Experimental and numerical investigation of the aerodynamic break-up of liquid droplets at diesel engine conditions

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In modern direct injection diesel engines in-cylinder pressure and temperature of the gas are very high and the density ratio of the droplet and the gas phase may be as small as 20. Since correlations for the break-up of droplets have been derived for atmospheric conditions with density ratios of about 1000 only, it is necessary to verify this data for diesel engine conditions.
Therefore, experimental investigations of the aerodynamic break-up have been performed at engine-like conditions. The measurements show that the mean diameter of the secondary droplets increases as the gas density is raised.
With a new break-up model implemented in the CFD-code FLUENT the agreement between the simulations and the measurements has been improved.

1 Introduction

Numerical methods are applied in engine design processes in order to optimise the combustion with respect to emissions and efficiency. Therefore, various phenomena within the cylinder have to be modelled in detail: atomisation of the fuel at the nozzle, mixture formation, ignition and combustion. Mixture formation is affected by the break-up of the spray and the evaporation of the fuel. For a precise description of the secondary break-up appropriate models for the dense two-phase flow are needed.

The correlations commonly used to predict the disintegration of the fuel droplets are based on experiments conducted at atmospheric pressure and temperature in shock tubes. The diameter of the secondary droplets is correlated to the Weber number We and the Ohnesorge number Oh. For Oh < 0.1 the influence of the Ohnesorge number is negligible.

$$\mathrm{We} = \frac{\rho u^2 d}{\sigma}, \quad \mathrm{Oh} = \frac{\eta}{\sqrt{\rho d \sigma}} \tag{1}$$

As the temperature and the pressure in the cylinder rise above the critical values of the fuel, the fuel droplets may reach the critical point prior to break-up. Thus, the surface tension of the droplets will decrease and break-up will be enhanced due to the increasing Weber number. To analyse these effects, experiments have been carried out to investigate the effect of gas density and temperature on the break-up.

Numerical simulations of the experiments using standard models taken from literature [1,2] for the aerodynamic break-up showed poor agreement with the experimental results especially at low Weber numbers. Implementing a new model into the FLUENT 4.48 code [3] resulted in improved accordance of experimental and numerical results.

2 Experimental investigations

The experiments were conducted using monodisperse droplets generated by a droplet chain generator [4] in a pressure chamber. The maximum pressure in the chamber is 5 MPa at gas temperatures of up to 800 K. The set-up used was proposed by Reitz and Liu [4] and is sketched in figure 1. The droplets are exposed to a high speed air flow aligned perpendicularly to the axis of the droplet chain. By varying the gas flow rate through the nozzle, break-up can be examined at different Weber numbers, gas-densities and temperatures. The diameter of the primary droplets was maintained at 95 µm, the fuels used were n-dodecane $C_{12}H_{26}$ and ethylbenzoate $C_9H_{10}O_2$.

The pressure chamber has three quartz windows which allow for backlight visualisations and Phase-Doppler-Anemometry (PDA) measurements at a scattering angle of 65° to minimise the influence of a varying refractive index of the fuel on the measurements [7,8]. This is important for the measurements at elevated temperature since the refractive index of the droplets depends on their temperature and is thus not known exactly during the experiments.

Visualisations of the break-up are made using a CCD-Camera with a long-distance microscope and spark-light illumination. The size and the velocity of the secondary droplets are measured using PDA.

2.1 Visualisations

Figure 2 shows images of the break-up taken at different Weber numbers and gas densities at a gas temperature T = 470 K. The primary droplets are shown in the upper left corner of the pictures. Increasing the gas density and keeping the Weber number constant results in larger secondary droplets (fig. 2a,b), whereas an increasing Weber number results in smaller droplets if the gas density is kept constant (fig. 2a,c). Similar results have also been obtained at ambient temperature and at a temperature T = 770 K

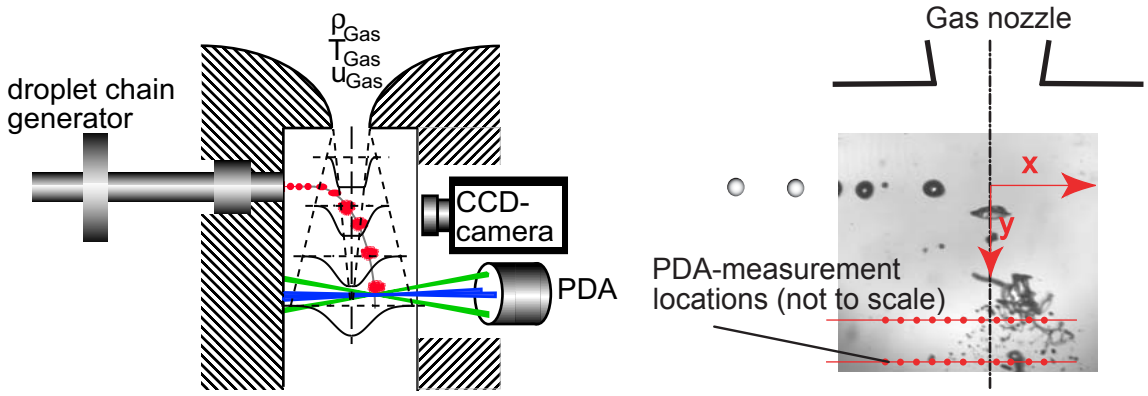

Figure 1: Sketch of the experimental set-up and PDA measurement locations

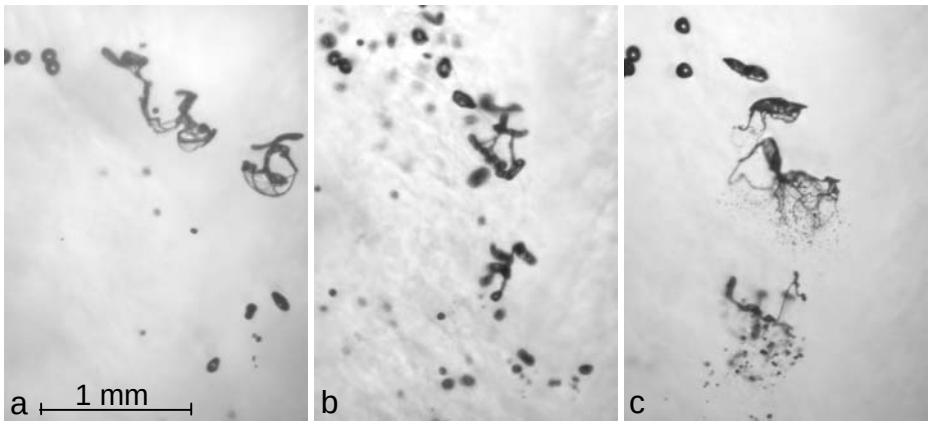

Figure 2: Visualisations of the break-up for different Weber numbers and gas densities, T_G = 470 K
a) We = 20, ρ = 5.8 kg/m³, b) We = 20, ρ = 20 kg/m³, c) We = 72, ρ = 5.8 kg/m³

2.2 PDA-measurements

PDA-measurements have been made at different positions downstream of the droplet chain. A Dantec [9] PDA system with an Ar^+-Laser was used. The focal length of the transmitting and the receiving optic were set to 310 mm so that the diameter of the measurement volume was 0.1 mm. Measurements were taken along lines parallel to the droplet chain axis as depicted in figure 1. The Weber number used to characterise the break-up in the following figures is calculated using the droplet properties at their initial temperature T_0 = 298 K.

Figure 3 shows the size distribution of the secondary droplets at y = 6 mm. For low Weber numbers the size distribution is monomodal at low gas densities and becomes bimodal as the gas density is increased. An increase in the density also results in an increase in the average diameter of the droplets. At higher Weber numbers this effect is less obvious, but still larger droplets are observed at higher gas densities.

In figure 4 the Sauter mean diameter (SMD) of the secondary droplets is shown versus the Weber number. As the Weber number increases the SMD is reduced. Increasing the gas density results in larger droplets whereas higher gas temperatures lead to smaller droplets. Due to the increased droplet temperature the surface tension decreases and the effective Weber numbers are higher. Numerical simulations predict, that the droplets temperature increases about 30 – 50 K prior to the break-up, thus reducing the surface tension by approximately 20%.

Increasing gas temperature and pressure above the critical values of the fuel (p_C = 1,8 MPa, T_C = 658 K for n-dodecane) did not result in enhanced break-up. The

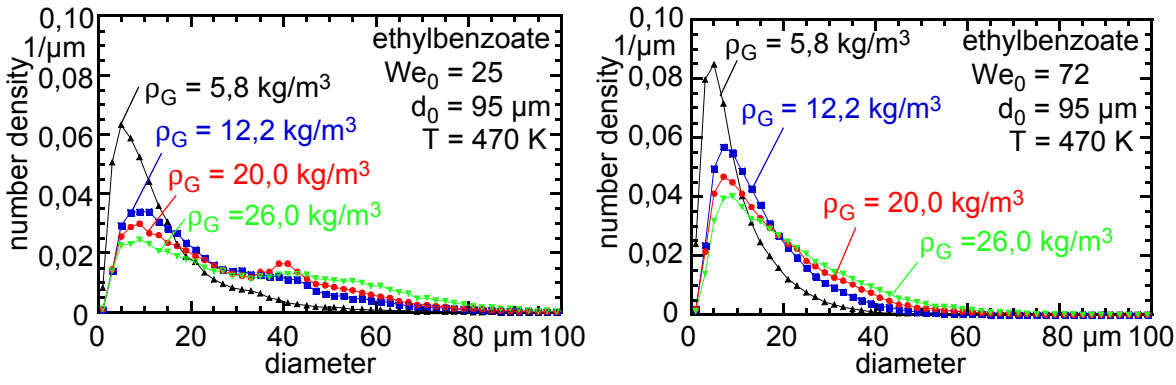

Figure 3: Diameter-pdf for different gas densities

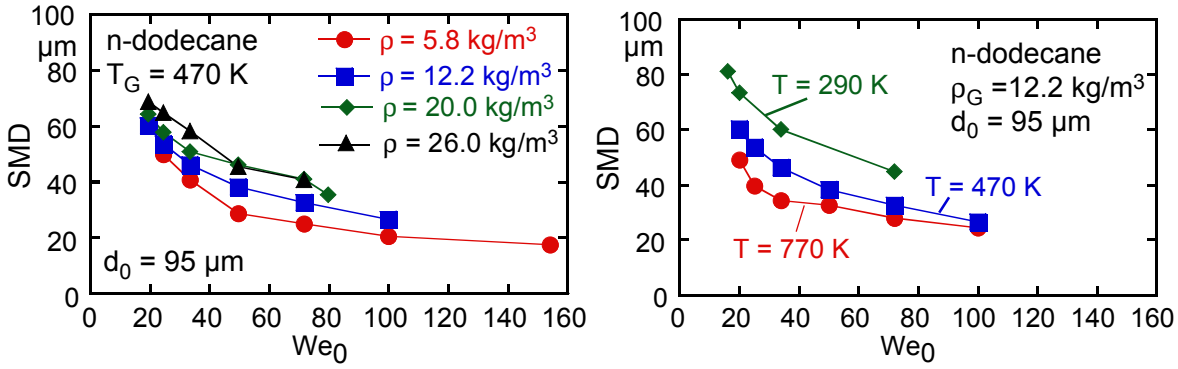

Figure 4: Influence of gas density and temperature on the Sauter diameter of secondary droplets

droplets did not become critical since they were exposed to the high temperatures for a short time only.

The most significant influence of the gas density on the size of the secondary droplets is observed at Weber numbers We < 50. At these Weber numbers bag-break-up takes place, as sketched below in figure 5. At higher gas densities the acceleration of the droplets will be faster, thus the time available for the droplets to break-up is shorter. As a consequence no bag will be formed and the break-up will be different as it can be seen from figure 2b. This explanation has been confirmed by numerical simulations using a Volume-Of-Fluid (VOF) method reported by Reichelt et al. [10].

3 Numerical simulation

The Euler/Lagrange method is used for the simulation of the two phase flow. The calculations were made using the finite volume code FLUENT 4.4.8 [3] which has been extended by various models for the simulation of fuel including real gas effects, droplet break-up and coalescence and models for the primary break-up of fuel sprays [7,11]. The calculations were performed on a 3D structured mesh with 36 × 41 × 22 cells. The size of the cells in the region where the break-up takes place is 220 µm, so that the length of a cell is about 2.2 times the diameter of the primary droplets.

3.1 Break-up models

Different models taken from the literature have been evaluated and compared to experimental results. The Taylor-Analogy-Breakup (TAB) model by O'Rourke and Amsden [1] calculates the break-up from an analogy between a droplet and a spring-mass-system. From the analogy the deformation of the droplets is determined for each time step. Break-up occurs if the deformation becomes larger than the droplets radius. The size of the secondary droplets can be found from an energy balance. Due to this analogy it is expected that the agreement will be good only for small Weber numbers. At higher Weber numbers bag- and shear break-up occur. The drag coefficients are calculated taking the droplet deformation into account.

The Wave-breakup Model by Reitz [2] is based on an analysis of instabilities at the droplet surface. From a numerical solution of the instability equations he derived

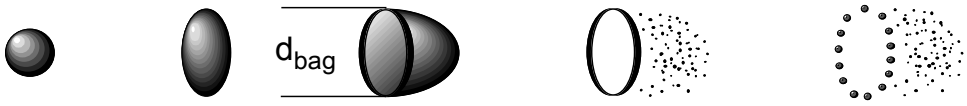

Figure 5: Bag break-up according to Pilch and Erdmann [6]

correlations for the wavelength Λ of the fastest growing disturbance and its growth rate as a function of the Weber and Ohnesorge number. The size of the secondary droplets is assumed to be proportional to the wavelength Λ. Since instabilities only occur at high relative velocities between the droplet and the gas, the Wave model will behave well for high Weber numbers. Both the TAB-model and the wave-model are implemented in various commercial CFD codes, e.g. KIVA[12], FIRE, FLUENT 6.0[13].

3.2 New break-up model

The calculations presented below in section 3.3 showed that the agreement between the simulations and the experiments is very poor for Weber numbers We < 60. For these Weber numbers a strong effect of the gas density on the break-up is observed. Chou and Faeth [14] conducted experiments on the break-up of single droplets in a shock-tube and provide very detailed data on the temporal evolution of the break-up. Based on these experimental data a new break-up model has been developed.

As long as the droplets do not break-up their deformation and drag coefficient are calculated using the TAB-model. If the deformation reaches the critical value for break-up the droplets are treated differently depending on their Weber number. For high Weber numbers the Wave-model is applied. For low Weber numbers the diameter of the rim of the bag (see fig. 5) is calculated from a correlation given by Chou and Faeth. Since the SMD of the droplets is mainly affected by large droplets, the contribution of the bag to the secondary droplets is neglected and the complete mass of the droplet is assumed to be in the rim.

As the diameter of the rim increases it will become thinner and finally break-up due to instabilities. Chou and Faeth [14] reported an equation to calculate the diameter of the secondary droplets d_S from the diameter of the rim. The break-up ends either if a characteristic time reported by Chou and Faeth has elapsed or if the relative velocity between the droplet and the surrounding gas vanishes. The equations necessary to calculate the diameter of the secondary droplets is given below in equation 2. The time t is taken from the beginning of the actual break-up, i.e. from the time when the droplets deformation becomes larger than its radius. ρ_L and ρ_G denote the density of the liquid and gaseous phase, respectively, and d_0 the initial diameter of the droplet.

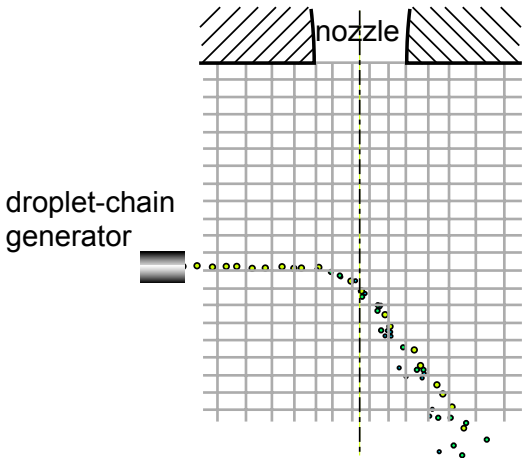

Figure 6: Sketch of the computational grid and the droplet break-up

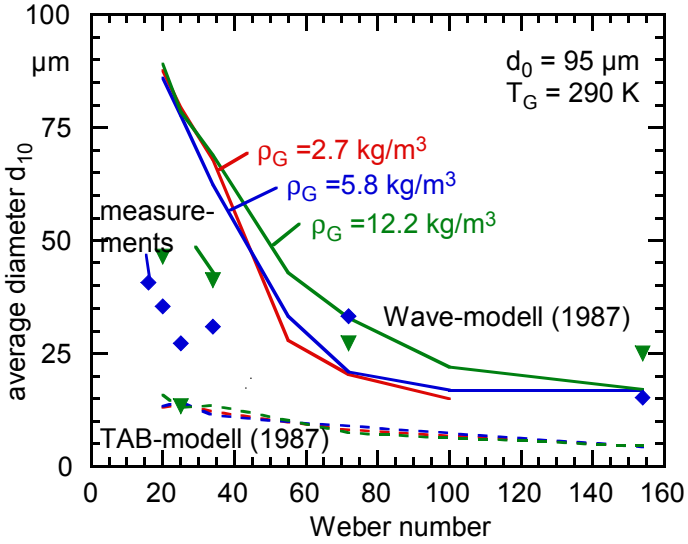

Figure 7: Comparison of experimental and numerical results using various break-up models

$$\tau \equiv \frac{t \cdot u_0}{d_0}\sqrt{\frac{\rho_G}{\rho_L}}$$
$$d^* = \frac{d_{bag}}{d_0} = \begin{cases} 1 + 0.5\tau & 0 \le \tau < 2 \\ 0.25\tau^2 - 0.18\tau + 1.43 & 2 \le \tau < 4 \end{cases} \qquad (2)$$
$$\frac{d_S}{d_0} = \frac{0.86}{\sqrt{d^*}}$$

3.3 Results and discussion

Numerical simulations of the break-up were carried out implementing boundary conditions comparable to the experiments. To get statistically significant results the break-up of up to 1000 droplets was simulated. The size of the secondary droplets was sampled at the same positions where the measurements were taken, i. e. 4 mm downstream of the droplet chain. Figure 7 shows a comparison of the experimental data with the numerical results. All models predict smaller secondary droplets as the Weber number increases, but both the TAB-model and the Wave model do not predict the influence of the gas-density on the mean diameter correctly. As expected the Wave model shows good agreement for larger Weber numbers whereas the behaviour of TAB-model is poor throughout the whole range of Weber numbers.

In figure 8 a comparison of experimental and numerical results using the new break-up model is shown. The new model predicts slightly too large droplets compared to experiments, but it can reproduce the effect of the gas density on the size of the break-up products for Weber numbers above 40. The too high value for the Sauter diameter is probably due to the assumption that the complete mass of the droplets is in the rim. In future work efforts will be made to improve the performance of the new model.

3.4 Application to spray simulations

PDA-measurements of diesel sprays at engine like conditions by Meingast et al. [15] have shown that 20 mm downstream of the nozzle the velocities of all droplets detected at a given

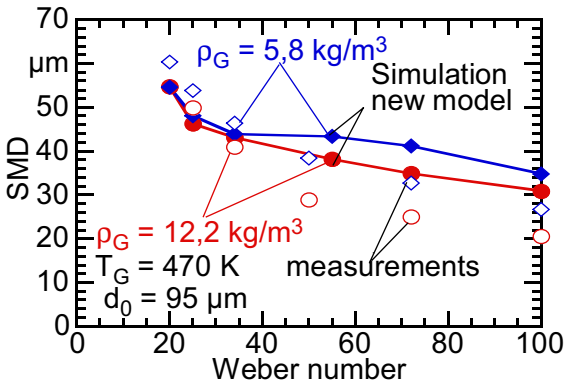

Figure 8: Comparison of experimental and numerical results using the new break-up model

position are almost identical. Since very small droplets reach nearly the velocity of the gas the relative velocity between the gas and the droplets is small. Thus break-up within the spray will only occur at low Weber numbers, so a model for the low Weber number regime is essential to predict fuel sprays accurately. Simulations of fuel sprays using the new break-up model also showed good agreement to the experimental data [16]. Thus the new model is useful for two phase flows where the concentration of the dispersed phase is as low as in the experiments presented here as well as for flows with a very high concentration of the secondary phase.

4 Conclusion

Measurements of the aerodynamic break-up of liquid droplets have been made at engine-like conditions. The results show that the gas density has an significant effect on the size of the secondary droplets especially at low Weber numbers. To account for this effect a new break-up model has been developed based on data found in literature. Computations made using this new model show satisfactory agreement with the measured data. The new model does not require more computational time compared to the Wave model and is suited for dense and dilute two phase flows.

5 Acknowledgements

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