnostics where soot precursors are minimal.

Kawahara et al. [31] evaluated the combustion of DME in an HCCI regime with a single cylinder using chemiluminiscence spectral analysis. It was observed that light emission from HCHO appeared at LTR as predicted by Emeleons cool flame band. The CO-O recombination spectrum was strong in the course of the main heat release. This signifies a strong correlation between rate of heat release (ROHR) and CO-O recombination.

Mancaruso et al. [32] studied the auto-ignition and combustion of HCCI in a CI engine using the common rail system. The fuel injection was staggered in five split succession. The ultra-violet-visible imaging and spectra indicated the presence of HCO and OH evenly distributed within the chamber. The process appears to be dominated by OH radicals and it was observed that the radicals significantly reduce PM in the chamber. Another observation was that OH radicals are a good indicator of the start of high temperature combustion.

Person et al. [33] studied the early development of flame in spark assisted HCCI by employing high speed chemiluminescence imaging. It was observed that even for large negative valve overlap (NVO), resulting from early closure of the exhaust valve and late opening of the inlet valve to achieve EGR strategy, it is the growing SI flame that controls the next HCCI combustion. It was concluded that spark timing could be deployed to phase the combustion timing despite the HCCI being responsible for the major heat release.

### 3.2.2. Planar Laser Induced Fluorescence (PLIF) Diagnostic

When an atom or a molecule has a laser beamed on it, the beam causes excitation which leads to emission of light (fluorescence) from the atom or molecules. Laser induced fluorescence (LIF) in its early stage of development was driven by single point measurements, but subsequent application of LIF in ICE has led to multi-point planar imaging. Planar laser induced fluorescence (PLIF) is a modern means by which flow can be visualized. PLIF is useful in qualitative as well as semi-quantitative characterization of flow. It provides spatial resolution of flow in a plane rather than integrating over line of sight. The PLIF has more fluorescence strength than Rayleigh and Raman [34] scattering and hence is more widely applied than the latter. Furthermore, PLIF can reveal the presence of intermediate species like formaldehyde (HCHO), making it possible to determine spatial as well as temporal detection of auto-ignition precursors prior to the observation of chemiluminescence early in the cool flame.

It has been determined from chemical kinetic mechanisms that in HCCI combustion, formaldehyde (HCHO) and OH radicals constitute important intermediate and active radicals prior to auto-ignition. This implies that ignition and the subsequent combustion process can be mapped by tracing the distribution of HCHO and OH.
Collin et al. [35] used a blend of iso-octane and n-heptane in an HCCI engine to simultaneously measure OH and formaldehyde (HCHO) using LIF. At the beginning of LTC, dense formation of HCHO was detected which continued to grow as LTC progressed. At the end of LTC, HCHO filled the entire measured region. OH signal was only picked up with PLIF when HCHO was absent. Peak OH was only observed when most fuel had been consumed (which occurred close to peak temperature). This, and the work of Sarner et al. [36], shows that HCHO is feasible as a fuel tracer for studying fuel visuals in HCCI at the LTR region.

4. HCCI MODEL STRATEGIES FOR BIODIESEL AND VALIDATION

A major concern for the application of biodiesel as transport fuel, on the performance and emission side, has been a reduced efficiency due to marginal differences between its heating value and that of diesel, and a tendency to emit higher NO\textsubscript{X} in comparative terms to diesel because of the oxygenated nature of the fuel which makes it susceptible to high NO\textsubscript{X} production at elevated temperatures. This challenge places HCCI in the spotlight as the most viable combustion strategy to deploy in biodiesel applications, going forward. The reason for this is fairly obvious, as the advantages of HCCI include a significant reduction of NO\textsubscript{X} emission (because HCCI is an LTC concept), the absence of soot in the exhaust, and, because it is an un-throttled operation, it produces a higher indicated thermal efficiency. Even the challenge of high UHC and CO emission in HCCI because of bulk quenching at low loads, wall quenching, and crevice flow at high load, can be addressed using the EGR strategy of negative valve overlap (NVO). The warm/hot EGR at steady state operation will effectively improve reactivity and the fear of oxygen starvation will not materialize because of the oxygenated nature of biodiesel. Numerical as well as experimental research in this direction is beginning to bring these points to light. HCCI does have some drawbacks, which have been highlighted earlier, but overall, its potential is significant. HCCI, through intense research, has evolved to include strategies such as early direct injection (DI), late direct injection and premixed/direct-injected HCCI combustion.

At the early stage of HCCI development, when diesel was used for HCCI combustion, difficulties were encountered in the preparation of homogenous mixtures because of low volatility, high viscosity and low resistance to auto-ignition. All these challenges exist even more strongly with the use of biodiesel HCCI combustion. As a result, conditions necessary to achieve diesel HCCI combustion must be given even greater attention in biodiesel HCCI. These conditions include mixture control (both charge component and temperature), and high pre-ignition mixing rate. Ryan et al. [37] and Grey et al. [38] used port injection in their study to achieve this. They, along with Christensen et al. [39], found out that port injection in HCCI for diesel reduced NO\textsubscript{X} emission but the smoke emission was significant and this was attributed to poor vaporization of the fuel leading to an inhomogeneous mixture. It was also observed that to reduce the likelihood of knock, the compression ratio had to be reduced. These early challenges were what informed the development of other injection strategies.

4.1. Early Direct Injection in HCCI

Early DI strategy was proposed in anticipation of its capacity to mitigate some of the challenges associated with port injection in HCCI. The strategy, in comparison to port injection, has three key advantages, including: (1) Injecting fuel during the compression stroke means that the high pressure and temperature effectively vaporizes the fuel and promotes good mixing. This permits cooler intake temperature and reduces the risk of early ignition; (2) With a carefully designed injector, fuel wall wetting is avoided which also reduces combustion inefficiency; (3) In theory, only one fuelling system is used for both
HCCI and conventional CI operation. However, early DI in HCCI increases the possibility of wetting, which constitutes the main disadvantage of this strategy. Several versions of this approach have been developed and are discussed below.

4.1.1. Premixed Lean Diesel Combustion (PREDIC)

Takeda et al. [40] and Nakagome et al. [41] described a DI HCCI strategy conducted by the New ACE institute in Japan. Early results from this study showed very low NO\textsubscript{X} and smoke emission but the UHC emission and fuel consumption increased beyond levels observed in conventional CI engines. This was attributed to poor combustion efficiency and advanced combustion phasing. In a bid to reduce fuel spray over-penetrating and wall wetting which produces UHC and combustion inefficiencies when injection is executed well ahead of top dead center (TDC) (when air density and temperature in the combustion chamber are low), three injectors were employed – one at the centre and two on the sides. The injectors on the sides were positioned such that their flows were made to collide at the centre to prevent wall wetting. The nozzle at the centre had its diameter reduced from 0.17 mm to 0.08 mm and hole number was increased from 6 to 16. To overcome early ignition, special fuel blends with cetane numbers between 19 and 40 were developed. Employing these changes, the engine could be operated with PREDIC. A subsequent work on the strategy reported the development of swirling flow achieved with a pintle-nozzle injector [42] which produced a more uniform mixture and improved efficiency.

A follow-up work to scale-up power density was initiated with a second injection near TDC [43]. This was achieved with dual side-mounted impinging-spray injectors to obtain a lean premix charge while a centre-mounted injector was deployed to execute the second injection near TDC. The NO and PM in this approach were much higher than in the normal HCCI but lower when compared to conventional CI strategy. Smoke emission was decreased but UHC was higher. Akagawa et al. [44] used this approach to study the effect of EGR rate and oxygenated fuels on fuel consumption, UHC and CO emission. Much higher loads were achieved at low NO\textsubscript{X} emission but at the cost of higher fuel consumption.

4.1.2. UNIBUS

Yanagihara et al. [45] used HCCI combustion with diesel fuel (Toyota UNIBUS). The UNIBUS approach adopted here was operated up to half load and half speed. Mixture preparation was key in this strategy. A piezo-actuator with a pintle size nozzle to reduce spray penetration was used. The strategy involved early injection around 50°BTDC (before top dead center) and late injection around 13°ATDC (after top dead center). Most of the data were obtained at a compression ratio of 12:1 to avoid early combustion of premixed charge. The parameters under investigation were: impact of injection timing, level of fuelling, EGR rate, double injections on emissions, torque, instantaneous heat release, and load. The results generally showed negligible PM emissions. 60 % EGR rate was shown to delay HCCI combustion by about 7° crank angle.

It was clearly established that a dual-injection strategy was feasible. At the second injection, 50 % of the fuel was introduced which significantly improved combustion efficiency of the first injection, reducing UHC emission by about 60 % and CO emission by about 75 %. The second injection can thus be considered as the trigger. Although, the NO\textsubscript{X} increased from a near zero level, the increase was still less than what was obtained with a conventional CI diesel strategy. However, fuel consumption penalties were still a challenge.

4.1.3. MULINBUMP
Su et al. [46] proposed a diesel HCCI strategy called MULINBUMP (so named because it is a flash mixing technology which evolved from the so-called BUMP combustion chamber designed with a special bump ring). These strategies combine premixed combustion with “lean diffusion combustion”. The premixed combustion was achieved using multi-pulse fuel injection. The start of pulse injection, pulse number, pulse injection period for each pulse, and the dwell between each pulse, were controlled. The main objective of the control was to prevent wall impingement of fuel and to enhance the mixing rate of each pulse parcel. The last pulse was set at TDC. The bump ring enhances the flash mixing and enables a fuel/air mixing rate higher than a conventional DI diesel engine. The auto-ignition and heat release rate for this strategy were investigated. By advancing the start of multi-pulse injection, noisy auto-ignition was avoided (reduced knock) but over advancing of start timing led to over-mixing resulting in higher THC emission. It was observed that a small amount of fuel in multi-pulse injection did not lead to a reduction in NOX emission hence, an increased amount was advocated.

This strategy has the potential to widen the operating conditions of the HCCI engine, the basic idea behind this strategy being that: (1) at low load HCCI control is established via multi-pulse fuel injection which enables very low NOX and PM emission (< 10 ppm) (2) At medium to high load the advantage of premixed combustion with “lean diffusion combustion” is improved further by super high injection pressure which ensures clean and high efficiency that can be achieved at the full load range. An indicated mean effective pressure (IMEP) of 0.93 MPa was achieved with this approach [24].

4.1.4. Small Angle Injection

It has been well establish that small angle (narrowing of angle) of the fuel spray cone reduces wall wetting and piston head wetting at early injection timing while maintaining high efficiency for HCCI combustion [47-50].

Kim and Lee [51] examined this phenomenon using two different injection nozzles with spray cone angle of 156° and 60° in HCCI combustion. In this study, the compression ratio was reduced from 17.8:1 to 15:1 in a bid to prevent early ignition of the early premix. Results obtained revealed that for a conventional CI engine the IMEP decreased rapidly as injection timing was advanced beyond 20° BTDC and indicated specific fuel consumption (ISFC) data became unacceptably high. Early injection helped create HCCI combustion but lead to poor fuel evaporation and piston bowl spray impingement leading to high UHC and CO emission.

It was further observed that there was a modest decrease in ISFC for the IMEP although the injection timing was advanced to 50° to 60° or the smaller cone angle injector. This shows that a small angle cone is effective for early injection in HCCI.

4.2. Late Direct Injection in HCCI

The modulated kinetic (MK) combustion system developed by Nissan motor company was the most successful late injection HCCI strategy. This strategy was discussed by Kawashima et al. [52, 53] and Kimura et al. [53]. To achieve the diluted homogenous mixture needed for HCCI, a long ignition delay and rapid mixing is required. In their study, Kimura et al. [53] achieved ignition delay by retarding injection timing from 7° BTDC to 3° ATDC and using a higher EGR to lower oxygen concentration of 15 % to 16 %. Rapid mixing was accomplished by using high swirl with toroidal combustion-bowl geometry. The operating range for the
first-generation MK was limited to 1/3 peak torque and 1/2 speed. This MK mode substantially reduced NO\textsubscript{X} to about 50 ppm without any increase in PM. Combustion noise was also reduced. In this strategy, combustion phasing is controlled by injection timing.

The second generation MK expanded the range of operation by means of several modifications [54]. Higher injection pressure (through a high pressure common-rail fuel supply) was executed to reduce fuel injection time at all speeds. The ignition delay was increased by reducing compression ratio and adding EGR cooling to reduce intake temperature. To reduce fuel spray wall impingement, the piston bowl was increased from 47 mm to 56 mm. This significantly reduced UHC emissions during cold start. It was observed that the second-generation MK strategy could be used for the entire range of engine operation, and met the targets of about 1/2 load and 3/4 speed. NO\textsubscript{X} emission was reduced by 98 % compared with conventional EGR, and PM emissions were similar to those of a conventional CI engine.

Recent work on MK by Kawamoto et al. [55] recommended higher CN fuel to reduce UHC in cold start conditions. The most strategic advantage of MK is that it does not require additional hardware and its operation with existing hardware does not negatively impact the engine’s specific power output. However, the injection timing retardation reduces engine cycle efficiency and gives rise to higher UHC emissions [24].

4.3. Premixed/DI HCCI

In this strategy, port injection is adopted as the primary fuel supply source to create a homogenous charge and the DI fuel injection subsequently is used to change the concentration and special position of the rich regions with the aim of controlling HCCI combustion.

Odaka et al. [56-59] proposed a homogenous charge compression ignition diesel combustion (HCDC) approach which used the premixed/direct-injected HCCI system. In this system, most of the fuel was injected into the intake manifold to form a homogenous premixture in the cylinder and a small amount of fuel was directly injected into the homogenous premix in the cylinder. This strategy reduced both NO\textsubscript{X} and smoke emission better than a conventional CI engine. It was also observed that smoke was reduced uniformly as the premixed fuel ratio increased.

Midlam-Mahler et al. [60-62] built a premixed/direct-injected HCCI system. A low pressure atomizer system was employed to achieve port/manifold fuel injection and a high pressure injection system was employed for the direct injection of fuel into the combustion chamber. In low load mode, the main torque came from the premixed lean homogenous fuel and the DI fuel only served to initiate ignition at high loads, the maximum homogenous charge was employed, and DI fuel proportion was increased to full load. Atomization to droplet size of less than 1 \( \mu \)m mean diameter allowed for fast evaporation during the compression stroke, making the heating of intake fuel unnecessary. Results obtained showed that by varying intake conditions, IMEP of up to 4.7 bar could be achieved at a speed range of between 1600 rpm to 3200 rpm. In addition, this strategy achieved very low NO\textsubscript{X} of less than 4 ppm and smoke emission of 0.02 FSN.

Foster et al. [63] and Berntsson and Danbratt [64] proposed various strategies incorporating the key components of the premix/direct-injected HCCI combustion with varying degree of success. The most interesting strategy was the use of different fuels for the different stages of the injection process in a bid to use fuel properties to greater advantage. This was developed by Inagaki et al. [65]. In this strategy gasoline (high octane, low CN) was used at the intake air-port for the homogenous premixed and diesel fuel (low octane, high CN) was injected directly into the combustion chamber at the DI stage to initiate ignition at timing BTDC. It was observed that ignition phasing of the combustion can be controlled via the
changing of fuel ratio for the two stages to the extent that combustion proceeds mildly. The operating load range where NO\textsubscript{X} and smoke emissions were 10 ppm and 0.1 FSN respectively were extended to an IMEP of 12 bars when an intake air boost system was employed.

4.4. Low-Temperature Combustion

Low-temperature combustion (LTC) is achieved in CI engines with the use of EGR. It uses a high level of dilution to reduce combustion temperature and increase ignition delay. The lengthened ignition delay gives ample time for fuel evaporation and increased fuel homogeneity in the reactant mixture, thus reducing NO\textsubscript{X} formation as a result of spikes in local temperature [24, 66]. This also inevitably reduces soot formation because of the absence of fuel rich zones. Alrikson and Dentbratt [56] calculated the Q-T map for soot and NO\textsubscript{X} concentration with the help of the SENKIN code using an n-heptane and toluene mixture as a diesel surrogate and concluded that to completely avoid NO\textsubscript{X} and soot formation regardless of equivalent ratio, local temperature must be kept below 1650 k. This is what is referred to as low temperature combustion [24]. However, research in HCCI combustion has warned that if local temperature falls below 1400 k, the oxidation rate from CO to CO\textsubscript{2} becomes too low [67]. The ideal temperature (1400 k < T\textsubscript{2} < 1650 k) becomes fairly obvious (see Figure 2). The challenge has been how to control this strategy and a significant number of research studies have been conducted with this objective in mind.

Natti [68] investigated soot and PM characteristic in a single cylinder HSDI diesel engine under CI and LTC regimes. The outcome observed that soot nucleation requires higher temperatures whilst surface growth proceeds at a lower temperature in the presence of the right hydrocarbon environment. Increased EGR was observed to kinetically slow down the reaction and give more scope for heat transfer. In conventional CI this reduced temperature sufficiently decrease oxidation but not accumulation. However, in LTC, other reactions are also hindered and as a result the accumulation mode begins to slow down and thus reduces the soot as EGR increases.

Henein et al. [69] and Choi et al. [70] studied the effect of injection pressure and swirl on engine emission under LTC. The injection pressure, swirl ratios and injection timing ranges investigated were broad in scope. Henein et al. [59] in their research used an EGR range that covered an engine operating range which encapsulated conventional CI engine and LTC regimes. They observed that combustion is sensitive to small variations in EGR particularly around the misfiring EGR limit in the LTC regime. Choi et al [70] conducted their study at 15 % O\textsubscript{2} concentration and found that an increase in injection pressure enhances mixing, resulting in increases in peak of heat release and decreased soot. The trade-off between soot and NO\textsubscript{X} at different injection pressure, swirl ratios and EGR rates, along with the misfiring threshold, were also identified. Other works on LTC are listed in the references [71-73].

5. HCCI CONTROL STRATEGY

Given the heavy dependence on charge composition, it is clear that for effective HCCI combustion, mixture and temperature control are essential tasks that require attention. Control measures for improving mixing rate of fuel include: (1) High pressure / ultra-high pressure injection and small nozzle holes, as investigated by Dodge et al. [74]; (2) High boost pressure as evaluated by Alfuso et al. [75]; (3) Design and reconfiguration of chamber geometry as studied by Su and Zhang [76]; and (4) Use of multi-pulse fuel injection using modulating injection as studied by Su et al. [46].

Aside from using mixing to control HCCI, ignition delay can also be deployed, and can be achieve by: (1) EGR using the MK system; (2) Varying of compression ratio and variable valve actuation as investigated by Reitz et al. [77]; (3) Fuel modification as studied by
Caterpillar Inc. in 2004 [78] and Scania Inc [79]. A summary of these strategies and their outcome are presented in table 1 below.

### Table 1 Combustion Strategies and Outcome

<table>
<thead>
<tr>
<th>Strategy</th>
<th>Test engine specifications</th>
<th>Outcomes</th>
<th>Reason</th>
<th>Remark</th>
<th>Ref</th>
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<tbody>
<tr>
<td>PREDIC</td>
<td>4-stroke, single cylinder, DI, NA, CI test engine</td>
<td>Low NOx, Increased CO, Higher UHC</td>
<td>Poor combustion efficiency, Advanced combustion phasing, Over-lean fuel/air mixture</td>
<td>Ensure homogeneous fuel/air mixture, Create partial load conditions</td>
<td>40</td>
</tr>
<tr>
<td>PREDIC</td>
<td>4-stroke, Single cylinder, NA, DI, CI engine</td>
<td>Low NOx, Gentle heat release pattern, Lack of ignition timing control, Higher fuel consumption, Combustion knocking</td>
<td>Self-ignition occurs near TDC, Near homogeneous fuel-air mixture</td>
<td>Proposed other methods to optimize ignition control, combustion velocity, and fuel injection system for reduction of UHC and CO.</td>
<td>41</td>
</tr>
<tr>
<td>PREDIC</td>
<td>4-stroke, Single cylinder, NA, DI, CI engine</td>
<td>Low NOx combustion near the rich limit, Improved fuel consumption, Better ignition delay</td>
<td>Use of oxygenated fuel, Gaseous fuels added to the intake air</td>
<td>KIVA-II software was adopted, Oxygenated fuel was used</td>
<td>42</td>
</tr>
<tr>
<td>MULDIC</td>
<td>4-stroke, Single cylinder, NA, DI, CI engine</td>
<td>Reduced NOx and smoke emissions, Higher fuel consumption, Improved thermal efficiency</td>
<td>Premature ignition and extremely late ignition for first and second stage combustion, Optimization of combustion led to increased constant volume combustion</td>
<td>Application of MULDIC reduced NOx emission with more than 50%</td>
<td>43</td>
</tr>
<tr>
<td>PREDIC and MULDIC</td>
<td>4-stroke, Single cylinder, NA, DI, CI engine</td>
<td>NOx reduced to 1 g/kWh, Reduced UHC and CO emissions, Improved fuel consumption</td>
<td>Application of EGR and oxygenated fuel</td>
<td>Modified KIVA-II used to improve autoignition, and combustion sub models</td>
<td>44</td>
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<td>UNIBUS</td>
<td>3 litre, 4-cylinder DI common rail, APIS</td>
<td>Extremely low NOx, Low temperature oxidation, Combustion image</td>
<td>Applications of Common Rail injection systems and multi-hole type nozzle</td>
<td>Application of UNIBUS and image intensifier</td>
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<td>MULINBUMP</td>
<td>Modified heavy-duty truck, DI CI engine</td>
<td>Reduced NOx and soot emissions, Higher UHC emissions</td>
<td>Advancing the start timing of multi-pulse injection</td>
<td>Use of BUMP-V combustion chamber</td>
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<td>Small Angle Injection</td>
<td>Single cylinder DI CI engine</td>
<td>Zero PM and NOx emissions, Improved fuel efficiency</td>
<td>Application of NADITM</td>
<td>Application of Valve Actuation (VVA), Variable Compression Ratio (VCR) engine or electric assisted turbocharger</td>
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<tr>
<td>Small Angle Injection</td>
<td>4-stroke, single cylinder, DI CI engine based on</td>
<td>Reduced NOx, smoke, and BSFC, Low UHC emission</td>
<td>Fuel injection timing near TDC, High cetane fuel</td>
<td>Application of dual mode combustion system is proposed</td>
<td>48</td>
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<tr>
<td>Strategy</td>
<td>Test engine specifications</td>
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<tr>
<td>Small Angle Injection</td>
<td>ISUZU 6H series</td>
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<td>localized bright soot incandescence</td>
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<td>reduction in dual injection conditions</td>
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<td></td>
<td>Low combustion efficiency</td>
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<td>Reduced NO PLIF signal levels</td>
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<tr>
<td>HCCI</td>
<td>Single cylinder SCORE</td>
<td>Reduced NOx and PM emissions</td>
<td>Application of numerical, optical, CFD calculations and experimental approaches</td>
<td>Application of optical diagnostics in transparent engines Application of SPACE LIGHT diesel HCCI concept</td>
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<td>Improved thermal efficiency</td>
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<tr>
<td>Narrow cone angle injection</td>
<td>Single cylinder DI, CI</td>
<td>Reduced NOx and CO emissions</td>
<td>Effective dual injection</td>
<td>Narrow spray cone angle injector with a dual injection strategy was effective in reducing NOx and CO emissions.</td>
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<td></td>
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<td>Improved combustion efficiency</td>
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<td>Variable swirl intake port</td>
<td>4-cylinder DI CI engine</td>
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<td>Use of experimental and analytical procedures</td>
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<td>Single cylinder DI engine</td>
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<td>Improved combustion efficiency</td>
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<tr>
<td>Modulated Kinetics</td>
<td>Single cylinder DI engine</td>
<td>Reduced NOx and smoke emissions</td>
<td>Application of low compression ratio, EGR cooling and high injection pressure Optimization of combustion chamber specifications</td>
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<td>Modulated Kinetics</td>
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<td>Reduced NOx, smoke and UHC</td>
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<td>HCDC</td>
<td>4-stroke single cylinder DI</td>
<td>Reduced NOx and extremely low smoke</td>
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<td>Effective combination of EGR and HCDC</td>
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<tr>
<td>HCDC</td>
<td>4-stroke single cylinder DI</td>
<td>Extremely low emission of NOx and smoke</td>
<td>Application of optical combustion phenomena and KIVA2 software</td>
<td>Impressive emission improvement with HCDC</td>
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<td></td>
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<tr>
<td>HCDC</td>
<td>4-stroke single cylinder DI</td>
<td>Reduced NOx and smoke emissions</td>
<td>Optimization of intake charge pressure and start of injection timing Use of oxygenated fuel</td>
<td>Homogeneous pre-mixture contributed to improvement of exhaust emissions</td>
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<td>diesel engine</td>
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<tr>
<td>HCDC</td>
<td>4-stroke single cylinder DI</td>
<td>Reduced NOx and smoke emission</td>
<td>DI fuel injection timing control and EGR</td>
<td>Application of EGR, and MTBE mixing</td>
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<tr>
<td>Mixed-mode HCCI/DI concept</td>
<td>4-stroke single cylinder DI diesel engine</td>
<td>Reduced NOx and UHC emissions 50% reduction in power consumption</td>
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<tr>
<td>HCCI</td>
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<td>Reduced NOx and PM emissions</td>
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<td>HCCI</td>
<td>4-stroke single cylinder DI diesel engine</td>
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<td>4-stroke DI common rail CI engine</td>
<td>Increased EGR led to slower reaction and more transfer of heat</td>
<td>High EGR rates in the LTC regime</td>
<td>Combination of EGR and LTC</td>
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<td>4-stroke single cylinder water cooled, 4-valve DI high speed diesel engine</td>
<td>Increased EGR led to reduced NOx, and soot but increased CO emissions</td>
<td>High EGR rates in the LTC regime</td>
<td>Combination of EGR and LTC</td>
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<td>4-stroke single cylinder High speed DI diesel engine</td>
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<td>Reduced injection pressure</td>
<td>Application of heat release analysis, spray analysis, and KIVA-3V CFD</td>
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<td>LTC and EGR</td>
<td>Modified 4-stroke, single cylinder light-duty diesel</td>
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<td>Application of KIVA software</td>
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<td>EGR</td>
<td>6 cylinder, turbocharged, intercooled diesel engine</td>
<td>Reduced soot emission Slight increase in NOx emission</td>
<td>Increased injection pressure Reduced hole size</td>
<td>Faster mixing of the fuel and air in the jet</td>
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<td>Evaporative and non evaporative</td>
<td>2 stroke single cylinder loop-scavenged CI engine with optical access</td>
<td>Tip penetration increased with the injection time under non-evaporative conditions Tip penetration reached a maximum early during the</td>
<td>Decrease of the jet kinetic energy</td>
<td>Effects of tip penetration Use of imaging techniques</td>
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<td>Strategy</td>
<td>Test engine specifications</td>
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<td>Kinetic model</td>
<td>N/A</td>
<td>injection and remains constant under non evaporative conditions</td>
<td>Use of computational singular perturbation and quasi-steady-state assumptions</td>
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<td>Single cylinder, 4-valve, DI SCOTE diesel engine</td>
<td>Effective control of combustion phasing and emissions Reduced CO and PM emissions</td>
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<td>Effects of injection pressures, EGR and IVC timing</td>
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</table>


**Conclusion**

Employing numerical evaluation along with experimental investigation in biodiesel combustion studies has fast-tracked research in this area and reduced costs significantly. It has also provided deeper insight into biodiesel combustion phenomena and their interrelations. From the trend observed in these studies, it has become obvious that biodiesel fuel sources can be competitively deployed with acceptable performance and emission levels. The concept of an ideal renewable fuel source with an ideal combustion strategy in a CI engine having acceptable performance and emissions is no longer far-fetched. Further, as the technical feasibilities converge, the cost (which still poses a significant challenge to biodiesel application) will exponentially decrease to economically acceptable levels.

Although significant progress has been made, research gaps in numerical studies of biodiesel combustion requiring bridging exist at almost every level of the research effort. These gaps are highlighted as follows:

1. The weakness of methyl butanoate (MB) as a suitable chemical kinetic mechanism surrogate in numerical studies has been highlighted in the review. Added to this is the fact that MB2D lacks extensive work on unsaturated alkyl mechanisms. More retooling is needed at this level to improve computational accuracies, considering that most biodiesel sources consist of various mixtures of saturated and unsaturated fatty acid methyl esters (FAME), and that the unsaturated components are the weak link in the formation of polycyclic aromatic hydrocarbons (PAH).

2. Significantly large chemical kinetic mechanisms for studying saturated and unsaturated FAME have been proposed with the most prominent being MDBio. But these large, often detailed mechanisms, are tailored either for low or high temperature reactions and are therefore unsuitable for 3D CFD application. A single reduced MDBio that can model both low and high temperature activities is needed to aid studies in low and high temperature reactions of biodiesel in 3D CFD numerical studies.

3. HCCI multi-blend strategy, at the computational level, has not been sufficiently explored in biodiesel combustion. Even at the experimental level, researches are scant, even though the potential to effectively solve the NO\textsubscript{X} and UHC (at low temperature) in biodiesel application is substantial. Very importantly, the reconfiguration of engines to allow biodiesel...
premixed and DI as control strategies could potentially lead to a breakthrough and open the door for a wider application of biodiesel as an alternative fuel.

(4) A potentially promising HCCI strategy that has not been vigorously pursued both at the computational as well as experimental level is the use of MK for multi-blend biodiesel. Modula kinetic (MK) deployed in an HCCI environment with higher unsaturated FAME blends for homogenous premix (to delay ignition) and the use of higher saturated FAME blends as DI near TDC or ATDC to trigger ignition, is proposed. The use of NVO is proposed to achieve a mild EGR (to avoid expensive engine retrofitting) and consequently LTC. It is possible to achieve high IMEP across the full load spectrum and near zero NOX and soot emission with this strategy. A good swirl number and sufficient thermal homogeneity will result in low UHC and CO (more so because of the oxygenated nature of the fuel).

REFERENCES


Potential Option for Computational Fluid Dynamic (Cfd) Scheme in Biodiesel Studies: A Review


Potential Option for Computational Fluid Dynamic (Cfd) Scheme in Biodiesel Studies: A Review


