

DETERMINATION AND INTRODUCTION OF THE TRANSPORT PROPERTIES OF SOYBEAN OIL BIODIESEL IN THE COMPUTATIONAL FLUID DYNAMIC CODE OPENFOAM

by

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In this work the determination and introduction of the transport properties of soybean oil biodiesel in the CFD code OpenFOAM has been studied. Additionally, effects of soybean oil biodiesel on the mixing process using CFD code OpenFOAM have been analyzed. In order to reach the objectives described, the most relevant transport properties of soybean oil biodiesel in the mixing process i. e. density, viscosity, surface tension, and vapor pressure have been determined. These transport properties were introduced in the CFD code OpenFOAM using coefficients obtained, which are based on the molecular structure of the fatty acids that composes the biodiesel and applying non-linear regressions. The main findings of the work were: the coefficients which are used in the proposed models by CFD code OpenFOAM for the introduction of the transport properties of soybean oil biodiesel have been obtained and the influence of the transport properties of soybean oil biodiesel on the mixing process has been confirmed.

Key words: *biodiesel, transport properties, diesel spray, mixing process, simulation, CFD code OpenFOAM*

Introduction

The use biodiesel in Diesel engines is one of the ways to fulfill on the one side, the demands of the customers and on the other side, the environmental regulations. It is the main reason why many researchers [1-6] have been focused on deepen in the knowledge of the effect of biofuel on the injection and combustion processes. The first step to study the combustion process, it is analysis of the injection process, specifically the mixing process, which is characterized through the macroscopic parameters of diesel spray: spray tip penetration, spray cone angle, and spray area. These macroscopic parameters can be experimentally determined, employing optically accessible constant volume chambers [7, 8], and numerically using CFD codes such as the CFD code OpenFOAM [9] among others. For accurate CFD simulation for biodiesel spray, the thermophysical properties of biodiesel (*i. e.* density, vapor pressure, heat of vaporization, liquid and vapor heat capacity, second virial coefficient, liquid and vapor viscosity, liquid and vapor thermal conductivity, surface tension and vapor diffusivity) must be determined appropriately, due to that these play an important role in defining the fuel spray development [10, 11]. According to Ismail *et al.* [12] the following transport properties: vapor

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pressure, vapor diffusivity, surface tension, liquid density, and liquid dynamic viscosity have significant effects on fuel spray structure, combustion, and emissions characteristics. In the following lines some examples where the mixing process has been characterized using the CFD code OpenFOAM will be described.

Yousefifard *et al.* [9] studied the effects of injection pressure and fuel properties on spray penetration, spray cone angle, and spray volume using the CFD code OpenFOAM, concluding that at ultra-high pressure, the geometrical properties of biodiesel fuel sprays are similar to those of diesel fuel sprays, also that biofuel have longer penetration at lower injection pressure. Ismail *et al.* [12] developed, validated, and applied the thermophysical and transport properties of biodiesel derived from three different feedstocks: coconut oil, soybean oil, and palm oil for fuel spray and combustion modeling in Diesel engine applications using OpenFOAM. They also found among other findings, a longer spray penetration for biofuel compared to those fossil diesel. Agudelo *et al.* [13] studied the effect of fuel type, injection pressure and ambient gas pressure on spray penetration, Sauter mean diameter (SMD) and evaporated fuel mass using OpenFOAM. They concluded that fuel properties significantly affected the atomization and evaporation processes and in a laser extent the spray fuel penetration. In each work previously described not report the way of the implementation of the transport properties in the CFD code OpenFOAM. Therefore, the objectives of the present study are: deepen knowledge related to determination and implementation of the transport properties of biodiesel in the CFD code OpenFOAM and to study the effects of soybean oil biodiesel on mixing process using the CFD code OpenFOAM.

Operating conditions of study cases

In the present study the mixing process will be studied through of the spray tip penetration, characteristic mixing parameter which will be characterized using the CFD code OpenFOAM. This code is based on the environment C++ which has a wide variety of spray sub-models and liquid library for simulation. More details of CFD code OpenFOAM are available in [14].

In order to carry out the characterization of the spray tip penetration in CFD code OpenFOAM is necessary to define several operating conditions: first of all the thermodynamic conditions at the control volume chamber during the injection event, injection parameters such as nozzle outlet diameter, injection pressure, injection time, injected mass, discharge coefficient and spray cone angle, numerical method and computational mesh, and the transport properties of soybean oil biodiesel. In the forthcoming lines will be given more details of the points previously described.

In base on Gimeno [15] the operating conditions for a diesel spray have been defined. It is worthy to note that Gimeno does not perform experiments using biodiesel. The thermodynamic conditions at the control volume during the injection event will be next:

- back pressure corresponds to pressure inside of control volume chamber. In the present study the back pressure will be fixed at 3.5 MPa,
- ambient gas corresponds to gas inside of control volume chamber; in the present study the ambient gas will be nitrogen due to it allows characterizing the spray diesel in non-reactive conditions, ideal conditions to study the mixing process, and
- control volume chamber temperature corresponds to temperature inside of control volume chamber; in the present work the temperature will be fixed at 306 K.

Regarding to injection parameters will be following: a nozzle outlet diameter of 112 μm , an injection pressure (pressure driven velocity) of 80 MPa and 184 MPa which are rep-

representative of those existing in current Diesel engine for both fuels in diesel and biodiesel and in order to reproduce a penetration by the premise of the increased injection pressure when using biodiesel due to its higher transport properties [16-19], an injection time of 1 ms, an injected mass of $5.7 \cdot 10^{-6}$ kg by nozzle orifice, a discharge coefficient of 0.8934, and a half spray cone angle for diesel and biodiesel of 18.955° and 15.886° , respectively. In tab. 1 the operating conditions previously described are summarized. As previously mentioned Gimeno [15] does not perform experiments using biodiesel, then the methodology employed to define the injection pressure and half spray cone angle for biodiesel case will be described.

Table 1. Operating conditions for diesel and biodiesel cases

Parameter	Diesel [B0] / biodiesel [B100]
Number of nozzle holes	6
Nozzle outlet diameter, [μm]	112
Spray cone angle, [$^\circ$] (diesel)	18.955
Spray cone angle, [$^\circ$] (biodiesel)	15.886
P_{inj} , [MPa] (diesel)	80
P_{inj} , [MPa] (biodiesel)	184
Ambient gas	N_2
Back pressure, [MPa]	3.5
Gas temperature, [K]	306
Injection time, [ms]	1
Mass injected by hole, [kg]	$5.7 \cdot 10^{-6}$
Discharge coefficient, [-]	0.8934

As already previously mentioned the injection pressure used for the biodiesel case should be increased to introduce the same of biodiesel mass that has been used in diesel case. The injection pressure is determined through of the eq. (1):

$$\dot{m}_f = AC_d U_{inj} \rho_f \quad (1)$$

where A is the effective area of the nozzle, C_d – the discharge coefficient, ρ_f – the fluid density, and U_{inj} – the injection velocity which is defined through of the eq. (2):

$$U_{inj} = \sqrt{\frac{2\Delta(P_{inj} - P_{back})}{\rho_f}} \quad (2)$$

The eq. (2) involves the transport properties related to the flow of biodiesel which increases in its absolute value, for this reason it is necessary to increase the injection pressure to obtain the same mass of biodiesel that has been determined in the diesel case.

The spray cone angle is one of the characteristic parameters which characterize the mixing process, in other words, a decrease in the spray cone angle impairs the efficiency of the air/fuel mixture [16, 20, 21]. The spray cone angle for biodiesel case will be determined through of eq. (3) which was proposed by Heywood [22] and taking into account the operating conditions described in tab. 1.

$$\tan \frac{\theta}{2} = \frac{4\pi}{A} \sqrt{\frac{\rho_g}{\rho_f}} \frac{\sqrt{3}}{6} \quad (3)$$

where A is a constant related to the nozzle geometry $A = 3.0 + 0.28 (L/D)$, L – the hole length where its value is around of 1 mm, D – the nozzle outlet diameter, and ρ_g and ρ_f are the gas and fuel density, respectively.

With regard to numerical method and computational mesh, the finite volume method will be used, and the computational mesh that will be used in the present study for both simulations (diesel and biodiesel cases) consists in a 3-D domain formed by hexahedral elements of $41 \cdot 41 \cdot 200$ computational cells and a simply grid (1, 1, 0.5) for a better definition in the axial direction.

Finally, the transport properties of soybean oil biodiesel must be determined. These in the CFD code OpenFOAM are defined through of next models:

- in eq. (4), the model for the density is described [23]:

$$\rho = \frac{A}{B^{1+\left(1-\frac{T}{T_c}\right)^D}} \quad (4)$$

- in eq. (5), the model for the viscosity is described [24]:

$$\mu = e^{\left(A + \frac{B}{T} + C \log T\right)} \quad (5)$$

- in eq. (6), the model for the surface tension is described:

$$\sigma = A(1 - T_r)^{(ET_r^3 + DT_r^2 + CT_r + B)} \quad (6)$$

- in eq. (7), the model for the vapor pressure is described:

$$P_{\text{vap}} = e^{\left(A + \frac{B}{T} + C \log T + DT^E\right)} \quad (7)$$

The transport properties are introduced in the CFD code OpenFOAM through of the coefficients A to E . In forthcoming section the transport properties of soybean oil biodiesel will be determined.

Determination of transport properties of soybean oil biodiesel

The determination of transport properties of soybean oil biodiesel consists in: determine the biodiesel composition, and determine the transport properties of biodiesel. In the following sections will be given more details of the points previously described.

Determination of soybean oil biodiesel composition

The biodiesel composition consists in the determination of which and in what proportion of fatty acid methyl esters are present in a biodiesel. In order to identify the biodiesel composition derived from soybean oil used in the present study, a gas chromatography was carried out using a gas chromatograph Bruker 450-GC which is composed by a separation column Bruker BR-S-WAX 30 mx0.32 mm of internal diameter (ID) and a flame ionization detector (FID). In the following lines more details about the methodology employed will be described. The 50 g of biodiesel and 1 mL of methyl heptadecanote solution with toluene were measured, then 1 μL of analyte was injected, using a bed of air to avoid the evaporation of volatile compounds and for clean the injector needle, next, a temperature of 260 $^{\circ}\text{C}$ was used in split less mode to evaluate high boil temperature in low boil temperature solvents, like fatty acid in toluene. Finally, helium with 99.99% of purity was used as a carrier gas with a constant flow set as 2.1 ml/min on the column.

Table 2. Soybean oil biodiesel composition

Fatty acid methyl esters	Mass fraction [-]
Palmitic	13.28
Stearic	4.66
Oleic	21.34
Linoleic	50.92
Linolenic	9.81

temperature of 260 $^{\circ}\text{C}$ was used in split less mode to evaluate high boil temperature in low boil temperature solvents, like fatty acid in toluene. Finally, helium with 99.99% of purity was used as a carrier gas with a constant flow set as 2.1 ml/min on the column.

A good determination of the fatty acid composition depends on the sample weight measurement, in order to reach this, five different repetitions for each measure will be carried out. In tab. 2 shows the soybean oil biodiesel composition obtained. It is worthy to note that the reached results are consistent with the literature [25].

Once determined the soybean oil biodiesel composition, the transport properties of soybean oil biodiesel will be determined.

Determination of the transport properties

Before to determine the transport properties of biodiesel, the critical properties of the fatty acids that composes the biodiesel must be determined due to that these are essential to apply the functional group correlations, to do that the Ambrose method [25, 26] will be used. With the critical properties of the fatty acids obtained and by applying the Kay's mixing rule [26] the transport properties of biodiesel will be determined. In tab. 3 the methods employed to determine the transport properties of biodiesel are shown.

Table 3. Proposed estimation methods for transport properties of biodiesel

Transport properties	Computation method
Liquid density	Ramírez-Verduzco equation [27]
Liquid viscosity	Ramírez-Verduzco equation [27]
Surface tension	Equation proposed by Allen <i>et al.</i> [28]
Vapor pressure	Ridel equation cited by Vetere [29]

Next, the coefficients needed to introduce the transport properties related to soybean oil biodiesel and diesel in the CFD code OpenFOAM will be obtained.

Obtaining the coefficients to introduce the transport properties of soybean oil biodiesel and diesel in the CFD code OpenFOAM

The empirical correlations cite in tab. 3 will be used to obtain non-linear regressions to adjust the transport properties, generating from this way, the coefficients which are used to introduce the transport properties of soybean oil biodiesel in the CFD code OpenFOAM. In fig. 1 the behavior of the transport properties of soybean oil biodiesel (B100) and diesel (B0) with the temperature is shown. In this figure also can be observed: an increase of the transport properties of soybean oil biodiesel in comparison with those transport properties of diesel, and a good agreement between the results reached from the empirical correlations and CFD code OpenFOAM models, therefore, can be concluded that the coefficients are consistent. In tabs. 4-7 presents the obtained coefficients.

Table 4. Density coefficients for soybean oil biodiesel; these are used in eq. (4)

Coefficients	Biodiesel [B100]	Diesel [B0]
A	32.08513	60.92023
B	0.1727497	0.2582
C	0.2581803	0.26628

Table 5. Viscosity coefficients for soybean oil biodiesel; these are used in eq. (5)

Coefficients	Biodiesel [B100]	Diesel [B0]
A	-12.16225	-18.96460
B	2009	2010.9
C	-4.284·10 ⁻⁷	1.0648

Table 6. Surface tension coefficients for soybean oil biodiesel; these are used in eq. (6)

Coefficients	Biodiesel [B100]	Diesel [B0]
A	144.2567	249.21
B	-1.3510·10 ⁴	-16,915
C	-17.84885	-35.195
D	-1.6657·10 ⁻⁵	0.028451
E	1.921481	1.0

Table 7. Vapor pressure coefficients for soybean oil biodiesel; these are used in eq. (7)

Coefficients	Biodiesel [B100]	Diesel [B0]
A	0.0914554	0.056436
B	3.652957	0
C	-5.737485	0
D	7.226804	0
E	3.896143	1.3658

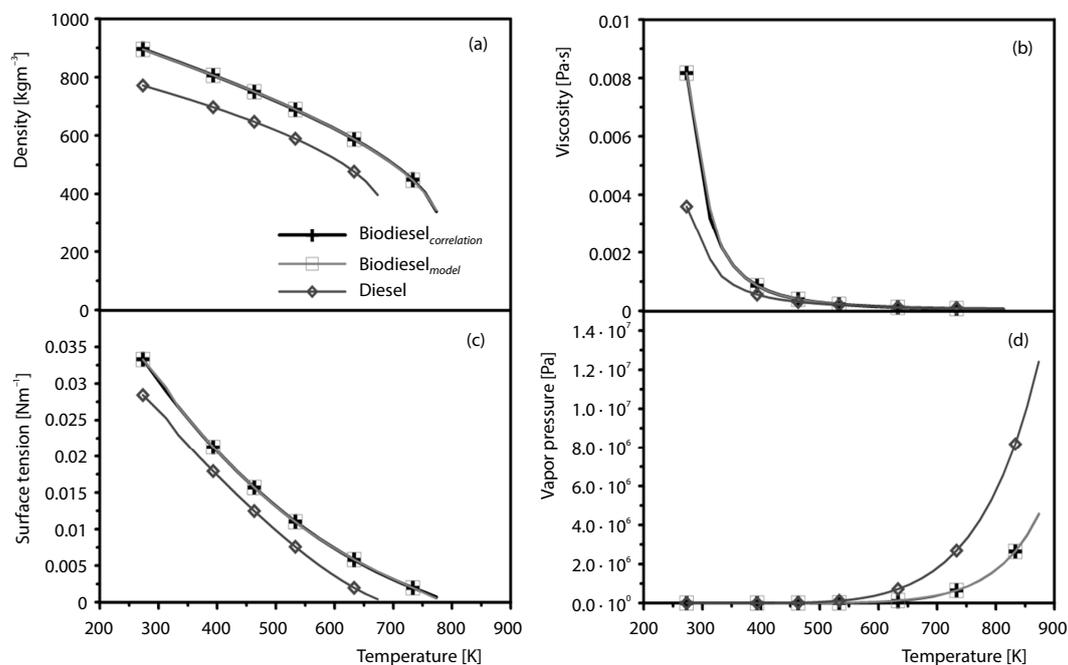


Figure 1. Comparison between empirical correlation and CFD code OpenFOAM models for the soybean oil biodiesel; a) density, b) viscosity, c) surface tension, and d) vapor pressure

Once obtained the coefficients to introduce the transports properties of soybean oil biodiesel in the CFD code OpenFOAM, effects of soybean oil biodiesel on the mixing process will be analyzed.

Effects of soybean oil biodiesel on the mixing process

As already mentioned in the section *Operating conditions of study cases* in the present study the mixing process will be studied through of the spray tip penetration, characteristic mixing parameter. Before showing the results related to mixing process. In fig. 2 the velocity of the surrounding gas for the soybean oil biodiesel and diesel is shown. From this figure can be seen qualitative way an increase in the velocity of the surrounding gas for soybean oil biodiesel case in comparison with diesel case. This behavior is due to that soybean oil biodiesel has a high droplet momentum which lead to an increased penetration.

Finally, in fig. 3 the temporal evolution of spray tip penetration is shown, in dashed line corresponding to diesel and continue line corresponding to soybean oil biodiesel. From this figure can be observed a higher penetration from the soybean oil biodiesel in comparison with the diesel, this behavior is due to higher viscosity of soybean oil biodiesel. It is worthy to note that this result is consistent with the literature [30].

Conclusions

Regarding the soybean oil biodiesel composition, the following fatty acids: palmitic, stearic, oleic, linolenic, and linolenic have been found. It is worthy to note that these results are consistent with the literature.

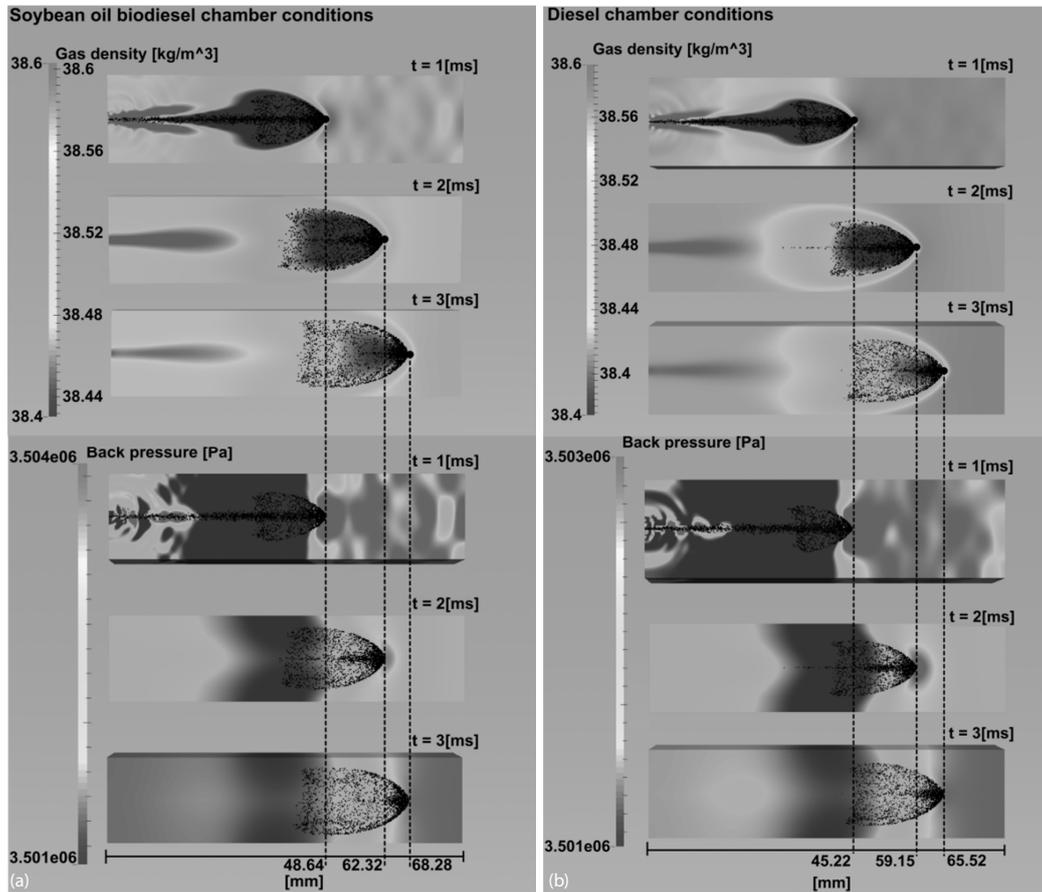


Figure 2. Chamber conditions for the (a) Soybean oil biodiesel, and (b) diesel

With regard to the determination of the most relevant transport properties of soybean oil biodiesel in the mixing process, the coefficients needed to introduce the density, viscosity, surface tension, and vapor pressure in the CFD code OpenFOAM have been obtained. A good agreement between the results reached from the empirical correlations and CFD code OpenFOAM models has been observed, therefore, can be concluded that the coefficients obtained are consistent. It is worthy to indicate that these coefficients have not reported in the literature yet. Therefore, these will be great utility for the people working on the study of the injection and/or combustion processes, through simulations carried out in CFD codes such as the CFD code OpenFOAM.

An increase of the transport properties of biodiesel in comparison with those of diesel has been observed. Finally, regarding the characterization of the mixing process through of the

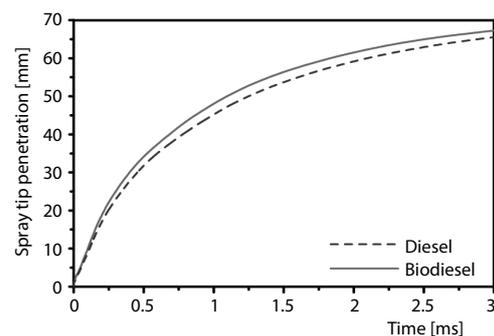


Figure 3. Evolution of the spray tip penetration vs. time; dashed line – correspond to diesel, continue line – correspond to biodiesel

spray tip penetration using a CFD code OpenFOAM, a higher spray tip penetration of the soybean oil biodiesel in comparison with the diesel has been noted. This behavior is due to higher viscosity of the soybean oil biodiesel.

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Nomenclature

A – effective area of the nozzle, [mm²]
 C_d – discharge coefficient, [–]
 D – nozzle outlet diameter, [μm]
 L – hole length, [mm]
 \dot{m} – mass-flow rate, [kg s⁻¹]
 P – pressure, [MPa]
 T – temperature, [K]
 U – velocity, [ms⁻¹]

Greek symbols

θ – spray cone angle, [°]
 μ – dynamic viscosity, [Pas]
 ρ – density, [kg m⁻³]

σ – surface tension, [Nm⁻¹]

Subscript

back – volume where the fuel is injected
 c – critical
 f – fuel
 g – gas
 inj – injection
 r – reduced
 vap – vapor

Acronym

SMD – sauter mean diameter

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