Modelling of turbulent atomisation with an Euler/Euler approach including the drop size prediction

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The aim of this project is the numerical calculation of the turbulent atomisation of liquids. For this a combined model will be used. The flow inside the nozzle and in the dense spray region is predicted using a two-fluid model. The dilute spray region will be calculated using an Euler/Lagrange approach. The required inlet data will be obtained from the two-fluid calculations, namely, gas and liquid velocities as well as the droplet concentration. Additionally, the droplet size distribution has to be predicted. The model used for the calculation of the drop size distribution is introduced and the results are compared with various experimental data. Further, the definition of the transfer boundary between both approaches is discussed. In the last part of this paper the in-house experimental facility and the performed measurements are described.

1. Introduction

Atomisation of fluids as well as the use of sprays is widespread in many industrial applications. This means, however, that very different requirements have to be fulfilled which are realised by different types of nozzles and operating conditions. Numerous experimental investigations of different atomiser types appeared in the literature during the last years [10], [16]. That is the reason why for many atomisers and working conditions empirical equations exist to calculate the main parameters, such as the characteristic droplet diameters. On the other hand, more and more analytical and numerical studies were carried out. Nevertheless, a complete theoretical description of the spraying process and especially of the dense spray region is not available up to now.
In the present study a new approach for the numerical prediction of atomisation and spray characteristics is developed. For the numerical calculation of the flow inside the nozzle and the atomisation a two-fluid approach is adopted which provides the droplet volume fraction and the velocities of droplets and air at the end of the dense spray region. The resulting droplet size distribution is predicted using a structure function approach. These data are used as inlet conditions for the Euler/Lagrange approach, which is more suitable to predict the spray propagation.

2. Modelling

2.1. General considerations

The Euler/Euler approach (also called two-fluid model) is widely used for predicting two-phase flows with high volume fractions. The advantage of this method lies in the use of similar equations for both phases. Therefore, this approach may be also applied for the numerical calculation of the atomisation of liquids, namely the flow inside the spray nozzle and in the dense spray region. Velocities and volume fractions of both phases can be obtained as output parameters. However, for nearly all technical applications knowledge of these parameters is not sufficient. At least the mean diameter of the spray (better the drop size distribution) should also be the result of the computation. Besides, the use of the Euler/Euler approach is not very well suited for the far spray region because here the droplet size distribution is of great importance. Therefore, the use of the Euler/Lagrange approach is much more promising in this region [14]. Hence, the development of a combined Euler/Euler Euler/Lagrange approach for the dense and dilute spray region, respectively, is the final objective of this project. To achieve this, the drop size distribution has to be predicted using the inlet variables, geometrical parameters and calculated results from the dense spray region.

2.2. Two-fluid model

A two-fluid model is used for calculation of the flow inside an atomiser nozzle and in the dense spray region. Reproduction of various nozzle geometries (pressure nozzles, air-blast atomisers etc.) is possible with this model. The programme package ELSA22 (Eulerian Lagrangian Solution Algorithm, 2 phases, 2 dimensional) is used for the calculation. Two-dimensional, axisymmetric calculations can be carried out with this tool. Turbulence of both phases is modelled using a k-ε turbulence model. Interactions between both phases are considered. A detailed description of the model is given in [12].

2.3. Prediction of drop size distribution

As explained before, the velocities and volume fractions of both phases – the dispersed and the continuous one – are predicted by the two-fluid model. These properties are, however, not sufficient for characterising the spray. Therefore, the prediction of a size parameter (the Sauter mean diameter or better the complete drop size distribution) is absolutely necessary for a better comparability with experimental data and coupling with the Euler/Lagrange approach. That is the reason why a model for the drop size distribution has to be used and implemented into the aforementioned code.

In general, there are two different possibilities for predicting the drop size distribution: experimental analyses and theoretical models. In the first case, a drop size distribution is measured for the considered nozzle type. The data can be reproduced by a distribution function (log-normal, Rosin-Rammler etc.) with empirically obtained parameters. Mostly, these parameters are calculated by similarity numbers comprising the inlet conditions and geometrical parameters.

Stability analyses and the maximum entropy formalism (MEF) belong to the second possibility. Stability analyses are used for calculation of the diameter after primary break-up. Having this diameter, a decay process (secondary break-up) is modelled and calculated to yield the final size distribution. A very promising approach is the use of the so-called maximum entropy formalism (MEF). This approach requires, however, the knowledge of a characteristic mean diameter (see e.g. [2]). Then the most probable distribution function can be calculated with the MEF. Therefore, this method is founded on a physical basis.

Another model is used in the present project. It originates from a work of Hartmann [7]. Using the maximum entropy approach, functions for drop size and volume distribution are obtained. In contrary to other MEF models (cf. [2], [3] and [6]) no mean diameter has to be provided as input parameter. The Sauter mean diameter and the drop size distribution are calculated iteratively using only known geometrical information and operating conditions. This is done assuming a structure formation process which is a function of the critical Weber number. There are three slightly varying functions differing in the number of drops in each class and in the function of the critical Weber number describing the number of classes formed. The general form for the calculation of the Sauter mean diameter d_{32} is [7]

$$\frac{d_{32}}{D} = \frac{\frac{C_1}{We} + C_2 \sum_{i=2}^{n} f(i)\left(\frac{1}{K_i} - \frac{1}{We}\right)}{\left(\frac{C_1}{We}\right)^{\frac{2}{3}} + \sum_{i=2}^{n} f(i)\left[C_2\left(\frac{1}{K_i} - \frac{1}{We}\right)\right]^{\frac{2}{3}}} \tag{1}$$

with $K_i = f(i, We_{crit})$ and $n = \frac{We}{K_i}$, (2)

where D is the nozzle exit diameter, i the counting variable, C_1 and C_2 are constants. $We_{crit} \approx 335$ is the critical Weber number, which arises from the equations describing the structure formation process for a three dimensional structure. We is the actual Weber number defined as

$$We = \frac{\rho \cdot d_{32} \cdot v^2}{\sigma} \tag{3}$$

with σ as surface tension, ρ as density and v as a characteristic velocity (the liquid velocity for pressure nozzles, the relative velocity for air-blast atomisers). Because of this definition equation (1) has to be solved iteratively to obtain the Sauter mean diameter. Additionally, the droplet number and droplet volume distribution of the spray considered can be obtained. They result from the calculated volumes and numbers of droplets at each structure level, i.e. in each class. As the equations show, the number of droplet classes formed depends only on the nozzle diameter and the operation conditions. Between 10 to 80 droplet classes were created for the cases studied so far.

Table 1: Comparison of the three different equations predicting the Sauter mean diameter d_{32}

	model equation I	model equation II	model equation III
number of newly formed droplets at each level (class)	n	1 (n = 1) $2 \cdot n - 2$ (n > 1)	2^{n-1}
Weber number for formation of a new structure	$335 \cdot n$	$670 \cdot n$	$335 \cdot 2^{n-1}$

Details of the aforementioned three different functions are given in Table 1, where n is a natural number. The table has to be read in the following way using equation I as an example: n is calculated using equation (2). It represents the level or class number. All droplets can be formed with equal probability up to this level. This means, the drop size distribution will consist of one droplet in class one, two droplets in class two up to n droplets in class n. All these differently sized droplets are also considered for the calculation of the Sauter mean diameter. The same can be done for the other two model equations, which can be understood as different drop formation processes. With this information it can be easily seen that the first line of Table 1 gives the values for f(i) in equation (1) and the second line the values for K_i in equation (2) for n larger than 1.

2.4. Possible couplings between the two-fluid model and the Euler/Lagrange approach

The complete model will describe the spray starting inside the nozzle up to the dilute spray region very far from it. The two-fluid model including the prediction of the drop size distribution is used for the first part and the Euler/Lagrange method for the second one. The coupling between these two model approaches is a decisive part of the whole model. That is the reason why its realisation is the main part of the current work.

There are different possibilities how this coupling can be done. First of all a simple geometrical transfer boundary is imaginable. It would be located in a certain distance from the nozzle and can

also be defined as a function of the radial coordinate in order to account for the liquid core and the disruption of the jet from outside as it is the case e.g. for air-blast atomisers. Although this condition is easy to handle, it will not be used because of a number of disadvantages. As one can imagine, this boundary depends on nozzle geometry and operation conditions like liquid properties and relative velocity. This means, the boundary has to be adjusted for each case considered.
The local volume fraction of the liquid offers another possibility for the determination of the transfer boundary. Using it, one can define a fixed value at which the liquid jet is considered to be atomised and where the model predicting the drop size distribution will be used. This boundary is independent of the nozzle geometry and experimental conditions. However, since no interface reconstruction algorithm (e.g. volume of fluid, VOF) is intended to be implemented, this approach would require relatively fine grids in order to limit the smearing of the interface. Nevertheless, the predicted break-up boundary would remain to be dependent on the grid resolution. This can be seen clearly in Fig. 1 were a schematics of a non-atomised jet is shown. The solid lines represent the real jet boundaries. The two-fluid model, however, would predict liquid volume fractions smaller than 1 in all hatched areas and therefore an earlier break-up of the jet than it occurs in reality. Actually, an approach is tested using the local value of liquid volume fraction as well as its gradient to avoid the previously named disadvantages.

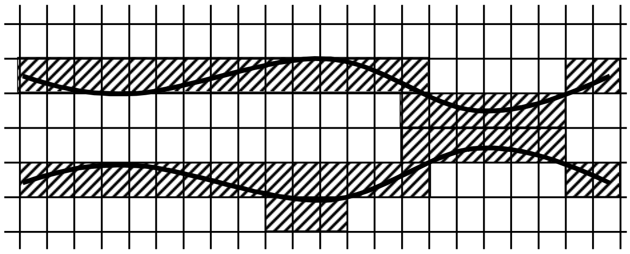

Fig. 1: Schematics of the numerical resolution of a non-atomised jet

3. Numerical results for model validation

3.1. Results of the two-fluid model

In a first step the whole spray region was calculated using the two-fluid model. The results were compared with experimental data of two different authors [1], [9]. Both of them investigated air-blast atomisers under ambient conditions and used water and air as working fluids. The experimental data from Scholz et al. [15] for a slit nozzle were used for the validation of the flow inside the nozzle.

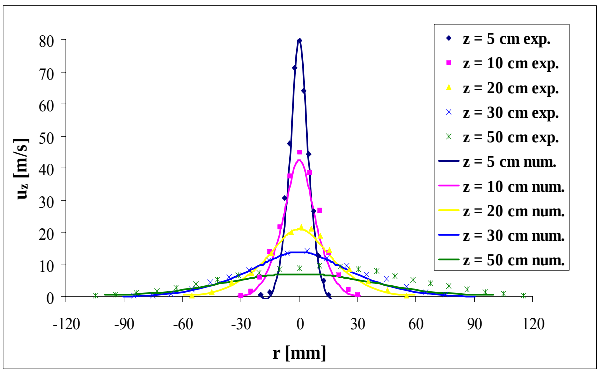

Fig. 2: Calculated radial profiles of axial gas phase velocity compared with experimental data of Bulzan et al. [1]

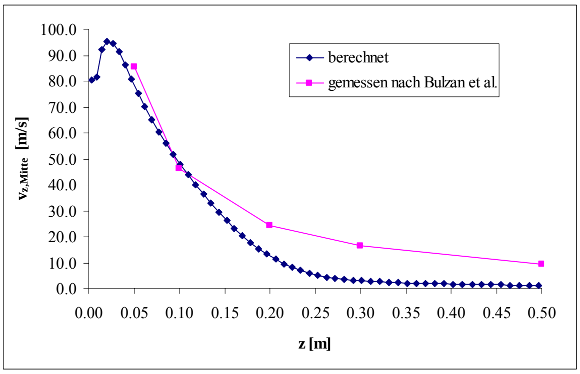

Fig. 3: Calculated axial liquid velocity at the spray axis as a function of the distance from the nozzle compared with experimental data of Bulzan et al. [1]

Numerical results of the two-fluid model were presented in detail previously [11], [12]. That is the reason why only a short overview is given here. The results for the liquid and gas velocity for the measurements of Bulzan et al. [1] are shown in Fig. 2 and Fig. 3 as an example. The agreement between experimental and numerical data is reasonably good. The data of Scholz et al. [15] measured inside the slit nozzle are also very well reproduced (cf. [11]).

3.2. Calculated drop size distributions

The model predicting droplet size distributions was tested for different conditions for further validation. Several data from literature were used for the assessment of the calculated Sauter mean diameter. A comparison of numerical and experimental data is presented in Fig. 4 showing a reasonable good agreement. The measurements as well as the results of the calculations have the same order of magnitude. The slope of the lines, however, is not the same. A reason for this is the fact that very different atomisers were considered. Besides, already the empirical correlations found in the literature have very different slopes.

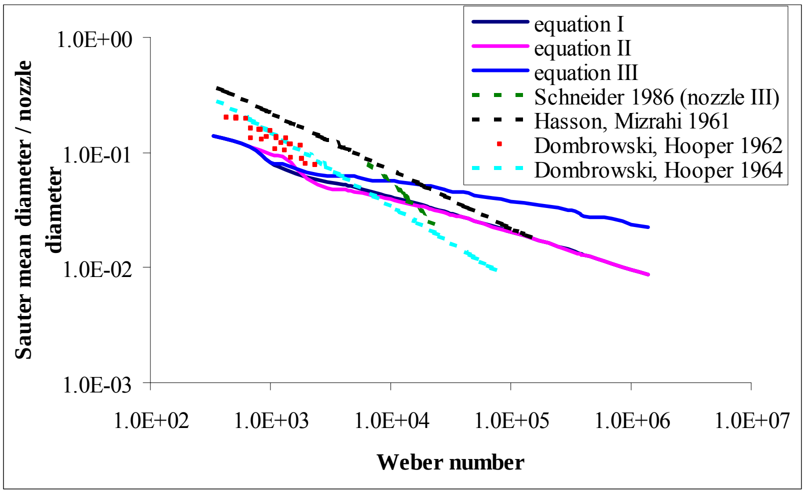

Fig. 4: Normalised Sauter mean diameter as a function of Weber number

As said before, not only the prediction of the Sauter mean diameter is necessary for coupling the two model approaches. That is the reason why the drop size distribution for the experimental cases calculated with the two-fluid model was also determined. The calculated droplet number distribution and its cumulative curve in comparison with the experimental data of Karl et al. [9] are given in Fig. 5 and Fig. 6. Three measured cumulative number distributions for different distances from the nozzle exit (X/D) are shown in Fig. 6. The differences between them are small, only a higher amount of small droplets can be observed for the distribution nearest to the nozzle exit. In the far field of the nozzle some of these small drops disappear due to coalescence. Additionally, three curves calculated with different combinations of the drop size prediction equations are shown. Ten to twenty different droplet size classes are calculated for the two-fluid nozzle and operation conditions investigated by Karl et al. [9] depending on the model equations used. Agreement between experimental and calculated data is very good. The same shape of the cumulative distribution and the same mean diameter are predicted. Only the existence of larger droplets is somewhat underpredicted. This, however, would improve if droplet collisions were considered as it will be done using the Euler/Lagrange approach for the dilute spray region.
The relative number distribution for the same case is shown Fig. 5. Only the experimental values measured at the nearest distance to the nozzle are given for comparison because effects like coalescence will be included later using the Euler/Lagrange approach. The results of equation I and a combination between model equations I and II are shown. Agreement between measurements and calculations is also good for this representation. Fluctuations in the combined curve appear

due to the facts that only discrete particle classes are formed and that both equations deliver new drops for multiples of 670 (cf. Table 1). Using the Euler/Lagrange approach for further calculations, these fluctuations should be flattened out, i.e. the distribution will become more continuous because of coalescence and further break-up. The interpolated curve, which shows a very good agreement with the measurements, underlines this fact.

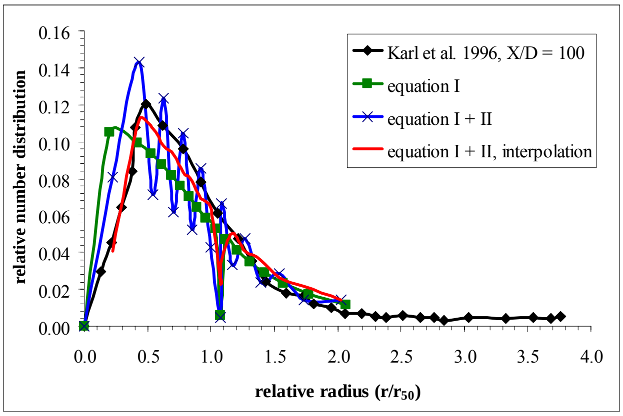

Fig. 5: Calculated droplet number distribution in comparison with experimental data of Karl et al. [9]

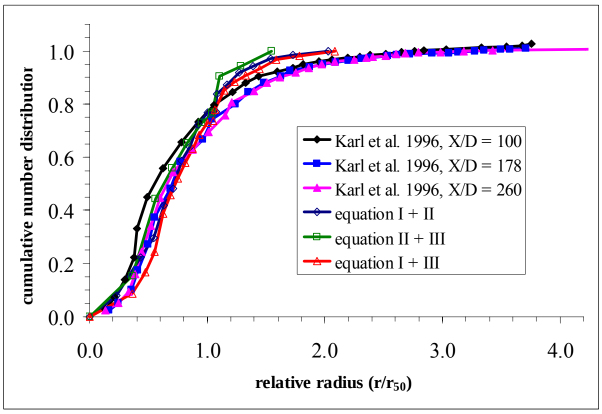

Fig. 6: Calculated cumulative droplet number distribution in comparison with experimental data of Karl et al. [9]

4. Experimental set-up

An experimental facility was built up to obtain more detailed measurements than accessible in literature. They are needed for a further validation of the models. Spray break-up could be visualised using a high speed camera (Ultra 8, DRS Hadland). Besides, measurements of drop size and velocity distributions were possible by applying a phase Doppler anemometer (Dantec). Experimental conditions are given in Table 2.

Table 2: Experimental conditions

nozzles used	pressure atomisers (full cone, hollow cone)
nozzle exit diameters	0.82 – 1.05 mm
ambient pressure	1 bar
injection pressures	5 – 12.5 bar
spray angles	80° (hollow cone); 30°, 45°, 60°, 80° (full cone)
working fluid	water
nozzle exit velocities	3 – 12 m/s

The facility itself (Fig. 7) consists of a spray chamber wherein the nozzle (3) was located. The position of the nozzle could be changed using a traversing system. There was also a suction system (4) installed to produce a low velocity downward flow preventing that small droplets remain in the measuring region for a long time. The liquid was delivered from a storage tank (2) to the nozzle (3) by a pump (1). The pressure was measured directly before the nozzle (6). The measuring system (5) was located on a fixed point outside the spray chamber.

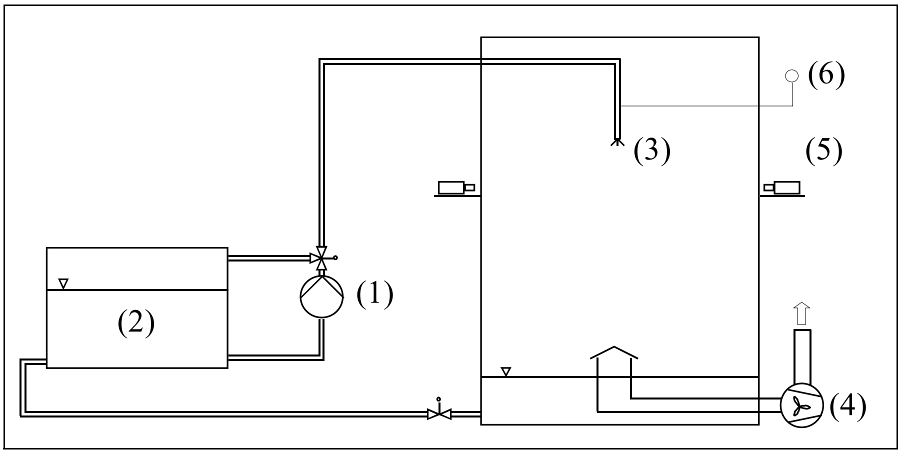

Fig. 7: Experimental facility, (1) pump, (2) storage tank, (3) nozzle, (4) suction system, (5) PDA or high speed camera, (6) pressure gauge

5. Experimental results

Using the previously described test facility, various measurements were carried out. A high speed camera was used to observe break-up behaviour of the sprays. Because of its poor resolution no single droplets could be registered. Therefore, the images were used for determination of the instabilities of the liquid sheet.

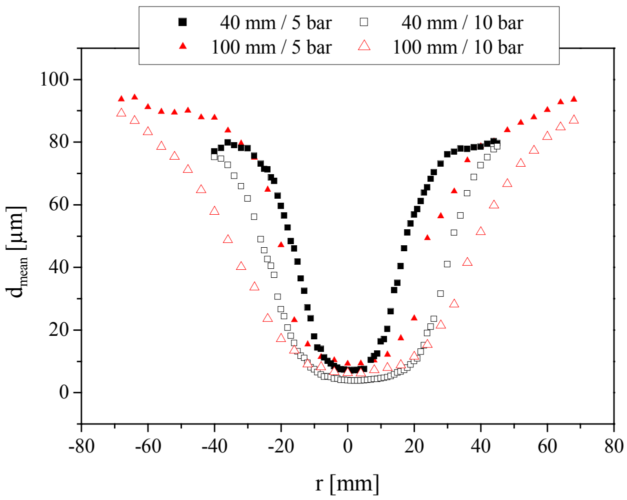

Fig. 8: Radial droplet size distribution for the hollow cone nozzle, different distances from the nozzle, different injection pressures

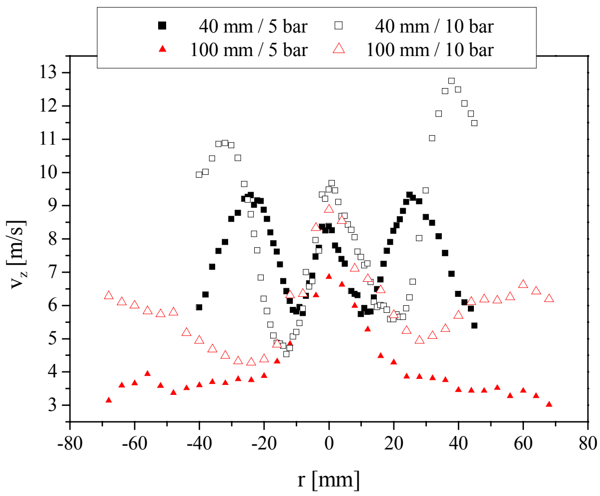

Fig. 9: Radial droplet velocity distribution for the hollow cone nozzle, different distances from the nozzle, different injection pressures

The drop number and drop volume distribution at different distances from the nozzles were measured using phase Doppler anemometry. The results for the hollow cone nozzle are shown in Fig. 8 and Fig. 9 as an example. One can see clearly the shape of the hollow cone spray in both figures. In the inner part, very near to the nozzle axis only small droplets can be found. They have such a small mass and such small Stokes numbers that they closely follow the air flow. That is the reason why in Fig. 9 high velocities in the middle of the hollow cone appear, caused by the air entrained from the environment. Big droplets produced by the decay of the conical liquid sheet can be found in the outer region of the jet. These droplets have a relatively high inertia and move in direction of the spray angle. One can see in both figures that rising the injection pressure leads to an increased spray angle. Besides, the droplet size decreases. This means, atomisation is enhanced because of the higher exit velocity. The positions of the maximum values are shifted outwards with increasing distance from the nozzle. This is due to the spray angle and the expansion of the spray. Fig. 9 shows also a decrease of droplet velocity with increasing distance from the nozzle and decreasing injection pressure. This is caused by deceleration of the drops by the quiescent ambient air. The nozzle exit velocity and therefore also the velocity measured in a certain distance is smaller for lower injection pressures.

6. Summary and further work

Turbulent atomisation of liquids was investigated in the presented work. The two-fluid model used for calculation of the flow inside the nozzle and in the dense spray region was discussed briefly. Afterwards the model for predicting the drop size distribution was explained and possible definitions for the transfer boundary were presented. Both theoretical approaches are necessary for getting a combined model describing the whole atomisation process. Results of the numerical calculations – obtained with the two-fluid model as well as with the model for drop size prediction – were shown and compared with various experimental data. A good agreement could be achieved and the applicability of the models could be proved. Besides, the in-house experimental facility was introduced and results of some measurements were discussed.
Further work comprises the implementation of the drop size prediction model into the numerical code used for two-fluid calculations. Additionally, the coupling between the two-fluid model and the Euler/Lagrange approach has to be established and tested. The results of the complete jet calculation have to be validated against measurements obtained from the in-house facility and from literature. Therefore, the experiments have to be continued, also with other types of nozzles.

7. Acknowledgement

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8. References

[1] Bulzan D L, Levy Y, Aggarwal S K and Chitre S 1992 *Atom. Sprays* **2** 445-62
[2] Cousin J, Yoon S J and Dumouchel C 1996 *Atom. Sprays* **6** 601-22
[3] Dobre M and Bolle L 2001 *ILASS-Europe 2001, Zürich*
[4] Dombrowski N and Hooper P C 1964 *J. Fluid Mech.* **18** 392-400
[5] Dombrowski N and Hooper P C 1962 *Chem. Eng. Sci.* **17** 291-305
[6] Dumouchel C, Sindayihebura D and Bolle L 2002 *ILASS-Europe 2002, Zaragoza* 443-8
[7] Hartmann D 1993 *Theoretische Untersuchungen zur Tropfenbildung bei Dispergierprozessen, Diss.* (Martin-Luther-Universität Halle)
[8] Hasson D and Mizrahi J 1961 *Trans. Inst. Chem. Eng.* **39** 415-22
[9] Karl J-J, Huilier D and Burnage H 1996 *Atom. Sprays* **6** (4) 409-34
[10] Lefebvre A H 1989 *Atomization and Sprays* (New York: Hemisphere Publishing Corporation)
[11] Platzer E and Sommerfeld M 2002 *7. Spray 2002, Freiberg* 41-50
[12] Platzer E and Sommerfeld M 2002 *ILASS-Europe 2002, Zaragoza* 509-14
[13] Schneider M H 1986 *Untersuchungen zum Einfluß der Zerstäubung auf die Verdampfung flüssiger Brennstoffe in turbulenten Sprayflammen, Diss.* (TH Darmstadt)
[14] Rüger M, Hohmann S, Sommerfeld M and Kohnen G 2000 *Atom. Sprays* **10** 47-81
[15] Scholz J, Brandt K and Beushausen V 2001 *6. Spray 2001, Hamburg* IV.2.1-IV.2.8
[16] Walzel P 1990 *Chem. Ing. Techn.* **62** (12) 983-94