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Numerical study on in-cylinder blending by means of a simultaneous direct injection of two liquid fuels in a heavy duty compression ignition engine

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Abstract

Dual fuel combustion has been recently of high interest, mainly in terms of utilization of fuels different than diesel fuel in compression ignition engines. Depending on the properties of a fuel which is additional to diesel fuel, and the type of the additional fuel supply method the combustion process may be strongly modified comparing to single fuel combustion. Nowadays the modification of the combustion process becomes the reason for implementing the dual fuelling process. However, still the main reason for its implementation remains the utilization of nonconventional fuels in compression ignition engines. Among different types of dual fuel systems the one based on simultaneous direct injection of two fuels seems to be most flexible one. It allows to stratify the charge in the cylinder, blend two different fuels at any ratio and does not decrease volumetric efficiency. Therefore, this study aims at mixture formation in a heavy duty engine employing simultaneous direct injection of two different liquid fuels. Special attention was paid to spray breakup and simultaneous evaporation of two fuels which are the key processes in mixture formation.

Keywords: Dual fuel; Injection; *n*-hexane; Heavy duty engine

1 Introduction

Dual fuelling process is not a new idea. However, it has been recently of high interest, mainly in terms of utilization of fuels different than diesel fuel

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in compression ignition engines, especially in the area of stationary diesel ignited natural gas engines [1]. It was also applied to natural gas bus engines [2]. In such engines natural gas, which has high octane number, is the main fuel. It is ignited by a small dose of diesel fuel injected directly into cylinder just before the TDC (top dead centre). This small dose of diesel fuel serves as a reliable ignition source.

Depending on the properties of the fuel, which is additional to diesel fuel, the combustion process may be strongly modified. In recent years the modification of the combustion started to be the reason for implementing the dual fuelling process. Combustion process modification by simultaneous fuelling with two fuels of different properties may allow to implement and control (by changing the blend ratio) the so called advanced combustion modes, which are recently of high interest. Kokjohn *et al.* [3] used dual fuel (DF) technology for controlling combustion phasing and rate of heat release in PCI (premixed controlled ignition) modes. They suggested that the fuel in-cylinder blending is capable of controlling combustion phasing because it changes the fuel reactivity. They stated that in order to control the rate of heat release at higher loads, the fuel stratification is needed. Wu *et al.* [4] used this approach due to the fact that it allows the in-cylinder blending of two different fuels at any blend ratio. They used gasoline as the PFI (port fuel injection) fuel, while various mass fractions of gasoline, ethanol and 2.5 dimethylfuran (DMF) have been directly injected. Based on the obtained results they concluded that the dual-injection strategy is a promising engine concept. It helps to utilize biofuels, reduce the dependency on fossil fuels, lower the emissions and improve the combustion process, especially at higher loads with less PFI mass fractions [4]. Their conclusions point out the advantage of DI (Direct Injection) over PFI–PFI decreases the volumetric efficiency.

Among different types of dual fuel systems the one based on simultaneous direct injection of two fuels seems to be most flexible one. It allows to stratify the charge in the cylinder, blend two different fuels at any ratio and does not decrease volumetric efficiency. Therefore, in this study a heavy duty engine equipped with simultaneous direct injection of two different liquid fuels was under investigation. Special attention was attached to droplet breakup and evaporation of two fuels, which are the key processes in mixture formation.

This fuelling concept could also be used for light hydrocarbons in CI (compression ignition) engines which are often regarded as a by-products of

the gas processing. Therefore, in this study n-hexane injection was investigated.

Computational fluid dynamics (CFD) methods are very useful tool in engine design and optimization process. However their accuracy is dependent on the models used and adopted assumptions. In engines employing direct injection the crucial element to model is the formation of the spray of the injected liquid. Although there are still some known drawbacks of the spray models, in general the accuracy of available models is sufficient to predict major characteristics of the sprays [5]. Therefore in this study the CFD method was selected for the assessment of the novel duel fuel system for light hydrocarbon utilization in CI engines.

2 Numerical model

The calculations were performed using AVL Fire 2013.2 [19], a commercial CFD software which is based on finite volume method.

The fluctuating parameters in turbulent conditions were averaged using the RANS (Reynolds averaged Navier-Stokes) method. In general, the global flow characteristics such as spray and vapour penetration, liquid length, ignition delay, flame liftoff length, heat release rates, pressure traces, etc., can be fairly well predicted by a RANS approach [5]. Moreover, RANS method is the most commonly used one in CFD tools for commercial applications due to its relatively low computational demands. For these two reasons, RANS approach was selected for presented simulations studies.

In RANS method, the local instantaneous values are averaged and therefore the closure model is required. There are several turbulence models proved to be reliable. In presented simulations the k-ζ-f model was used. This model was developed by Hanjalic *et al.* [6]. It is based on Durbin's elliptic relaxation concept, which solves a transport equation for the velocity scales ratio $\zeta = \overline{v^2}/k$ instead of the equation for $\overline{v^2}$ [6], where $\overline{v^2}$ is the velocity scale and k is the turbulence kinetic energy. Detailed description of Durbin's model can be found in [7]. Hanjalic *et al.* [6] claim that due to a more convenient formulation of the equation for elliptic function f and especially of the wall boundary condition for this function, it is more robust and less sensitive to nonuniformities and clustering of the computational grid than Durbin's model. The advantages of this model were important especially around nozzle region, where the velocity gradients are very high. Therefore, this model was chosen for the simulations.

Liquid fuel spray is a two phase flow in which the liquid phase is strongly dispersed. Spray simulation requires a multiphase model. There are two methods, which are commonly used for multiphase flow representation. One is Euler-Euler – CDM (continuous droplet model) method and the other one is Euler-Lagrange – DDM (dispersed droplet model). In CDM method, the groups of droplets with different sizes are treated as a different phases and are represented mathematically as interpenetrating continua. When the droplet size range is very wide, the number of phases in CDM model needs to be high as well. In case of high number of phases computational demand becomes very high. Therefore CDM is most suitable for modeling multiphase flows with low number of phases. Nevertheless, there were some attempts in the past to use this approach for modeling of n-hexane ($CH_3(CH_2)_4CH_3$)) spray [8]. In DDM method the droplets are tracked in a Lagrangian way through the computational domain. This method was firstly used in a stochastic form for liquid sprays by Dukowicz [9]. It allows individual attributes, such as particle size, composition, etc., to be statistically assigned for each particle. In this method the ordinary differential equations for the trajectory, momentum, heat and mass transfer of a single droplet are solved. However, the droplets of the same properties are grouped in parcels. Each parcel is introduced in the flow domain with initial conditions of position, size, velocity, temperature and number of particles in the parcel. The equations are not solved for every single droplet but only for representative one for the parcel [10]. Therefore significant reduction of the computational requirements is achieved with this approach. In combination with the reasonable accuracy the relatively low computational demands were the main reason for using this approach in this study.

Injected liquid enters the gaseous medium as a more or less continuous phase, which after certain distance disintegrates. There are different forces acting on the liquid jet, and thus there are different mechanisms of the liquid jet breakup possible. According to Arcoumanis *et al.* [11] three different mechanisms of jet breakup can be distinguished: the aerodynamic-induced atomization, the jet turbulence-induced atomization and the cavitation-induced atomization. The internal flow plays also huge role in jet disintegration, especially when cavitation appears. Simple spray models assume that the injected liquid enters the computational domain (gaseous medium) as a collection of droplets. In order to include the cavitation effects on spray formation in that simple approach, Nurick [12] proposed a model which accounts for internal flow effects basing on geometrical properties of

the injector nozzle, nozzle length to diameter ratio and entrance radius. This approach was applied in this study. When the injected liquid jet is disintegrated into droplets, the droplets may undergo further breakup. According to Pilch and Erdman [13], the droplet breakup nature is dependent on the Weber number. In high pressure direct injection systems Webber number is very high. Then the droplet is expected to undergo catastrophic breakup. In such conditions the most suitable breakup model is the Wave model. This model is based on the Kelvin-Helmholtz instability of a liquid jet, where the viscous forces produce waves on the liquid surface and new droplets are formed from the surface waves. Waves grow on the droplet surface with a growth rate Ω and a wave length Λ, and the sizes of the newly-formed droplets are determined from the wave length and growth rate of this instability [14].

Breakup of the initial droplet results in both, production of new droplets and the reduction of the size of the parent droplet. The rate of change of the parent droplets is given by following relation [14]:

$$\frac{dr}{dt} = -\frac{r - r_{stable}}{\tau_\alpha} \quad , r_{stable} \leq r \ , \tag{1}$$

where r is the radius of the parent droplet, t and τ_α are the time and breakup time, respectively, and r_{stable} is the breakup droplet radius and is described by following relation:

$$r_{stable} = B_0 \Lambda \ , \tag{2}$$

where Λ is the wave length and B_0 is the droplet radius constant. The breakup time is dependent on wave growth rate and wave length according to the following formula:

$$\tau_\alpha = 3.726 B_1 \frac{r}{\Lambda \Omega} \ . \tag{3}$$

The rate of breakup in this model can be adjusted by two constants: B_0 – droplet radius constant and B_1 – droplet breakup time constant. These values were specified according to recommendations provided by the author of the model [15]. In the study constants B_0 and B_1 were set to 0.61 and 20, respectively.

At the same time when the jet disintegrates the injected liquid undergoes evaporation. This process is the most intensive in highly dispersed region of spray where the droplets are small and interface surface is high. In this study

conducted the Dukowicz model [16] was used in all investigated cases. This model was created basing on the analogy between heat and mass transfer processes in the vicinity of the droplet surface. This model has several assumptions: the flow near the droplet is spherically symmetrical, there is a quasi-stationary layer of liquid vapor near the droplet surface, the droplet temperature is uniform, the properties of the surrounding gas are constant, vapor and liquid on the droplet surface are in thermodynamic equilibrium. The rate of change of droplet temperature depends on the heat balance, which assumes that the heat convection from the gas to the droplet either heats up the droplet or supplies heat for vaporization.

3 Computational mesh

The computational domain includes the whole cylinder. The full cylinder geometry was used to compose the computational mesh. The geometry was created basing on real engine parameters and included the piston movement. The geometrical parameters of the engine cylinder and selected engine parameters needed for creating the deforming mesh are presented in Tab. 1.

Table 1: Parameters of the engine needed for creating the deforming mesh.

Parameter	Value
Cylinder diameter	320 mm
Stroke	350 mm
Conrod length	740 mm
Compression ratio	13.8

The computational mesh was created in a way to avoid strong stretching and compression of the cells during the mesh deformation according to piston movement. Therefore depending on the crank angle (CA) the mesh was composed of different number of elements. The cross-section of the deforming mesh at different crank angles is shown in Fig. 1.

The created mesh at BDC (bottom dead centre) consisted of 300 000 elements, among which the majority was of hexahedral shape. There was also low number of tetrahedron, pyramid and prism cells. One outer layer of the cells was created according to the outer surface. The maximum size of the mesh element was 5 mm. Mesh at TDC consisted only of 33 000 elements.

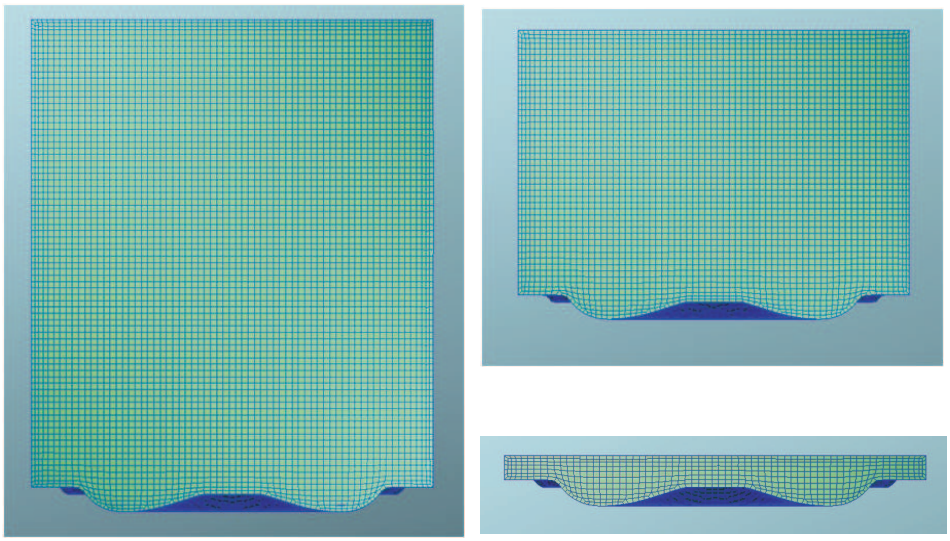

Figure 1: Cross-section of the deforming mesh at 180, 90, and 0 CA degrees before TDC, respectively from left up.

4 Initial and boundary conditions

The aim of the study was to investigate the spray and mixture formation in the dual fuel system employing simultaneous direct injection of two different fuels. However the reference case was needed to draw any conclusions about the mixture formation in terms of conventional CI engine. Therefore two cases were calculated. All the parameters beside the fuel injection were the same: the engine speed, compression ratio. The engine speed was 750 rpm. The other parameters like, fuel mass injected, initial temperature and pressure were set according to the measured values on engine dyno. Due to the fact that the geometrical model did not include the intake ports and the intake stroke was not simulated, the rotational charge motion was applied as an initial condition. The initial rotational speed of the air was set to 1125 rpm. The other initial conditions and injection parameters in calculated cases are presented in Tab. 2. The simulations were started at BDC therefore the parameters in the cylinder presented in the Tab. 2 are the parameters at this piston location.

In previous work Kapusta [18] calculated that the fuel mass flow rate of n-hexane is 0.116 kg/s, thus the mass of the hexane supplied to the cylinder through a single injector is 0.464 g. This value appeared to be in

Table 2: Summary of analyzed cases.

Case no.	Chamber pressure at BDC, MPa	Chamber temperature at BDC, K	Start of injection (before TDC), CA deg	Injection duration diesel fuel and hexane, (in brackets), CA deg	Injected mass of diesel fuel (per cycle, per cylinder), g	Injected mass of hexane (per cycle, per cylinder, g
1	0.35	343	12.5	4 (18)	0.17	0.465
2	0.35	343	12.5	28.5	3.644	–

accordance with the real engine measurements [20]. Although this amount of hexane was not sufficient to reach 100% load, the hexane injection system was a part of a dual fuel system and the rest of energy could be delivered in diesel fuel. However in this study the dose of the diesel fuel was minimal – just for ignition. All cylinder walls were assumed to be adiabatic. The simulations did not include combustion in order to avoid its influence on mixture formation.

5 Results

The obtained results were analyzed mainly in terms of spray development. The spray parameters were compared for two different cases characterized in Tab. 2. The results were averaged over the whole domain. Additionally, 3D spray clouds were compared in order to visualize the differences in spray formation and development.

The Sauter mean diameter (SMD) averaged over the whole domain is presented in Fig. 2.

Presented graph clearly shows that in dual fuel operation droplet diameter is higher. The bigger droplets increase the time needed for fuel to evaporate and under reacting conditions may result in increased soot formation. Normalized evaporated mass of injected liquid fuel is shown in Fig. 3.

The graph showing the evaporation process of the liquid fuel indicates that at the beginning the evaporation in dual fuel mode is faster. It probably results from the fact that at the beginning both fuels are injected at the same time, so actually the liquid fuels leave injector through almost double number of nozzle holes. After the initial stage the poor breakup of *n*-hexane makes the evaporation prolonged. Moreover, in Fig. 4 one can

clearly notice that the spray penetration of the n-hexane is not as high as those of diesel fuel.

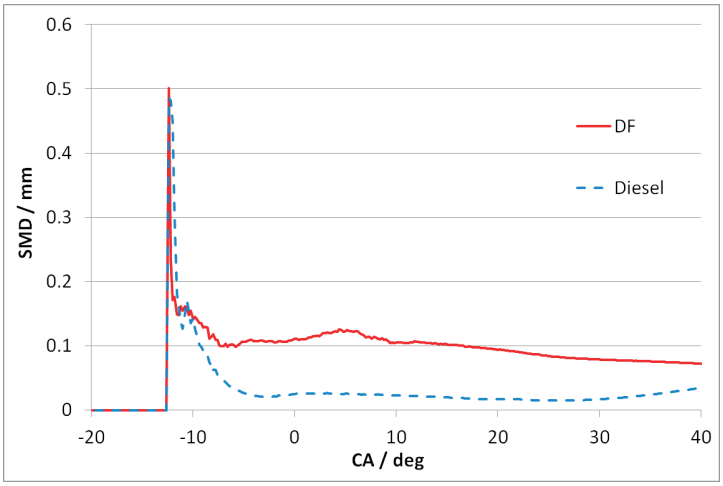

Figure 2: SMD averaged over the whole domain; DF - dual fuel, Diesel – diesel fuel.

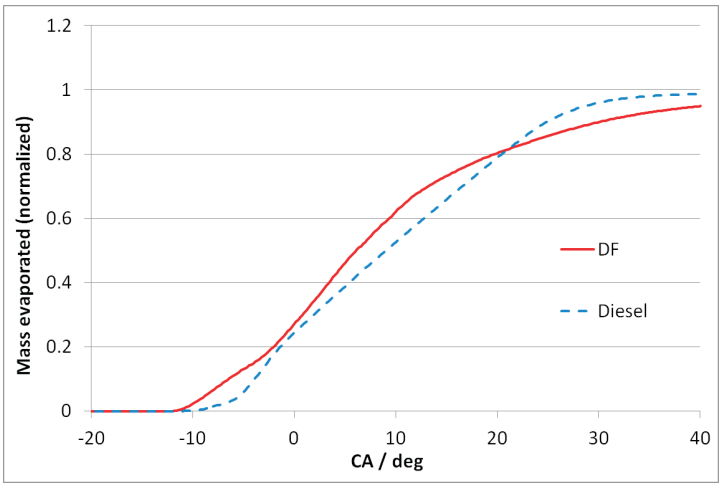

Figure 3: Normalized evaporated mass of liquid fuel.

The spray penetration shown in Fig. 4 indicates that the n-hexane distribution over the chamber may not be sufficient to provide effective mixture formation. In order to visualize the spray formation and development the

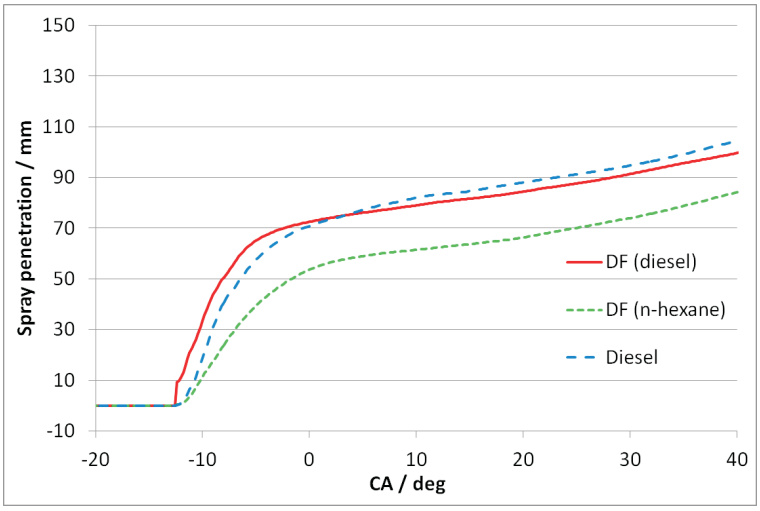

Figure 4: Spray penetration.

spray clouds were presented in Fig. 5. Presented spray clouds differ between each other. One can observe that the spray cloud for conventional single fuel CI engine looks much denser than the one for DF operation. This however, can be linked with higher mass injected during the same injection time. The brightness of the droplets presented in Fig. 5 indicates their velocities. Dark droplets have low velocity while the bright ones high velocity. The velocities of the spray droplets for diesel fuel were much higher than for *n*-hexane. This again can be linked with the difference in injection pressure, and it is in accordance with poor droplet breakup and lower spray penetration noticed for *n*-hexane injection.

6 Conclusions

Numerical simulations were performed in order to compare the injection process in novel dual fuel system for light hydrocarbon utilization in CI engines with the injection in conventional single fuel CI engine operated on diesel fuel. Calculated results for all cases were analyzed and the following conclusions were made:

- The bigger droplets were observed in DF mode. This increases the time needed for fuel to evaporate and under reacting conditions may result in increased soot formation.

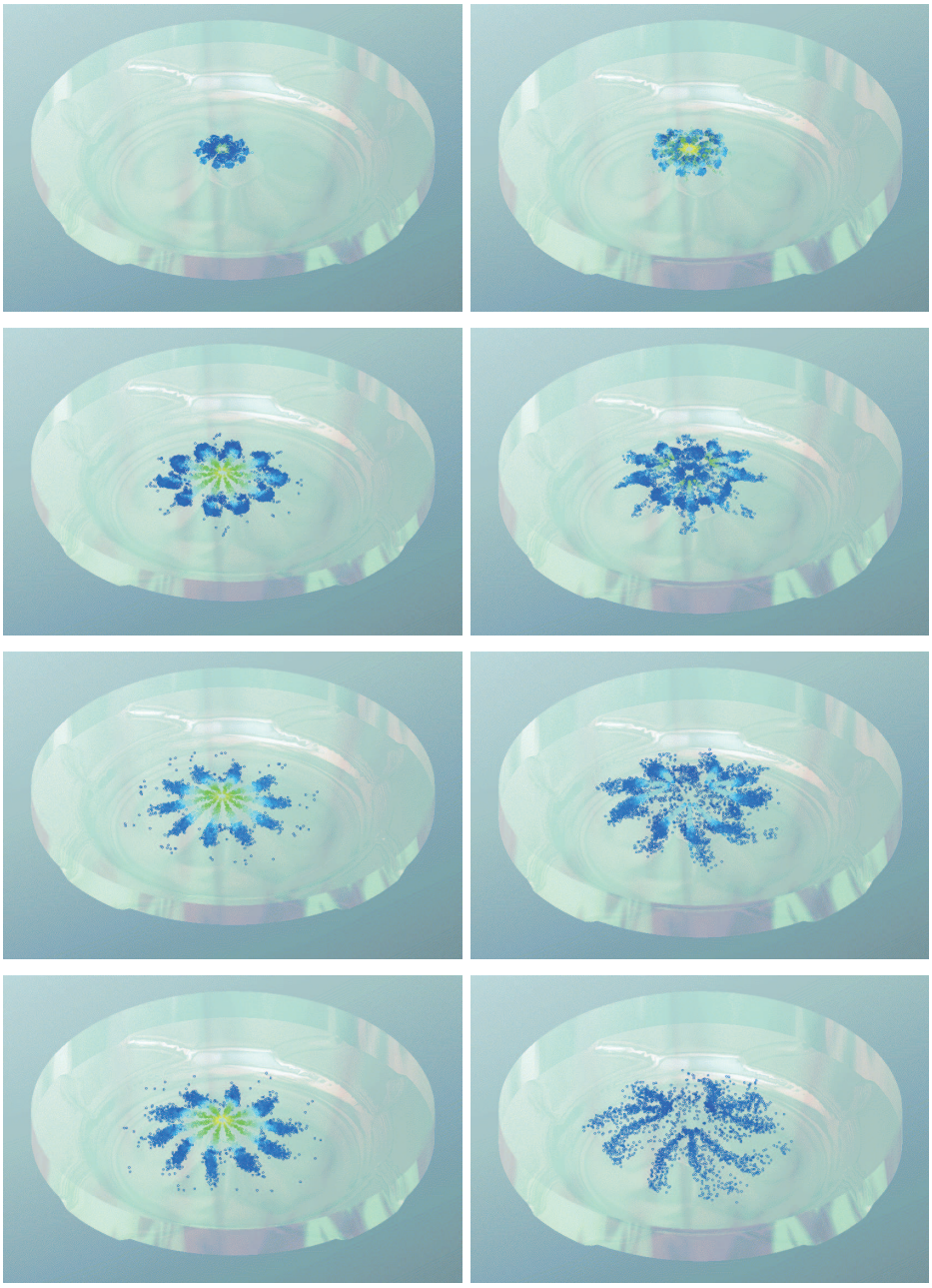

Figure 5: Spray clouds visualization; left – conventional single fuel CI engine, right – dual fuel. The images were recorded at: -10, -5, 5, 15 CA degrees after TDC, respectively from top to bottom.

- The observed poor breakup of n-hexane droplets makes the evaporation process prolonged.
- Lower spray penetration for n-hexane indicates that the n-hexane distribution in the chamber may not be sufficient to provide effective mixture formation.
- The appearance of the spray in DF mode is completely different to those in conventional diesel operation. The spray for diesel operation is much denser, what can be linked with higher mass injected during the same injection period.
- The velocities of the spray droplets in case for diesel fuel were much higher than for n-hexane. This may result from the difference in injection pressure, which is in accordance with poor droplet breakup and lower spray penetration.

Combining these observations made one can draw a conclusion that the injection pressure in n-hexane fuel line should be higher. Higher injection pressure results in lower SMD as well as decreases spray penetration.

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