MODELLING OF TURBULENT ATOMISATION WITH A COMBINED EULER/LAGRANGE EULER/EULER APPROACH: STARTING WITH A TWO-FLUID MODEL IN THE DENSE SPRAY REGION

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Abstract
This paper deals with the numerical calculation of the atomisation of a turbulent round jet. First, an overview of the maximum entropy formalism is given. This approach will be used to predict the drop size distribution. For the calculation of the velocities and the volume fractions of the continuous and the dispersed phase an Euler/Euler method (two-fluid model) is used. The basic equations used for the applied two-fluid formulation are provided. For validation, the calculated results are compared with two sets of experimental data for two fluid atomisers. The agreement is reasonably well and shows the applicability of the model. Further work will include the introduction of the maximum entropy formalism in order to obtain the drop size distribution and, for the second part of the study, the coupling between the two-fluid model and an Euler/Lagrange method for predicting the spray evolution.

Introduction

Two different approaches exist for the numerical simulation of liquid atomisation and spray systems: the Euler/Lagrange and the Euler/Euler method (also called two-fluid model). In both cases the continuous phase is calculated with the Eulerian method. This approach uses a stationary frame of reference and enables the calculation of all field variables in every control volume for every time step. For the dispersed phase the Eulerian (quasi continuous) or the Lagrangian approach (tracking of particle trajectories) are used. The Lagrangian method groups the real particles into numerical parcels consisting of a certain number of droplets having the same properties (size, velocity, ...). These parcels are tracked through the calculation area implying that the frame of reference is moving. Usually this calculation method is applied to describe dilute flows where the volume fraction of the dispersed phase is low enough to allow numerical calculation.

If the volume fraction of the dispersed phase is high and interfaces exist in the flow domain as it is the case in the dense spray region very near an atomiser nozzle, the Euler/Lagrange method is not applicable. For this region the two-fluid model is used which yields good solutions in areas where two separate fluids or very dense mixtures can be found. Using this approach similar conservation equations for both phases and an additional relation for the volume fraction of one phase are solved. An important parameter, however, can not be predicted with the Euler/Euler method: the droplet size distribution. But, it is necessary for judging the performance of different atomisers. In some recent publications (v. Berg et al. [2], Tomiyama [13]) a modified two-fluid model can be found. There the conservation equations are solved not only for each phase but for the continuous phase and each droplet size fraction. A disadvantage of this method is that the number of equations to be solved dramatically increases when the droplet size distribution becomes wider and therefore the number of droplet size classes increases. This is the reason why in the present study the particle size distribution will be predicted using a maximum entropy formalism. The droplet size distribution, their volume fraction and velocities will be eventually used as inlet conditions for a Lagrangian method which allows a reliable prediction of sprays by accounting for all the relevant physical effects.

The Maximum Entropy Formalism (MEF)

For spray applications it is very important to know the droplet size distribution of the nozzle used. However, up to now in most cases extensive experimental measurements have to be carried out to get this information. A best-fit procedure is then applied to these experimental results to find an analytical probability density function (PDF) describing the spray of this nozzle. Although this method is used very often, it has no physical basis [7].

This is the reason why nowadays many different maximum entropy formalisms are used to predict the size and velocity distributions of the droplets in a spray. Such approaches were initially proposed by Jaynes [8], [9] and have the advantage that the selection of the distribution function is put on a physical basis. This is done in a way that the most probable distribution function is chosen. To get this function all information available about

the process under consideration are taken as constraints. Therefore, if all relevant information are known and considered, a physically reliable distribution function can be obtained.

Beginning from the first papers about the MEF (Jaynes [8], [9]) nowadays more and more publications appear about this topic. A good review of some of the older literature is given by Ahmadi and Sellens [1]. Beside the description of own research the authors provide the equations of the distribution functions of several other working groups. In this review not only size distribution functions but also combined size-velocity distribution functions are considered. However, as shown and proved in [1] it is possible to treat the size distribution independently from the velocity distribution.

Some recent publications come from the working group of Dumouchel (Cousin and Dumouchel [4], [5]; Cousin et al. [6]) and from Dobre and Bolle [7]. The first authors developed two different size distribution functions for the number and volume distributions. As shown in [4], there is a difference between both distributions and this difference (caused by the fact that the volume distribution contains additional information about the particle shape) has to be taken into account during the application of the MEF. If this is done, droplet number and volume distributions consistent with each other can be obtained. The corresponding functions are developed in [4] and it is shown that for the number distribution the Shannon entropy is usable whereas for the volume distribution the Bayes entropy has to be applied. In the second part of their paper [5] the developed equations are used to predict the size distributions of two different pressure atomisers. The Sauter diameter can be used as a good estimate for the theoretically determined drop diameter.

Dobre and Bolle [7] deal with ultrasonic atomisation. They used a combination of the Shannon and the Tsallis entropy to predict the bimodal number distribution. The Shannon entropy in this case provides a good fit for the drops produced by the wave instability mechanism whereas the size of the droplets formed through cavitation effects can be predicted by the Tsallis entropy.

Definitions of Several Entropy Functions

There are several types of entropy functions that can be used in a MEF. Two of them are described by Dobre and Bolle [7]: the Shannon and the Tsallis entropy. The type widest used is the Shannon entropy defined as:

$$S(p_i) = -k_e \sum_{i=1}^{n} p_i \ln p_i \quad , \tag{1}$$

which leads after maximisation with constraints to an exponential distribution. The more general case is the Tsallis entropy, which is given by:

$$T(p_i) = -k_e \left(\frac{1 - \sum_{i=1}^{n} p_i^q}{q-1} \right) , \tag{2}$$

and leads after maximisation to a power law distribution. The Tsallis entropy includes the Shannon entropy as a limiting case because $S(p_i)$ equals $T(p_i)$ if $q = 1$. Both entropies have their maximum value if all events are equally probable ($p_i = 1/n$ for all i) and are minimum when the outcome is certain, that means one event will happen definitely [7].

An extended survey of the possible kinds of entropy formulations can be found in [10]. The author gives a detailed description of the mathematical background and the application of the MEF. Beside the aforementioned two types of entropy functions some additional approaches are described. This is for example the Bayes entropy defined as:

$$B(p_i) = -\left(\sum_{i=0}^{n} p_i \ln \frac{p_i}{\alpha_i} \right) - \ln(\alpha_i)_{min} \quad . \tag{3}$$

This entropy is not a measure of the probability of a certain event (as the other two entropies) but a measure if a previously defined distribution will occur or not. The α_i in equation (4) are the previously defined probabilities and $(\alpha_i)_{min}$ is the probability of the event that is most unlikely to occur. If this $(\alpha_i)_{min}$ certainly happens the Bayes entropy is minimum whereas it has its maximum when the prescribed probabilities occur.

The Two-Fluid Model Used for the Calculations

For the calculation of the turbulent atomisation of a round jet the in-house flow calculation program ELSA22 (Eulerian Lagrangian Solution Algorithm, 2 dimensional, 2 phases) was used. This two-dimensional code is based on the SIMPLE algorithm [12] and allows calculations with cartesian and cylindrical coordinates. This code was extended by a two-fluid approach. The method should enable to calculate the liquid flow inside the nozzle, the region of atomisation (dense spray) and the air entrainment. At the end of the break-up region the two-fluid approach should provide the velocities of both phases, i.e. air and droplets, as well as the droplet size distribution through either a heuristic approach or the maximum entropy formalism. These results will be used as inlet condition for a Lagrangian calculation of the spray dispersion (Figure 1).

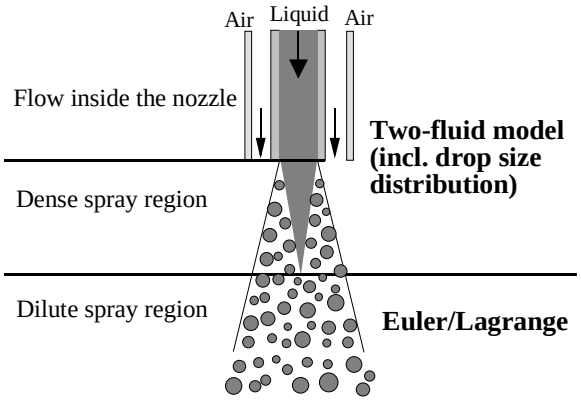

Figure 1. Schematic description of the different spray regions and the models applied there

Hence, the following general modelling equations are used for the continuous gas phase (4) and for the dispersed liquid phase (5), the used quantities to obtain the equations for all conservation variables are given in Table 1:

$$\frac{\partial}{\partial z}\left(\rho u_z \Phi\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho u_r \Phi\right)=\frac{\partial}{\partial z}\left[\Gamma\frac{\partial \Phi}{\partial z}\right]+\frac{1}{r}\frac{\partial}{\partial r}\left[r\Gamma\frac{\partial \Phi}{\partial r}\right]+S_\Phi \tag{4}$$

$$\frac{\partial}{\partial z}\left(\rho_d v_z \Phi\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho_d v_r \Phi\right)=\frac{\partial}{\partial z}\left[\Gamma\frac{\partial \Phi}{\partial z}\right]+\frac{1}{r}\frac{\partial}{\partial r}\left[r\Gamma\frac{\partial \Phi}{\partial r}\right]+S_\Phi\,. \tag{5}$$

Table 1. Definition of the quantities in equation (4) and (5)

Φ	Γ	S_Φ
φ	-	0
φ_d	-	0
$\varphi\cdot u_z$	$\mu+\mu_t$	$-\varphi\frac{\partial p}{\partial z}+\frac{\partial}{\partial z}\left(\left(\mu+\mu_t\right)\left[\frac{1}{3}\frac{\partial}{\partial z}\left(\varphi u_z\right)-\frac{2}{3}\frac{1}{r}\frac{\partial}{\partial r}\left(r\varphi u_r\right)\right]\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\mu+\mu_t\right)\frac{\partial}{\partial z}\left(\varphi u_r\right)\right)+\varphi_d\rho_d C_D\left(v_z-u_z\right)+\varphi\rho g_z$
$\varphi\cdot u_r$	$\mu+\mu_t$	$-\varphi\frac{1}{r}\frac{\partial p}{\partial r}+\frac{\partial}{\partial z}\left(\left(\mu+\mu_t\right)\frac{\partial}{\partial r}\left(\varphi u_z\right)\right)+\frac{1}{3r}\frac{\partial}{\partial r}\left(\left(\mu+\mu_t\right)\left[r\frac{\partial}{\partial r}\left(\varphi u_r\right)-2\varphi u_r-2r\frac{\partial}{\partial z}\left(\varphi u_z\right)\right]\right)-2\left(\mu+\mu_t\right)\frac{\varphi u_r}{r^2}+\varphi_d\rho_d C_D\left(v_r-u_r\right)+\varphi\rho g_r$
$\varphi_d\cdot v_z$	$\eta+\eta_t$	$-\varphi_d\frac{\partial p}{\partial z}+\frac{\partial}{\partial z}\left(\left(\eta+\eta_t\right)\left[\frac{1}{3}\frac{\partial}{\partial z}\left(\varphi_d v_z\right)-\frac{2}{3}\frac{1}{r}\frac{\partial}{\partial r}\left(r\varphi_d v_r\right)\right]\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\left(\eta+\eta_t\right)\frac{\partial}{\partial z}\left(\varphi_d v_r\right)\right)+\varphi_d\rho_d C_D\left(u_z-v_z\right)+\varphi_d\left(\rho_d-\rho\right)g_z$
$\varphi_d\cdot v_r$	$\eta+\eta_t$	$-\varphi_d\frac{1}{r}\frac{\partial p}{\partial r}+\frac{\partial}{\partial z}\left(\left(\eta+\eta_t\right)\frac{\partial}{\partial r}\left(\varphi_d v_z\right)\right)+\frac{1}{3r}\frac{\partial}{\partial r}\left(\left(\eta+\eta_t\right)\left[r\frac{\partial}{\partial r}\left(\varphi_d v_r\right)-2\varphi_d v_r-2r\frac{\partial}{\partial z}\left(\varphi_d v_z\right)\right]\right)-2\left(\eta+\eta_t\right)\frac{\varphi_d v_r}{r^2}+\varphi_d\rho_d C_D\left(u_r-v_r\right)+\varphi_d\left(\rho_d-\rho\right)g_r$
$\varphi\cdot k$	$\mu+\frac{\mu_t}{\sigma_k}$	$\varphi\left(P_k-\rho\varepsilon\right)-C_D\varphi_d\rho_d\left(k\theta-k_d\right)$
$\varphi_d\cdot k_d$	$\eta+\frac{\eta_t}{\sigma_{k,d}}$	$\varphi_d\left(P_{k,d}-\rho_d\varepsilon_d\right)+C_D\varphi_d\rho_d\left(k\theta-k_d\right)$
$\varphi\cdot\varepsilon$	$\mu+\frac{\mu_t}{\sigma_\varepsilon}$	$\varphi\frac{\varepsilon}{k}\left(C_{\varepsilon1}P_k-C_{\varepsilon2}\rho\varepsilon\right)$
$\varphi_d\cdot\varepsilon_d$	$\eta+\frac{\eta_t}{\sigma_{\varepsilon,d}}$	$\varphi_d\frac{\varepsilon_d}{k_d}\left(C_{\varepsilon1}P_{k,d}-C_{\varepsilon2}\rho_d\varepsilon_d\right)$

Besides, the following relations are required:

$$P_k = \mu_t \left(2\left[\left(\frac{\partial u_z}{\partial z} \right)^2 + \left(\frac{\partial u_r}{\partial r} \right)^2 + \frac{u_r^2}{r^2} \right] + \left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z} \right)^2 \right), \quad \varphi + \varphi_d = 1 \quad \text{and} \tag{7}$$

$$P_{k,d} = \eta_t \left(2\left[\left(\frac{\partial v_z}{\partial z} \right)^2 + \left(\frac{\partial v_r}{\partial r} \right)^2 + \frac{v_r^2}{r^2} \right] + \left(\frac{\partial v_z}{\partial r} + \frac{\partial v_r}{\partial z} \right)^2 \right). \tag{8}$$

In the dispersed dense spray region it is assumed that only drag and gravity act on the droplets. The correlation of the drag coefficient is given by:

$$C_D = \frac{18\mu}{\rho_d d_p^2} \left(1 + 0.15 \mathrm{Re}^{0.687} \right) . \tag{6}$$

Results

The calculated results were compared with measurements available from the literature for validating the implementation of the two-fluid model. Two different cases were chosen as a source for experimental values (Karl et al. [11] and Bulzan et al. [3]). In both of them air-assisted atomisers as well as water and air (as the atomised and the atomising phase, respectively) were used. The following figures show the calculated velocity profiles in comparison with the experimental data.

In Figure 2 and Figure 3 the radial profiles of the streamwise velocity component of the continuous gas phase for the two different cases are compared with the calculated results. It can be seen that the shape of the profiles is well predicted although the values in the centre of the jet are slightly overpredicted for the first case (Karl et al. [11]). For the second test case [3] the agreement of the calculated and the measured axial velocity profiles along the spray is much better.

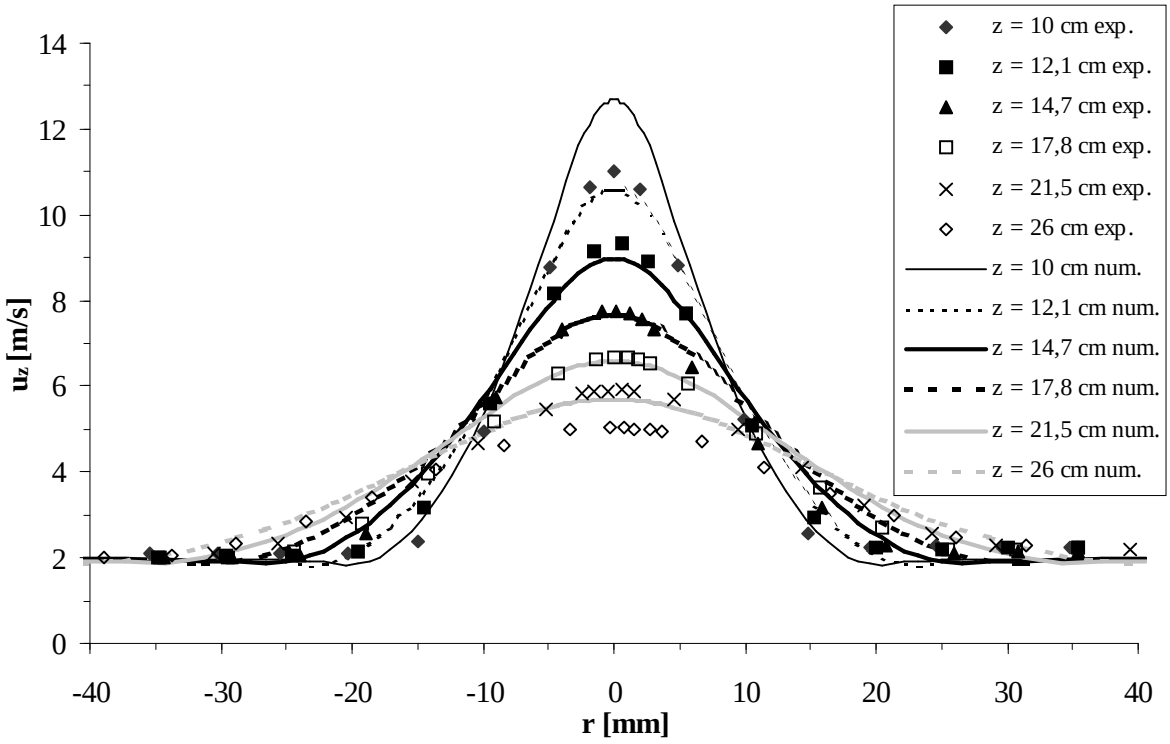

Figure 2. Comparison of the radial profiles of the axial gas phase velocity at different distances from the nozzle (experimental data from Karl et al. [11] as symbols, calculated results as lines)

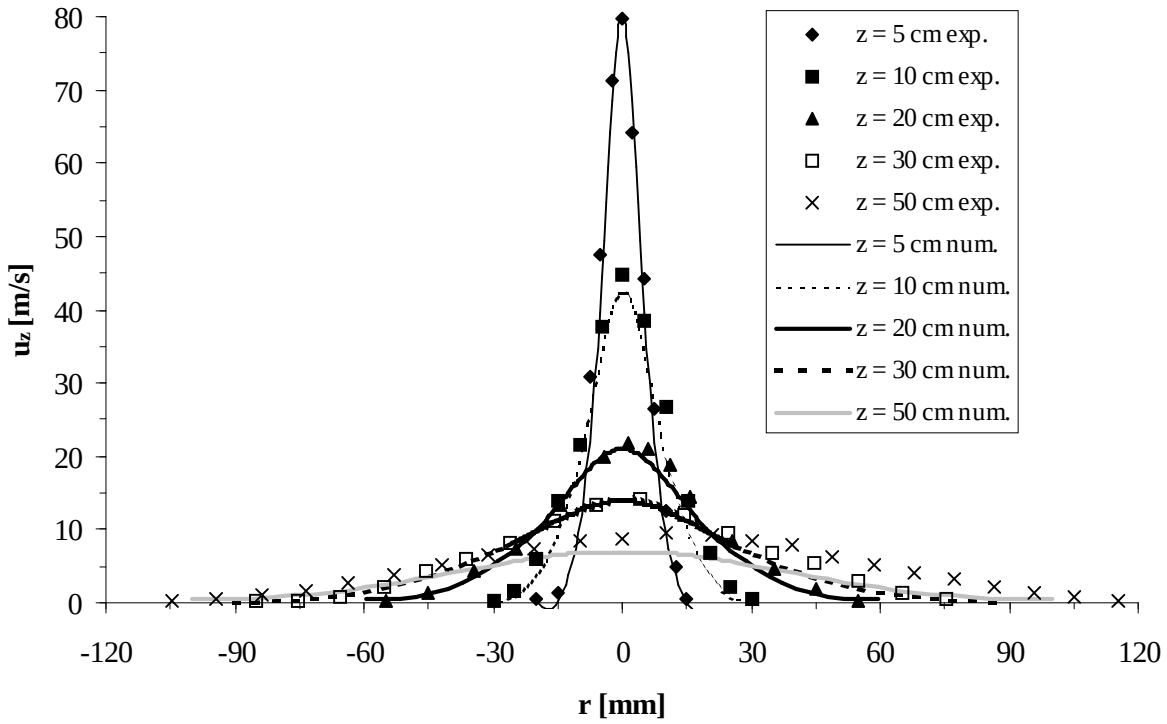

Figure 3. Comparison of the radial profiles of the axial gas phase velocity at different distances from the nozzle (experimental data from Bulzan et al. [3] as symbols, calculated results as lines)

In Figure 4 and Figure 5 the change of the axial velocity of the droplets along the spray centre line is shown. Again, the agreement is better for the experimental data of Bulzan et al. [3]. But also for the fluid velocity the model gives reasonable results, only the jet length is underpredicted. One should notice that, because of the high density of the dispersed phase directly behind the atomiser orifice and the bad accessibility with optical measurement techniques, experimental data are only available at a certain distance from the nozzle exit while the best numerical results with the two-fluid model can be obtained in the dense spray region.

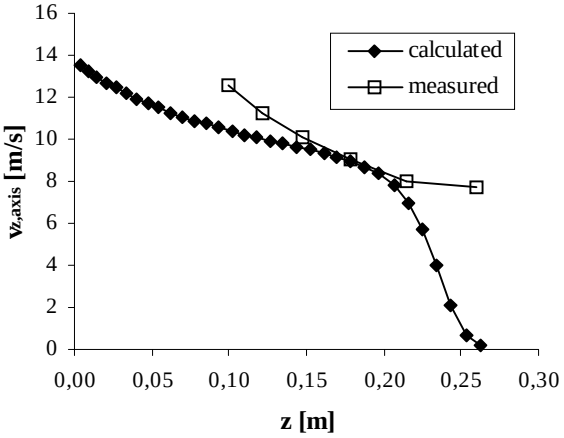

Figure 4. Axial liquid phase velocity at the jet axis as a function of the distance from the nozzle (experimental data from Karl et al. [11])

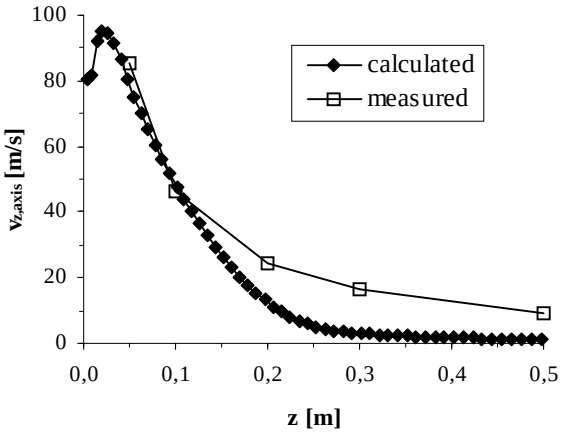

Figure 5. Axial liquid phase velocity at the jet axis as a function of the distance from the nozzle (experimental data from Bulzan et al. [3])

Discussion and further work

A two-fluid modelling approach for predicting the jet atomisation of liquids was introduced. In general, it can be concluded that this two-fluid model is able to predict different experimental data on spray atomisation. The test cases considered were two-fluid atomisers with central liquid injection. Both, the liquid as well as the air phase velocities developing downstream the nozzle exit could be predicted reasonably well.

To improve the present model also the droplet size distribution will be calculated. Therefore, an heuristic model and the maximum entropy formalism will be included in the numerical code. In the later stage, the two-fluid model will be used only in the dense spray region while for the dilute region an Euler/Lagrange method will be applied. Both numerical methods have to be appropriately coupled to allow effective calculations of the entire spray.

Acknowledgement

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Nomenclature

B	Bayes entropy
C_D	drag coefficient (inverse particle relaxation time)
$C_{\varepsilon 1}$, $C_{\varepsilon 2}$	constants for the calculation of the dissipation
d_p	mean droplet diameter
g	gravitation constant
k	turbulent kinetic energy
k_e	information entropy constant
n	number of outcomes
p	pressure
p_i	probability of a certain outcome
P	production term
q	Tsallis law exponent
r	radial distance from the jet axis
Re	Reynolds number
S	Shannon entropy
S_Φ	general source term
T	Tsallis entropy
u	velocity of the continuous phase
v	velocity of the dispersed phase
z	axial distance from the nozzle
α_i	previously described probability of a certain outcome
Γ	general diffusion coefficient
ε	dissipation of the turbulent kinetic energy
η	dynamic viscosity of the dispersed phase
θ	interaction coefficient, function of the Lagrangian liquid and the particle relaxation time scale
μ	dynamic viscosity of the continuous phase
ρ	density
σ	turbulent Schmidt number
φ	volume fraction
Φ	general quantity

Subscripts

d	dispersed phase
k	turbulent kinetic energy
min	minimum
r	radial
t	turbulent
z	axial
ε	dissipation of the turbulent kinetic energy

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