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Diesel/biodiesel proportion for by-compression ignition engines

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Abstract

Nowadays, computational combustion (CC) presents complex mathematical models where the fuel physical properties are important parameters. Most research on biodiesel aims at reducing pollutant emissions placing little emphasis on the relation between the fuel physical properties and its internal combustion. In this work it is presented a brief review on the importance of the physical properties and their relation to the internal combustion proposing a method to determine the volumetric proportion of biodiesel which will have efficient combustion in compression engines. The main injection and atomization properties related to the quality of ignition were measured, such as: density, viscosity and surface tension for mineral diesel (B0), biodiesel (B100) and other eleven mixtures BXX. With the proposed method, it was found that mixtures of diesel/soybean ethylic biodiesel from B2 to B30, present satisfactory internal combustion. The method may be used to predict the behavior of BXX proportions from other animal or vegetable sources and even be used as a preliminary or complementary criterion for the biodiesel certification.

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1. Introduction

Diesel engines are the axis of world industry. With high torque, durability and economical on fuel under several conditions, they dominate sectors like road and train transport, agricultural, military, construction, mining, maritime propulsion and stationary electricity production. The ignition in these engines occurs by compression and since their invention, besides mineral diesel, they have used from crude or transesterified vegetable oils (biodiesel) to alcohols of short chain. They also work with hybrid fuels which are binary mixtures (diesel/vegetable oil) or ternary (vegetable oil, ethanol, and diesel) in the most varied proportions. In this sense, biodiesel is a binary hybrid fuel (diesel/methylic ester, ethylic, etc.). B2, for instance, indicates mixture of 98%v of diesel with 2% of ester.

2. Physical properties and internal combustion

In the internal combustion, the fuel is submitted to thermodynamic conditions that involve flow, heat exchange, phase change and chemical reaction. In the simulation and computational combustion, the fuel properties are frequently combined into dimensionless or non-dimensionless groups as shown in the brief review that follows.

Breuer [1], states that the fuel properties interfere in the dynamics of heat release and in the conversion into mechanical energy. He considers the combustion as occurring in two phases, one of pre-mixture and another of diffusion. The model for canola oil and its methylic esters, considers the viscosity, cetane number, distillation curve and the proportion of the air/fuel mixtures. According to Egolf and Jurs [2] this proportion is a function of the autoignition temperature (AIT). Fig. 1 shows that effectively flammable mixtures appear between the flash (FT) and fuel autoignition temperatures.

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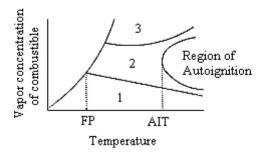


Fig. 1. Flammability regions of fuel vapor/air mixtures: (1) mixtures too lean to burn; (2) flammable mixtures; (3) mixtures too rich to burn [2].

The model of Kim et al. [3] describes the self-ignition and gaseous jet propagation, in turbulent flame under high pressure, being combustion heat $(\Delta H_c, kJ/kg)$, mass diffusivity $(D_{AB}, mm^2/s)$, specific heat $(C_p, J/mol K)$ and density $(\rho, kg/m^3)$, the physical properties used in the model.

Matsui et al. [4] modeled the injection characteristics before the atomization. One of the parameters is the dimensionless Reynolds number ($Re = v_0 d_0/v$) being the properties: density, kinematic viscosity (v, m/s²) besides the speed of sound (v_s , m/s) in the flow.

For Bertoli and Migliaccio [5], the diffusive mechanism of Fick's Law observed in the evaporation of sprays with chemical reaction on the surface of the drops, depends on the density, specific heat, vaporization enthalpy ($\Delta H_{\rm v}$, kJ/kg), thermal conductivity (k, W/m K) and heat convection coefficient (h, W/m² K).

The research of Goodrum and Eiteman [6] and Allen et al. [7] on disintegration of liquid jets uses the dimensionless group of atomization $K_a = [We/Re(\rho_L/\rho_G)]^{1/3}$, where $\rho_{\rm I}/\rho_{\rm G}$ is the relation of the fuel densities (L) and the gaseous phase (G) in the combustion chamber. Re and We are the numbers of Reynolds and Weber. d_0 and v_0 are the diameter and velocity of the jet in the injection. In the combustion of drops under reduced gravity carried out at the National Aeronautics and Space Administration (NASA), Dee and Shaw [8] created drops of constant diameter by mixing liquids of different surface tension (propanol and glycerol) and developed a model, based on Fick's Law, to describe the heat and mass transient transport during the combustion. They used the density, thermal conductivity, vaporization heat and the diffusivities (mm²/s) of the three transport phenomena: mass (D), heat (α) and of momentum (v), which are some of the properties in the dimensionless group of Peclet $(Pe = v_0 d_0 / \alpha = RePr)$ that is the time relation between the heat transport by convection and diffusion in a fluid.

Eaton et al. [9] on their review on software about combustion reports lagrangian formulations and CFD approaches (computer fluid dynamics) of the equation of Navier–Stokes expressed as tensorial systems. The properties of these models are combustion enthalpy, radiation intensity, speed of sound and others included in the numbers of Reynolds, Prandtl ($Pr = \mu C_p/K$), Schmidt ($Sc = \mu/\rho D_{AB}$) and Mach ($Ma = v_0/v_S$). Pr and Sc relate the dif-

fusivities of momentum/heat and of momentum/mass respectively. Ma is the relation of fluid velocity and speed of sound in the liquid. Ma^2 relates the kinetic and thermal energies in the flow.

Domingo et al. [10] developed a DNS model (direct numerical simulation) for low turbulence flames produced by gaseous fuels or atomized liquids. The evolution of the gaseous phase is approached with the equations of Navier–Stokes extended to flows with chemical reaction. The physical properties required in this case are density, viscosity, diffusivity, thermal conductivity, specific heat, speed of sound and vaporization enthalpy. Most of them in the Re, Pr, Sc and Nu groups ($Nu = hd_0/k$). Besides these, the model also uses the number of Strouhal ($Sr = fd_0/v_0$) which determines the frequency (f, Hz) with which the current lines are separated in the laminar flows; and the number of Lewis ($Le = k/\rho C_p D_{AB} = Sc/Pr$) which relates the thermal and mass diffusivities of the fluid.

Aggarwal [11] in an extensive review on the ignition and self-ignition phenomena of atomized fluids also emphasizes the importance of the fuel properties. According to him, ignition occurs in the thermal limit layer which may be three ways: droplet ignition, ignition of a cloud, and spray ignition. The properties are: viscosity, diffusivity and thermal conductivity, gathered in *Re*, *Pr* and *Nu*.

MacLean and Lave [12] indicate, besides the above properties, others (cetane number, volatility, air/fuel stoichiometric ratio, flash point, flammability limits, corrosivity, lubricity, etc.) as determining in the quality of ignition and on the engine's life. They also point out that the combustion of diesel fuels is more complex than the gasoline's due to greater variability in the composition and consequently in the physical properties. In addition, the low level of sulfur of the biofuels from vegetable sources improves the quality of the emissions but noticeably harms the stability of the fuels, that is, the capacity to keep its properties and composition constant in time. The electrical conductivity and the lubricity of biofuels are the properties affected by the reduction of the sulfur level and shall be corrected with additives.

Aiming at the internal combustion of crude vegetable oil, Morón-Villarreyes [13] developed QSPR models (quantitative structure property relationships) to estimate the internal combustion properties by using just triglyceride molecular characteristics.

3. Indicative parameters of internal combustion efficiency

In the diesel engine with operational cycle of four strokes, temperatures of 813 K and pressures of up to 2000 bar [14] are common. These conditions interfere with the properties of the fuel affecting the injection, atomization, combustion and finally the transformation of the chemical energy into mechanical energy. As it is observed, the internal combustion implies, simultaneously, inertial, viscous and surface effects. For instance, the average diameter of the drops (d) depends on the speed (v_0) with which

the liquid is injected and on the fuel properties. This influences the mechanical project of the injector nozzles that must produce homogeneous sprays that facilitate the quick mixture of the vaporized fuel with the air.

Goodrum and Eiteman [6] indicated the density. dynamic viscosity, surface tension, specific heat and vapor pressure as being the most relevant properties. In another work, Flores-Luque et al. [15] delimitated the study for the density ρ (g/cm³), dynamic viscosity μ (mPa s) and surface tension σ (mN/m) combined into five dimensional groups called indicative parameters of internal combustion efficiency or also combined functions of physical properties, being $A = \mu/\rho$, $B = \sigma/\mu$, $C = \sigma/\rho$, $D = \sigma^2/\mu\rho$ and $E = \mu^2/\sigma\rho$. The mathematical form of each of these groups was originated in the modeling equations of injection and atomization dynamics of Schweitzer [16]. The idea of combining properties in dimensional groups was also used by Othmer and Jaatinen [17] who, for instance, defined the group $\sigma \rho / \mu$ (kg/m² s) to study the thermal/hydraulic behavior of vegetable oil/solvent mixtures (micela) aiming at optimizing the industrial oil extraction process.

3.1. Parameter A

This dimensional group relates μ and ρ through the known expression:

$$A = \frac{\mu}{\rho} \quad [\text{mm}^2/\text{s}] \tag{1}$$

which is just the definition of kinematic viscosity ($v = \mu/\rho$, mm²/s). The value of v along with the values of speed v_0 of the fuel through the injector of diameter d_0 characterize the flow of liquids through the Reynolds number, if the injection occurs in a laminar (Re < 2300) or turbulent ($Re > 10^4$) regime.

3.2. Parameters B and C

The time (t_d) necessary for a liquid jet to disintegrate into microdrops is determined through the equation of Schweitzer [16]:

$$t_{\rm d} = k_2 \left[\left(\sqrt{\frac{6}{(\sigma/\mu)}} \right) d_0 + \left(\sqrt{\frac{8}{(\sigma/\rho)}} \right) d_0^{3/2} \right],$$

disregarding the k_2 constant and the jet diameter (d_0) and grouping the physical properties it is obtained:

$$B = \frac{\sigma}{\mu} \quad [\text{m/s}],\tag{2}$$

$$C = \frac{\sigma}{\rho} \quad [\text{cm}^3/\text{s}^2] \tag{3}$$

These parameters influence the synchronization of the engine cycles. Nowadays, the time variable is evaluated with the cetane number (CN) which permits to predict the time interval (ignition delay time, ID) up to the self-ignition of the air/fuel mixture, confirming the dependence of the ID on the autoignition temperature (AIT). The time interval

in milliseconds, from the injection to the autoignition is estimated with the equation, $ID = 1.512 + 840.15/(CN-3.547)^{1.52}$ resulting in values from 3.9 to 4.2 ms [18,19]. The current standards for biodiesel demand the same specifications of mineral diesel which must present a minimum cetane number of 40. The biodiesel must present either 47 or 51 according to ASTM D6751 and EN14214 standards respectively [19].

3.3. Parameter D

The diameter of the drops (d) after atomization (Fig. 2), is calculated through the expression

$$d = \frac{k_1}{v_0^3} \frac{\sigma^2}{\mu \rho}$$

which defines group D:

$$D = \frac{\sigma^2}{\mu \rho} \quad [dm^4/s^3] \tag{4}$$

Aggarwal [11] shows that the present models predict details like the heating quickness of the drop surface and the time in which ignition will occur (ID) in relation to the number of spray drops (see Fig. 3b). These phenomena depend mainly on the statistical distribution of the drop diameters [20]. The dimensionless groups representative of these phenomena are the numbers of Weber and Bond. $We = v_0^2 d_0 \rho / \sigma$, relates inertial and surface forces in the atomization. $Bd = d_0^2 \rho g / \sigma$, relates gravitational and surface forces in the dropping. The Ohnesorge number $(Oh = \mu / \sqrt{\rho \sigma d_0} = \sqrt{We}/Re)$ relates viscous and surface forces.

In another study, Morin et al. [21] observed the total vaporization of suspended drops of canola methylic biodiesel. Before changing the phase, the drop is heated by natural convection depending on the dimensionless numbers of Nusselt, Prandtl, Grashoff ($Gr = g\beta\Delta T\rho^2d_0^3/\mu^2$) and Rayleigh (Ra = GrPr). Besides density, viscosity and surface tension, these groups contain the specific heat, thermal expansion (β , T⁻¹), thermal conductivity and heat transfer coefficient.

The application of this experimental procedure may quantify the deposits on the engine, being able to complement the standards for carbon residuals (ASTM D183) and

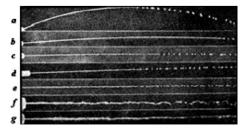


Fig. 2. Disintegration patterns of liquid jets (water, $d_0 \approx 1.0$ mm): (a) $v_0 = 3.1$ m/s; (b) $v_0 = 4.7$ m/s; (c) $v_0 = 7.8$ m/s; (d) $v_0 = 10$ m/s; (e) $v_0 = 24$ m/s; (f) $v_0 = 34$ m/s; (g) $v_0 = 40$ m/s [16].

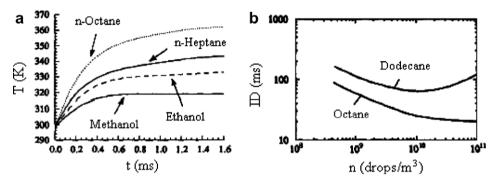


Fig. 3. (a) Time variation of the surface temperature of atomized drops. (b) Effect of the number of drops in a cloud on the ID [11].



Fig. 4. Injector after EMA Engine test cycle-200 hours (ethyl canola): (a) clean injector; (b) B0; (c) B50; (d) B100 [22].

ashes (ASTM D482). Impurities, in general, form deposits (see Fig. 4) that retard ignition and alter the engine cycle.

3.4. Parameter E

Until the jet atomization occurs, its diameter is not constant and oscillates until disintegrating into a homogeneous spray (see Figs. 2 and 5).

Spray homogeneity is obtained if the wave length (λ, m) with which the oscillations in the jet diameter propagate reaches an optimal value determined through the equation,

$$\lambda = \sqrt{2}\pi d_0 \sqrt{1 + \sqrt{\frac{2}{d_0} \frac{\mu^2}{\sigma \rho}}}$$

that contains the E parameter:

$$E = \frac{\mu^2}{\sigma \rho} \quad [\mu \text{m}] \tag{5}$$

Yoon [23] researched the pattern evolution of continuous and intermittent sprays varying the number of We (see Fig. 6).

Alterations and disturbances in the spray pattern may occur due to impurities; catalyst, reactant and byproduct remainders, from the biodiesel synthesis; especially glycerin (see Figs. 4 and 7).

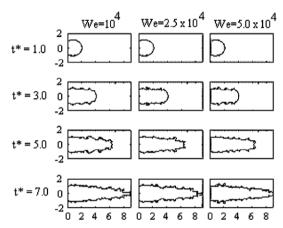


Fig. 6. Simulation of a jet evolution in relation to the number of Weber $(t^* = v_0 t/d_0)$ [23].

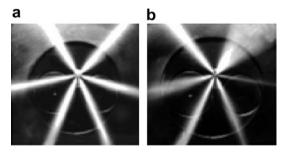


Fig. 7. Diesel atomization patterns (a) clean injector (b) injector with deposits [14].

For the efficient performance of fuel under the conditions that prevail in the engine, the five parameters must remain within an adequate interval. Taking as reference the efficient mechanical work of agricultural diesel engines, Flores-Luque et al. [15] established the intervals shown in Table 1.



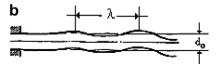


Fig. 5. Oscillation of the jet diameter before atomization: (a) symmetrical rotational disturbance; (b) wave inducing disturbance [16].

Table 1
Intervals of efficient performance of diesel engines [15]

T(K)	288	298	313
$A \text{ (mm}^2/\text{s)}$	5.03-7.02	3.82-5.46	2.64-4.39
B (m/s)	4.64-6.55	6.07 - 8.11	8.25-10.8
$C \left(\text{cm}^3/\text{s}^2 \right)$	30.2-34.2	29.6-33.5	28.7-32.5
$D \left(dm^4/s^3 \right)$	1.37-2.21	1.73-2.67	2.30-3.43
$E (\mu m)$	0.66-1.51	0.31 - 1.01	0.05 - 0.65

4. Materials and methods

The diesel/biodiesel mixtures were prepared with diesel from a private gas station (Esso, Florianópolis, SC) and soybean ethyl biodiesel produced through alkaline catalysis at the GEQ/FURG, analyzed and certified at the Fuel and Lubricant laboratory of ISATEC-IPIRANGA, Rio Grande, RS [24].

Density was obtained by picnometry at room temperature (\approx 298 K) through sample weighing on analytical scale. The picnometer volume was gauged with distillated water and calibrated with ethanol.

The kinematic viscosity (v) was directly measured at 298 K (± 0.01) in a Cannon-Fenske viscosimeter no. 100 with Schott optical reader which uses the equation v = K(t - v), where $K = 0.01511 \text{ mm}^2 \text{ s}^{-2}$ is a constant provided by the manufacturer and v is a correction factor. The flow time t was determined in triplicate.

The surface tension was determined at room temperature (≈298 K) through the drop weight method by applying Tate's Law, using water as reference liquid. The method of Tate for measuring surface tension is reliable despite having been proposed in 1864. It was improved in 1919 by the correction factor of Harkins–Brown; discussed in 1994 by Garandet et al. [25] and most recently by Yildirim et al. [26].

5. Results and discussion

Table 2 shows the values for the five indicative efficiency parameters of internal combustion (Eqs. (1)–(5)). The numbers in bold indicate the mixtures with satisfactory combustion according to the criterion of Table 1.

The values of parameter A indicate that the pure diesel and the mixtures of B2 up to B30 are satisfactory as to the injection when kinematic viscosity is directly measured. In contrast, in the measurement separated from dynamic viscosity at 298 K (with Brookfield reometer of digital cone, model DV-III with spindle number 42) and density (by picnometry at ~298 K) the mixtures B2 up to B20 were satisfactory. However, it is important to point out that the direct measurement of kinematic viscosity is more reliable, meets ASTM D445 standard and applies to newtonian fluids as the mixtures BXX. Commercial diesel (diesel no. 2), for instance, must have a viscosity of 2.7 mm²/s at 311.7 K [27]. At lower temperatures as 298 K, 4.71 mm²/s in measurement involving picnometry and 4.62 mm²/s in the

Table 2
Indicative parameters of fuel efficiency of diesel/biodiesel mixtures at 298 K

BXX	$A \text{ (mm}^2/\text{s)}$	B (m/s)	$C \left(\text{cm}^3/\text{s}^2 \right)$	$D \left(dm^4/s^3 \right)$	<i>E</i> (μm)
B0	4.62	7.0230	32.446	2.2787	0.6578
B2	4.67	6.9516	32.464	2.2568	0.6718
B5	4.72	6.9346	32.732	2.2698	0.6806
B10	4.82	6.8007	32.780	2.2293	0.7087
B20	5.06	6.5461	33.123	2.1683	0.7730
B30	5.24	6.3169	33.100	2.0909	0.8295
B40	5.48	6.0898	33.372	2.0323	0.8999
B50	5.54	6.0677	33.615	2.0397	0.9130
B60	5.78	5.8643	33.896	1.9877	0.9856
B70	5.90	5.7703	34.045	1.9645	1.0225
B80	6.48	5.2831	34.234	1.8086	1.2266
B90	6.57	5.3313	35.026	1.8674	1.2324
B100	6.82	5.2650	35.907	1.8905	1.2954

direct measurement were obtained. BXX mixtures presented differences of 0.27 mm²/s on the average.

The jets of pure diesel and of B2 up to B40 mixtures, injected in the combustion chamber, disintegrate at the adequate time as indicate parameters B and C.

The values of *D* show that the atomization of diesel and of all mixtures (from B2 to B100) presents sprays with drop diameters in an adequate distribution.

The values of E indicate that mixtures with up to 60% of soybean biodiesel inject with the best conditions to disintegrate before ignition.

According to the criteria of Table 1, the mixtures from B0 to B30 satisfy simultaneously all the parameters, agreeing with the Brazilian Biodiesel Program as to the lack of need to tune-ups when using mixtures of up to B20.

6. Conclusion

The study of the fuel physical properties is important in the engine performance as shown by the several computational combustion models. Independently of the approaches or complexity of the models [28], such properties are generally the same ones. The method, being of easy application with low cost measurements, when compared to others [29], can aid preliminary quality control in small scale biodiesel production or used to predict the behavior of any specific proportions of diesel with vegetable or animal biodiesel and even be used as preliminary or complementary criterion for the biodiesel certification.

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