JET AND DROPLET BREAKUP MODELLING APPROACHES

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Abstract

Three-dimensional computational fluid dynamics (CFD) plays important role in engines development. The mixture formation in a direct-injection piston engines poses a huge challenge in successful simulations of the engine processes. It is due to the fact that the spray as a two-phase flow complicates the computational process. Moreover, this multiphase flow is not uniform. Three main zones, depending on the distance from the nozzle exit are visible when a liquid is injected. Very dense so called "thick" in a direct vicinity of the injector hole, than "thin" as a result of primary breakup downstream the injector and finally in the certain distance from the injector appears "very thin" region as a result of secondary breakup. It is important to take into account that the liquid phase in various regimes behaves differently and is under influence of different phenomena. The modelling approach needs to take in to consideration all those elements. This paper focuses on presentation of the theory and numerical models for primary and secondary breakup phenomena. The primary breakup is a process that results from a combination of three mechanisms: turbulence within liquid phase, implosion of cavitation's bubbles and aerodynamic forces acting on a liquid jet. Secondary breakup regime occurs mainly due to the aerodynamic interactions between the liquid and the gaseous phase.

Keywords: spray, modelling, simulation, breakup, injection, CFD, computational fluid dynamics

1. Introduction

Spray appears in many power and energy systems such as industrial burners, gas turbines, furnaces and engines. Sprays are also present in aftertreatment systems (urea-water solution injection), fire extinguishers, medical atomizers, agriculture atomizers, and others. Therefore, their significance is very high.

Spray is a two-phase flow of gas and liquid in which the liquid phase is strongly dispersed in the gaseous one. As a two-phase flow, spray requires a multiphase model. In general, there are two approaches for multiphase flow modelling:
– CDM (Continuous Droplet Model) – Euler-Euler approach,
– DDM (Dispersed Droplet Model) – Euler-Lagrange approach.

In Euler-Euler approach, the collections of droplets with different sizes are described as a different phases, which are treated as interpenetrating continua. For sprays where the droplet diameters ranges from very small to the large ones high number of phases is required in order to provide proper spray representation. However, each additional phase requires addition of set of the equations. When the number of phases becomes high the computational power requirements becomes enormous. Therefore, Euler-Euler approach is recommended for modelling multiphase flows with low number of phases.

In Euler-Lagrange approach, the droplets are tracked in a Lagrangian frame of reference. This method was firstly applied in a stochastic form for liquid sprays by Dukowicz [1]. This method allows individual attributes, such as particle size, composition, etc., to be statistically assigned for each particle [18, 19]. The droplets with similar properties can be collected in groups named parcels, while the ordinary differential equations for the trajectory, momentum, heat and mass transfer are solved for a single droplet. The parcels are introduced into the computational 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 [2]. Thus, the significant reduction of the computational demands is observed. This feature together with the reasonable accuracy makes this approach perfect for engineering use therefore the study focuses on this approach.

2. Breakup regimes

In engine fuel injection systems, the fuel typically leaves the injector nozzle in a more or less continuous liquid phase that can obviously not be reproduced with the Lagrangian discrete droplet approach. Therefore, additional submodels are necessary in order to describe the breakup processes, which lead to the formation of droplets, before the DDM can be applied [3].

In high pressure, liquid sprays there are visible three main regions depending on the distance from the nozzle exit when a liquid is injected. The first one is very dense, so-called "thick", and it is observed in a direct vicinity of the injector hole. In a slightly higher distance from the injector as a result of primary breakup, the "thin" region is observed. And finally in the higher distance from the injector appears "very thin" region as a result of secondary breakup.

One can see that two different types of breakup are involved in spray formation, primary breakup and secondary breakup. The primary breakup occurs near the nozzle exit where the liquid core disintegrates into ligaments and droplets. The secondary breakup occurs at larger distance where the initially large droplets brake up into smaller ones. The regions of different spray breakups are shown in Fig. 1. These regions include different phenomena and thus they cannot be covered by one common description.
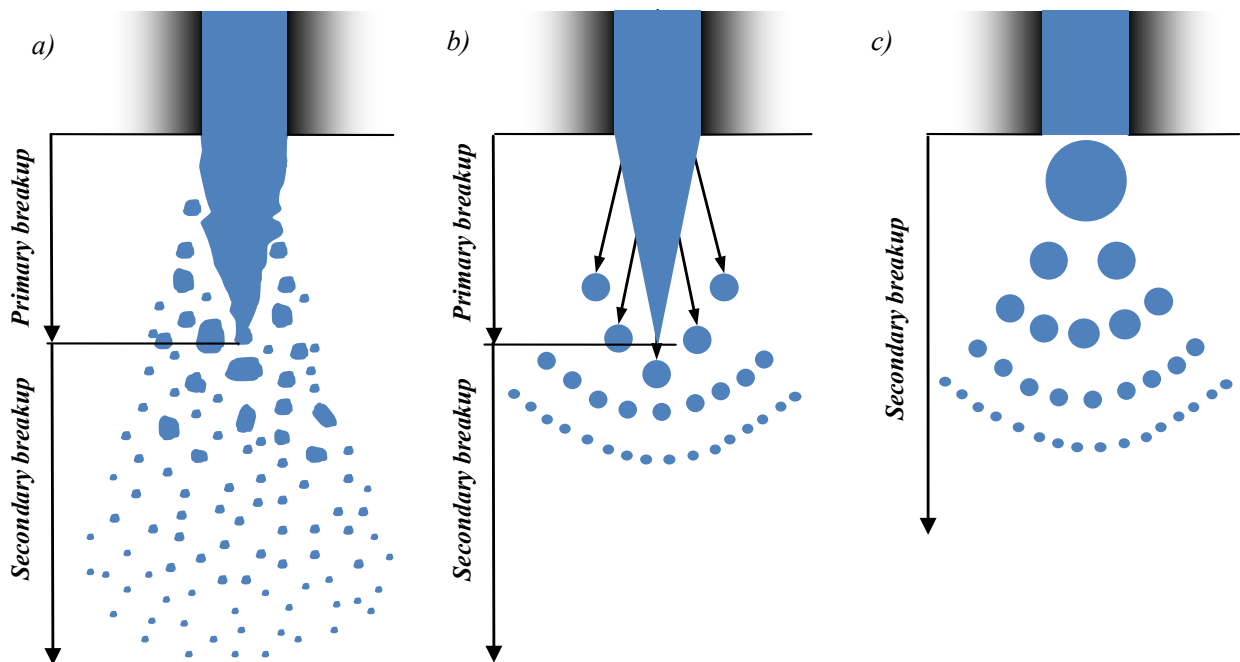

Fig. 1.   *Breakup regimes (a) and spray representation for different modelling approaches, with primary breakup (b) and without primary breakup (c)*

According to Arcoumanis et al. [4], due to the various forces acting on the liquid jet, there are different mechanisms of the liquid core breakup, the aerodynamic-induced atomization, the jet turbulence-induced atomization and the cavitation-induced atomization. Cavitation within the injector nozzle is one of the major factors influencing the structure of the spray. On the other hand, in secondary breakup only the aerodynamic-induced breakup plays a role. Therefore, the modelling of the primary breakup requires additional information on the liquid flow at the nozzle outlet. This information often cannot be obtained; therefore, in many studies the primary breakup is not included. Such approach limits the accuracy of the results but for many engineering problems, it is still sufficient [16, 17].

In general, the spray formation can be modelled in two ways, including and excluding the primary breakup. The difference in spray representation in these two approaches is shown schematically in Fig. 1.

A more simple approach (Fig. 1c) omits the primary breakup and assumes that the injected liquid after exiting the nozzle outlet is initially composed of droplets which undergo only

In high-pressure diesel injectors often cavitation occurs. This phenomenon has strong influence on spray formation. There is possible three different flow regimes trough the nozzles, which are shown in Fig. 2. One is pure liquid flow (Fig. 2a). The second one involves cavitation but the cavitation does not reach the nozzle exit (Fig. 2b). In the third one, the cavitation is so intense that it reaches the nozzle exit (Fig. 2c).
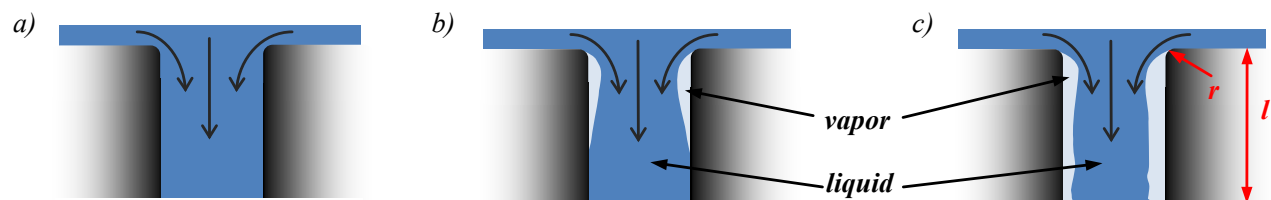

Fig. 2. Flow regimes through the nozzle (a) and spray representation for different modelling approaches, with primary breakup (b) and without primary breakup (b)

In order to include the cavitation effects on spray formation in blob method, Nurick [5] proposed a model, which accounts these effects basing on geometrical properties of the injector nozzle, nozzle length to diameter ratio and entrance radius. The geometrical parameters of the nozzle used in this model are shown in Fig. 2. (marked with red).

The modelling approach, including primary breakup is more complex. In this approach, primary breakup is modelled and in-injector effects are included. It is arranged in two steps. In the first step, internal flow in the injector is simulated and fluid parameters and its properties at the outlet are collected. In the second step, the spray process is simulated with the use of the results obtained during the first step. The simulation procedures for different modelling approaches and required input data are shown in Fig. 3.

The modelling approach, which includes primary breakup, seems to be much more complex and that it requires much more data. However, one needs to be aware that successful implementation of blob method (either with Nurick's model or without) requires injection rate diagram. This can be only determined experimentally and usually this data is not available. In such cases injection rate can be assumed as constant or trapezoid, but then the results may significantly differ. The influence of the injection rate assumption on spray formation was shown by Kercheva et al. [6].

3. Primary breakup modelling

The primary breakup is a process that results from a combination of three mechanisms: turbulence within liquid phase, implosion of cavitation's bubbles and aerodynamic forces acting on liquid jet. In secondary breakup, the aerodynamic forces play the main role in the breakup process.
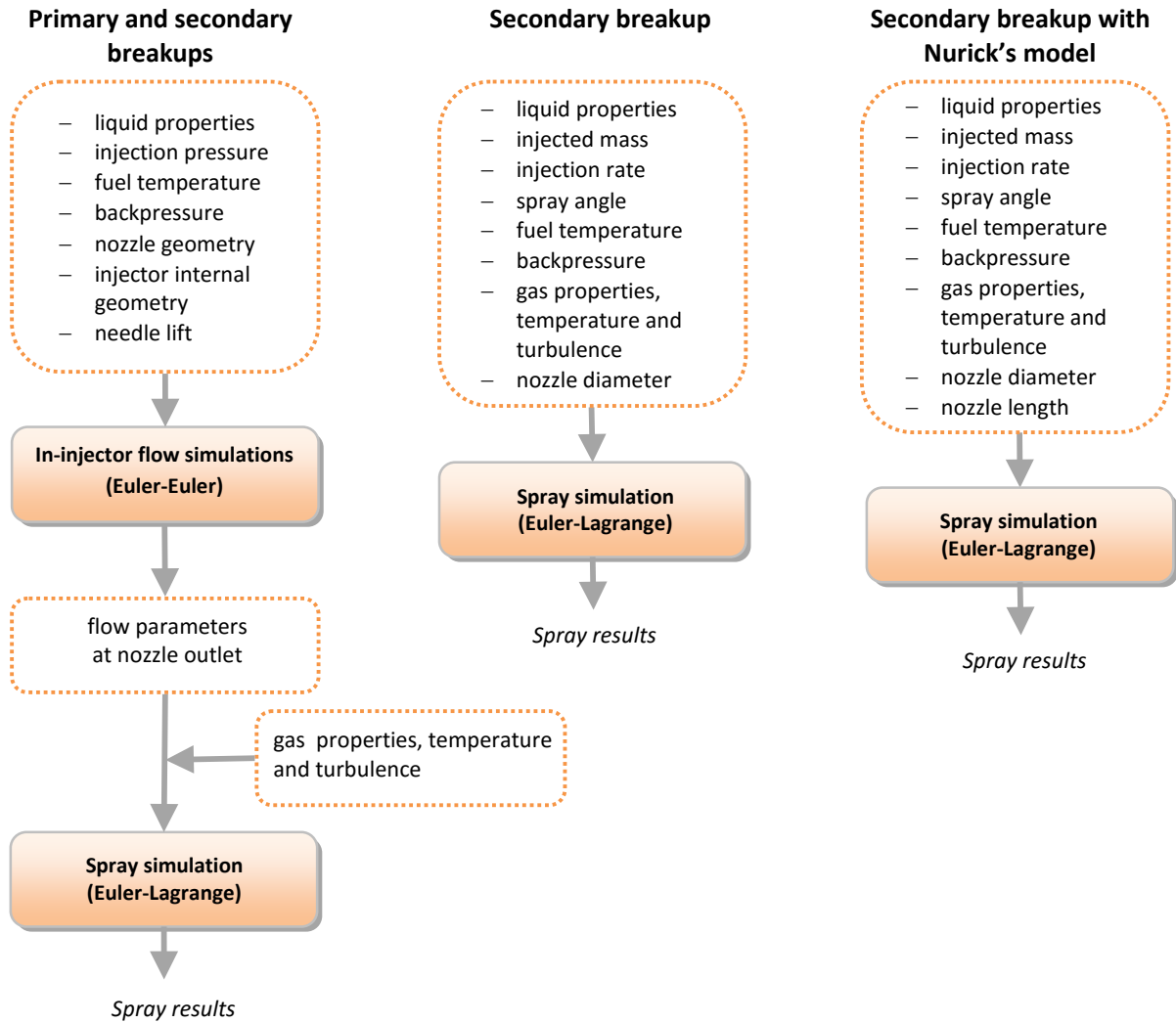
Primary and secondary breakups

- liquid properties
- injection pressure
- fuel temperature
- backpressure
- nozzle geometry
- injector internal geometry
- needle lift

In-injector flow simulations (Euler-Euler)

flow parameters at nozzle outlet

gas properties, temperature and turbulence

Spray simulation (Euler-Lagrange)

Spray results

Secondary breakup

- liquid properties
- injected mass
- injection rate
- spray angle
- fuel temperature
- backpressure
- gas properties, temperature and turbulence
- nozzle diameter

Spray simulation (Euler-Lagrange)

Spray results

Secondary breakup with Nurick's model

- liquid properties
- injected mass
- injection rate
- spray angle
- fuel temperature
- backpressure
- gas properties, temperature and turbulence
- nozzle diameter
- nozzle length

Spray simulation (Euler-Lagrange)

Spray results

Fig. 3. The simulation procedures and input parameters required for different modelling approaches

Therefore, the models for primary breakup regime need to be different from for secondary breakup.

The primary breakup needs to take into account all these three mechanisms. In general, there are two different approaches to primary breakup modelling.
− blob injection,
− core injection.

These two breakup models are schematically shown in Fig. 4. Blob injection primary breakup model should not be mixed up with blob method (shown in Fig. 1c).
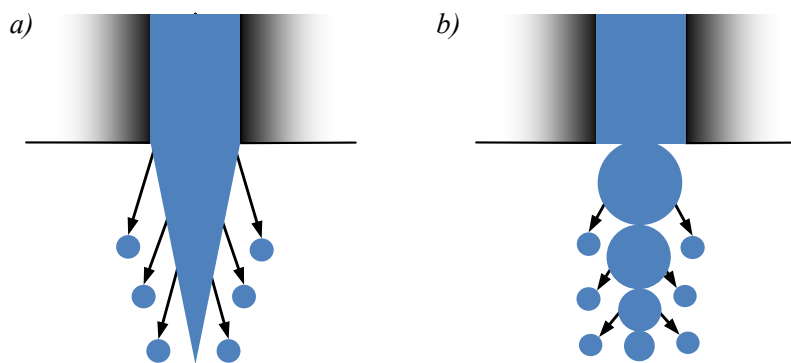

Fig. 4. Primary breakup modelling approaches, core injection (a) and blob injection (b)

In the blob, injection model the liquid core is represented by a group of blobs of size gradually decreasing with increasing distance from nozzle exit due to detachment of child droplets. The diameter of the biggest droplet located at the nozzle exit is equal to nozzle diameter. The child droplets are detached from the initial collection of blobs according to Wave model described in chapter 4.1. The detachment of drops from initial blobs in primary breakup is thus similar to detachments of child drops from large drops in secondary breakup. The droplets released from initially introduced large blobs in the primary breakup additionally receive radial velocity.

In core injection, the liquid core is represented by a cone which erosion depends on the released droplets. The core injection primary breakup model results in much smaller droplets than the nozzle diameter.

One important remark is that the primary and secondary breakup models do not act the same time on the same parcels but subsequently [7]. In AVL Fire, a commercial CFD software the criteria for switching from primary to secondary break-up are a check on critical transition Weber number and checks on stable or minimum diameter [7].

4. Secondary breakup modelling

After the jet disintegrates into droplets, the droplets can break up and form smaller droplets. According to Pilch and Erdman [8], there are different mechanisms of droplet breakup, which are dependent on the Weber number. Moreover, the breakup models can be based on different theories. Therefore, there are broad varieties of secondary breakup models among which following ones need to be mentioned:
– O'Rourke and Amsden [9] TAB model,
– Reitz and Diwakar [10] Wave model,
– Pilch and Erdman [8] FIPA model,
– Huh and Gosman [11] model,
– Su et al. [12] KH-RT model.

As for the engine application, the TAB and Wave models are the most widely used ones and covers all the regimes of engine sprays starting from gasoline PFI (Port Fuel Injection) low-pressure injection ending with high-pressure diesel sprays. Therefore, only these two models will be discussed in details.

4.1. Wave model

For high-pressure direct injection, where the Weber number is very high, the most suitable breakup model is the model named Wave, which is based on the wave theory implemented for blobs by Reitz [13] and used for the first time for liquid spray by Reitz and Diwakar [10]. 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 wavelength Λ, and the sizes of the newly formed droplets are determined from the wavelength 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 droplets. The rate of change of the parent droplets is given by following relation [14]:

$$\frac{\mathrm{d}r}{\mathrm{d}t} = -\frac{r_p - r_{stable}}{\tau_\alpha}, \qquad r_{stable} \le r_p, \tag{1}$$

where r_p is the radius of the parent droplet τ_α is the breakup time 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 wavelength and B_0 is the droplet radius constant. The breakup time is dependent on the wave growth rate and wavelength according to the following equation:

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

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 B_0 and B_1 recommended by the authors of the model [10, 13] are 0.61 and 20, respectively.

4.2. TAB model

The TAB model also known as Taylor Analogy Breakup model originally developed by O'Rourke and Amsden [9] is based on the analogy between deforming droplet and oscillating mass on a spring.

The spring force corresponds to the surface tension forces, while the external forces acting on the oscillating mass correspond to the aerodynamic forces. The damping forces represent the viscosity of the liquid. The general formulation of TAB model is shown below:

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} = \frac{C_F \rho_g u^2}{C_B \rho_l r^2} - \frac{C_K \sigma}{\rho_l r^3} y - \frac{C_d \mu_l}{\rho_l r^2} \frac{\mathrm{d}y}{\mathrm{d}t}, \tag{4}$$

where C_F, C_K, C_d and C_B are dimensionless model constants, ρ_g and ρ_l are the densities of gas and liquid, respectively.

The size of the droplet emerging during the breakup process from the parent drop is determined basing on energy balance between parent and child drops. Derived formula for droplet diameter is shown below:

$$\frac{r}{r_{32}} = 1 + \frac{8K}{20} + \frac{\rho_l r^3}{\sigma} \left(\frac{\mathrm{d}y}{\mathrm{d}t}\right)^2 \left(\frac{6K-5}{120}\right), \tag{5}$$

where r is the size of the child droplet, r_{32} is the Sauter Mean Radius (SMR) of the parent drop and K is the model constant.

In distinguish from the Wave model, the TAB model results in a distribution of droplet sizes after the breakup.

One needs to be aware that the important model limitation is resulting from the fact that the breakup is connected with one oscillation mode. Such representation is sufficient for low Weber numbers. For the spray regimes with higher Weber numbers, other oscillation modes become important in the breakup process.

5. Evaporation modelling

Beside the liquid ligaments and droplets breakup simultaneously in the spray region, the evaporation process is ongoing. It has influence on global spray parameters and on secondary breakup as well. It results from the fact that the evaporation process leads to decrease of the droplet diameters while they move along the gaseous environment. The most frequently used in engineering applications evaporation model is the Dukowicz model [15]. This model is based on the assumption of analogy between heat and mass transfer processes in the vicinity of the droplet surface. Moreover, there are several additional assumptions in this model:
– the flow near the droplet is spherically symmetrical,
– there is a quasi-stationary layer of liquid vapour in the vicinity of the droplet surface,
– droplet temperature is uniform,

– the properties of the surrounding gas are constant,
– vapour and liquid are in thermodynamic equilibrium on the droplet surface.

The rate of droplet temperature change is determined by the heat balance, which states that the heat convection from the gas to the droplet either heats up the droplet or supplies the heat for vaporization process.

5. Conclusions

The mixture formation by a direct-injection becomes very important issue in piston engines development. Therefore, the spray modelling becomes one of the crucial elements in engine processes CDF simulations. The study summarized the approaches to spray modelling, especially in terms of high-pressure injection systems. The theory and numerical models for account primary and secondary breakup phenomena were briefly presented.

One can conclude that even the simple approach to spray modelling based on blob method requires detailed data on injection in order to provide reliable results. However, for initial engineering studies some assumptions can be made to provide useful results.

Acknowledgements

6. References

[1] Dukowicz, J. K., *A particle-fluid numerical model for liquid sprays*, J. Comput. Phys, Vol. 35, pp. 229-53, 1980.
[2] Heywood, J. B., *Internal Combustion Engine Fundamentals*, McGraw-Hill, 1988.
[3] Stiesch, G., *Modeling Engine Spray and Combustion Processes*, Springer, 2003.
[4] Arcoumanis, C., Gavaises, M., French, B., *Effect of fuel injection processes on the structure of diesel sprays*, SAE Tech. Pap., 970799, 1997.
[5] Nurick, W. H., *Orifice cavitation and its effect on spray mixing*, J. Fluids. Eng., Vol. 98, pp. 681-687, 1976.
[6] Kercheva, B., Kapusta, Ł. J., Teodorczyk, A., *LES numerical study on n-hexane injection in a compression ignition engine*, Arch. Combust., 2, 2014.
[7] *Spray Module, AVL fire version 2013.1*, AVL List Gmbh, Graz, Austria 2013.
[8] Pilch, M., Erdman, C., *Use of breakup time data and velocity history data to predict the maximum size of stable fragments for acceleration-induced breakup of a liquid drop*, Int. J. Multiph. Flow., Vol. 13, pp. 741-757, 1987.
[9] O'Rourke, P. J., Amsden, A. A., *The TAB method for numerical calculation of spray droplet break-up*, SAE Tech. Pap., 872089, 1987.
[10] Reitz, R. D., Diwakar, R., Structure of high-pressure fuel sprays, SAE Tech. Pap., 870598, 1987.
[11] Huh, K. Y., Gosman, A. D., *A phenomenological model of diesel spray atomisation*, Proc. Int. Conf. Multiph. Flows, Tsukuba, Japan 1991.
[12] Su, T. F., Patterson, M. A., Reitz, R. D., Farrell, P. V., *Experimental and numerical studies of high pressure multiple injection sprays*, SAE Tech. Pap., 960861, 1996.
[13] Reitz, R. D., *Modeling atomization processes in high-pressure vaporizing sprays*, At. Spray Technol., Vol. 3, pp. 309-337, 1987
[14] Vujanović, M., *Numerical modelling of multiphase flow in combustion of liquid fuel*, PhD thesis, University of Zagreb, 2010.
[15] Dukowicz, J. K., *Quasi-steady droplet phase change in the presence of convection*, 1979.

[16] Jankowski, A., *Modelling of Combustion Processes of Liquid Fuels,* Journal of KONES, Powertrain and Transport, Vol. 19, No 4, pp. 239-244, Warsaw 2012.

[17] Jankowski, A., *Laser Research of Fuel Atomization and Combustion Processes in the Aspect of Exhaust Gases Emission,* Journal of KONES Vol. 15, No. 1, pp. 119-126, Warsaw 2008.

[18] Jankowski, A., Siemińska-Jankowska, B., Sandel, A., Bocheński, C., *Investigation of the Fuel Spray Atomization Spectrum in Common Rail System for Diesel Engines*, Journal of KONES, Vol. 10, No. 1-2, pp. 53-64, Warsaw 2003.

[19] Żurek, J., Jankowski, A.: *Experimental and Numerical Modelling of Combustion Process of Liquid Fuels under Laminar Conditions,* Journal of KONES, Vol. 21, No. 3, s. 309-316, Warsaw 2014.