

Modeling of Combustion and Emissions Formation in Heavy Duty Diesel Engine Fueled by RME and Diesel Oil

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ABSTRACT

A comparative study on engine performance and emissions (NO_x , soot) formation has been carried out for the Volvo D12C diesel engine fueled by Rapeseed Methyl Ester, RME and conventional diesel oil. The fuel and combustion models used in this paper are the modifications of those described in [1–3].

The numerical results for different load cases illustrate that for both fuels nearly 100% combustion efficiency was predicted; in the case of RME, the cumulative heat release was compared with the RME LHV, 37.2 kJ/g. To minimize soot and NO_x emissions, 25–30% EGR levels depending on the engine loads and different injection timings were analyses. To illustrate the optimal engine performance conditions, a special technique based on the time-transient parametric ϕ -T maps [4] has been used.

INTRODUCTION

Bio-diesel fuels refer to non-petroleum based diesel fuels consisting of long chain alkyl esters produced by transesterification of vegetable oils, and proposed to be used (as neat or blended with conventional fuels) in unmodified diesel engines. The usage of bio-diesel fuel and their blends with conventional diesel oil promises substantial reduction of greenhouse and PM emissions in diesel engines, resulting in that engine combustion processes were investigated both numerically and experimentally. However, it was demonstrated (see Figure 1) a decrease of soot level, albeit an increase of NO_x emissions.

To analyze different strategies for reducing NO_x emissions, a realistic numerical simulation is required. A critical point of the modeling is the use of accurate bio-diesel fuel properties and combustion mechanism.

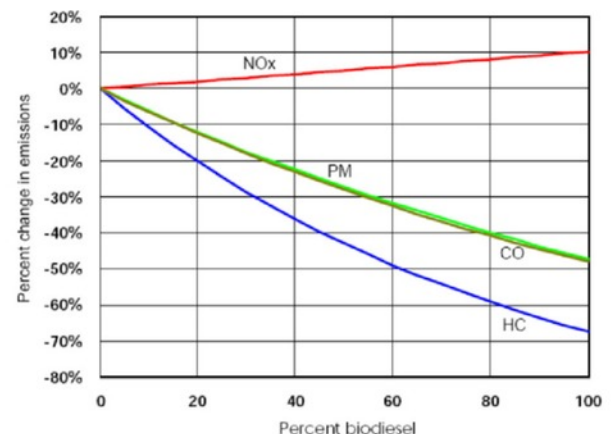


Figure 1 Trends in percentage change in pollutant emissions with bio-diesel content as estimated from published in the EPA study [5].

Bio-diesel is the name given to the esters of the structure $\text{R}-(\text{C}=\text{O})-\text{O}-\text{R}'$, where R and R' are chains of alkyl and alkenyl groups with as many as 17–19 carbon atoms. The five components of the real bio-diesel fuel are: methyl palmitate, methyl stearate, methyl oleate, methyl linoleate and methyl linolenate; their contents in the fuel are shown in Table.1 [6].

Table.1: Average compositions of rapeseed bio-diesels

Esters	Formulas	Rapeseed biodiesel,RME
methyl palmitate	$C_{17}H_{34}O_2$	4.3%
methyl stearate	$C_{19}H_{38}O_2$	1.3%
methyl oleate	$C_{19}H_{36}O_2$	59.9%
methyl linoleate	$C_{19}H_{34}O_2$	21.1%
methyl linolenate	$C_{19}H_{32}O_2$	13.2%

Table 2: Diesel oil and RME typical properties

Property	Diesel	RME
Calorific Value (kJ/kg)	42,600	~37,200
Cetane number	>50	~52
Carbon Content (%M)	86.1	75.8

Some typical properties of RME compared to those for diesel oil are listed in Table 2. For the methyl oleate ($C_{19}H_{36}O_2$), the carbon content calculated as ~77.03 % is in agreement with that presented in Table 2. In [2], another RME formula was proposed ($C_{21}H_{39}O_2$) which carbon content is equal to ~78.02%. Currently, there are few papers (see e.g. [7, 8]) in which the theoretical models for bio-diesel were developed. In this work, the main liquid fuel properties were taken as those of methyl oleate, $C_{19}H_{36}O_2$ [9]. The main fuel vapor thermal properties were taken as those of methyl oleate in the NASA polynomial form of the Burcat [10] database.

Special global reactions were introduced to “crack” the main fuel into its constituent components, $C_{11}H_{22}O_2$, $C_5H_{10}O_2$ and C_3H_4 , then, to C_7H_{16} and $C_4H_6O_2$, which sub-mechanisms were collected in a general (309 species, 1472 reactions) one which includes also soot and NO_x formation/destruction processes. The mechanism was reduced (99 species, 411 reactions) for the CFD engine modeling based on the shock-tube data at the diesel-like conditions and applied to the experiments [11] in the Volvo D12C diesel engine at 25% and full loads. Simulations were carried out by the KIVA-3V [12] engine code modified to account for detailed chemistry. Comparisons of the in-cylinder parameters as well as out-emissions levels for diesel oil and bio-diesel fuel are made.

COMPUTER MODELS

BIO-DIESEL THERMO-PHYSICAL PROPERTIES

Bio-diesel surrogate fuel model consists of two parts describing the thermal and transport properties of the liquid fuel and its vapor, and the ignition and combustion properties of constituent components. To model the fuel spray atomization, droplets breakup and evaporation, and finally, combustion the fuel physical properties were compiled. The physical properties of RME (methyl oleate): enthalpy, latent

heat of vaporization, vapor pressure, liquid viscosity, surface tension and thermal conductivity can be found in [3]. For comparison, in Figure 2, some physical properties of the primary reference component of diesel oil (hexadecane, $C_{16}H_{34}$), diesel oil surrogate, DOS, ($C_{14}H_{28}$) [13] and RME are plotted. The difference among the properties was found to be not drastic that opens the prospects to use RME in the diesel engines without hardware modifications.

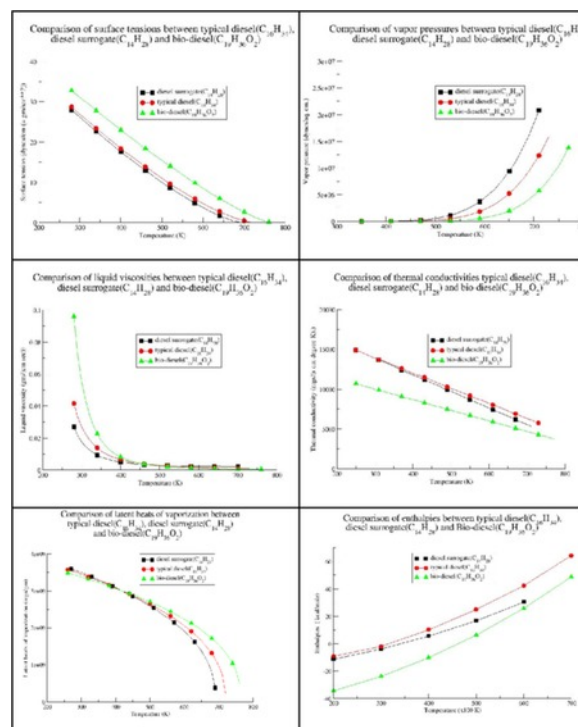
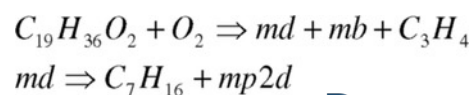


Figure.2: Comparison of physical properties of different fuels

The RME properties were approximated and included into a fuel library of the KIVA-3V code.

RME SURROGATE COMBUSTION MECHANISM

The long chain methyl ester, $C_{19}H_{36}O_2$ will generate a lot of species during combustion process. The reaction mechanism was proposed in a form of a bio-diesel surrogate as a 1:1:1 (volume ratio) blend of methyl decanoate (md, $C_{11}H_{22}O_2$), methyl butanoate (mb, $C_5H_{10}O_2$) and allene (C_3H_4), md and mb represent long chain and short chain esters, respectively. Allene represents a short-chain alkenyl group. To describe the bio-diesel surrogate decomposition into the constituent components, two global stages were added to the kinetic mechanism of elementary reactions as follows:



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where md decomposes into n-heptane and methyl propanoate, mp2d ($C_4H_6O_2$). The new LLNL species notations are described in the [Appendix](#).

The detailed mechanisms for the three constituent components are existing: the mb mechanism taken from the LLNL web site [8] contains 264 species participating in 1219 reactions, the n-heptane and allene sub-mechanisms were taken in the form [14] involving 72 species and 325 reactions. Combined together, that leads to the RME mechanism consisting of 309 species taking part in 1472 reactions. For CFD applications, the mechanism was reduced to 99 species participating in 411 reactions as described in [3].

The sub-mechanisms matched shock-tube experimental data for the constituent components. Predicted ignition delay times simulating shock-tube experiments are shown in [Figure 3](#). In the plot 3a) the detailed LLNL mb mechanism was compared with the reduced mechanism for engine modeling; in the plot 3b) auto-ignition of md was calculated and compared with that of n-decane [6]. The ignition delays for RME, its constituent components and DOS are presented for comparison in [Figure 4](#).

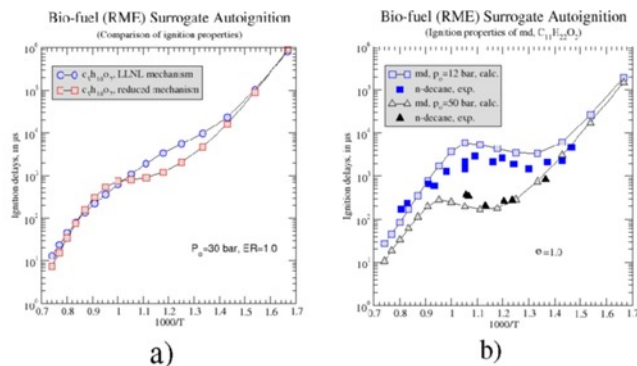


Figure 3: Calculated auto-ignition properties of a) mb based on detailed and reduced chemical mechanisms; b) md compared with the experimental data

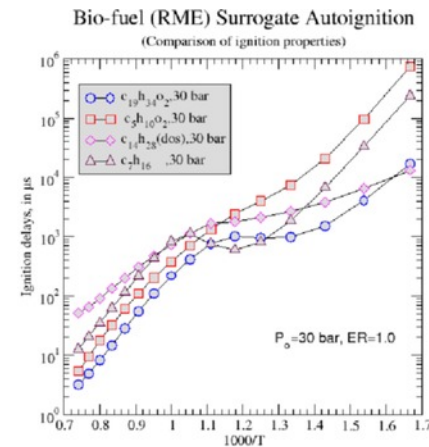


Figure 4 Auto-ignition properties of RME, its constituent components, n-heptane, mb, and DOS

Since different chemical formulas for RME were suggested (see [2], [6]), the global reactions presented above can facilitate to match the number of carbon and hydrogen atoms in the fuel molecule by proper selection of the third species in the first reaction.

TURBULENT COMBUSTION MODELING

To simulate turbulent combustion, the Partially Stirred Reactor (PaSR) method [15] has been employed. To outline the main features of the approach, let us consider the average gas phase equations for a chemically reacting mixture of ideal gases with embedded condensed liquid droplets written as

$$\frac{\partial \rho_i}{\partial t} + \nabla \left[\rho_i \bar{u} - \frac{\mu_i}{Sc_i} \nabla \rho_i \right] = \dot{\rho}_i^c + \delta_{i1} \dot{\rho}_i^s, \quad i = 1, \dots, N_s \quad (1)$$

where ρ_i is the density of the i -species, $\dot{\rho}_i^c$ is the chemical sources defined by combustion mechanism, $\delta_{i1} \dot{\rho}_i^s$ is the source term due to a presence of a spray, δ_{i1} is the Kronecker delta function, i.e. species 1 is the species of which the spray droplets are composed; μ_i is the turbulent viscosity, Sc_i is the Schmidt number, and N_s is the number of species.

Since the KIVA-3V code is based on the operation-splitting procedure applied to the mass conservation equations [Eq. \(1\)](#) for species participating in the multi-step reaction mechanism, the third step of the computational procedure accounting for the chemical kinetics coupled with micro-mixing can be interpreted as representing combustion in a constant volume partially stirred reactor of a computational cell size, where reactions occur in a fraction of its volume described in the term of the system of ODEs

$$\frac{dc^1}{dt} = \frac{c^1 - c^0}{\tau} = f_r(c) \quad (2)$$

where τ is a the time integration step, $f_r(c)$ is the chemical source term calculated at some unknown (virtual) concentrations, c , the parameters of a sub-grid scale reaction zone.

The model distinguishes between the concentration (in mean molar density) at the reactor exit, c^1 , the concentrations in the reaction zone, c , and in the feed, c^0 . When time proceeds, c^1 trades place for c^0 . The species indices are omitted for simplicity. To close the model, the additional equation for the reaction volume can be used

$$\frac{dc}{dt} = -\frac{c - c^1}{\tau_{mix}} + f_r(c) \quad (3)$$

where τ_{mix} is the micro-mixing time.

The difference between [Eq. \(3\)](#) and that from the PSR (Perfectly Stirred Reactor) [\[16\]](#) model of the Chemkin code [\[17\]](#) is that the residence time in the reactor equation of the PSR model is replaced by the micro-mixing time. Taking this equation in a steady-state form, the basic equations of the PaSR model are as follows

$$\frac{dc^1}{dt} = f_r(c) = \frac{c - c^1}{\tau_{mix}} \quad (4)$$

There are a number of micro-mixing models based on different principles; the review of those can be found in [\[18\]](#). One of the simplest and widely used micro-mixing model is “Interaction by Exchange with the Mean” (IEM) approach [\[18\]](#). In this approach, the scalar variable c relaxes to its mean c^1 value according to the linear term in the equation [Eq. \(4\)](#). Then, rewriting the reaction rate $f_r(c)$ in [Eq. \(4\)](#) in terms of reactor exit parameters:

$$f_r(c^1) + \left(\partial f_r / \partial c\right)_{c=c^1} (c - c^1) = f_r(c^1) - \frac{c - c^1}{\tau_c} \quad (5)$$

using its Taylor's expansion at the value c^1 . Then assuming that the reaction time can be defined as a reciprocal value of the Jacobian matrix diagonal elements evaluated at the grid resolved values $c=c^1$, i.e., $\tau_c \sim [\partial f_r / \partial c]^{-1}$ and accounting for the fact that $(\partial f_r / \partial c)_{c=c^1} < 0$. After algebraic manipulation with the second pair of [Eq. \(4\)](#) it leads to the relation

$$f_r(c^1) - \frac{c - c^1}{\tau_c} = \frac{c - c^1}{\tau_{mix}}$$

and then, to the main relation of the PaSR model.

$$f_r(c) = f_r(c^1) \frac{\tau_c}{\tau_c + \tau_{mix}} \quad (6)$$

This means the chemical source terms can be calculated using the averaged species concentrations, if multiplied by the model rate parameter ratio $\tau_c / (\tau_c + \tau_{mix})$. The application of [Eq. \(6\)](#) to the chemical mechanisms of the arbitrary complexity is straightforward. The model parameters such as τ_c and τ_{mix} are calculated as described in [\[19\]](#). With these values, the final rate expression takes form

$$\frac{c^1 - c^0}{\tau} = \frac{c^0 f_r(c^0)}{c^0 + term_r^\ominus \tau + term_r^\ominus \tau_{mix}} \quad (7)$$

where $term_r^\ominus$ represents the species destruction rate in $f_r(c^0)$ rate expression similar to [\[17\]](#).

MODIFIED SPRAY MODELS

The 3D-CFD model based on the KIVA-3V code has been used to calculate the engine process in a feasible complexity (using a detailed chemical mechanism) with a special tracking of “chemical” equivalence ratio [\[20\]](#) for multi-component mixture in each computational cell. This information was used to construct the emission parametric maps in the combustion process analysis. In order to improve the accuracy of calculations, the original KIVA-3V spray sub-models for fuel injection, spray atomization were also modified. The primary atomization depends on the spray's interaction with the ambient gas, leading to the formation of ligaments close to a liquid core that further disintegrates into parent droplets. After primary atomization has been completed, a secondary stage starts dependent on the parent droplet parameters (sizes, velocities, etc.)

In this paper, a combination of K-H, Kelvin-Helmholtz, and R-T, Rayleigh-Taylor [\[21\]](#), models coupled with the “blob” injection model were modified, validated and applied. The spray core is represented as a region close to the injector orifice with large droplets (blobs) to the size equal to the effective nozzle diameter. Based on spray instability theory, new droplets are formed from a parent droplet or the blob. It is assumed that small droplets are formed from the parent drops with the size proportional to the K-H wavelength.

In high pressure diesel spray, the droplets span a wide range of Weber numbers that requires to approximate different breakup mechanisms in the modeling. Secondary droplet atomization taking place as a result of the primary atomization process is described in terms of the R-T model. The hybrid K-H/R-T model was realized in such a way that it only affects droplets beyond the breakup length determined in terms of the R-T model,