MODELLING OF SPRAY ATOMISATION AND DISPERSION

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ABSTRACT

The present paper describes a model combining a two-fluid method and an Euler/Lagrange approach to calculate the liquid atomisation from the flow inside the nozzle up to the dilute spray region far away from the nozzle exit. Additionally, a drop size distribution model is used. In the first part, a short overview of the method is given. Special emphasis lies on the coalescence model for the Lagrangian part and on the coupling between the two different approaches. Experimental data from the literature and measurements carried out at an in-house test facility were used for the validation of the numerical computations. The influence of the consideration of the coalescence in the Lagrangian part of the model was discussed. Besides, the results obtained with the fully coupled model were compared to those obtained when the two-fluid model was used for the calculation of the whole atomisation region.

INTRODUCTION

The atomisation of liquids is subject of scientific research for many decades now. Although there exist many experimental investigations for very different operational conditions and working fluids, the theoretical description of the atomisation process and especially of the dense spray region is not completed up to now. During the last years and because of the fast development of the computational fluid dynamics, the insight into these processes increased significantly. Nevertheless, many questions remain open and a complete, universal description of the whole atomisation process including the dilute spray is still impossible.

MODELLING

Overview of the model

In the present paper a combined model is presented for predicting the whole atomisation process. This includes the prediction of the flow inside the nozzle, the atomisation, the behaviour in the dense spray region, and the dilute spray far from the nozzle exit. Different methods are used for the different regions. The flow inside the nozzle is assumed to be a single phase flow. It is calculated using the Eulerian approach which considers the fluid as a continuous phase moving through a fixed coordinate system. For the atomisation and in the dense spray region a two-fluid model is used. This means the Eulerian approach is extended to both phases which are both considered as continuous fluids. The results of these calculations are the velocities and the volume fractions of both phases at the end of the dense spray region. There, a transfer boundary is defined since the results serve as input parameters for the Euler/Lagrange approach. This method is used for the description of the dilute spray region farther away from the nozzle exit where the strict conditions of the dense spray are no longer valid. The Lagrangian approach is applied for the disperse phase. However, the data obtained by the two-fluid model are not sufficient to establish the coupling. A very important characteristics of the spray – the drop size distribution resulting from the atomisation – must also be known. Therefore, a structure function approach is combined with the two-fluid model. This approach is based on a kind of maximum entropy formalism (MEF) and provides the Sauter mean diameter of the spray as well as the droplet volume and the number distribution [1].

Two-fluid model

All computations were carried out with the in-house program package ELSA22 (Eulerian Lagrangian Solution Algorithm, 2 phases, 2 dimensional). This code allows two-dimensional calculations in cartesian and cylindrical coordinates. It is based on the finite volume approach [2] and the solution of the Reynolds-averaged conservation equations. It was extended by the equations of the Eulerian approach for the second phase that are similar to those of the continuous phase. The well known k-e turbulence model is used for both phases. The interaction terms were considered only for the momentum equations. It is assumed that only drag and gravity act on the droplets in the dense spray region. The complete modelling equations used for the stationary, rotational symmetric case without mass transfer are given in a previous publication [3].

Euler/Lagrange approach

In contrary to the two-fluid model, the treatment of both phases is different when the Euler/Lagrange approach is used. The continuous phase is solved at a fixed coordinate system (Euler approach) whereas the particles are tracked through the flow field. Both phases are coupled by interaction terms. An extensive overview of this method is given in [4]. The same equations for isothermal conditions and without evaporation are used here.

The calculation of collisions and possible coalescence is an important part of the Euler/Lagrange approach [4]. In the stochastic collision approach it is not necessary to track all particles simultaneously as this must be done for a deterministic method [5]. Instead of this, the droplets are tracked sequentially and possible collision partners are generated by sampling its properties from the local statistical distribution functions calculated in the previous time step. A collision will occur, if both droplets – the real and the fictitious one – are located inside a collision cylinder. This yields the following definition of the collision probability [4]

$$p_{coll} = 0.25 \cdot p\left(d_1 + d_2\right)^2 \frac{N_2}{Vol}\left|v_{rel}\right| Dt \quad . \tag{1}$$

If a random number between zero and one is smaller than p_{coll}, a collision will occur. Then, two possible collision modes can take place: permanent coalescence and grazing collision leading to one or two droplets after the collision, respectively. The decision which collision mode occurs is made using the classical model of Brazier-Smith [6]. They define the critical collision angle as

$$F_{crit} = min\left(arcsin\left(\sqrt{\frac{s\,e}{d_2\, r_d v_{rel}^2}}\right); \frac{p}{2}\right) \quad \text{with} \tag{2}$$

$$e = \frac{4.8\left(1+\left[\frac{d_1}{d_2}\right]^2 - \left(1+\left[\frac{d_1}{d_2}\right]^3\right)^{\frac{2}{3}}\right)\left(1+\left[\frac{d_1}{d_2}\right]^3\right)^{\frac{11}{3}}}{\left[\frac{d_1}{d_2}\right]^6\left(1+\frac{d_1}{d_2}\right)^2} \quad . \tag{3}$$

The actual collision angle F is a result of the stochastic collision model. It is a function of the lateral displacement between the two droplets – the real and the fictitious one – which itself is a function of two random numbers in the range of [0…1] (cf. [7]). If $F < F_{crit}$ is valid, permanent coalescence will occur. In all other cases a grazing collision will take place. The velocity of the real droplet after a grazing collision is given according to [4]

$$v_{ac} = \frac{v_{1,i}m_1 + v_{2,i}m_2 + m_2\left(v_{1,i} - v_{2,i}\right)\frac{sinF - sinF_{crit}}{1 - sinF_{crit}}}{m_1 + m_2} \quad . \tag{4}$$

It is smaller than the velocity before the collision due to energy dissipation. The direction of the droplet motion, however, remains the same. The droplet velocity and the diameter after coalescence are calculated according to [4] using Eqs. (5) and (6)

$$v_{ac} = \frac{v_{1,i}m_1 + v_{2,i}m_2}{m_1 + m_2} \quad , \tag{5}$$

$$d_{ac} = \sqrt[3]{d_1^3 + d_2^3} \quad . \tag{6}$$

In the case of permanent coalescence, the number distribution has to be updated, too. For this, a trick is used to achieve the droplet mass conservation. If the generated fictitious collision partner has a smaller diameter than the real droplet, the collision event will be valid and the calculation is continued. In the opposite case, the resulting droplet disappears (see [4]).

Prediction of the drop size distribution and coupling between the model approaches

A model originating from Hartmann [8] and the structure formation process proposed by Naue [9] is used in the present work for providing a drop size distribution. Naue [9] assumes that a slowly or not moving fluid is molecularly dispersed, i.e. it consists of fluid molecules which move because of the acting driving forces. If a stability criterion is exceeded, some structures will appear in the fluid. Their length scale is larger than that of the molecular motion, i.e. the mean free path length. These structures can be for instance eddies in a turbulent flow. Their properties differ from those of the unstructured regions. Increasing the total energy of the system leads to the formation of further structures at higher levels which exist additionally to all previously formed ones. Once some structures appeared, the fluid properties are not equally distributed any longer. They differ for regions with different levels of structuring. The motion of the structures (averaged in time and space) is considered in the balance equations. The structure size is a function of the corresponding level. It depends on the momentum and the energy of the whole system. The information entropy first proposed by Shannon [10] is a measure for evaluating this process. It becomes maximum for optimal processes and is a function of the total effort for the structure formation.

The atomisation of a liquid is considered as such a structure formation process. The continuous liquid inside the nozzle is divided in differently sized droplets. Each size class has a different structure level. The total effort for the structure forming process

is calculated with the function given in [9]. The resulting equations when the entropy is maximised are given in [3]. The general equation can be used for the calculation of the Sauter mean diameter. It can be understood as the relation between the micro and the macro length scale or between the forming and the formed volume, respectively. The droplet number and the volume distribution are obtained, too. They result from the calculated volumes and numbers of the droplets at each structure level, i.e. in each size class. One assumes that all droplet classes exist with the same probability up to the computed structure level. This leads to a distribution function. Since the drop size distribution is calculated using only known geometrical information and operation conditions, no mean diameter has to be provided as input parameter. This is a big advantage over other MEF models [11, 12]. Hartmann [8] gives also three slightly varying cases that are further explained in [3]. They can be taken as different drop formation mechanisms. It is possible to use combinations of two cases. For this, the different forms of the general model equation are multiplied by two factors between zero and one giving one when added. These new forms are added to yield the combined Sauter mean diameter.

Having the results of the two-fluid model and the drop size distribution, a transfer boundary between the two different approaches has to be defined. At this boundary, the variables of the liquid phase obtained in the dense spray region have to be transferred into the Lagrangian frame of reference. The transfer boundary is found by checking the actual values of the volume fraction of the liquid phase in each control volume. If a certain value is reached, the jet will be considered as atomised, i.e. only drops exist. Besides, it has to be assured that atomisation occurs for the considered case. For this, a criterion depending on similarity numbers was used [13]. With this, the behaviour of liquid jets can be assigned to three regimes: the Rayleigh break-up, the sinuous wave break-up and atomisation. The Reynolds number $Re = \frac{vDr_d}{h}$ and the Ohnesorge number $Oh = \frac{h}{\sqrt{r_d s\ D}}$ are used for characterising these regimes. The boundary between the sinuous wave break-up and the atomisation region is important for this study. Only if it is exceeded, atomisation will occur. It is given as

$$Oh = 100 \cdot Re^{-0.92} \quad . \tag{7}$$

RESULTS OF THE NUMERICAL CALCULATIONS

Different experimental data were used for the validation of the numerical calculations. The measurements of Karl et al. [14] made at an air-blast atomiser were considered first. The authors give the experimentally obtained values of the liquid and the gas phase velocity for different experimental conditions. Additionally, the drop size distributions are presented. Because the nozzle geometry is complex and difficult to reproduce with numerical grids, own measurements were carried out using pressure nozzles with and without swirl. The flow in the whole region of atomisation starting from the single phase flow inside the nozzle up to the dilute spray region far away from the nozzle exit can be computed for these geometries.

Influence of the coalescence

The influence of the coalescence was analysed to assess the Lagrangian method. For this, the spray behaviour far away from the nozzle exit was calculated using the Euler/Lagrange approach. Measurements made at the in-house test facility provide the experimental data for the validation of the calculations and the input parameters at the beginning of the dilute spray region. A commercial full cone pressure swirl atomiser with a spray angle of 60° was used at first. It was operated at 5 bar. The resulting radial profiles of the axial drop velocity are compared to the measured ones in Fig. 1. The profiles 40 mm away from the nozzle exit are given. The agreement between the measurements and the calculations is very good near the spray axis. The spreading of the jet, however, is underestimated by the numerical computations.

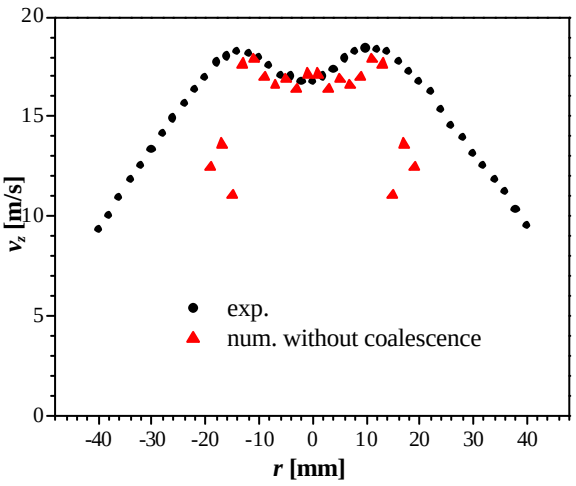

Fig. 1 Comparison of the calculated and the measured radial profiles of the axial drop velocity of a pressure swirl atomiser (60° cone angle, 40 mm from the nozzle exit); calculations with the Euler/Lagrange approach

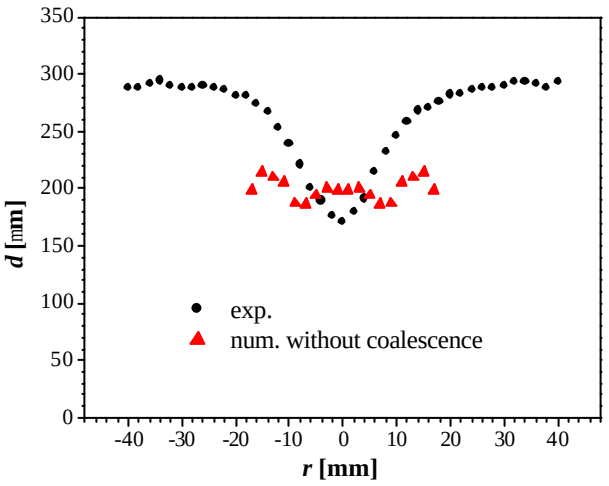

Fig. 2 Comparison of the calculated and the measured radial profiles of the mean drop diameter of a pressure swirl atomiser (60° cone angle, 40 mm from the nozzle exit); calculations with the Euler/Lagrange approach

The comparison of the radial distribution of the mean droplet diameter is shown in Fig. 2. The measurements give a minimum value at the spray axis and an increase of the drop size towards the outer edges of the spray. At the spray axis the numerical calculations give nearly the same value as the measurements. The increase of the drop diameter towards the spray edges, however, is underestimated and only a slight maximum can be seen. The agreement will improve, if the droplet collisions and coalescence is considered. To demonstrate this, the comparison of the radial distribution of the mean droplet diameter for another pressure swirl atomiser (45° cone angle) is shown in Fig. 3. In this case, the measurements predict a slight maximum of the drop size at the spray axis. This behaviour will not be reproduced, if the computations are carried out without consideration of droplet coalescence. If this effect is taken into account, the agreement is much better. It is clear, however, that the asymmetry of the measurements cannot be reproduced by the two-dimensional calculations.

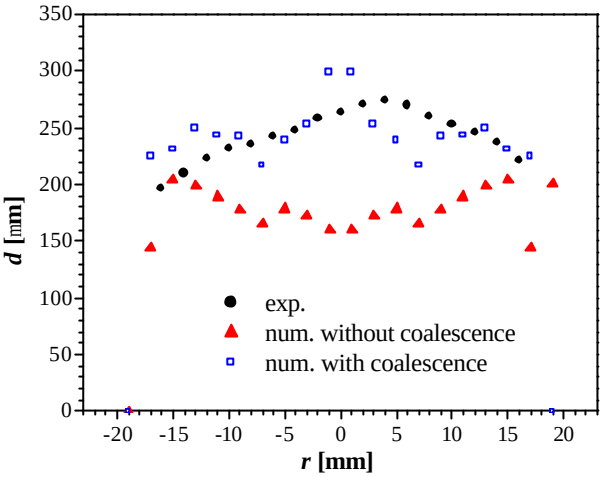

Fig. 3 Comparison of the calculated and the measured radial profiles of the mean drop diameter of a pressure swirl atomiser (45° cone angle, 40 mm from the nozzle exit); calculations with the Euler/Lagrange approach

Results of the fully coupled model

At the beginning of this project the two-fluid model was used to calculate the entire spray. The corresponding results of these computations were discussed extensively in previous publications [3, 15]. The agreement between the measured and the calculated values for the gas phase velocity was very good, already for this method. The liquid phase velocity, however, was only poorly predicted by the computations. This can be seen in Fig. 4, where the numerical results obtained with the two-fluid model are compared to the experimental data of Karl et al. [14].

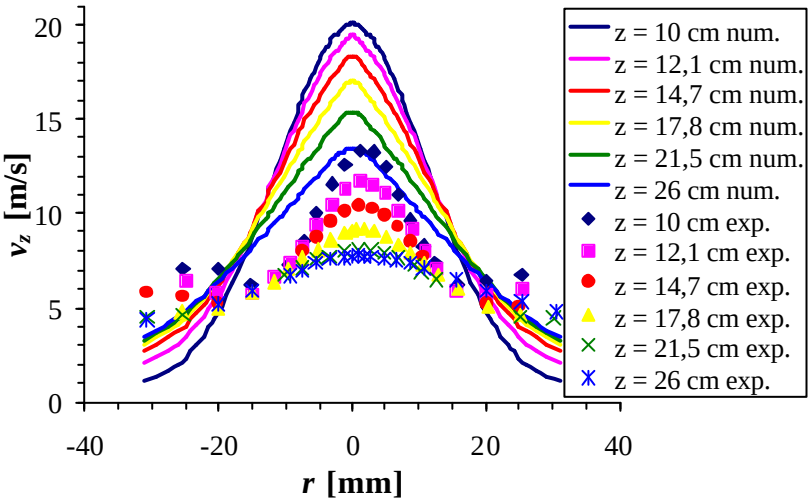

Fig. 4 Radial profiles of the axial liquid phase velocity at different distances from the nozzle exit, experimental data of Karl et al. [14] vs. numerical calculations with the two-fluid model

To enhance this prediction of the liquid phase velocity, the coupled model was applied now. It has the big advantage that no initial drop size distribution function has to be known at the beginning of the calculation and provided as input. In contrary to this, the actual distribution function for the considered case is calculated by the drop size prediction model. This information as well as the velocities and the volume fractions computed in the dense spray region by the two-fluid model serve as input parameters for the coupled Euler/Lagrange approach. Behind the transfer boundary, the liquid phase is tracked as parcels that move through the gas flow field. The velocity of the liquid phase in each control volume is obtained by statistical averaging of the velocities of all parcels that crossed this control volume. Hence, the profiles of the liquid velocity at different distances from the nozzle exit can be

determined. These profiles are given in Fig. 5 and compared with the same experimental values as before. As it can be seen, the agreement between the numerical and the experimental data is much better than before. The width of the calculated velocity profiles matches very well with the experiments. The computations with the two-fluid model deliver too high velocities in the core of the spray for all distances from the nozzle exit (cf. Fig. 4). If the coupled model is used, the peak value will be only sligthly overestimated for the profiles closest to the nozzle and slightly underestimated for the profiles at large distances from the nozzle exit. For the behaviour at the edge of the spray the agreement is not so good. As before, all numerical values are smaller than the measured ones. And another point has to be mentioned: The experimental profiles show a slight asymmetry. This behaviour can of course not be reproduced by the two-dimensional calculations, but has to be taken into account in the discussion of the results. The fluctuations in the calculated curves are caused by the relatively small number of tracked parcels (1800 parcels). They will disappear, if a larger number of parcels is used.

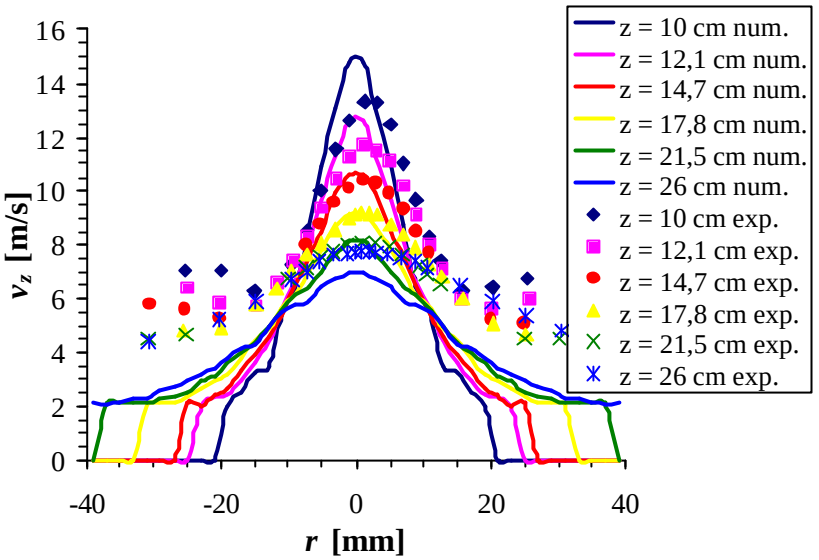

Fig. 5 Radial profiles of the axial liquid phase velocity at different distances from the nozzle exit, experimental data of Karl et al. [14] vs. numerical calculations with the coupled model

SUMMARY AND FURTHER WORK

The present paper describes a model combining a two-fluid method and an Euler/Lagrange approach to calculate the liquid atomisation. In the first part, a short overview of the model is given. Special emphasis lies on the coalescence model for the Lagrangian part and on the coupling between the two different approaches. Experimental data from the literature and measurements carried out at an in-house test facility were used for the validation of the numerical computations. The influence of the consideration of the coalescence in the Lagrangian part of the model was discussed. The results show that the neglection of the coalescence leads to a wrongly predicted spray behaviour. Besides, the results obtained with the fully coupled model were compared to those obtained when the two-fluid model was used for the whole spray. The latter leads to a strong overestimation of the liquid phase velocities, whereas the agreement for the coupled model is much better.

Further work comprises the implementation of a model for the secondary break-up in the Lagrangian part of the model. Different approaches were introduced in a recent paper [16]. These have to be tested and validated against experiments.

NOMENCLATURE

symbol	meaning	unit
d	droplet diameter	m
D	nozzle diameter	m
e	function for the calculation of the critical collision angle	-
m	mass of the droplet	kg
$\frac{N_2}{Vol}$	number density of the smaller droplets in a control volume	$1/m^3$
Oh	Ohnesorge number	-
p_{coll}	collision probability of two droplets	-
r	radial coordinate	mm
Re	Reynolds number	-
Dt	time step	s
v	liquid velocity	m/s
z	axial distance from the nozzle exit	cm
h	dynamic viscosity of the disperse phase	Pa s
r	density	kg/m^3
s	surface tension	N/m

F	collision angle	rad

Indices

1	larger droplet
2	smaller droplet
ac	after the collision
crit	critical
d	disperse phase (droplet)
i	direction of the velocity in the coordinate system
rel	relative
z	axial

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