DEVELOPMENT OF A COMBINED VOF-LPT METHOD TO SIMULATE TWO-PHASE FLOWS IN VARIOUS REGIMES

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ABSTRACT

The breakup of a liquid jet into irregular liquid structures and droplets leading to the formation of a dilute spray has been simulated numerically. To overcome the shortcomings of certain numerical methods in specific flow regimes, a combined approach has been chosen. The intact liquid core, its primary breakup and the dense spray regime are simulated using the Volumes of Fluid (VOF) method in combination with Large Eddy Simulation (LES), while the Lagrangian Particle Tracking (LPT) approach in the LES context is applied to the dilute spray regime and the secondary breakup of droplets. A method has been developed to couple both simulations on a statistical basis. This statistical coupling approach allows to reflecting the dominating physical mechanisms of the two-phase flow in each regime to a high degree, but is at the same time computationally more efficient than comparable approaches. The coupling approach applies for the atomization of a fuel jet in a high pressure chamber, demonstrating the efficiency of the computations.

NOMENCLATURE

Roman symbols

d	diameter (m)
F	force (N)
L	characteristic length scale (m)
m	mass (kg)
n_i	interface unit normal $(-)$
p	pressure $(\mathrm{N}/\mathrm{m}^2)$
Q	heat flux $(\mathrm{J}/(\mathrm{m}^2 \cdot \mathrm{s}))$
R	specific gas constant $(\mathrm{J}/(\mathrm{kg} \cdot \mathrm{K}))$
r	position (m)
T	temperature (K)
t	time (s)
U	characteristic velocity scale (m/s)
u	velocity (m/s)
Z	mixture fraction $(-)$

Greek symbols

α	liquid phase volume fraction $(-)$
δ	Dirac function $(1/\mathrm{m}^2)$
κ	interface curvature $(1/\mathrm{m})$
μ	dynamic viscosity $(\mathrm{kg}/(\mathrm{m} \cdot \mathrm{s}))$
ν	kinematic viscosity $(\mathrm{m}^2/\mathrm{s})$
ρ	density $(\mathrm{kg}/\mathrm{m}^3)$
σ	surface tension (N/m)

Subscripts

amb	ambient
d	droplet
g	gas
inj	injection
jet	jet
l	liquid
noz	nozzle
p	parcel
rel	relative
s	source
spa	spamwise
str	streamwise
x,y,z	spatial coordinates

Abbreviations

FDM	Finite Difference Method
LES	Large Eddy Simulation
LPT	Lagrangian Particle Tracking
pdf	Probability Density Function
RANS	Reynolds Averaged Navier-Stokes
SGS	Sub Grid Scale
VOF	Volumes of Fluid
WENO	Weighted Essentially Non Oscillatory

Non-dimensional Numbers

Re	Reynolds number
We	Weber number

INTRODUCTION

A typical two-phase flow developed from an injection nozzle passes through various flow regimes. At the nozzle the *intact core* of the liquid jet can be observed. Instability mechanisms, dominantly cavitation in the injection nozzle, turbulence in the liquid jet and aerodynamic instabilities, cause the primary breakup of the jet (Farth *et al.* (1998)). The region, where the jet is completely disintegrated but the liquid volume fraction is still high, is called the *dense spray* region. Due to turbulent dispersion, the spacing between the droplets increases and the liquid volume fraction decreases. Secondary breakups lead to decreasing droplet sizes and an enhancement of the evaporation of the droplets. This is called the *dilute spray* region.

The primary breakup, the dense spray region, and the structure of dilute sprays has been studied experimentally (e.g. in Faeth *et al.* (1995), Naber & Siebers (1996), Martinez-Martinez *et al.* (2007) and Wu *et al.* (2006)), but as this region is optically dense it is difficult to measure and measurements are limited to identifying rather large liquid structures or more global parameters of the spray. Thus, to obtain a higher spatial and temporal resolution, numerical simulations need to be performed.

Due to different phenomena that are dominating and which have to be covered in simulations in the different regimes, different numerical methods show to be the most appropriate. The aim of this paper is to simulate two-phase flows in various flow regimes. Therefore it is chosen to apply an approach which combines the VOF method for the dense spray region and the LPT method for the dilute spray region. To study the flow time resolved and to capture the dynamic effects of the spray breakup, a LES is performed.

Another VOF-LPT coupling approach has been developed in Tomar *et al.* (2010). Here it has been decided for each liquid structure individually, whether to treat it with the LPT or VOF method. The decision is taken based on the size and shape of the droplet. The approach leads to a very good physical modelling of the flow of both phases, while maintaining high computational efficiency. A major aim of this current work is, to develop a coupling method of a very high computational efficiency and at the same time to reflect the physical principles of the flow to a high degree. Thus a coupling method is developed to couple both simulations on a statistical basis. This leads, compared to the above mentioned approach, to a computational significantly faster method, but the physical applicability is only slightly reduced.

GOVERNING EQUATIONS AND NUMERICAL METHODS

Primary Breakup and Dense Spray Region

The VOF method is used to handle the liquid and the gaseous phase. The flow field is described in Eulerian framework by the incompressible, isothermal Navier-Stokes equations for multiphase flows without phase changes. To assume constant temperature is reasonable as evaporation can be neglected in the dense spray region (Faeth *et al.* (1995)). Mass conservation is given by Eg. 1 and momentum conservation by Eq. 2.

$$\frac{\partial \rho}{\partial t} + \frac{\partial u_i \rho}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial u_i \rho}{\partial t} + u_j \frac{\partial u_i \rho}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{1}{Re_{jet}} \frac{\partial}{\partial x_j} \left(\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) + \frac{\kappa \delta n_i}{We_{jet}} \tag{2}$$

The last term on the right hand side of the momentum equation represents the effect of the surface tension of the liquid at phase interfaces, where κ is the interface curvature, δ is a Dirac function and n_i the interface unit normal. The jet Reynolds number Re_{jet} and Weber number We_{jet} are defined as

$$Re_{jet} = \frac{U_{inj} d_{noz}}{\nu_l} \tag{3}$$

and

$$We_{jet} = \frac{\rho_g U_{inj}^2 d_{noz}}{\sigma} . \tag{4}$$

To compute the phase interface, additionally a transport equation for the liquid volume fraction α in a computational cell is solved,

$$\frac{\partial \alpha}{\partial t} + \frac{\partial u_i \alpha}{\partial x_i} = 0 , \tag{5}$$

where $\alpha = 1$ represents a computational cell which is fully filled by liquid and $\alpha = 0$ represents a computational cell which is fully filled by gas. The viscosity μ and density ρ in the momentum equation are obtained from the constant liquid and gas densities and viscosities, assuming a linear dependency on α. The governing equations are discretized by the Finite Difference Method (FDM). The convective terms are approximated by a third-order accurate scheme, the diffusive and pressure terms by forth-order schemes and the time derivatives by a second order upwind scheme. The large scale structures in the flow field are simulated by an LES. The residual stresses are modelled by the so-called 'implicit' Sub Grid Scale (SGS) modelling (Pope (2000)), where no explicit SGS expression is used.

Dilute Spray Region

The continuous gaseous phase is described in Eulerian framework by the Navier-Stokes equations with constant diffusivities. As the spray is dispersed and its droplets are small,

the isothermal assumption taken in the dense spray region does not suit any longer. Low Mach number flow is assumed, which means that the density is function of the temperature only. The continuous phase volume fraction is assumed to be unity. Mass conservation is given by Eq. 6, momentum conservation by Eq. 7, energy conservation by Eq. 8 and mixture fraction conservation by Eq. 9.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = \dot{m}_S \tag{6}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\mu \frac{\partial u_i}{\partial x_j} + \dot{F}_{s,i} \tag{7}$$

$$\frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_j T}{\partial x_j} = \frac{\partial}{\partial x_j}\rho \alpha_c \frac{\partial T}{\partial x_j} + \dot{Q}_s \tag{8}$$

$$\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_j Z}{\partial x_j} = \frac{\partial}{\partial x_j}\rho D_c \frac{\partial Z}{\partial x_j} + \dot{Z}_s \tag{9}$$

Source terms for mass, momentum, energy and mixture fraction, $\dot{m}_S$, $\dot{F}_{s,i}$, $\dot{Q}_s$ and $\dot{Z}_s$, are introduced, which account for the coupling from the liquid to the gaseous phase. The system of equations is closed by the equation of state for incompressible flows,

$$p_0 = \rho RT, \tag{10}$$

where p_0 is the constant reference pressure.

The convective terms are approximated by an up to fifth-order WENO scheme, the diffusive and pressure terms by forth-order central differences and the time derivatives by a second order upwind scheme. The large scale structures in the flow field are simulated by an LES. The residual stresses are modelled by the so-called 'implicit' SGS modelling Pope (2000), where no explicit SGS expression is used.

The dispersed phase is described by stochastic parcels which are is tracked individually in Lagrangian framework. Only aerodynamic forces are taken into account for the momentum exchange between gaseous and liquid phase. For secondary breakup the bag breakup and the stripping breakup regimes are assumed to be dominant. They are modeled according to D. *et al.* (2000), which combines the Wave Breakup model and the Taylor Analogy Breakup Model. The evaporation of liquid mass is taken into account by an evaporation model, which assumes that the droplet is composed of a single-component and has a spherical shape with uniform properties.

Coupling from VOF to LPT

In the VOF method all liquid structures are resolved by the computational grid, therefore no models are needed besides the modelling of the surface tension term and the SGS terms. This makes the method physically adequate to simulate a two-phase flow in all above described regimes. The drawback is that, especially in the dilute spray regime, where the droplets are small, high spatial resolution is needed to resolve each droplet. Thus the computational costs are too high to simulate a complete spray using the VOF method.

In the LPT method the volume of computational cells is assumed to be much larger than the volume of the droplets. The droplets are assumed not to displace any fluid and are considered as mathematical particles, which allow one to track the droplets individually in the Lagrangian framework. This makes the method computationally fast, but models for the droplet related processes, like breakup, evaporation, aerodynamic interaction with the surrounding gas or droplet-droplet interaction, need to be introduced. These models are usually derived in experiments or analytically for simplified flow situations. The simplifying assumptions that are taken when deriving such models include that the droplets are spherical and they do not interact with each other. Thus, the droplets in the dilute spray regime are assumed to be small (i.e. the droplet-droplet spacing is large as compared to the droplet size and surface tension tends to give the droplets a spherical shape). In such regimes the LPT is a good approximation. In the intact liquid core and dense spray regime, where primary breakup occurs, the liquid structures are of irregular shape and collisions and aerodynamic interaction between liquid structures are frequent, the physical processes of the flow are poorly reflected by the LPT method.

To overcome the drawbacks of both methods, coupling approaches have been developed, which link a VOF simulation of the liquid core and the dense spray regime to an LPT simulation of the dilute spray regime. The straightforward approach, where the physical domain of both simulations are overlapping, has been chosen in Tomar *et al.* (2010) and Herrmann (2009). Due to the overlapping, it is possible to decide for each liquid structure individually whether it is adequately described by the VOF or by the LPT method.

The coupling approach developed in this work is on a statistical basis: A layer, called the coupling layer, is introduced close to the outlet of the VOF simulation where the liquid mass, which passes by, is analysed. This layer is considered to be far enough downstream from the injector, that the spray is dilute enough to be simulated with a LPT approach. At this layer the statistical parameters of the droplet distributions are extracted and used as starting conditions for the LPT simulation. The drawback of this approach compared to the straightforward approach is, that the coupling layer is fixed in space. Therefore it can not be at the ideal position for all liquids to be transferred from the VOF to the LPT simulation, which reduces the physical applicability of the method. The advantage of the method is, that the VOF simulations only need to run until statistical convergence of the droplet distributions. This can be used in the LPT simulation as starting condition for much larger time scales. Thus the statistical coupling is computationally more efficient than the straightforward approach, where the LPT simulation has to 'wait' for each single droplet to be transferred.

A snapshot of the penetrating jet and the schematic location of the coupling layer are shown in Fig. 1.

The algorithm used at this layer to identify connected liquid structures is based on Herbert D.A. (2008), but extended to time dependent problems. This algorithm calculates the equivalent radius of a spherical droplet, as well as its centre of gravity and its average velocity vector. Three test cases, a spherical droplet, an ellipsoid representing a distorted droplet and a rotating ellipsoid, have been run on different grid resolutions to test the accuracy of the extraction method applied

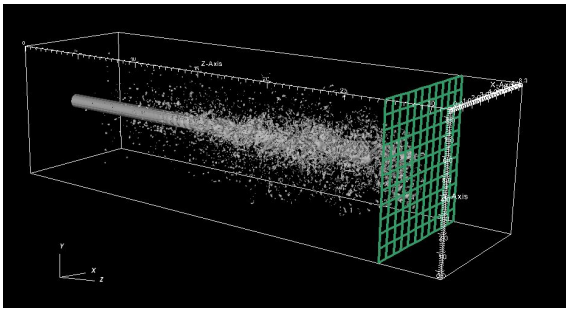


Figure 1. Snapshot of the jet and location of the coupling layer.

at the coupling layer. It has been shown in Grosshans H. (2010) that if the droplet diameter is resolved by at least 3 cells ($d/h > 3$) the results are considered to be sufficiently accurate. For this resolution the testcases showed an error in the identified liquid volume between 10% and 30%.

The droplet injection in the LPT simulation uses the statistical parameters extracted from the VOF simulation by performing Monte-Carlo simulations. Rotational symmetry is assumed and the streamwise position of the droplet is already defined by the location of the coupling layer. Thus four parameters need to be given at injection: the droplet diameter, the streamwise velocity, the spanwise velocity and the spanwise position. The evaluation of the correlation coefficients for each combination of these parameters shows that they are independent of each other, except the correlation found between spanwise position and streamwise velocity. This relation is given by:

$$u_{str} = 0.61 - 0.17 \cdot |r_{spa}| \; . \tag{11}$$

Hence three statistical distributions, for the droplet diameter, streamwise and spanwise velocity, were obtained from the VOF simulation and used to perform three independent Monte-Carlo simulations in the LPT part. The spanwise position is then obtained by a linear relationship from the streamwise velocity.

The gaseous phase is also coupled at the location of the coupling layer. The average streamwise velocity is obtained from the VOF simulation and applied to the LPT simulation as a steady gas inlet. This is a simplified approach as turbulent fluctuations are neglected. This simplification is supposed to be justified, as the turbulent structures, which influence the droplet trajectories significantly, are assumed to be larger in the dilute spray regime than in the dense spray regime.

PROBLEM SET-UP

The injection speed U_{inj} of the simulated spray is 500 m/s, the nozzle diameter d_{noz} is 10^{-4} m, the results are normalised to these values. The jet Reynolds number Re_{jet} equals 14964, the jet Weber number We_{jet} is 10000, the liquid-gas density ratio is 10 and the liquid-gas viscosity ratio is 3.42. The ambient gas density is 14.8 kg/m^3, the ambient gas temperature is 1000 K.

The examined geometry is a confined cubical domain of an edge length of $1080\,d_{noz}$. The region up to 40 nozzle diameters downstream after injection, where the primary breakup is expected to occur, is simulated using the VOF method. The rest of the domain is simulated using the LPT approach.

RESULTS

Primary breakup creates a large amount of small droplets, their statistical data being extracted at the coupling layer. The droplet diameter distribution resulting from the VOF simulation is shown in Fig. 2(a). It is interesting to note that there is a two peak distribution: one peak at $d_d/d_{noz} \approx 0.02$ and a second one at $d_d/d_{noz} \approx 0.08$. This is an indication that there are two instability mechanisms dominating: The Kelvin-Helmholtz instability, stripping small droplets away from the surface of the jet, and the Rayleigh-Taylor instability, creating larger liquid structures. In a pure LPT simulation, a distribution of the droplet diameters has to be assumed as a starting conditions. Usually a standard distribution, e.g. a Rosin-Rammler distribution, is chosen for that, which does not show such a two peak distribution. Thus this acting of two different breakup mechanisms during primary breakup is clearly a physical mechanisms that is commonly not captured by a pure LPT simulation. Such two peak distributions have also been found experimentally in Lubarsky *et al.* (2010).

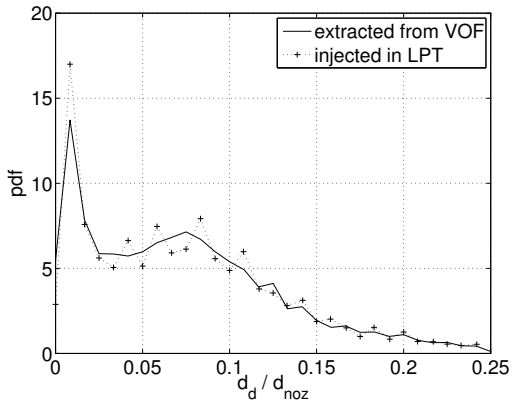
The distribution of streamwise velocities in Fig. 2(b) shows a peak at $u_{str}/u_{inj} \approx 0.1$ and an approximately linear decreasing curve until the point where the streamwise velocity equals the droplet injection velocity. The spanwise velocities in Fig. 2(c) show also a peak at $u_{spa}/u_{inj} \approx 0.1$, but the gradient of the curve towards the higher velocities is much steeper than the one for the streamwise velocities. This is caused by the fact that the spanwise velocities are not related to the momentum given to the droplet at injection, but it is purely caused by turbulent dispersion, i.e. the trajectory of the droplets is changed due to aerodynamic interaction with turbulent eddies in the surrounding gas.

The LPT simulations are started with the above described statistical distributions, by performing Monte-Carlo simulations. The results of these Monte-Carlo simulations are shown as well in Fig. 2(a) to Fig. 2(c). The distributions resulting from the Monte-Carlo simulations show to converge to the distributions from the VOF simulation, which demonstrates the accuracy of the developed coupling algorithm.

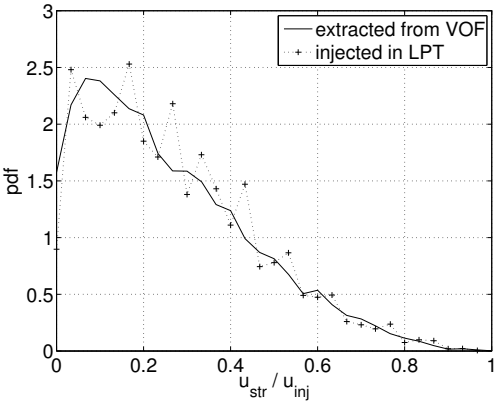
After injection in the LPT simulation, the droplets experience further secondary breakups, get smaller and finally evaporate. This results in an increase of the mixture fraction in the gaseous phase (see Fig. 3) and in an increase of the gas density (see Fig. 3(a)). At the same time, energy is needed to evaporate the liquid, thus, due to energy conservation, the surrounding gas is cooled down. This effect can be seen in Fig. 3(c).

SUMMARY AND CONCLUSIONS

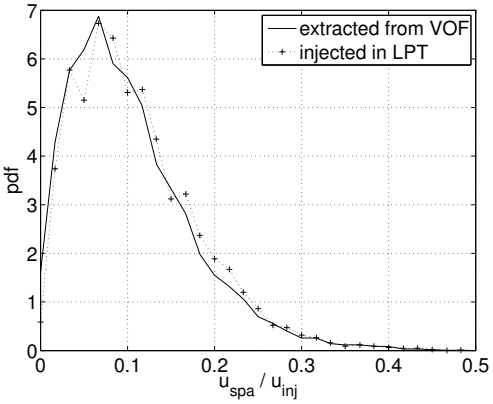
A two-phase flow has been simulated in various flow regimes using a combination of the VOF and LPT methods. The disintegration of the liquid core into ligaments and droplets due to aerodynamic instabilities has been shown. By introducing a coupling layer close to the outlet a method has



(a) Droplet diameter distribution.



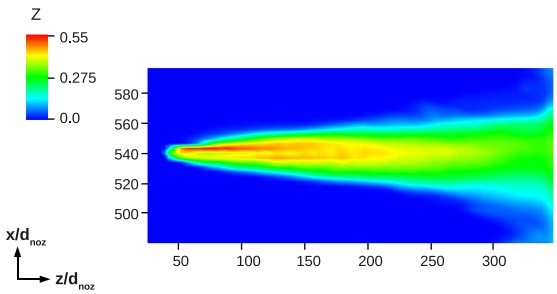
(b) Streamwise velocity distribution.



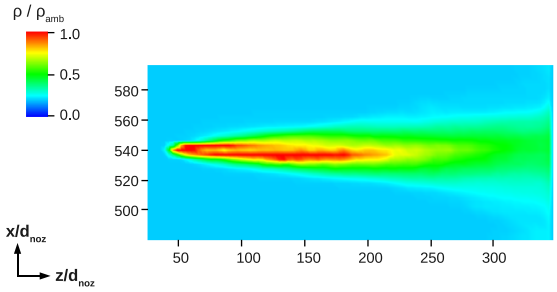
(c) Spanwise velocity distribution.

Figure 2. Droplet distributions extracted from the VOF and injected in the LPT simulations.

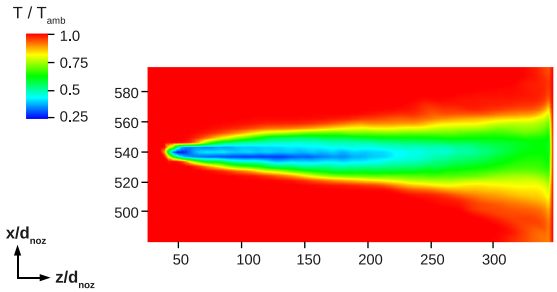
been developed to identify droplets, their radius, position and velocity. This coupling layer was shown to deliver accurate results if a droplet is resolved by at least 3 computational cells over the diameter. The extracted data was used to build up datasets, which can in the following be used to start a simulation of a dilute spray using the LPT method. The statistics of the droplets injected in the LPT simulation were shown to converge to the statistics extracted from the VOF method, thus



(a) Average gas mixture fraction.



(b) Average gas density.



(c) Average gas temperature.

Figure 3. Results of the LPT simulation, detail of the cross-section at $y = 540\ d_{noz}$.

the coupling works accurately.

The method, developed in this paper, to simulate two-phase flows in various flow regimes is qualitatively compared to other methods in Fig. 4. The simulation presented in this paper is judged to be computationally much more efficient than a pure VOF simulation and physically much more applicable than a pure LPT simulation. Compared to previous coupling approaches, the developed method is judged to be more efficient while the modelling penalty is small.

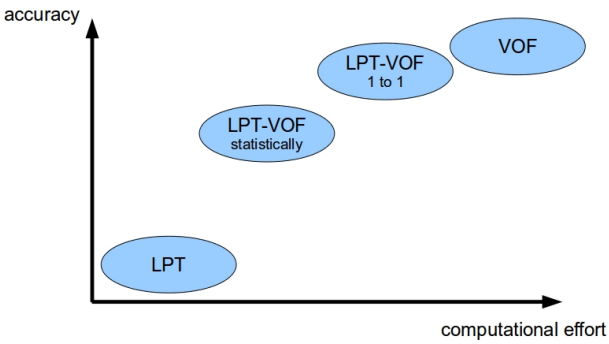


Figure 4. Qualitative comparisons of methods to simulate two-phase flows

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