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Performing Computational and Experimental Evaluation of Biodiesel in Homogeneous Charge Compression Ignition Using Combined Modula Kinetic and Premixed/Direct Injection Strategy

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Abstract : Biodiesel as a renewable alternative to diesel with the capacity to reduce emissions and broaden energy access is restrained by some performance and emission concerns. A comparatively marginal drop in thermal efficiency due to lower heating value, susceptibility to emit higher oxides of Nitrogen (NO_X) at high temperatures in addition, to a higher carbon – monoxide (CO) and unburnt hydrocarbon (UHC) emission at low temperature constitutes some of the challenges. Homogenous charge compression ignition (HCCI) holds significant potential to mitigate these challenges. Modula kinetic and premixed/DI strategy in the HCCI environment is hereby proposed. Using a higher proportion of unsaturated fatty acid methyl ester (FAME) for the premix port injection as a bulk charge to delay ignition, a higher proportion of saturated FAME is proposed for use in small quantity direct injection (DI) around the top dead center (TDC) to trigger ignition. Low-temperature combustion (LTC) is achieved by exhaust gas recirculation (EGR) via negative valve opening (NVO). On the computational side, the Reynolds average Nervier – stoke turbulent model will be used to compute the physics of the flow events and MDBio in KIVA-3V will compute the chemistry. The computational model proposed is the 3D CFD with multi-zone detail chemistry (20 zones at the least). It is anticipated that high indicated mean effective pressure (IMEP) will be achieved because of the high heat release rate (HHRR) of the unsaturated FAME and the high spontaneity of combustion. Near zero NO_X and soot are envisioned since the 1650k mark will not be breached. Also, high homogeneity and the oxygenated nature of the mix will provide a designed ceiling for UHC and CO emissions.

Keywords : Thermal efficiency, Emission, Homogenous charged compression ignition (HCCI), Modula kinetic, premixed/DI, Fatty acid methyl ester (FAME), Low-temperature combustion (LTC), Biodiesel Surrogates.

1.0 Introduction

In the global energy scene, the challenge of increasing demand, accelerating depletion rate of fossil and the negative environmental impact of unregulated use of conventional energy sources makes advocacy for renewable energy sources (RES) a global imperative. On the demand segment, based on British petroleum estimates, global energy consumption is estimated to be 9.7 Gtoe with a significant proportion consumed in North America [1]. This region's demand is projected to grow at 1.5% from 2002 to 2030. The Asia Pacific will grow at 3.9% within the same period and global energy demand is expected to peak at 16487 Mtoe by the year 2030 [1]. The observed trend in demand growth shows that developing and underdeveloped regions have a higher scope for demand growth than developed regions such as North America and Europe. Indicating that demand strain will only get more challenging. On the supply side, finite fossil (petroleum, natural gas and

coal) account for 80% of global energy sources. Nuclear energy as of 2009 accounts for about 13% leaving renewable energy sources to account for the rest [2]. Petroleum-derived energy source has the most chequer of history, 63% of global oil reserves occur in the Middle East and given its finite nature, peak oil is projected to occur between 2015 – 2030 [1]. The highly localized nature of oil finds comes with significant geopolitical risk and this has often precipitated conflict, price fluctuation and supply uncertainty. The existential threat posed by any potential accident ensuing from the use of nuclear energy has heightened public resistance to its proliferation. After Chernobyl and Fukushima, a phased-out policy was adopted in Japan and Germany [3]. This indicates that in the energy spectrum, supply from fossil and nuclear sources is constrained, going forward. Added to these is the issue of environmental sustainability. Griffin [4] and many others have stated that increasing the use of petroleum fuel will intensity global warming caused by carbon dioxide (CO_2) emission not to mention the other countless health risks posed by the unregulated emission oxides of Nitrogen (NO_X), soot, carbon monoxide (CO), unburnt hydrocarbon (UHC) and aldehydes [5]. Against these backgrounds, renewable energy sources (RES) have been identified presently, 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 engine is a key component, the renewable energy source option available in that sector, will play a vital role in the sustainability drive.

1.1 Biodiesel and Novel Combustion Strategies

Biodiesel is composed of fatty acid methyl ester (FAME) produced from vegetable oil or animal fat through a transesterification process. This is achieved using alcohol in the presence of an alkaline catalyst. Besides being carbon neutral, the use of Biodieselin internal combustion engines has been reported to result in the reduction of carbon monoxide (CO), unburnt hydrocarbon (UHC), particulate matter (PM) and soot precursors emission [6]. Its primary challenge has been the marginal drop in engine power [7, 8], increase in oxides of nitrogen (NOx) emission at high combustion temperature [9, 10] and poor reactivity leading to higher emission ofCO and UHC at start-up or low load condition due to poor flow properties at low temperature.These advantages and challenges have triggered intense research efforts aimed at finding combustion strategies that could harness the potentials of biodiesel and mitigate the challenges obstructing itswider applications. Alrikson and Denbratt [11] in their computation of the equivalent ratio – Temperature (– T) map for soot and NO concentration using the SENKIN code observed that NO_X and soot emission could be eliminated regardless of equivalent ratio if the combustion temperature is kept below 1650k. The term, low-temperature combustion (LTC) is theprocess by which combustion temperature is kept below the NO_X and soot production threshold. Thisis often achieved via exhaust gas recirculation (EGR) to reduce oxygen concentration [12]. In another study, a temperature floor has also beendetermined to be 1400k [13]. Below this temperature, it has been observed that the oxidationrate of CO to CO_2 becomes too low leading tounacceptable levels of CO and UHC emission.

In the 1990s, a strategy with the best potential to reduce NO_X and so emissions came to light and began to receive wide research attention. Homogenous charge compression ignition (HCCI) sometimes called control auto-ignition (CAI) is acombustion strategy that relies heavily on the chemical kinetic of the fuel for the start of ignition. It is characterized by the induction of premixed charge and ignition in the combustion chamber, because of elevated temperature and pressure, during the compression stroke near the TDC. Because the charge is premixed, the equivalent ratio is calibrated near stoichiometric air and, given that combustionis spontaneous with multiple flame fronts, a higher thermal efficiency was observed in comparison to a compression ignition (CI) engine. All HCCI studies have consistently reported a significant reduction in NO_X and soot emissions because of the low-temperature regime [12]. But HCCI also facessome challenges which include combustion phasing, UHC and CO (mostly in diesel fuel runs) emission and problems with a cold start. The motivation here is that given the biodiesel oxygenated nature, warm EGR achieved via negative valve opening (NVO) could deliver sufficient heat intothe cylinder to improve charge homogeneity and a higher combustion efficiency which could eliminatethe UHC and CO emissions. Given the array of parameters that need to be observed and controlled, the most cost-effective way to conduct the study will be through numerical means, using very specific experimental data for result validation.

1.2 Numerical Study and Validation Tools.

Given the size of parameters, properties and systems features that need to be controlled, monitored and evaluated in combustion studies, direct physical experimentation is often unhelpful.The most efficient means, in terms of cost and research time, to conduct combustion studies is through numerical methods. This is often accompanied with well-targeted experiments to obtain data for validation purposes. The 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 a significant level of thermal and charge stratification. As a result of these, a surrogate chemical kinetic mechanism that closely represents the chemical properties and processes of the charge to compute the chemistry is selected. The physics of the flow process and thermal exchange in the HCCI also guides the selection of the model that will compute the flow and thermal behavior of the charge.

The study involves a proportionally high unsaturated FAME at the premixed sage of HCCI as the main fuel injection stream with a smaller DI near TDC of a proportionally high saturated FAME to serve only as an ignition trigger as proposed in the MK [14, 15] strategy. The fuel injection strategy at the premix stages is through port injection hence the detailed MDBio surrogate chemical kinetic mechanism of LLNL [16] which has been successfully reduced to 77 species and 209 reactions by Brakora et al [17] and, coupled to KIVA – 3V (which is now available as an open source code) is here proposed to compute the chemistry. The quazi-dimensional, multi-zone reduced chemical kinetic code built into the 3D –CFD code (KIVA) proposed by Aceves et al [18-20] will be used to compute the physical flow process along with MDBio to solve the ID spray phenomena and SOI. The species concentration and emission trend, it is hoped, will be adequately resolved in the special and temporal domain. Data obtained from previous HCCI or CI combustion strategies with proximity in test features to the proposed strategy could be used as effective engine diagnostic tools to validate the numerical results. Or where funding permits, a suitable optical engine diagnostic test – rig with a fully fitted PLIF test – kit [21] could be used to obtain specific data for validation purposes.

2.0 Background of CFD Method and Engine Diagnostics.

The computational approach to research in internal combustion engine (ICE) and engine development has had a long and successful history. The progressive application of models with increasingly higher fidelity alongside state-of-the-art engine diagnostic tools has resulted in the full resolution of the most important process in fuel combustion in ICE, making it possible to predict engine performance and emissions with increasing levels of accuracy. Most importantly, proposing a novel combustion strategy that improves performance and mitigates or eliminates undesirable emissions. The convergence of biodiesel potential with CFD capability is increasingly foretelling the possibility of a perfectly 'green ICE'. A concept where a carbon-neutral fuel source produces zero UHC, CO, NO_X and PM with a higher cycle efficiency in an internal combustion engine. 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 for any given combustion strategy.

2.1 Chemical Reaction Pathways and Surrogates

Onishi [22] and Noguchi [23] suggested that, unlike SI combustion which is spark-assisted and relies strongly on flame propagation and, CI on air/fuel mixing, HCCI relies exclusively on chemical kinetics for SOI hence chemical reaction pathways and LTK plays a crucial role in its processes. And since it is not practicable to adopt the chemical composition of actual biodiesel in numerical studies to compute the chemistry owing to its complexity, simple and well-characterized chemical kinetic are used as surrogates to mimic the behavior of the actual fuel [24]. Biodiesel surrogates are grouped into small (short carbon chain, < 5) or large (long carbon chain, >5) [25]. Small surrogates have been used more extensively because of their inherent advantages which include short CPU runtime, availability of a wide range of in-cylinder engine validation data and the flexibility of use. But it also faces significant challenges which include reduced accuracies, lack of low-temperature reactivity, unclear NTC region and differences in auto-ignition characteristics from actual biodiesel amongst others. Large surrogate mechanism fully addresses these challenges but with their own new set of difficulties

which include an unwieldy and complex structure, heavydependence on smaller sub-mechanisms longer CPU run time and limited in-cylinder engine validation data [25].

Biodiesel is defined as a fuel comprised of mono-alkyl esters of long chain fatty acids derived from vegetable oils or animal fats [73]. Biodiesel is typically created by reacting fatty acids with an alcohol in the presence of a catalyst to produce the desired mono-alkyl esters and glycerin. After the reaction, the glycerin, catalyst, and any remaining alcohol or fatty acids are removed from the mixture. The alcohol used in the reaction is typically methanol, although ethanol and higher alcohols also have been used. Most of the biodiesel currently produced in the U.S. is made from soybean oil [74], and soy biodiesel typically consists of the five methyl esters shown in Fig. 1 [75]. While neat (i.e., 100%) biodiesel can be used, a blend of between 2 and 20% (by volume) of biodiesel with diesel fuel is recommended to avoid engine compatibility problems [73].

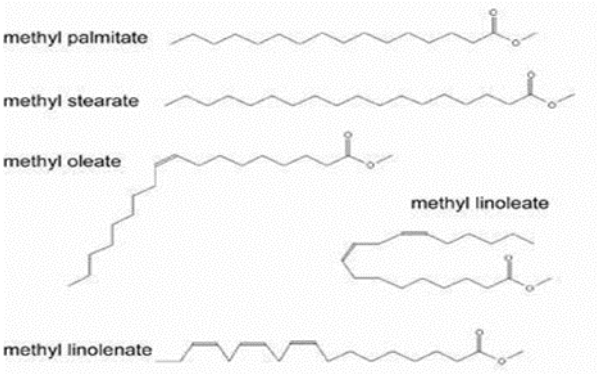

Figure 1: Molecular structures of the five methyl esters that typically comprise soy biodiesel [74]

i. Small surrogates include:

(1) Methyl butanoate (MB< C_5 H_{10} O_2), developed by Brakora et al [26], Golovitchev and Yang [27], Fisher et al [28] and has been coupled to KIVA – 3,CHEMKIN.

(2) Methyl (E) – 2 butenoates (MB2D, D5 H8 O2), developed by Gail et al [29] to mimic unsaturated FAME which MB failed to properly do. It has been complied with CHEMKIN.

(3) MBBio developed by Mohamed Ismail et al [30]. It is generic and could be tailored further for any specific application. It has been complied to open FOAM.

ii. Large surrogate includes:

(1) Methyl Decanoate (MD, C_{11}, H_2 O_2) developed by Glaude et al [31] through the use of EXGAS. It has been complied with CHEMKIN. The unsaturated verson, methyl – 5- decanoate (MD5D, C_{11} C_2 O_2) and methyl – 9 – decanoate (MD9D, C_{11} C_{20} O_2) have also been developed.

(2) MD Bio developed in LLNL [32] and reduced by Luo et al [33]. It has complied with CONVERGE, CHEMKIN AND KIVA -3V.

(3) Methyl stearate (C_{19} H_{38} O_2) developed by Herbinet et al [34] through the use of EXGAS. Same prodedure was used to develop methylpalmitate (C_{17} H_{34} O_2) by Hakka et al [35].

(4) Westbrook et al [36] also developed methyloleate, stearate, palmitate, linoleate and linolenate.

2.2 CFD Flow Model.

Numerical technique developed for flow studies ranges from highly refined to coarse grain depending on the level of fidelity required for a given investigation [Basic research need]. Among the fine grains, Quantum Mechanics (QM) occupies the prime position followed by Molecular Dynamic (MD) and Kinetic Monte Carlo (KMC) with spatial and temporal domains ranging from 10^{-12}m x 10^{-12}s (Pico scale) to 10^{-9}m x 10^{-9}s (Nanoscale). These computations can capture processes ranging from intra-atomic processes for a small number

of atoms to intermolecular activities. The effort required to compute at this level, in terms of computing resources and CPU runtime is quite rigorous but additional information obtained as benefits do not necessarily make any substantial difference in prediction capability, particularly for CFD application in biodiesel studies.

Direct numerical simulation (DNS), large eddy simulation (LES) and Reynolds averaged Nervier–Stokes (RANS) are the band most often mentioned in CFD studies and, their spatial and temporal domain ranges from Nanoscale (10^{-9}m x 10^{-9}s),through micro-scale (10^{-6}m x 10^{-6}s) to milli scale (10^{-3}m x 10^{-3}s). RANS, which has the coarsest grain size in combustion studies. But LES is gaining an increasing foothold with power and data storage capacity [37]. There are primarily five categories of application in biodiesel computation. They are summarized below.

2.2 Zero Dimension, Single Zone withDetail Chemistry.

This is the simplest model, applying the first law of thermodynamic in engine simulation. Often, heat exchanged between charges and mass – blow - by are neglected. Both the thermodynamic and transport properties are considered homogenous. This model often overestimates results because thermal and charge stratification constitute significant process-altering realities in ICE. The model gives good result in estimating ID and NO_X formation because both events are linked to the highest temperature which is close to the mean gas temperature. Brakora and Reitz [38] used this model to estimate NO_X formation from biodiesels.

2.2.2 Quazi Dimensional, Multi-Zone withDetail Chemistry.

The over simplification of combustion processes in the single zone model was addressed by the proposal for a multi – zone model which divides the combustion chamber into several regions or zones with each having uniform thermodynamic and transport properties. Different initial parameters are used for each zone. Normally, crevices and boundary layers (low-temperature zones) are included to obtain a good resolution of UHC and CO for HCCI processes. They are described as quazi – dimensional because the dimension arephenomenologically determine to represent crevices, core adiabatic zones and boundary layers. Fiveland and Assanis [39] developed and used this model to predict performance and emissions under turbocharge conditions. Figure 2 details the scheme.

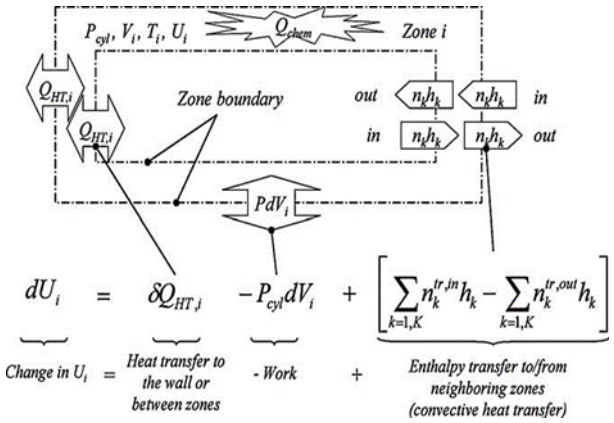

Figure 2: Quazi-dimensional, multi-zone model.

2.2.3 1D Full Engine Cycle with Detail Chemistry.

Zero and quazi dimensional computation only capture engine processes at the start of intake valve closure (IVC) and the end of exhaust valve opening (EVO). Implying that parameters have to be specified at IVC creating substantial scope of computational error. This is because average mixture temperature, equivalent ratio and residual gas fraction (RGF) are difficult to determine. To overcome these challenges 0D and quazi dimensional model are combined with engine cycle simulation codes which computes the parameters and IVC. These 1D codes predict engine parameter from air intake to exhaust pipe making it possibleto model the gas exchange processes. Ogink [40] produced the BOOST – SENKIN, single zone model which predict auto ignition timing and heat release rate for a HCCI gasoline engine using this approach. Milovanovic et al [41] studies the

variable valve timing (VVT) impact on gas exchange processes in HCCI using the sameapproach.

2.2.4 3D CFD, Multi-zone with Detail Chemistry.

Despite the improvement recorded with 1D full engine cycle with detail chemistry, some challenge still persisted. These include poorly specified charge and thermal stratification and RGF at IVC. Aceves et al [18-20] proposed that to overcome these challenges and achieve the finer resolution that the CFD model could provide while at the same time avoiding computational stiffness or reducing computation time that could result if the chemistry is computed in 3D CFD, a segregated sequenced multi-zone model needs to be adopted. This procedure used 3D CFD code (KIVA) for the flow computation and a quazi–dimensional multi-zone detail chemical kinetic code to compute the chemistry. The KIVA code is a transient, 3D, multiphase, multi-component scheme that analyses chemical reacting flows with sprays. This code is under development at the Los Alamos National Laboratory [42] and is open-sourced. The approach requires that the fluid mechanic code is first executed to evaluate temperature distribution withinthe cylinder without combustion between the zones. This information is then used in the chemical kinetic code. Hence, every zone in the multi-zone chemical kinetic code is ascribed differential initial temperature and parameter obtained from the CFD code. These steps fully account for the thermal gradient. It initially used 10 zones but was later increased to 40 for higher resolution. Babajimopoulos et al [43] and Flower et al [44] used this model with good results. The only mentioned drawback is its overestimation of CO. This is the model that is being proposed for this work.

2.2.5 3D CFD with Detail Chemistry

Multi–dimensional computational fluid dynamic with detail chemistry possess the best potential to predict more accurately engine activities when the complete geometry of the combustion chamber is fully resolved and detail kinetic chemistry isemployed to evaluate chemical events. The computational resources for such a procedure are significant and depend on CFD mesh resolutions and the size of the chemical kinetic mechanism. Agarwal and Assanis [45] performed a simulation of natural gas ignition consisting of the detailed chemical kinetic mechanism of 22 species and 104 reactions using the multi-dimensional CFD reacting flow code KIVA – 3V. The purpose was to explore the auto-ignition of natural gas injected into a quiescent chamber in CI like condition. The complete kineticwas executed up to the ignition point.

2.3 HCCI Strategies

Homogenous charge compression ignition (HCCI) potential to significantly reduce NO_X (because it is an LTC concept) and soot emission in the exhaust, its unthrottled operation leading to higher indicated thermal efficiency and operation at near stoichiometric places it in a good position to address some of the drawback associated with the use of biodiesel in CI engine. The challenges of engine control, load scaling and UHC/CO emission are currently being addressed through variousresearch strategies. UHC and CO emissions particularly, occur because of bulk quenching at low loads, wall quenching and crevice flow at high loads. But those are being resolved using a plethora of strategies that include warm/hot EGR at steady-state operation to improve reactivity. These strategies are useful for FAME combustion inICE. The fear of oxygen starvation resulting from tight EGR regime is mitigated by the oxygenated nature of FAME. This clearly, is the focus of this proposal.

HCCI strategies are broadly categorized into; early direct injection, late injection and premixed/DI injection. The early direct injection includes premixed lean diesel combustion (PREDICT) developed by Takeda et al [46], UNIBUS developed by Yanagihara et al [47], MULINBUMP developed bySu et al [48] and small angle injection strategy developed by Kim and Lee [49]. The late injection strategies include, modulated kinetic (MK) developed by Nissan Motor Company and describedby Kawashima et al [14] and the second generation MK recommended by Kawamoto et al [50]. The other HCCI strategies are the premixed/DI HCCI and the LTC HCCI strategy. Given the focus of thispaper, the strategies that will be described are the modulated kinetic and the premixed/DI strategies.

2.3.1 Modulated Kinetics (MK)

The modulated kinetic (MK) combustion system was developed by Nissan Motor Company as a late injection HCCI strategy. Kawashima et al [14] and Kimura et al [51] gave details of this strategy. To achieve the diluted homogenous mixture needed for HCCI, a long ignition delay and rapid mixing were required. The ignition delay was achieved by retarding injection timing from 1°BTDC to 3°ATDC and using a higher EGR to lower oxygen concentration to 15 – 16%. Rapid mixing was accomplished by using a high Swirl with toroidal combustion bowl geometry. The operating range for the first-generation MK was limited to 1/3 peak torque and ½ speed. This strategy effectively reduced NO_X to about 50ppm with increase in PM for gasoline combustion. Combustion phasing was achieved by injection timing.

The second-generation MK expanded the operating range through various modifications [15]. Higher injection pressure (through a high-pressure common-rail fuel system) was executed to reduce fuel injection time at all speeds, the ignition delay was increased by reducing the compression ratio and adding EGR cooling to reduce intake temperature. To reduce fuel spray wall impingement, the piston bowl was increased from 47 to 56mm. This significantly reduced UHC emission during cold start. It was observed that the second-generation MK strategy could be used for the entire range of engine operations. And met the target of about ½ load and ¾ speed. NO_X emission was reduced by 98% compared to conventional EGR and PM emission was like conventional CI engine. The most strategic advantage of MK is that it does not require additional hardware and its operation with existing hardware did not negatively impact the engine's specific power output. But the injection timingretardation reduced engine cycle efficiency and gave rise to higher UHC emissions [12].

2.3.2 Premixed/DI HCCI

This strategy incorporates port injection as the primary fuel supply source to create a homogenous charge and the DI fuel injection is used at the secondary stage to change the concentration and spatial position of the rich regions with the sole purpose of triggering ignition and as a means of HCCI combustion control.

Odaka et al [52] proposed a homogenous charge compression ignition diesel combustion (HCDC) which used the premixed/direct–injection 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 premixed in the cylinder. Thisstrategy reduced both NO_X and smoke emissions better than the conventional CI engine. It was also observed that smoke was reduced uniformly as the premixed fuel ratio increased.

Midlam – Mohler et al [53, 54] also built a premixed/direct-injected HCCI system. 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 comes from the premixed lean homogenous fuel and the DI fuelonly serves to initiate ignition at high loads. The maximum homogenous charge is employed, and the DI fuel proportion is increased to the fuel load. Atomization to droplet size of less than 1mm mean diameter allows fast evaporation during the compression stroke, making the heating of intake unnecessary. Result obtained showed that by varying intake condition, IMEP of up to 4.7bar can be achieved at speed range of between 1600 – 3200 rpm. In addition, the strategy achieved very low NO_X of less than 4ppm and smoke emission of0.02FSN.

The most interesting strategy in the premixed/DI HCCI was proposed by Inagaki et al [55]. In this strategy, gasoline (high octane, low cetane number)was used at the intake port for the homogenouspremixed and diesel fuel (low octane high cetane number) was injected at DI to initiate ignition at timing BTDC. It was observed that ignition phasing of the combustion can be controlled via thechanging of fuel ratio for the two stages to the extent that combustion proceeds mildly. The operating load range where NO_X and smoke emission were 10ppm and 0.1FSN respectively were extended to an IMEP of 12bar where an intake air boost system was employed.

2.4 Biodiesel Properties Solver

The thermo-physical properties of FAME to be used in CFD computation required good accuracies for

prediction to achieve high fidelity and given their large number and cost associated with experimental determination, the best option is to compute their value using well-validated correlations [1]. The properties could either be transport or thermodynamic. It is well known that both transport (viscosity, density, bulk modulus, surface tension) and thermodynamic (heat capacities, conductivities, vapour pressure, latent heat of vaporization etc.) properties have a strong coupling to FAME structure. For example, densities increase in the carbon chain and are higher with high unsaturated esters [56], kinematic viscosity increases with increased carbon chain lengthand decreases as unsaturation increases [57], etc.

Given that thermophysical properties are key determining factor in the outcome of combustion processes and which subsequently determine engine pre-combustion strategy, engine performance and emissions, it is important to obtain good accuracies in determining their values in an efficient and cost-effective manner. Two handbooks are useful in the estimation of FAME properties when developing a code to compute biodiesel properties. They include the work of Reid et al [58, 59] and Poling et al [60] which provide a useful reference for the comprehensive compilations of group contributions and experimentally determined correlations. Software has also been developed for use in the estimation of hydrocarbon thermo-physical properties. They include Knovel critical tables [61], DIPPR [62] and BDProp [63, 64]. Mixing rules [65, 66] are also considered because they are important considerations when computing FAME properties.

2.5 Engine Diagnostic and Experimental Validations

Model fidelities are often validated with a plethora of engine diagnostic tool and well-designed experiments. Since 1979 when optical diagnostic was discovered, it has continued to play an important role in in-cylinder process observation [12]. This tool has been refined to such a degree that comprehensive information on flow patterns, species, and temperature distribution with high spatial and temporal resolution can now be obtained, very importantly, their non-intrusive, in-situ capability enables process observation without distortion [21]. Consequently, their use has been widespread. Richter et al [67] used planar laser-inducedfluorescence (PLIF) in HCCI to evaluate distribution of fuel and OH radicals in the combustion chamber. Glassman [68] used chemiluminescence at low temperatures to observe fuel oxidation and heat release for diesel in a study to test the efficacy of chemiluminescence and spectral analysis in in-cylinder observation.

PLIF was also used to study NO emission from engines by Dec and Canacin [69]. Laser-induced incandescence (LII) was used by Singh et al [70] and Huestis et al [71] to study soot propagation anddestruction processes by applying two – a color optical pyrometer in LTC. Musculus [72] also used LII in the study of soot luminosity and soot laser-induced incandescence.

A significant database of engine test result exists, which can be used to perform validation studies of model results but, where specific data set are needed for a narrow band of engine test protocol, building a test rig with sufficient diagnostic tool do not pose any serious challenge.

3.0 Method/Test Protocol and ExpectedOutcome.

Broadly stated, the proposed strategy is a partial merger of the premixed/DI and Modula Kinetic to improve cycle efficiency, increase IMEP, eliminate NO_X and soot emissions, and reduce UHC and CO emissions. The fuel is a multi-blend FAME of saturated and unsaturated mix. At the premixed injection stage, less reactive and low cetane unsaturated FAME will constitute the bulk of the fuel to be introduced via port injection. The purpose being to delay ignition to enable the formation of a diffused homogenous charge. This will also be helped by the EGR via NVO so that ignition delay will be retarded from 7^o BTDC to approach 1^o - 0^o BTDC. A small quantity of high proportion saturated FAME blend will be injected via DI around 2^o - 1^o BTDC to change charge mix, creating rich zone that will trigger ignition and form the spark kernel at just about the time that the rest of the charge is about to ignite. Thespontaneous global combustion that will ensue will be rapid and deep given the milder thermal andcharge stratification. Peak temperature will be calibrated not to exceed 1650^ok via the EGR means to achieve zero NO_X and soot formation. It is envisioned that with good bowl geometry selection, swirl level and the partially warm EGR, a controlled thermal stratification will create a temperature floor of 1400k and prevent build-up of UHC and CO from wall quenching and crevices region. Cycle efficiency

will improve since the charge mix is near stoichiometric and ignition is calibrated to occur BTDC.

The following are proposed for the work.

1. **Model type**: 3D CFD, multi-zone with detail chemistry.
2. **Surrogate**: methyl Decanoate bio (MDBio)built into KIVA 3V with proportion alteration for premix and DI stage.
3. **Property solver**: A developed property solver code coupled to the model tocompute on demands properties for the chemistry and physics of the process.
4. **Validation**: The existing validation code for the ID NOx map will be used to validate the ID and NOx formation data. The resultingscale quantities will be used to computethe IMEP and is ISFC.
5. **Test Rig**: A suitable diagnostic test rig withPLIF capability will be used to fully resolve and validate the CO and UHC history. PM formation, if any, will also bedetermined through the same method.
6. **Post-processing and Optimization**: After validation, a broad range of parameter grids will be simulated to optimize output and make useful predictions.

4.0 Conclusion

Given the tool currently available for biodiesel combustion studies, it is now technically possible to determine the best combustion strategy that can increase engine performance, eliminate emission and more importantly the right mix of FAME that can achieve that. The latter is a very important fact. Biodiesel is simply a mixture of varying components of FAME. If through numerical studies, we can determine the mixture with the best outcome in each engine strategy, it becomes possible in the short term, to mix that proportion for use from existing biodiesel and, in the long term, genetically engineer a plant algae source that could produce an exact oil copy. This is the future of renewable energy research, walking backward from the answer to the problems that prevent us from obtaining the answer we desire is the key to unlocking the potentialsinherent in biodiesel fuel sources.

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