LP-model for ECN Spray A penetration

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Abstract

Any alternative fuel that can replace diesel fuel in internal combustion engines needs to have the same spray parameters as diesel fuel has. Spray penetration is important and a simple parameter that can easily be measured experimentally. It is known that spray penetration increases with increasing injection pressure and depends on ambient gas conditions. However, the influence of fuel properties on spray penetration is not clear yet.
A recently developed LP-model for diesel spray penetration based on a length parameter (LP) takes into account the physical properties of fuels such as viscosity, density and surface tension. The length parameter is related to the liquid jet breakup, ligament creation, and necking.
In this paper, the model has been applied to the ECN Spray A conditions (n-dodecane with injection pressure 150 MPa and ambient gas density 22.8 kg/m^3). The spray penetration under Spray A conditions calculated using the LP-model shows a good agreement with experimental data.
In addition, the LP parameter was also used to calculate the Sauter mean diameter (SMD) of droplets under the ECN Spray A conditions. The fuel viscosity has more influence on the SMD values than the density or surface tension. As a rule experimental data shows that SMD increases when the surface tension is increased. But in the case of high ambient pressure we can ignore the surface tension influence on SMD. This tendency was included in the new LP model for SMD.

Keywords
Spray penetration, LP-model, ECN Spray A**,** Sauter mean diameter, biofuels

Introduction
Any alternative fuel that can replace diesel fuel in internal combustion engines needs to have the same spray parameters as diesel fuel has. Spray penetration is an important parameter that can easily be measured experimentally.
In [1] progress was made with ongoing experimental investigations of the atomisation of n-dodecane ($C_{12}H_{26}$) using microscopic imaging and high-speed video with an ECN 'Spray A' injector. The experimental conditions were a gas density of 22.8 kg/m^3, an in-cylinder pressure of 4.8 MPa and a fuel temperature value of approximately 700 K. A long working distance dual-frame microscope was used for the near-nozzle region and the periphery of the dense spray. The study was focused on the primary atomisation during the start, the steady-state and the end of the injection process.
Very often Diesel fuel is approximated by n-dodecane. In [2] n-dodecane was chosen as the surrogate for diesel fuel with density of 750 kg/m^3. Results from the baseline WSR and PDF models for n-dodecane are shown in [3]. Spray penetration and liquid length as well as lift of and ignition delay for Spray A were analysed. For n-dodecane, large differences were observed between two models: the WSR and PDF. The PDF model gives a closer agreement with experimental data (within 5%) of ignition delays and lift-off lengths at an initial temperature of 900 K (for 22.8 kg/m^3 and 15% O_2 ambient density and oxygen level, respectively). The WSR model predicted an ignition delay that was three times higher than the measured value.
But as was shown in [4], the estimation of the evaporation of diesel fuel by only one component (n-dodecane) in droplet evaporation models leads to the underestimation of the evaporation time.
A simple LP-model for spray penetration of biodiesel and diesel fuels has been developed [5]. This model is based on a length parameter (LP) that takes into account the physical properties of fuels such as viscosity, density and surface tension. The length parameter is related to the liquid jet breakup, ligament creation, and necking [5]. A model was developed in [6], but this was created for different types of low-volatility biofuels (for ethanol) and different type of engines, and they cannot be used for high- volatility fuel in a consistent manner. Liquid length, spray penetration and droplet size were carried out for diesel, biodiesel, pentanol and their blends in [7]. They found that the lower volatility fuel has the longer spray penetration. The liquid length for pentanol was shorter than that for other fuels. The influence of different mixtures of diesel fuel, biodiesel (RME) and ethanol for

fuel injection and combustion were investigated in [8]. They found that mixture formation is independent of temperature and physical properties of the fuel components because the spray can be taken as a gas flow with the main component nitrogen in the system used for the study.
In the work presented in this paper, the LP-model has been applied to the ECN Spray A conditions (n-dodecane with injection pressure 150 MPa and ambient gas density 22.8 kg/m^3). This is to assess the capabilities of the model in evaluating well considered experimental conditions.

Material and methods

The Engine Combustion Network (ECN) is an international collaboration among experimental and computational researchers in engine combustion established to provide experimental data, obtained under controlled and standardised operating conditions, as well as to provide a collaborative comparison of measured and modelled results of diesel spray experiments and alternative fuels at engine conditions [1, 9]. In the current work experimental data from the ECN Spray A conditions were used. These were obtained from experiments conducted at the Sandia National Laboratories. The facility at this laboratory is able to measure ambient gas temperatures from 450 K to 1400 K, densities from 1 kg/m^3 to 60 kg/m^3, and at injection pressures values up to 350 bar [9]. In the liquid spray penetration experiments, fast Mie scattering and Schlieren (for vapour penetration) were used. The operating conditions for the ECN 'Spray A' are shown in Table 1.

Table 1. Summary of experimental conditions used for the ECN Spray A [9]

Experimental conditions	n-dodecane
Ambient gas temperature [K]	900
Ambient gas pressure [MPa]	near 6.0
Composition	O_2 = 15.00; N_2 = 75.15; CO_2 = 6.22; H_2O = 3.62
Ambient gas density [kg/m^3]	22.8
Nozzle diameter [mm]	0.090
Number of holes	1 (single hole)
Fuel injection pressure [MPa]	150, prior to start of injection
Duration of injection [ms]	1.5
Fuel temperature at nozzle [K]	363

As seen from Table 1, the experiments were carried on with an injector with a single hole. We need keep in the mind that spray penetration results will be different when the number of holes is increased. Also, both ambient pressure (6 MPa) and injection pressure of Spray A (150 MPa) are high.

Properties of n-dodecane

The n-dodecane has a higher cetane number but lower density and viscosity compared with diesel fuels. The properties of n-dodecane compared with #2 Diesel fuel from [9] are presented in Table 2.

Table 2. N-dodecane (nC12) properties comparing with #2 Diesel fuel [9]

Fuel properties	n-dodecane	#2 Diesel fuel
T100 [°C]	216	350
Cetane number	87	46
Cetane index		47
Low. Heat. Value [MJ/kg]	44.17	42.975
Fuel density at 15°C [kg/m^3]	752.1	843
H_2 mass %	15.3	13.28
Kin. Visc. (40°C) [mm^2/s]	1.5	2.35
Sulphur [ppm]	0	9
Aromatics Vol. %	0	27

Table 3 shows the properties of n-dodecane delivered by different authors.

Table 3. Properties of n-dodecane.

n-dodecane properties	Manin et al. [10]	Chiboub et al. [11]
Density [kg/m^3]	750	753
Kinematic Viscosity [mm^2 s^{-1}]	1.36	1.335
Dynamic Viscosity [mPa.s]		0.97954
Surface tension [mN/m]	25.4	
Boiling point [K]	489	489.5 [12]
Critical temperature [K]	658	
Critical pressure [MPa]	1.82	

The surface tension of heavy *n*-alkanes including n-dodecane was investigated in [13]. We need keep in the mind as the pressure exceeds the critical value, the enthalpy of vaporization disappears, and surface tension effects diminish [14].

Results and discussion

Length parameter (LP)

Eggers [15] introduced two parameters for modelling of droplets breakup that are based on liquid properties: time parameter and *length parameter*. The *Length parameter* (LP) takes into account the viscosity, density and surface tension of the liquid:

$$LP = \frac{\nu_f^2 \rho_f}{\sigma};\ LP = \frac{\mu_f^2}{\sigma \rho_f}. \quad (1)$$

LP is related to liquid ligament creation after jet breakup and necking [15]. LP has a dimension of [m].

The thermo-physical properties of n-dodecane compared to different pure liquids are shown in Table 4. The data of density, dynamic viscosity and surface tension are taken from [16]. LP is calculated using Eq. 1.

Table 4. Comparison of physical properties of pure liquid and LP

Fuel	Density	Dynamic viscosity	Surface tension	LP [m]	LP $^{0.1}$
Water	998.2	0.89 ×10^{-3}	72.75×10-^{3}	0.11×10^{-7}	0.16
n-decane	764.4	0.84×10^{-3}	23.83×10^{-3}	0.39×10^{-7}	0.181
n-dodecane	755.2	1.35×10^{-3}	24.69×10^{-3}	0.98×10^{-7}	0.199
n-hexadecane	770.3	3.06×10^{-3}	27.15×10^{-3}	4.48×10^{-7}	0.232

Spray penetration.

It is known that spray penetration increases with increasing injection pressure and depends on ambient gas conditions. The analysis of correlations for spray penetration has been presented previously [17]. However, the influence of fuel properties on spray penetration is not clear yet.

Our analysis shows that the spray penetration of biodiesels will be proportional to $LP^{0.1}$ [5]:

$$S_{tip} = A_{LP}\left(d_{noz}^{0.5} P_{inj}^{0.36} \rho_a^{-0.29}\right) LP^{0.1} t_{inj}^{0.5}, \quad (2)$$

where time t_{inj} is in [ms].

An application of equations 1 and 2 to the ECN Spray A conditions allows us to predict the spray penetration and to assess the applicability of the LP-model. Figure 1 shows the spray penetration of n-dodecane vs. time predicted by LP-model (see Eq.1, Eq.2) compared to those measured by [9].

We found that A_{LP} = 0.146 for the LP-model (see Eq. 2) for the case of the ECN Spray-A based on n-dodecane properties (see Table 4). This is different from A_{LP} = 0.066 based on diesel and biodiesel properties at t = 80°C [5]. When the LP-model was used for diesel and biodiesel at lower temperature values (see [5]) A_{LP} was varied from 0.23 to 0.3 depending on the experimental conditions.

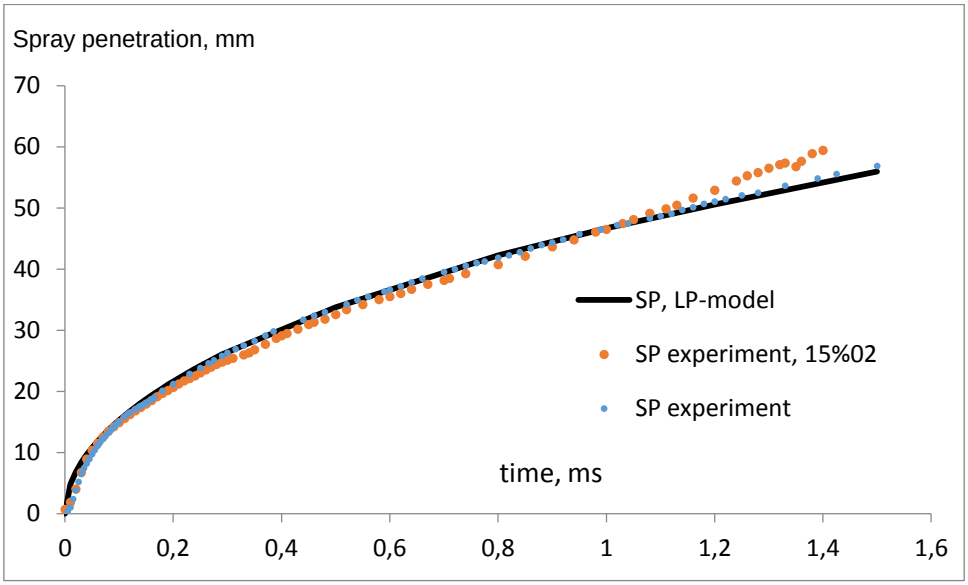


Figure 1. Spray penetration of n- dodecane vs. time predicted by LP-model and measured [9] (SP-experiment)

Comparing acetone-butanol-ethanol & n-dodecane blend (ABE20) and n-dodecane Spray A it was considered in [18] that the vapour spray penetration depends mainly on the spray momentum which in turn depends on the injection pressure, the fuel density and the gas density, "whatever the ambient temperature". There was no significant difference (1% of variation in average) in the spray penetration of ABE20 and n-dodecane [18]. The liquid length (i.e. liquid phase penetration length) is another important spray parameter.

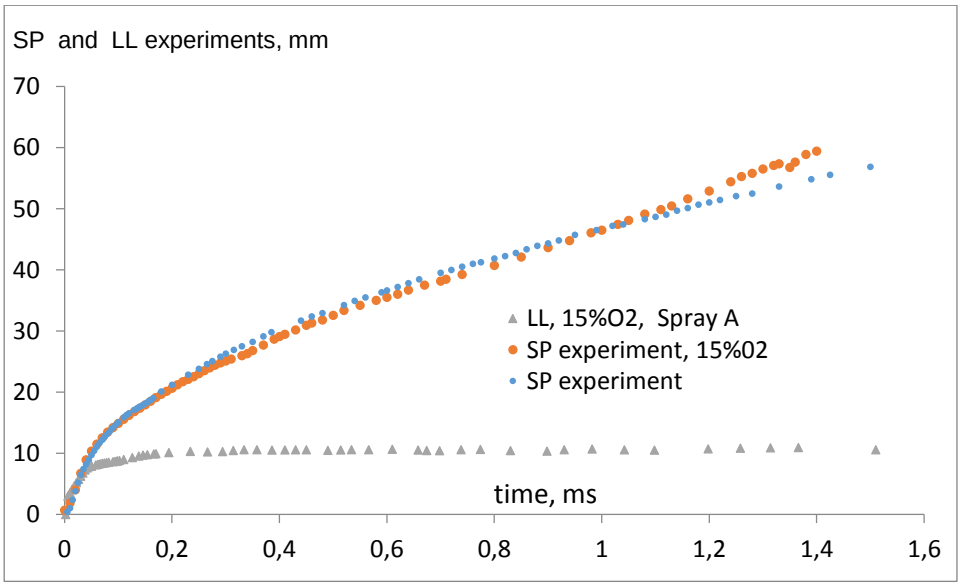
Liquid length (LL)

Martınez-Martınez et al. [19] noticed that for diesel fuel an increase in fuel density increases the resistance to liquid penetration and shortens the penetration length. Eq. (3) is recommended in [19] as the best for predicting the LL in the fuel injection process before the second break-up regime (mm)

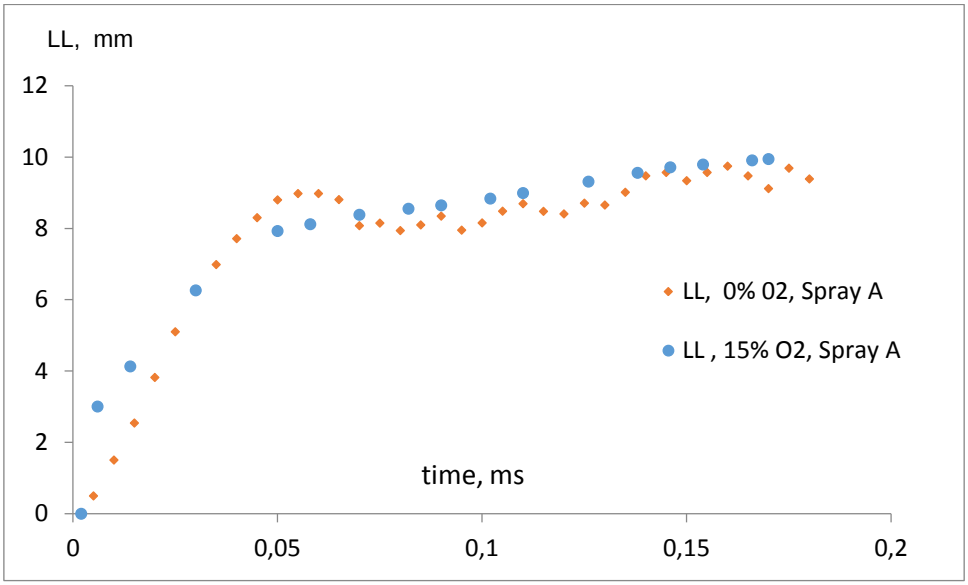
$$0 < t < t_r \;\; LL(t) = 6.47 d_{noz}^{0.56} \rho_a^{-0.27} P_{inj}^{0.23} C_d^{0.08} t^{0.5}, \qquad (3)$$

where t is time from start of injection (μs), t_r is time for the second break-up regime (μs), d_{noz} is nozzle diameter (μm).

It was found [19] that the discharge coefficient causes a maximum variation of the LL of only about 3% under experimental conditions ($0.58 < C_d < 0.87$). Liquid length with 15% O_2 of n-dodecane under ECN Spray A experiments compared with vapour spray penetration vs. time measured [9] are shown in Figure 2 a). Figure 2 b) compares the Liquid length for n-dodecane with 15 % and 0% of O_2 for an injection time that is less of 0.2 ms.



a)



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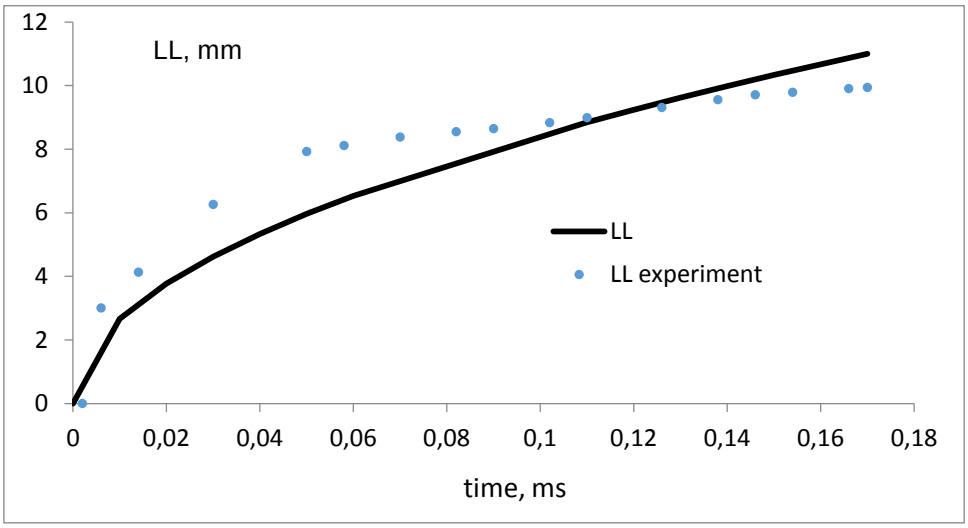

c)

Figure 2. Liquid length of n- dodecane vs. time measured [9] a) compared with SP for dodecane b) LL at different % of O2; c) LL from Spay A and LL that was fitted to Eq. 3

We found that Eq. 3 doesn't fit the experimental data [9] for LL of Spray A even with different coefficients other than 6.47 that was used in the equation (see Fig. 2 c)).
The liquid length (LL) at different temperature values for acetone-butanol-ethanol mixture, blended with n-dodecane in a volume ratio of 20% (ABE20) was analysed in [18]. Table 5 shows maximum LL for different temperature values in comparison to the reference fuel, n-dodecane [18].

Table 5. Comparison of liquid length of n-dodecane and ABE20

Temperature, (K)	LL (mm) n-dodecane	LL (mm) ABE20
800	12.0	11.4
850	11.5	10.6
900	10.4	10.2

It is known, that the LL is longer at lower ambient temperature than at high temperature values because more energy is entrainment on the liquid fuel. Also higher temperature values lead to an increase in the evaporation rate, with the surface tension and viscosity of the fuel lower, and the atomization process enhanced [2].

The LL of ABE20 was shorter than those of n-dodecane for all ambient conditions, mainly due to the higher volatility of ABE20 [18]. The boiling point of the fuel components of ABE20 was 32.7%, 20.2%, and 28.2% lower than that of n-dodecane for acetone, butanol, and ethanol, respectively. Moreover, the vapor pressure of acetone, butanol, and ethanol was 30.8 kPa, 0.58 kPa, and 7.9 kPa, which is much higher than that of n-dodecane (0.018 kPa). So, the evaporation rate of ABE20 was higher than n-dodecane one [18].

Sauter mean diameter (SMD).

The LP- model was also used to calculate the Sauter mean diameter (SMD) of droplets using the ECN Spray A conditions. The fuel viscosity has more influence on the SMD values than the density or surface tension [5]. It was shown in [20] how the LP model can be used for the modelling of SMD for biodiesel sprays:

$$SMD = B_{LP} d_0^{0.35} LP^{0.1} \Delta P^{-0.54} \rho_g^{0.06} \quad (4)$$

with B_{LP} = 23 for biodiesel.

The SMD of biodiesel according to [21]

$$SMD = 2.25 m^{0.25} \mu_f^{0.25} \sigma^{0.25} \rho_g^{-0.25} \Delta P^{-0.5} \quad (5)$$

where m is mass of fuel injected.

The formulae of Elkotb from [22] can be used to calculate the SMD of diesel and biodiesel:

$$SMD = 6156 \rho_f^{0.737} \nu_f^{0.385} \sigma^{0.737} \rho_g^{0.06} \Delta P^{-0.54}. \quad (6)$$

Notice, that ΔP is in bar, and SMD is in μm in Eq. 6.

ECN Spray A can be under critical conditions as we can see from Tables 1- 3. For example, at critical conditions, n-hexane spray forms finger-like structures that were observed on the jet surface in the experiment of [14]. Similar phenomena occur in multi-component sprays [14].

Figure 3 shows the computed SMD values of n-dodecane using the LP-model (see Eg.4) compared to [22] (see Eg.6) for different fuels (see Table 6). Notice that the value of the SMD for ECN Spray A (n-dodecane) in Figure 3 is not real because probably spray doesn't create proper droplets in this case. At the conditions presented in Table 1 for n-dodecane it is suggested [23] that a different type of spray break-up occurs as they found no evidence of drops or ligaments. Vanishing surface tension might lead to diffusion determined spray break-up according to [23].

As a rule the fuel viscosity has more influence on the SMD values than the density or surface tension. Sometimes the experimental data show that SMD increases when the surface tension increases. But in the case of high ambient pressure cases we can ignore the surface tension influence on SMD. This tendency was included in the new LP model for the SMD (see Eq.1 and Eq.4). As we can see from these equations if the surface tension goes to zero the SMD will be extremely large. This shows the deference of the LP concept for SMD from other empirical models. From Eq. 5 and Eq.6 as σ = 0 then SMD = 0.

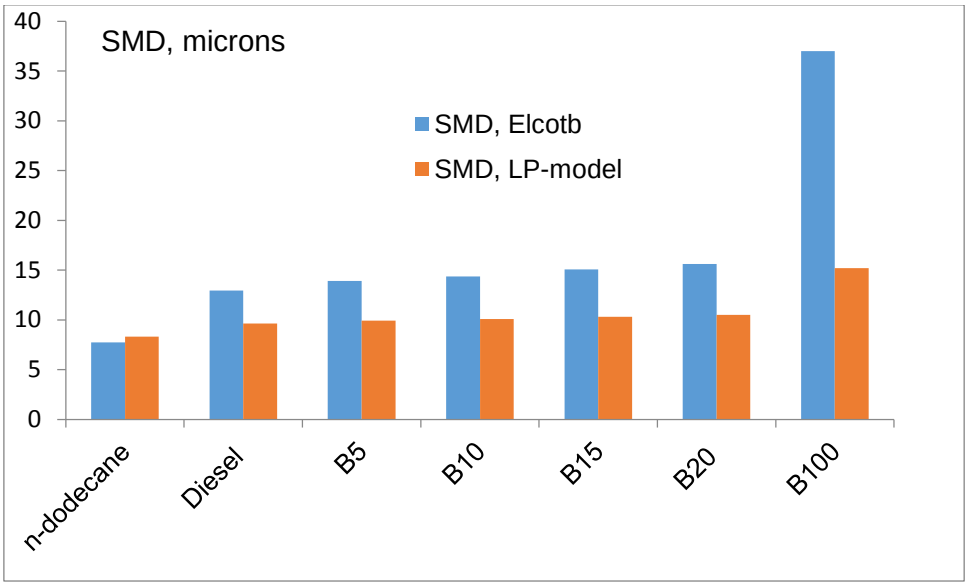

Figure 3. SMD of n- dodecane compared with different fuels using Eg.4 (LP-model) and Eq. 5.

It is important to calculate the spray penetration, liquid length and SMD of different alternative fuels and their blends with diesel. Tables 6-7 show the physical properties [7, 21] and LP that were calculated using Eq. (1) for different blends of biodiesel, diesel and pentanol.

Table 6. Comparison of physical properties [21] and *LP* of biodiesel (PME) and PME blends

Fuel	Density	Dynamic viscosity	Surface tension	*LP* [m]	$LP^{0.1}$
Diesel	828.7	0.03	0.00324	4.22E-07	0.23
B5	832.2	0.03045	0.0038	5.7E-07	0.237
B10	836.1	0.03048	0.0041	6.6E-07	0.241
B15	838.9	0.03054	0.0046	8.26E-07	0.246
B20	842	0.03055	0.00504	9.88E-07	0.251
PME	901.2	0.0345	0.00352	3.99E-05	0.363

It was investigated in [7] that diesel or pentanol and blend of diesel, biodiesel and pentanol (DBP) have almost the same SMD at ambient pressure of 1.8 MPa as well as at injection pressure of 80 MPa. When ambient pressure was increased to 2.5 MPa, the SMD for DBP was larger than for diesel fuel. For low ambient pressure (1.2 MPa) the SMD for DBP was smaller than for diesel.

Table 7. Comparison of physical properties [7] and *LP* of biodiesel (PME), diesel and DBP blend

Fuel	Density, 20°C	Kinematic viscosity, 20°C	Surface tension	*LP* [m]	$LP^{0.1}$
PME	871.4	7.159×10^{-6}	30.3×10^{-3}	1.47E-06	0.261
Diesel	830.4	4.127×10^{-6}	27.5×10^{-3}	5.14E-07	0.235
Pentanol	815	2.89×10^{-6}	24.7×10^{-3}	2.76E-07	0.221
DBP	-	3.9×10^{-6}	26.9×10^{-3}		

As we can see from Table 7 the $LP^{0.1}$ for diesel and pentanol is close to each other. The same tendency shows from the LP-model for SMD as well as the experimental measurements [7] at both middle ambient and injection pressure values. The calculation of the LP for another mixture (diesel, biodiesel and ethanol) shows the same tendency for liquid length. According to our calculation of LP based on the data of [8] good agreement with experimental data for maximum liquid length will be an $LP^{0.32}$ for biodiesel, diesel, and ethanol that equal to (0.01; 0.008; 0.004) respectively. In other words, maximum liquid length (during second break-up regime) will be proportional to $LP^{0.32}$.

So, the maximum liquid length for alternative fuels can be calculated as:

$$LL_{\max} = C_{LP}\left(d_{noz}^{0.5} P_{inj}^{0.36} \rho_a^{-0.29}\right) LP^{0.32}. \quad (7)$$

All parameters in Eq.7 are in SI units. Eq. 7 was adapted for maximum LL calculation from Eq. 2 and was checked out against the experimental data of [8] for biodiesel, ethanol and their blends (ambient temperature of 700° C, ambient pressure of 6MPa and injection pressure of 120 MPa). It was found that the best agreement with the experimental data was when C_{LP} = 0.253 for gas density of 22.8 kg/m^3 and nozzle diameter of 90 μm, that is as shown in Table 8.

Table 8. Comparison of maximum liquid length of diesel, biodiesel, ethanol and their blends

Fuel	LL (mm) Experiment [8]	LL (mm) Eq. (7)
Biodiesel	25	25
Diesel and blends	20	20
Ethanol	10	13

Notice that Eq. 7 cannot predict LL very well for ethanol. Ethanol is not suitable as fuel for diesel engines because it has very low cetane number (about 6-8).

Conclusions

A recently proposed the correlation, the LP-model, was used for the calculation of the ECN Spray A penetration values under conditions relevant to internal combustion engines. This model uses a length parameter that accounts for the effects of the thermo-physical parameters of a fuel on the fuel spray penetration. The spray liquid

length and SMD values were also predicted using this model. The LP-model gives a good agreement with experimental data from the ECN Spray A for the fuel spray penetration values.

Nomenclature

A_{LP}	coefficient in Eq. 2
B_{LP}	coefficient in Eq. 4
C_{LP}	coefficient in Eq. 7
C_d	discharge coefficient
d_{noz}	nozzle diameter [m]
LL	liquid length [mm]
LP	length parameter [m]
P_{inj}	injection pressure [Pa]
S_{tip}	tip spray penetration [m]
t_{inj}	time after the start of injection [ms]
t	time after the start of injection [s]
ν_f,	fuel kinematic viscosity [m^2 s^{-1}]
μ	fuel dynamic viscosity [Pa s]
ρ_f	fuel density [kg m^{-3}]
ρ_g	gas density [kg m^{-3}]
σ	fuel surface tension [N m^{-1}]

Abbreviations

DF	diesel fuel
LP	length parameter
PDF	probability density function
PME	palm methyl ester
SMD	Sauter mean diameter
SP	Spray penetration
WSR	well-stirred reactor

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