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INVESTIGATION OF HEAT RELEASE RATE OF BIODIESEL PILOT FUELLED NATURAL GAS ENGINE WITH STOCHASTIC REACTOR MODEL

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Abstract
In this study, heat release rate (HRR) characteristics of natural-gas (NG) dual-fuel (DF) engine using biodiesel pilot fuel were investigated by stochastic reactor model (SRM). SRM Engine Suite software having solution method in zero-dimensional was used to apply stochastic reactor model into the DF engine. Results of the study were validated by the experimental data obtained from biodiesel pilot fuelled NG engine. Biodiesel surrogate fuel was considered as a mixture of methyl decanoate (25 v%), methyl-9-decenoate (25 v%) and n-heptane (50 v%) and its skeletal kinetic mechanism includes 71 species and 217 reactions. In addition, it is shown that biodiesel surrogate fuel chemical kinetic mechanism could represent soy biodiesel fuel. Case studies were realized under 50, 100, 150 and 200 stochastic particles with 120 MPa pilot fuel injection pressure and 17°BTDC pilot fuel injection timing conditions in the simulations. It was observed that SRM method is a good tool to investigate HRR of biodiesel pilot fuelled DF engine.

Keywords: Dual fuel engine, Biodiesel pilot fuelled natural gas engine, Stochastic Reactor Model, Monte Carlo stochastic particle method, Probability Density Function

1. Introduction

Effects of air pollution and climate change on life quality of people have been inclusively discussed by the authorities, scientists and researchers during the last decades. One of the most significant sources of this deterioration is exhaust emissions stemmed mainly from road vehicles, marine-, and jet engines. Exhaust emissions from these engines are caused by combustion of hydrocarbon fuels and composed of Carbon monoxide (CO), Nitrous oxides (NO_x), unburned hydrocarbon (UHC), Sulphur oxides (SO_x), and Carbon dioxide (CO_2) in general [1]. There are various legislations and regulations to control and to mitigate harmful exhaust emissions. European Emission Standards (i.e. Euro VI) [2] and International Maritime Organization (IMO) MARPOL Annex VI [3] are fundamental standards for road vehicles and maritime field, respectively.

The ódual fuelô engine concept is developed to enhance engine emissions. Two different fuels (i.e. LPG, biogas, natural gas as the main fuel and diesel, DME, etc. as the pilot fuel) are simultaneously admitted into combustion chamber [4] in DF engines. They are either originally produced by factory or converted from available compression ignition (CI) engines. They can be operated on either conventional liquid fuels or gaseous fuel (NG) [5,6].

Diesel fuel is conventionally used as a pilot fuel in DF engines since it does not require major modifications in the engine fuel system. Recently, biodiesel has also been commonly used as a pilot fuel in DF engines since its properties are similar to diesel fuel. Furthermore, biodiesel has higher cetane number than conventional diesel fuel. It decreases ignition delay and is an environmentally friendly fuel with low smoke emissions as it contains 10% oxygen [7,8,9].

Nowadays, NG is conventionally used as a main fuel in DF engines. Natural gas has lower carbon-to-hydrogen ratio and higher auto-ignition temperature according to other hydrocarbon fuels. Therefore, using NG in DF engines lowers the CO_2 emissions. In addition, when NG amount entered into the combustion chamber is increased, oxygen ratio in the combustion chamber decreases. Hence, biodiesel pilot fuel can be considered for starting ignition to increase oxygen ratio.

It was investigated impacts of pilot injection pressure on engine performance and exhaust emissions characteristics in a single cylinder diesel engine and also aimed to obtain a simultaneously reduction of PM and NO_x emissions [7]. It was found by author that biodiesel pilot fuel injection at high pressure had lower indicated mean effective pressure (IMEP) than diesel fuel injection. As pilot fuel injection pressure of biodiesel was increased, smoke and NOx emissions are decreased and increased, respectively. It was investigated effects of pilot injection timing on combustion and exhaust

emissions with a biodiesel-CNG dual fuel combustion system in a single cylinder diesel engine [8]. It was found that performance could be optimized for biodiesel-CNG dual fuel combustion by adjusting the pilot injection timing at low loads and retard injection timing at high loads. Smoke was reduced and NO_x was increased by advanced pilot injection timing in biodiesel-CNG dual fuel combustion. It was performed an experimental investigation about the use of Jojoba Methyl Ester as a pilot fuel and natural gas or LPG as a primary fuel under dual fuel mode in Ricardo E6 variable compression diesel engine [10]. They found that Jojoba Methyl Ester fuel revealed improved dual fuel engine performance, reduced the combustion noise, extended knocking limits and reduced the cyclic variability of the combustion. It was extensively tested natural gas combustion to obtain performance and emissions maps in a direct injection CI engine [11]. Diesel and Rapeseed Methyl Ester (RME) were used as a pilot fuel. It was found that thermal efficiency of dual fuel mode was lower except from highest powers than that of single diesel fuel operation and speciýc NO_x contours of diesel and RME based single fueling were signiýcantly different when these fuels were used to pilot natural gas combustion. Also, it was found that RME piloted speciýc NO_x at the highest speeds were the only exception to this trend and higher speciýc UHC and lower speciýc CO_2 emissions were observed in case of natural gas based dual fueling. An experimental investigation is carried out to compare engine performance and emissions in natural gas dual fuel engine being originally CI engine. In their study, Pongamia pinnata methyl ester (PPME) and Diesel were used as a pilot fuel. It was found that PPME-CNG dual fuel operation was more effective than Diesel-NG dual fuel operation in terms of engine performance and emission characteristics and also PPME-CNG operations slightly increased NOx when compared to Diesel-CNG operation [12].

It is carried out an experimental study to investigate effect of eucalyptus biodiesel on engine performance and exhaust emission of NG dual fuel engine. They found that biodiesel as pilot fuel shows similar pressureï time history, with highest peak, as diesel fuel in conventional and dual fuel modes and also the use of eucalyptus biodiesel as pilot fuel decreased the high emission levels of UHC, CO and CO_2 particularly at high engine loads. NO_x emissions increased since eucalyptus biodiesel has lower heating value and the oxygen presence in the molecules [13].

There are a several studies on biodiesel pilot fuelled DF engines being NG as a main fuel, but it could be not found any stochastic based theoretical study on NG-DF engines with biodiesel pilot fuel in available literature. Thus, in this study, a theoretical model is developed and HRR of DF engine, having biodiesel being a pilot fuel and NG being a main fuel is investigated by using a SRM.

2. Model Description

Stochastic reactor model, its algorithm and numerical method for engine simulation are introduced in this section.

2.1. Stochastic Reactor Model for dual fuel engine

For general dual fuel engines simulated, it must be chosen Dual Fuel-SRM mode. The SRM is a spatially zero dimensional model of the contents of the combustion chamber based on Probability Density Function (PDF) transport methods. SRM in ICEs is realized by dividing the mass within the cylinder into an arbitrary number of virtual packages called particles. Each of these particles has a chemical composition, a temperature and a mass and can mix with other particles and exchange heat with the cylinder walls [14, 15, 16, 17, 18, 19].

The contents of the cylinder are subjected to pressure and volume changes, etc.. All quantities of interest are space independent and calculated from these processes. Solutions were obtained for SRM equations by Monte Carlo particle method. [14].

The global quantities in the SRM model are the total mass, volume, mean density and mean pressure. They are assumed not to vary spatially in the combustion chamber. These quantities are calculated based on known engine geometry, density and pressure [16,19].

Scalars, temperature and mass fractions for each species are local quantities. They are considered as random variables. These variables are expressed by MDF [16].

The fuel injection model includes fuel mass, which was injected, and the injection rate proýle. The injected fuel is assumed to be vaporized at the moment of injection and introduces new fuel particles into the ensemble. This changes the total mass inside the cylinder and causes a change in the mass fractions and temperatures of the current set of particles [16, 19].

2.2. Main Equation

SRM Model calculates the evolution of the N_S chemical speciesô mass fractions, Y_1, é ,Y_{Ns}, and the temperature, T, as a function of time.

The N_S+1 random scalar variables are put together into the vector

$$\psi = \left(\psi_1,\ldots,\psi_{N_S},\psi_{N_S+1}\right) = \left(Y_1,\ldots,Y_{N_S},T\right)$$

whose distribution is given by the PDF, f. Mean quantities may be calculated using the PDF by:

$$\left\langle \psi_j(t) \right\rangle = \int \psi_j f(\psi;t)\, d\psi \quad (1)$$

In engine context, the in-cylinder density varies during an engine cycle, so it is more convenient to use the Mass Density Function rather than the PDF. The MDF is associated with the PDF by:

$$F(\psi;t) = \rho(\psi) f(\psi;t) \quad (2)$$

where ρ is the mass density. The time evolution of the MDF in the SRM is described by the following PDF transport equation:

$$\frac{\partial}{\partial t}F(\psi;t) = \underbrace{-\sum_{j=1}^{N_S+1}\frac{\partial}{\partial \psi_j}\left[G_j(\psi)F(\psi;t)\right]}_{\text{chemical reaction}} + \underbrace{\sum_{j=1}^{N_S+1}\frac{\partial}{\partial \psi_j}\left[A_j(\psi)F(\psi;t)\right]}_{\text{turbulent mixing}}$$
$$\underbrace{\frac{1}{V}\frac{dV}{dt}F(\psi;t)}_{\text{piston movement}} \underbrace{-\frac{\partial}{\partial \psi_{N_S+1}}\left[U(\psi_{N_S+1})F(\psi;t)\right]}_{\text{convective heat transfer}} \quad (3)$$
$$\underbrace{+\frac{F_C(\psi;t)}{\tau_{crev}}}_{\text{crevice flow}} \underbrace{-\frac{F(\psi;t)}{\tau_{cyl}}}_{\text{crevice flow}} \underbrace{+\frac{F_f(\psi;t)}{\tau_f}}_{\text{fuel injection}}$$

with the initial conditions:

$$F(\psi;0) = F_0(\psi) \quad (4)$$

The right hand side of Equation (3) introduces the physical in-cylinder processes of chemistry, turbulent mixing, heat transfer, piston movement, crevice þow and fuel injection [16].

2.3. Solution Method

Equation (3) is solved using a Monte Carlo stochastic particle method [14, 16]. An ensemble of N_{par} stochastic particles make up a statistical representation of the PDF, which is approximated by:

$$f(\psi;t) \approx \frac{1}{N_{par}} \sum_{i=1}^{N_{par}} \delta\left(\psi - \psi^{(i)}(t)\right) \quad (5)$$

where superscripts attribute individual particles. Equations (1) and (5) combine to give an approximation of the mean quantities:

$$\left\langle \psi_j(t) \right\rangle \approx \frac{1}{N_{par}} \sum_{i=1}^{N_{par}} \psi_j^{(i)}(t) \quad (6)$$

To solve Equation (3), an operator splitting technique is employed so that each term can be treated separately [14, 20]. The operator splitting loop is described below:

1. Initialized t=0, Δt, CAD=IVC. Determine temperature, composition, mass, volume and pressure of particle ensemble.
2. Progress in time tŸ $t+\Delta t$. If CADÓEVO or t Ót_{stop} then save the detailed exhaust composition as input EGR and stop.
3. Perform volume change due to piston movement.
4. Perform gas exchange between bulk and crevice volumes.
5. Perform the first half of the turbulent mixing splitting step.
6. Perform stochastic heat transfer splitting step.
7. Perform the pressure equilibration step.
8. Perform the chemistry step.
9. Perform the pressure equilibration step.
10. Perform the second half of the turbulent mixing splitting step.
11. Perform the direct injection splitting step.
12. Go to step (2).

3. Results and Discussions

3.1. Biodiesel Chemical Kinetic Mechanism Feasibility

Chemical kinetic mechanisms for each biodiesel have not been developed yet. Hence, biodiesel surrogate fuel chemical kinetic mechanisms were used available studies. Firstly, these mechanisms were developed as detailed chemical kinetic mechanism, but use of this mechanism in CFD or SRM Software is very time-consuming. Therefore, reduced chemical mechanisms using some reduction methods were used instead of detailed chemical mechanisms. Thanks to reduced chemical kinetic mechanisms, simulations with CFD or SRM software has been very fast in terms of time. Surrogate fuel mixture considered for biodiesel in this study is composed of 25% of methyl-decanoate (MD), 25% of methyl-9-decenoate (MD9D), and 50% of n-heptane [21]. Reduced chemical kinetic mechanism, given by [22], for aforementioned fuel mixture was used during simulations. It was made a comparison between soy methyl ester lower heating value and the biodiesel surrogate fuel chemical kinetic mechanism lower heating value to show representability of soy biodiesel. While defined lower heating value for soy biodiesel, given by [7, 8], is 40.001 MJ/kg, defined lower heating value for biodiesel surrogate fuel chemical kinetic mechanism is 37.7 MJ/kg [22]. As mentioned above, it was demonstrated that biodiesel surrogate fuel chemical kinetic mechanism could represent soy biodiesel fuel.

3.2. Energy Audit for natural gas and biodiesel surrogate fuel

In this section, it was calculated as 36.443 MJ/m^3 thermal energy of natural gas used in SRM Engine Suite software and also calculated for

different conditions thermal energy of biodiesel surrogate fuel used in SRM Engine Suite software. Table 1 shows these results. Finally, calculated the energy audit for natural gas and biodiesel surrogate fuel is shown in Table 2. As seen in Table 2, biodiesel energy share has low values in terms of percentage and these values are allowable level.

Table 1. Released thermal energy amounts for injected pilot fuel cases

Thermal energy amounts for different pilot injection timings		
Pilot injection timings	Injected amounts of pilot fuel [kg]	Thermal energy for biodiesel pilot fuel [MJ]
11^0 BTDC	3.8127E-5	0.001437388
14^0 BTDC	3.85151E-5	0.001452018
17^0 BTDC	3.92305E-5	0.001478991
20^0 BTDC	3.88978E-5	0.001466448
23^0 BTDC	3.94592E-5	0.001487611

Thermal energy amounts for different pilot injection pressures		
Pilot injection pressures	Injected amounts of pilot fuel [kg]	Thermal energy for biodiesel pilot fuel [MJ]
30 MPa	2.75624E-5	0.001039102
60 MPa	3.18815E-5	0.001201932
90 MPa	3.50035E-5	0.001319634
120 MPa	3.92728E-5	0.001480586
150 MPa	4.1864E-5	0.001578274

Table 2. Calculated thermal energy values for dual fuel engines

Thermal energy for different pilot injection timings		
Pilot injection timings	Total thermal energy [MJ]	Biodiesel energy share [%]
11^0 BTDC	36.44443739	0.003944052
14^0 BTDC	36.44445202	0.003984196
17^0 BTDC	36.44447899	0.004058204
20^0 BTDC	36.44446645	0.004023789
23^0 BTDC	36.44448761	0.004081855

Thermal energy for different pilot injection pressures		
Pilot injection pressures	Total thermal energy [MJ]	Biodiesel energy share [%]
30 MPa	36.4440391	0.002851227
60 MPa	36.44420193	0.003298005
90 MPa	36.44431963	0.003620958
120 MPa	36.44448059	0.00406258
150 MPa	36.44457827	0.004330615

3.3. Heat Release Rate Characteristics

The number of particles governs the precision of predictions. Normally, 100 particles are sufficient in many applications according to previous study [23]. However, simulations were carried out for 50, 100, 150 and 200 stochastic particles to see the effect of different stochastic particles on solution. Firstly, Figure 1 and 2 show the history of heat release rate (HRR) vs. crank angle for 14°BTDC pilot injection timing and 17°BTDC pilot injection timing, respectively. The simulation results were obtained in 100 stochastic particles. Secondly, Figure 3 and 4 show the history of heat release rate (HRR) vs. crank angle for 90 MPa pilot injection pressure and 120 MPa pilot injection pressure, respectively. The simulation results were obtained in 100 stochastic particles. Finally, Figure 5 and 6 show the history of heat release rate (HRR) vs. crank angle for 120 MPa pilot injection pressure and 17°BTDC pilot injection timing, respectively. The simulation results were obtained in 50, 100, 150 and 200 stochastic particles. Simulation results are in good agreement with experimental data. However, deviations of model results from experimental data can be rooted in lacking of fully chemical kinetic mechanisms of biodiesel fuel and some unknown operating parameters of engine requested by this software. In addition, these skippings are due to stochastic jump process into the solution algorithm [24]. Characteristics of HRR of the Figures between 1 and 6 also resembles to the results given in [25, 26, 27, 28]. Thus, it was observed that the SRM method is a good tool to investigate HRR of biodiesel pilot fuelled dual fuel engine.

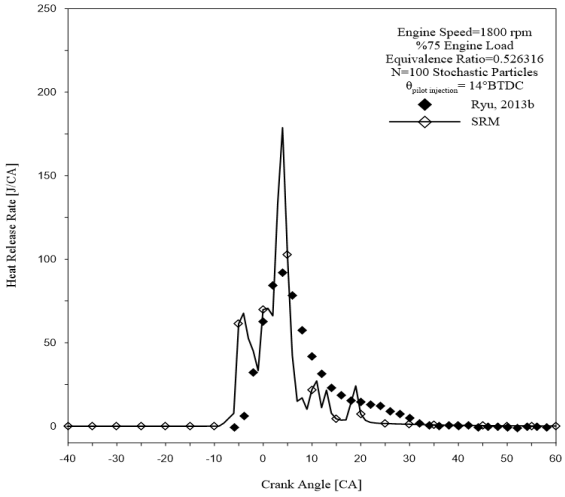

Fig. 1. HRR vs. Crank Angle for the 14°BTDC pilot injection timing

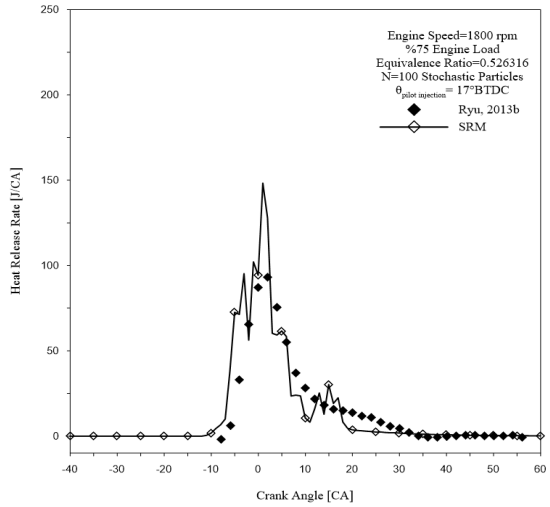

Fig. 2. HRR vs. Crank Angle for the 17°BTDC pilot injection timing

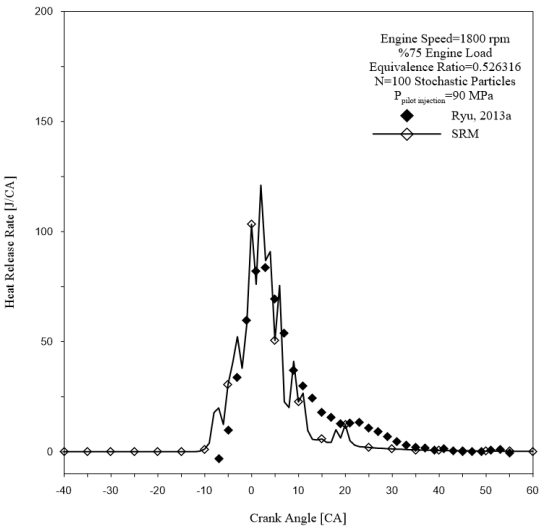

Fig. 3. HRR vs. Crank Angle for the 90 MPa pilot injection pressure

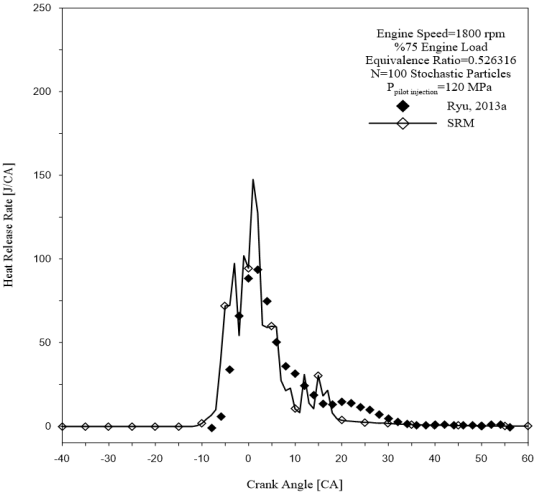

Fig. 4. HRR vs. Crank Angle for the 120 MPa pilot injection pressure

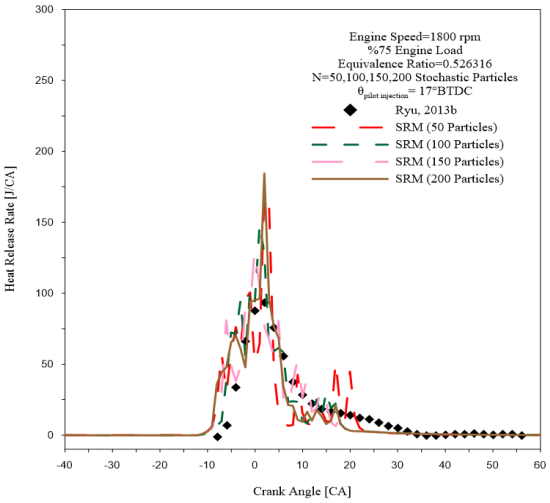

Fig. 5. HRR vs. Crank Angle for the 17°BTDC pilot injection timing for different stochastic particles

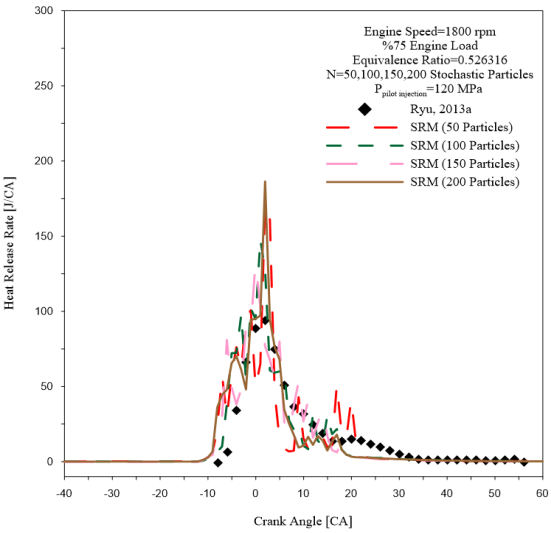

Fig. 6. HRR vs. Crank Angle for the 120 MPa pilot injection pressure for different stochastic particles

4. Conclusions and Future Work

It was firstly used a novel dual fuel-SRM model based on the probability density function (PDF) approach to simulate biodiesel pilot fuelled natural gas engines. This approach was performed with ókinetics & srm engine suite v8.2.9ô software. In this software, due to the fact that some parameters (inlet temperature, inlet manifold pressure, piston head, cylinder head, cylinder liner temperatures) are not absolutely specified, it was approximately predicted using ótrial-and-errorô method. Furthermore, crevice volume (%) parameter which affected ómaximum pressure locationô was nearly calculated by benefitting engine geometry.

The simulation results showed in good agreement with experimental data. However, deviations of model results from experimental data

can be rooted in lacking of fully chemical kinetic mechanisms of biodiesel fuel and some unknown operating parameters of engine requested by this software. SRM method (SRM Engine Suite Software) is a good tool to investigate HRR of biodiesel pilot fuelled dual fuel engine. When detailed chemical kinetic mechanisms for each biodiesel (soy bean, canola, rapeseed methyl esters) is developed, maybe we will gained more better agreement in experimental data.

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Nomenclature and Units

BTDC	: Before Top Dead Center [°CAD]
CAD	: Crank Angle Degrees
CFD	: Computational Fluid Dynamics
EVO	: Exhaust Valve Opening [°CAD]
HRR	: Heat Release Rate [J/°CAD]
IVC	: Intake Valve Closing [°CAD]
MD	: Methyl decanoate
MD9D	: Methyl-9-decenoate
MDF (F)	: Mass Density Function
N_{par}	: Stochastic particle numbers
PDF	: Probability Density Function
RPM	: Revolution per minute
SRM	: Stochastic Reactor Model
t_{stop}	: Iteration stop time
°	: Degree
(i)	: Individual particle
ρ	: Mass Density [kg/m^3]
ψ	: Chemical species

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