

THEORETICAL ANALYSIS OF ATOMIZATION IN A DIESEL ENGINE FUELED WITH SOYBEAN OIL

Nury Nieto Garzón

Edson Bazzo

Amir A. M. Oliveira Jr.

Laboratory of Combustion and Thermal Systems Engineering, Federal University of Santa Catarina,
Florianópolis-SC, 88.040-900, Brazil.

nury@labcet.ufsc.br; ebazzo@emc.ufsc.br; amir.oliveira@gmail.com

Abstract. The use of straight vegetable oils to replace diesel fuel in compression ignition engines is hampered by their poor atomization which leads to higher emissions and fouling of the surfaces of the combustion chamber. Here, the measured dynamic viscosity, density, and surface tension of soybean oil and its blends with diesel oil are used to predict the required temperature and blend proportion that would place the liquid fuel mixture within the atomization regime for common mechanical injectors with passage length/diameter of the nozzle of 2 to 6. The sprays are assumed to be injected in the pressurized air conditions typical of the combustion chamber of a small, naturally aspirated, single cylinder, four strokes, direct injection diesel engine operating under nominal conditions, namely, fuel temperature from 90 °C to 150 °C, injection pressure from 160 bar to 200 bar, injection timing from 335 to 345 crankshaft angle, compression ratio of 17.3, and speed of 2200 rpm. The observed spray parameters were spray cone angle and average (SMD) droplet diameter. Influence of injection parameters and physical fuel properties was analyzed through the Analysis of Variance (ANOVA) of the results. Optimal operating conditions with soybean oil blends were identified.

Keywords: biofuels, soybean oil, compression-ignition engines, atomization.

1. INTRODUCTION

Environmental and energy security concerns have encouraged studies on the use of straight vegetable oils (SVO) and fatty acid methyl esters (FAME) application to replace diesel fuel in compression ignitions (CI) engines. To be used as a drop in fuel, the alternative fuels must closely match the thermophysical properties of diesel fuel. For the use in compression ignition engines, the key properties are viscosity, density and lower heating value (LHV). The former affect directly the fuel atomization in the combustion chamber, while the last is related to the power produced during the combustion stroke.

Fuel atomization influences significantly the performance and emissions of CI engines. The fuel spray is commonly characterized by the spray tip penetration, cone angle, droplet velocity, average droplet size, and droplet size distribution (Chen *et al.*, 2013). Ideally, the spray should evolve within the atomization breakup regime. This regime is attained when the fuel jet forms a cone-shaped spray at the nozzle exit and produces droplets with sizes much smaller than the nozzle exit diameter (Heywood, 1988; Reitz and Bracco, 1979).

Vegetable oils are mostly formed by polyunsaturated triglycerides. The unsaturation bonds of the carbon chains in these compounds and the large molecular size lead to high dynamic viscosity, high density, low volatility and low LHV when compared to diesel oil (Agarwal *et al.*, 2008; Rakopoulos *et al.*, 2006). High dynamic viscosity causes poor atomization, large droplet size, and longer penetration of the jet. The fuel is not well distributed and mixed with air for burning in the combustion chamber, leading to poor combustion with loss of power and production of gas and particulate emissions (Agarwal *et al.*, 2008; Franco and Nguyen, 2011).

In this work, the influence of the injection pressure, injection timing, passage length/diameter (L/d_o) of the nozzle, and fuel temperature on the spray observed variables as tip penetration, cone angle, and average (SMD) droplet size are analyzed using semi-empirical correlations developed for mechanically injected CI engines, fuelled by heavy fuels. The sprays are supposed to be injected in the conditions that prevail in the combustion chamber of small, naturally aspirated, single cylinder, CI engines, operating with compression ratio of 17.3, and speed of 2200 rpm. The analysis provides the needed fuel temperature and blending ratio with diesel fuel that places the spray in the atomization regime. The analysis of variance (ANOVA) is used to assess the importance of the spray parameters in the observed variables.

2. CHARACTERIZATION OF FUEL THERMOPHYSICAL PROPERTIES

Density, dynamic viscosity, and surface tension are the fuel properties that more significantly affect the spray behavior. Here, these properties were measured at pressure of 1 bar and temperature from 25 °C to 85 °C, both for the pure fuels as well as for their blends.

Azian et al. (2001) used a modified Andrade-type equation to account for the effect of temperature $T(^{\circ}\text{C})$ on dynamic viscosity $\mu(\text{Pa.s})$,

$$\mu = \exp\left(a + \frac{b}{T} + \frac{c}{T^2}\right) \quad (1)$$

where a , b and c are constants. This model was curve fitted to the dynamic viscosity of soybean and diesel oils measured in the temperature range of 25 $^{\circ}\text{C}$ to 85 $^{\circ}\text{C}$. Table 1 presents the values of the curve-fitted parameters. The values of the coefficient of determination, R^2 , very close to 1 suggest that the model provides an adequate fitting of the measurements.

The dynamic viscosity of the blends of soybean and diesel oils $\mu_m(\text{Pa.s})$ can be predicted from the Grunberg-Nissan mixing rule (Reid et al., 1987),

$$\ln \mu_m = \sum_i^n x_i \ln \mu_i + \sum_i^n \sum_j^n x_i x_j G_{ij} \quad (2)$$

where μ_i is the dynamic viscosity of pure i^{th} component, x_i and x_j are the concentrations (in mass, mol or volume fraction) of the i^{th} and j^{th} components, G_{ij} is the interaction parameter, and n is the number of components in the mixture. When the components of a mixture have similar chemical structure, it is expected that they do not interact with each other and consequently the interaction parameter can be neglected (Benjumea et al., 2008). Vegetable and diesel oil blends form completely miscible solutions at all proportions within the temperature range tested. Therefore, as a first approximation, the interaction parameter is neglected and the dynamic viscosity of the binary mixture becomes

$$\ln \mu_m = x_1 \ln \mu_1 + x_2 \ln \mu_2 \quad (3)$$

This expression was used to predict the viscosity of the blends and the results are compared to the measurements in Fig. 1(a). The concentrations were used in volume fraction of each component. A reasonable agreement is found.

From the measurements, the density of the pure fuels varied linearly with temperature. Therefore a simple linear relation,

$$\rho = \alpha + \beta T \quad (4)$$

where α and β are constants, is used. Figure 1(b) presents the comparison of the curve fitted linear model and the measurements, and an excellent agreement is observed. Table 1 presents the curve-fitted constants.

The density of the blend is assumed to follow a simple ideal mixture rule,

$$\rho_m = \phi \rho_v + (1 - \phi) \rho_d \quad (5)$$

where ϕ is the volume fraction of each component and the subscripts v , d and m correspond to vegetable oil, diesel oil and blend, respectively. ρ_v and ρ_d follow Eq. (4).

Surface tension measurements of soybean and diesel oils resulted in a linear dependency with temperature, as also obtained by Esteban et al. (2012). Therefore, a simple linear fit

$$\sigma = AT + B \quad (6)$$

where A and B are constants, is used. Table 1 presents the values of the curve-fitted constants.

Mixture surface tensions can be estimated from the modified Macleod-Sugden correlation presented in Reid et al. (1987), which, for a binary mixture, simplifies to

$$\sigma_m = \left[\phi_1 \sigma_1^{1/4} + \phi_2 \sigma_2^{1/4} \right]^4 \quad (7)$$

where ϕ is the volume fraction of each component. Figure 1(c) presents the comparison of the predictions and the measurements in the temperature range from 25 $^{\circ}\text{C}$ to 50 $^{\circ}\text{C}$. Maximum deviations of 4 % are found between predictions and measurements. Although clearly the model does not follow the behavior suggested by the measurements, due to its simplicity, this model will be used as a first approximation for this narrow temperature range.

Table 1. Values of the constants curve-fitted to the measurements of dynamic viscosity, density, and surface tension.

Dynamic viscosity, μ (Pa.s)			Density, ρ kg/m ³			Surface tension, σ (N.m)		
	Soybean oil	Diesel oil		Soybean oil	Diesel oil		Soybean oil	Diesel oil
a	1.3999	-0.8988	α	930.67	844.98	A	-0.1148	-0.128
b	-1882.65	-585.37	β	-0.6421	-0.6493	B	36.47	32.6
c	783832	366101						
R ²	0.99997	0.99925	R ²	0.9979	0.9976	R ²	1	1

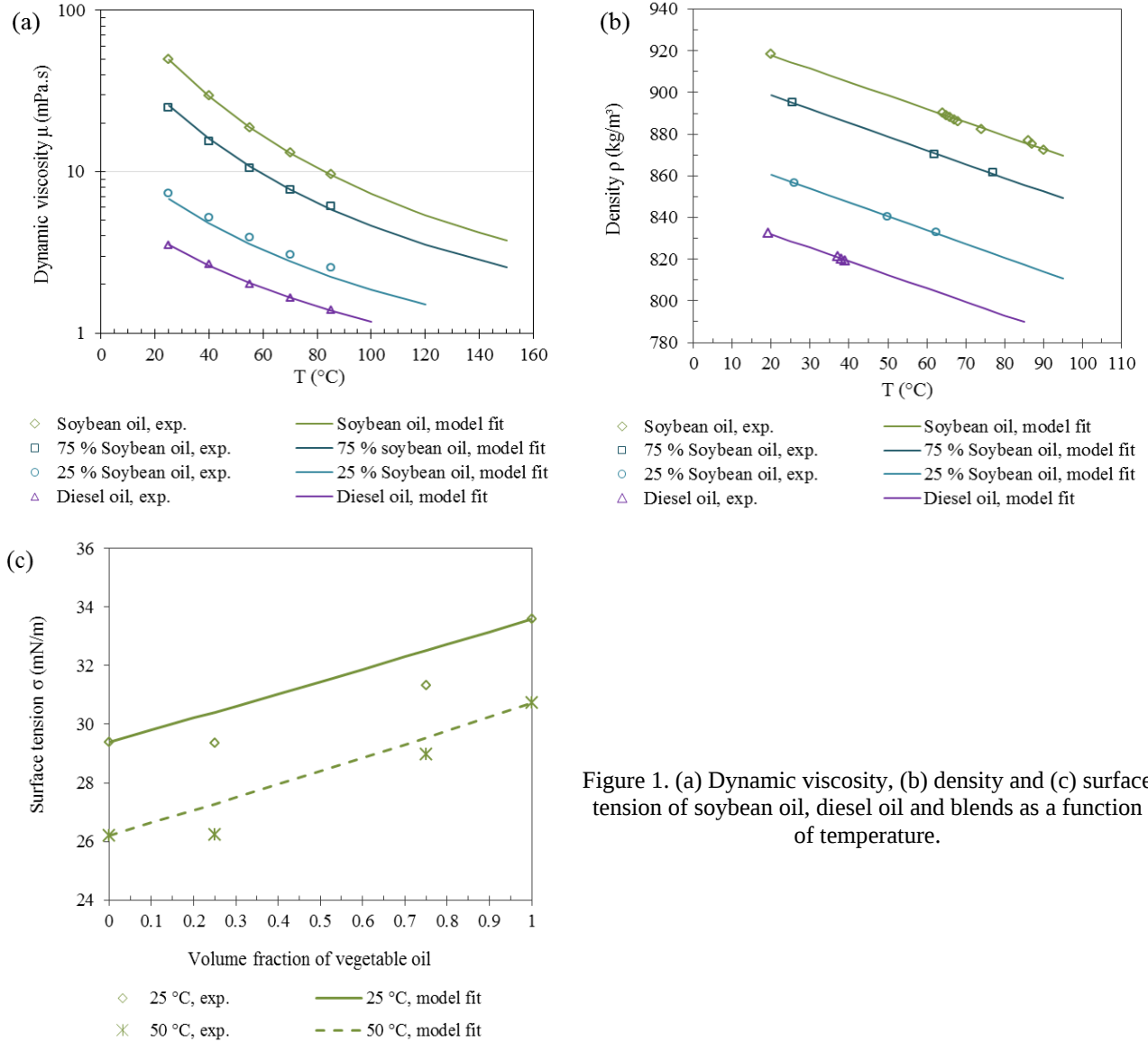


Figure 1. (a) Dynamic viscosity, (b) density and (c) surface tension of soybean oil, diesel oil and blends as a function of temperature.

3. ATOMIZATION BREAKUP REGIME

This is the regime of interest for internal combustion engines. In this regime, the injected fuel forms a cone-shaped spray at the nozzle exit, and it produces droplets with sizes very much less than the nozzle exit diameter (Heywood, 1988). Atomization of fuel favors mixture formation and consequently the performance of the diesel engine. Different jet atomization mechanisms have been proposed. Reitz and Bracco (1979) conducted experiments to study jet atomization. A spray chamber was used for testing different operating conditions, including the conditions commonly found in automotive applications. The spray chamber allowed to change injection pressure, gas density, liquid viscosity, nozzle L/d_o ratios, and it allowed observing the breakup process photographically. The authors found that aerodynamic effects, liquid turbulence, jet velocity profile effects, and liquid supply pressure oscillations, each could not alone explain the experimental results. The aerodynamic effects at the liquid/gas interface, supplemented by cavitation and/or wall boundary layer velocity profile relaxation effects are the major components of the atomization mechanism.

Reitz and Bracco (1979) based on the aerodynamic hypothesis and their experimental results described a criterion for the onset of jet atomization, which establishes:

$$\sqrt{\frac{\rho_l}{\rho_g}} \leq k \quad \text{when} \quad \frac{\rho_l}{\rho_g} \left(\frac{Re_l}{We_l} \right)^2 > 1 \quad (8)$$

$$\left(\frac{\rho_l}{\rho_g} \frac{We_l}{Re_l} \right)^{1/3} \leq k \quad \text{when} \quad \frac{\rho_l}{\rho_g} \left(\frac{Re_l}{We_l} \right)^2 < 1 \quad (9)$$

where ρ_l , ρ_g are the liquid and gas densities, respectively. We_l and Re_l are the dimensionless number of Weber and Reynolds expressed for the liquid phase as

$$We_l = \frac{\rho_l u d_o}{\sigma_l}, \quad Re_l = \frac{\rho_l u d_o}{\mu_l} \quad (10)$$

The constant k is a parameter obtained empirically related to the ratio of the length L and the diameter d_o of the orifice as

$$k = \frac{18.3}{\sqrt{A}} \quad A = 3 + \frac{L/d_o}{3.6} \quad (11)$$

This criterion incorporates the effects of gas density, liquid properties, the geometric characteristics of the orifice, and the operating conditions through the liquid velocity u . The velocity of the jet at the outlet plane of the orifice is

$$u = C_d \left[\frac{2(p_{inj} - p_g)}{\rho_l} \right]^{0.5} \quad (12)$$

where C_d is the coefficient of discharge, p_{inj} is the injection pressure, and p_g is the gas pressure. According to Lefebvre (1989), the coefficient of discharge can be estimated for round orifices as

$$C_d = \frac{1}{\left[\frac{1}{C_{d,max}} + \frac{20(1+2.25L)}{Re_l} \right]}, \quad C_{d,max} = 0.827 - 0.0085L \quad (13)$$

The spray can be mostly simply described by its Sauter mean droplet diameter (SMD) and spray cone angle (θ). The SMD is the diameter of a model drop whose volume-to-surface-area ratio is equal to the ratio of the sum of all droplet volumes in the spray to the sum of all droplet surface areas (Baumgarten, 2006). From the literature, the SMD is usually estimated from the fuel properties, injection pressure, and the dimensionless numbers of Weber and Reynolds. Elkoth (1982) proposed a correlation using the fuel properties at 20 °C. Ejim *et al.* (2007) used the same correlation for calculating the SMD of different biodiesel at 80 °C. This correlation, which is used here, is given as

$$SMD = 6156 \nu^{0.385} \sigma_l^{0.737} \rho_l^{0.737} \rho_g^{0.06} \Delta p^{-0.54} \quad (14)$$

where ν (m²/s), σ_l (mN/m) and ρ_l (kg/m³) are the kinematic viscosity, surface tension, and density of the liquid and ρ_g (kg/m³) is the density of the gas. $\Delta p = p_{inj} - p_g$ (bar) is the difference between the pressure in the injection line and the pressure in the combustion chamber. This correlation returns SMD in μm . Similarly, the spray cone angle is estimated using the correlation (Baumgarten, 2006),

$$\tan\left(\frac{\theta}{2}\right) = \frac{4\pi}{A} \left(\frac{\rho_g}{\rho_l} \right)^{0.5} f(\gamma) \quad (15)$$

where $f(\gamma)$ is an empirical scaling function given by

$$f(\gamma) = \frac{\sqrt{3}}{6} (1 - \exp(-10\gamma)), \quad \gamma = \left(\frac{Re_l}{We_l} \right)^2 \frac{\rho_l}{\rho_g} \quad (16)$$

One can observe that when γ becomes large, $f(\gamma)$ tends asymptotically to $\sqrt{3}/6$.

4. ENGINE OPERATION CONDITIONS

The analysis was carried out at typical conditions prevailing in the combustion chamber of a direct injection diesel engine. The engine geometric characteristics are presented in Tab. 2. The gas properties in the cylinder were calculated assuming polytropic compression with polytropic coefficient $n = 1.3$. At the beginning of the compression stroke, air properties were fixed at $T_1 = 300$ K and $p_1 = 101$ kPa. The volume occupied by the gas V_g is expressed as a function of crank angle θ as (Heywood, 1988)

$$V_g = V_c \left[1 + \frac{(r_c - 1)}{2} \left\{ R + 1 - \cos(\theta) - [R^2 - \sin^2(\theta)]^{0.5} \right\} \right] \quad (17)$$

where V_c is the dead volume of the cylinder, r_c is the compression ratio, and R is the ratio of connecting rod length to crank radius. Gas pressure and temperature, p_g and T_g , are calculated from polytropic relations assuming ideal gas behavior,

$$p_g = p_1 \left(\frac{V_1}{V_g} \right)^n, \quad T_g = T_1 \left(\frac{p_g}{p_1} \right)^{\frac{n-1}{n}}, \quad \rho_g = \frac{p_g}{R_g T_g} \quad (18)$$

where V_1 corresponds the volume of air in the beginning of compression and R_g is the gas constant, calculated assuming standard, simplified, dry air.

Table 2. Geometric specifications of the diesel engine.

Bore (mm)	115
Stroke (mm)	115
Compression ratio	17.3
Connecting rod (mm)	185.5
Displacement volume (cm ³)	1,194
Minimum cylinder volume (cm ³)	73.3

The 3⁴ factorial design was proposed for the theoretical analysis. This design presents four variables of test or factors assessed in three levels or conditions. Table 3 presents the factors and levels considered in the experimental design proposed. All tests assumed constant nozzle diameter $d_o = 0.0003$ m.

Table 3. Factors and levels of experimental design.

	Factors			
	Fuel temperature T , (°C)	Injection pressure p , (bar)	Injection angle θ_{inj} , (°)	Ratio L/d_o of nozzle
Levels	90, 120, 150	160, 180, 200	335, 340, 345	2-4-6

The experimental design involved 81 combinations of the analyzed factors (T , p , θ_{inj} , L/d_o). Both the factors themselves as well as their square terms were tested as important parameters. The assessed responses were the maximum percent vegetable oil (VO) in the blend to achieve adequate spray atomization according the criteria presented in last section, the spray cone angle (θ), and the average droplet diameter (SMD). The equations providing the relations between factors and responses were solved in MATLAB software. The Analysis of Variance (ANOVA) was used to estimate the statistical significance of the parameters on the assessed responses. The statistical analysis was performed considering a confidence interval of 95% using the Statistic software.

5. RESULTS AND DISCUSSIONS

Table 4 presents the statistical significance of each parameter in the assessed responses as evaluated by ANOVA. The values of probability p are also shown. A parameter is considered significant when $p < 0.05$.

Table 4. Importance of each parameter as evaluated by ANOVA. The values of probability p are also shown.

Parameter	Soybean oil		
	VO	SMD	θ
T	++++ (p<0.0001)	++++ (p<0.0001)	-- (p=0.1272)
p	++++ (p<0.0001)	++++ (p<0.0001)	--- (p=0.8415)
θ_{inj}	++++ (p<0.0001)	++++ (p<0.0001)	++++ (p<0.0001)
L/d_o	++++ (p<0.0001)	++++ (p<0.0001)	++++ (p<0.0001)
T^2	+++ (p=0.0024)	---- (p=0.8875)	---- (p=0.9465)
p^2	--- (p=0.6745)	-- (p=0.1471)	---- (p=0.9930)
θ_{inj}^2	- (p=0.0529)	++ (p=0.0050)	++++ (p<0.0001)
$(L/d_o)^2$	++ (p=0.0092)	++ (p=0.0098)	--- (p=0.7630)

From Tab. 4, it is observed that the significant parameters for VO are T , p , θ_{inj} , L/d_o , T^2 , and $(L/d_o)^2$. For SMD, they are T , p , θ_{inj} , L/d_o , θ_{inj}^2 , and $(L/d_o)^2$. Finally, for θ the significant variables are θ_{inj} , L/d_o , and θ_{inj}^2 , indicating that temperature and injection pressure do not influence significantly in the spray cone angle.

Figure 2 presents the maximum allowed volume fraction of soybean oil in the blend at the boundary of the atomization regime, following Reitz and Bracco (1979) rules. Each curve corresponds to a given θ_{inj} / p condition. Figure 2(a) was obtained for $L/d_o = 2$ and Fig. 2(b) for $L/d_o = 6$. For both ratios L/d_o , the maximum percent vegetable oil in the blend to achieve adequate spray atomization increases with the increasing of the temperature, and it decreases when the injection pressure rises. The values of the physical properties decrease when the temperature rises and low viscosity and surface tension favor the breakup the liquid jet in the atomization regime. The effect of the injection pressure is explained in the interaction of the jet velocity and the gas. Increasing the injection pressure increases the jet velocity which lowers the aerodynamic effects that influence on the atomization regime. Similarity, when the fuel injection is advanced (low injection timing), the gas pressure is low, increasing the pressure differential across the nozzle and thus the jet velocity. Therefore, when the fuel injection occurs closer of the position of top-dead-center the maximum percent vegetable oil increases. In figure 4a, one can also observe that this effect on the maximum percent vegetable oil is more significant than the effect of the variation of pressure. Results of figure 4b indicate that the maximum percent of vegetable oil decreases with the increasing of the ratio L/d_o of nozzle, resulting that, in the condition of $L/d_o = 6$, there is no blend with adequate spray atomization at the injection timing of 335.

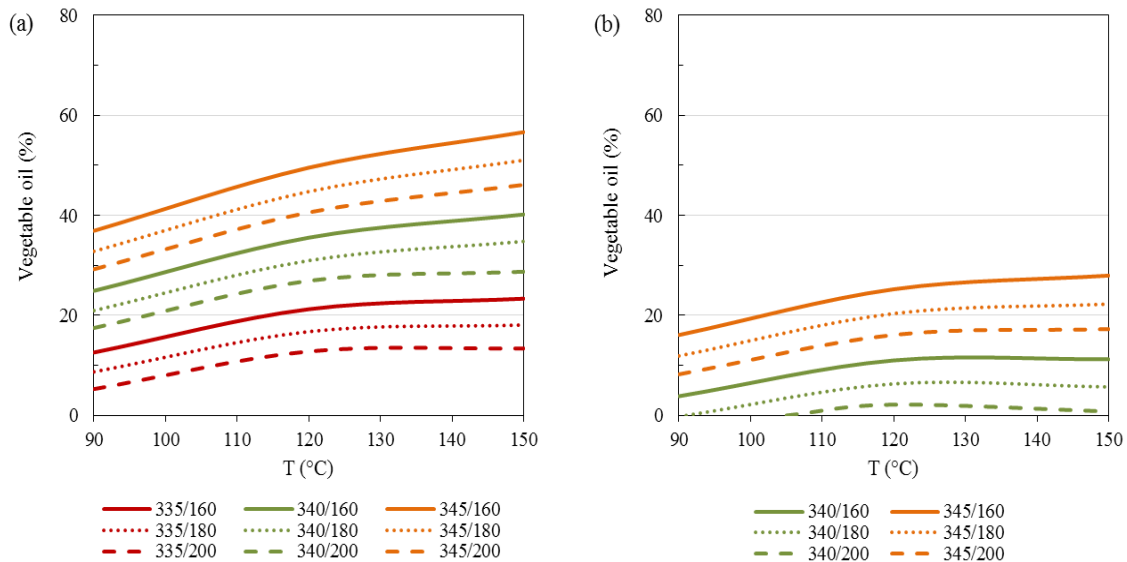


Figure 2. Maximum allowed percent of soybean oil in the blend as a function of injection temperature, for pressures $p = 160, 180, 200$ bar at injection timing $\theta_{inj} = 335, 340, 345$: (a) $L/d_o = 2$. (b) $L/d_o = 6$. The legend for the curves indicates injection timing / pressure.

Figure 3 presents the average droplet diameter at given θ_{inj} / p conditions. Figure 3(a) was obtained for $L/d_o = 2$ and Fig. 3(b) for $L/d_o = 6$. For both ratios L/d_o , SMD decreases with the increasing of injection temperature and pressure. One can be observed the advanced injection increases the SMD, and similar effect is presented when the ratio L/d_o of nozzle is low. Decreasing of physical properties and high injection pressure favor the of liquid jet break in small

droplets. Conversely, the injection in a denser medium, close injection to the position of top-dead-center of piston, inhibits the formation of small droplets.

The significant influence of all variables on the results of VO and *SMD* demonstrates the interaction of the fuel properties and the conditions into combustion chamber as gas pressure or density on the regime of liquid jet breakup.

Spray cone angle is mainly influenced by the injection timing and the ratio L/d_o of nozzle. Spray cone angle increases with the injection timing, which indicates gas pressure into combustion chamber is a significant factor in the spray cone angle. Furthermore, spray cone angle decreases with the increasing ratio L/d_o of nozzle. Fuel temperature and injection pressure do not influence significantly in this parameter.

Optimization of responses were developed in Statistica Ultimate Academic software, considering as criteria to maximize the percent vegetable oil in the blend with similar *SMD* and spray cone angle than diesel oil at 85 °C, which were calculated as 25 µm and 15.1°, respectively. Results of optimization are presented in Fig. 4. It was found, with desirability of 94 %, that the following conditions satisfy the goal: $T = 135$ °C, $p = 160$ bar, $\theta_{inj} = 345$, and $L/d_o = 2$. In these conditions, the responses are 49 % of vegetable oil in the blend, *SMD* of 24.2 µm, and 14° of spray cone angle.

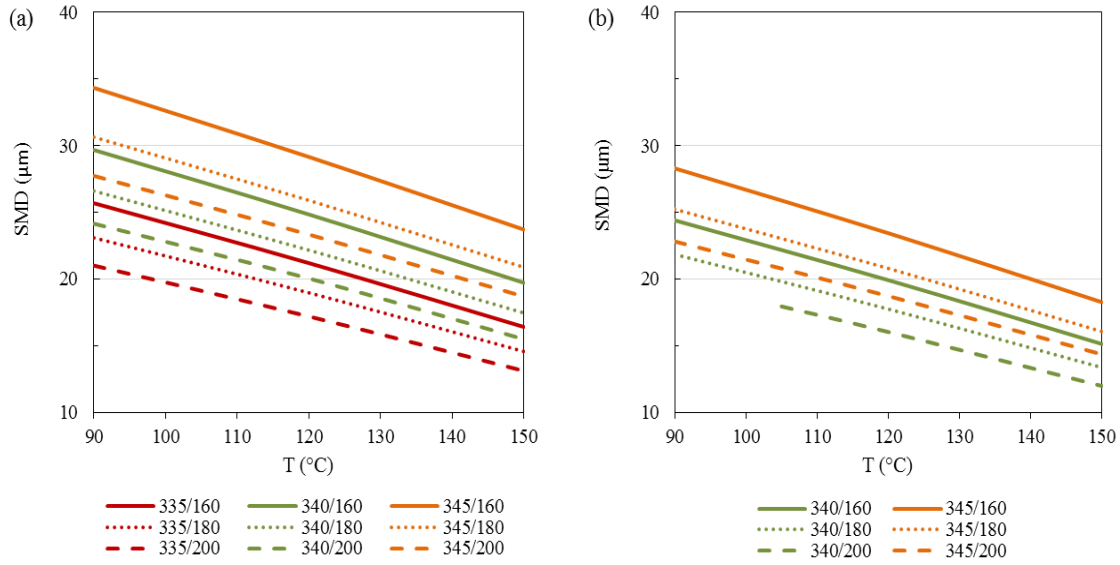


Figure 3. Average droplet diameter as a function of injection temperature, for pressures $p = 160, 180, 200$ bar at injection timing $\theta_{inj} = 335, 340, 345$: (a) $L/d_o = 2$. (b) $L/d_o = 6$. The legend for the curves indicates injection timing / pressure.

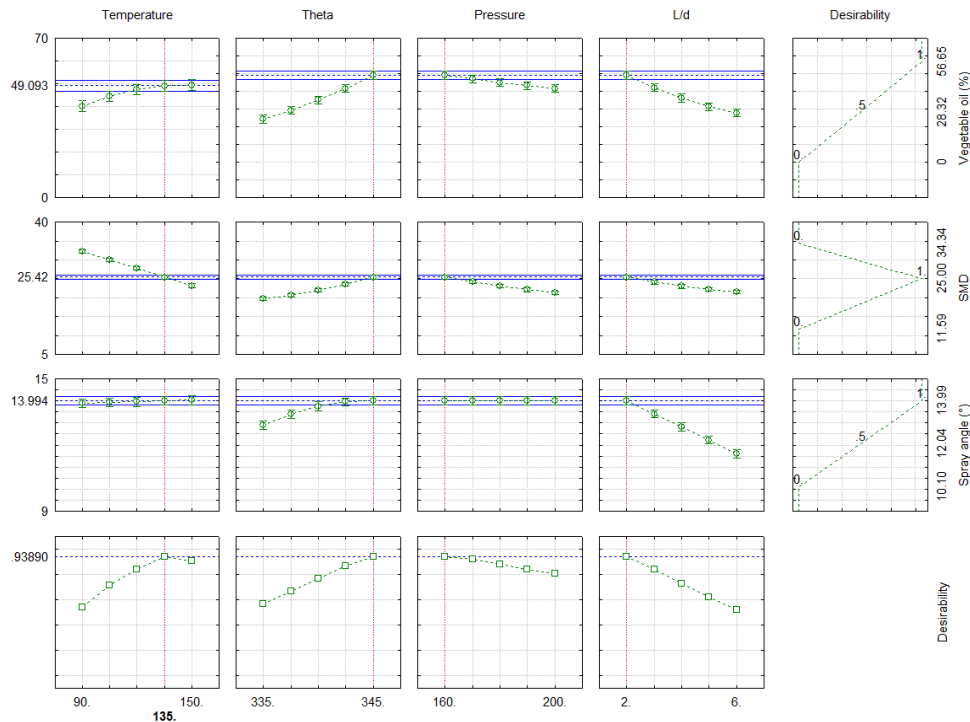


Figure 4. Optimization of responses.

6. CONCLUSIONS

A theoretical analysis of the atomization of soybean oil blends with diesel oil was developed. Density, dynamic viscosity and surface tension were assessed for soybean and diesel oils and curve-fitted to correlations to calculate these physical properties for binary blends with different proportions of vegetable oil. Criteria from the literature that define the boundaries of the atomization regime were then used to estimate the maximum allowable concentration of vegetable oil in the blend under several typical conditions of the injection system. A 3^4 factorial design was proposed for the theoretical analysis. The design involved four variables of test or factors assessed in three levels or conditions. The tested variables were fuel temperature, ratio L/d_o of nozzle, injection pressure, and injection timing. The assessed responses were maximum allowable concentration of vegetable oil in the blend to achieve adequate spray atomization, spray cone angle and average droplet diameter. The significance of the estimates was assessed using Analysis of Variance.

The results showed the interaction of the fuel properties and the conditions into combustion chamber as gas pressure or density on the regime of liquid jet breakup. The maximum percent vegetable oil in the blend to achieve adequate spray atomization increases with the increasing of the temperature, and it decreases when the injection pressure rises or the ratio L/d_o of nozzle increases. Decreasing of physical properties and high injection pressure favor the of liquid jet break in small droplets. Consequently, SMD decreases with the increasing of injection temperature and pressure. Spray cone angle increases with the injection timing, indicating the influence of gas pressure into combustion chamber. Fuel temperature and injection pressure do not influence significantly in this parameter.

Optimization process was developed in Statistica Ultimate Academic software, considering as criteria to maximize the percent vegetable oil in the blend with similar SMD and spray cone angle than diesel oil at 85 °C. It was found 49% of vegetable oil as the maximum percent in the blend, and $T = 135$ °C, $p = 160$ bar, $\theta_{inj} = 345$, and $L/d_o = 2$ as the optimal operating conditions for this blend.

7. ACKNOWLEDGEMENTS

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