Large-Eddy Simulation of the Primary Breakup of a Spatially Developing Liquid Film

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Atomization of liquid jets is of fundamental interest for the automotive industry, gas turbines, medicine, agriculture, etc. However, the physical phenomena leading to the disintegration of jets are still not very well understood. Direct numerical simulation is a useful tool for understanding the physics of primary breakup but, because all scales in the flow must be resolved, it is computationally expensive, especially if the Reynolds number is high. On the other hand, in the absence of walls, LES is only a weak function of *Re*. Therefore the focus of our work is to develop a LES methodology for two phase flows, following the ideas in the literature. This paper constitutes a first step in this direction. Quantitative results are presented for a three-dimensional LES of a liquid film exhausting into a gaseous atmosphere.

1 Introduction

Contemporary three dimensional, time dependant models for two phase flows with moving interfaces are, for engineering applications, mostly based on solutions of the Reynolds-averaged Navier-Stokes equations ([14, 20]). Shortcomings of such RANS models have been documented by several generations of researchers. On the other hand direct numerical simulation provides a useful tool for understanding the detailed physics of two phase flow problems, but because all scales in the flow must be resolved, DNS is restricted to moderate Reynolds numbers and therefore to fundamental research ([7, 11, 13, 24]). Large eddy simulation (LES) offers a compromise between RANS approaches and DNS. In the LES methodology one only resolves those eddies that are large enough to contain information about the geometry and dynamics of the specific problem under investigation, and regards all structures on a smaller scale as "universal" following the viewpoint of Kolmogorov. The LES equations are derived by applying a filter function to eq. (1)-(3). While LES of mono-phasic flows has reached a sophisticated standard, an application of the LES formalism two two-phase flows with moving interfaces is hard to find in the literature. Recently Wörner et al. [25] presented volume averaged conservation equations for volume-of-fluid interface tracking. Because the volume averaging in there equations is equivalent to a filtering in physical space, their approach is conceptually related to the LES method. Also Alajbegovic [1] applied the LES formalism to the multiphase flow equations. In contrast to the previously mentioned work he separates the capillary force into a resolved and an unresolved part and shows that due to the interfacial subgrid-scales an additional force appears. The present work constitutes a first step in applying the above mentioned formalisms in a numerical simulation.

2 Governing equations

We deal with the following set of conservation equations in their instantaneous, local form. The continuity equation in an incompressible formulation

$$\frac{\partial u_i}{\partial x_i} = 0\,, \tag{1}$$

and the Navier-Stokes-equation

$$\begin{aligned} \frac{\partial}{\partial t}(\rho u_i) &= -\frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial}{\partial x_j}\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \\ &\quad -\frac{\partial p}{\partial x_i} + \frac{\partial T_{s(ij)}}{\partial x_j}\,. \end{aligned} \tag{2}$$

Here ρ denotes the density and μ the molecular viscosity. In equation (2) the consideration of two phase flows is included through the interfacial stress tensor $T_{s(ij)}$ to be modeled below. The interface between the two immiscible fluids is implicitly given by the volume fraction F which is advected by the following equation

$$\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial x_i} = 0\,. \tag{3}$$

At the interface, continuity of fluid velocity is assumed, that means the limiting values of velocity $\mathbf{u}_L$ and $\mathbf{u}_G$ are identical. In (2) the interfacial tension stress acting between the two fluid phases is usually modeled by considering only the inviscid term and assuming it to be a constant ([12])

$$\boldsymbol{T}_s = \sigma(\boldsymbol{I} - \boldsymbol{n}\boldsymbol{n})\delta_s \quad \text{and} \quad \nabla \cdot \boldsymbol{T}_s = 2\sigma\kappa\boldsymbol{n}\delta_s\,, \tag{4}$$

where σ denotes the surface tension, $\boldsymbol{n}$ the unit normal on the surface, κ the mean curvature, δ_s a Dirac function concentrated on the surface and $\boldsymbol{I}$ the unit tensor. An extension of this formulation, in which a surface deformation rate has been taken into account, may be found in [8].

Following the work of Wörner et al. [25] the LES-VOF equations can be derived by applying the following procedure. In order to differentiate between the components in phase $k \in 1, 2$ residing in domains Ω_k we first introduce the phase indicator function χ_k

$$\chi_k = \begin{cases} 1 & \text{if } x \in \Omega_k \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

The filtered multiphase quantity Ψ_k is then defined as

$$\overline{\Psi_k}^k(x) = \int\limits_{V_k} \chi_k(x)\Psi_k(x) \tag{6}$$

where V_k denotes the part of a volume V which is solely occupied by phase k. Multiplying equations (1) and (2) with χ_k for each phase, averaging over V and applying the Gauss and Leibnitz rules for averaging yields the volume averaged separate field equations. Defining a mixture density and a center of mass velocity and summing the averaged mass conservation and momentum equations, yields finally the volume averaged single field equations (for details see [25]). Besides the well known subgrid scale stress

$$\tau_{ij}^{sgs} = \alpha_1 \tau_{1,ij}^{sgs} + \alpha_2 \tau_{2,ij}^{sgs} \quad \text{where} \quad \alpha_k = V_k/V \quad \text{and} \quad \tau_{k,ij}^{sgs} = \rho_k \left(\overline{u_i\, u_j}^k - \overline{u_i}^k\, \overline{u_j}^k \right) \qquad (7)$$

which arises from filtering the non-linear convective term, two additional subgrid scale terms appear, depending on the relative velocity $\boldsymbol{u_r}$ between both phases. They are called momentum drift flux term and interfacial friction term. In the following we use the assumption that both phases share the same velocity field in the interfacial transition region (homogenous model, $\boldsymbol{u_r} = 0$). From DNS data (see [11]) it is known that the dominant wavelength at the interface is of the order of the nozzle diameter. Therefore the interfacial topology is well resolved by our grid and we have not to take into account a subgrid contribution to the capillary force as in [1]. Applying these assumptions we obtain finally the filtered governing equations which are known from mono-phasic LES (see e.g. Sagaut [21]).

3 Numerical Technique

Equations (1) and (2) are solved, using a finite volume technique on a cartesian mesh. The variables are located on a staggered grid. For spatial discretization a TVD scheme is used. Temporal discretization is an explicit Runge-Kutta-method of third order accuracy. The Poisson equation is inverted with a Multigrid-Solver. A Volume-of-Fluid scheme, with PLIC interface reconstruction ([4], [7], [22]), is used to advect the interface (see equation (3)) so that droplet formation and ejection away from the liquid jet can be captured. The code has been validated at several test cases including capillary waves and a Rayleigh Taylor instability ([6]). The results are in favorable agreement with those of the literature (see [4] and [19]).

For the generation of the inflow data we followed a new procedure, based on digital filtering of random data, developed by Klein et al. [9], to obtain velocity fluctuations $\mathcal{U}_i$ which approximate a prescribed autocorrelation function. These fluctuations are conditioned such that each distribution has zero mean, unit variance and zero covariance with the other distribution. Then the velocity field is constructed according to $u_i = U_i + a_{ij}\mathcal{U}_j$ where U_i denotes the mean velocity profile and the coefficients a_{ij} are related to the Reynolds stress tensor which should be matched by the inflow data ([18]). The axial mean velocity profile was taken from the experimental work of Heukelbach et al. [5] and is plotted in figure 3 (left). The inflow length scale was set to $1/10D$ and the fluctuation level to 2%, constant over the nozzle.

4 Subgrid scale models

We consider in this work two models of Smagorinsky type [23]. Here the influence of the unresolved motion on the resolved scales is treated as an additional viscosity

$$\nu_t = (C_s \Delta)^2 |S_{ij}|, \quad \text{with} \quad S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \qquad (8)$$

the filter width Δ and the model coefficient C_s.

Germano et al. [3] proposed a procedure for evaluating the model coefficient from information contained in the resolved field. By introducing a second, so called test filter, one can obtain the subgrid stresses for two different filter widths, the difference of which is a second order tensor L_{ij}, which can be thought of a stress resulting from motions at intermediate scales. Introducing the modeling approximations, a second tensor M_{ij} can be defined, which is like L_{ij} directly computable from resolved quantities. Relating both tensors the model constant can be determined by minimizing a certain error function, following the work of Lilly [16].

5 Flow Configuration

A water jet exhausting into air is simulated with a Reynolds number of $Re = U_0\ D/\nu = 6000$, where U_0 denotes the bulk velocity at the inlet, D the nozzle diameter and ν the kinematic viscosity. The extension of the computational domain in axial (x) and homogeneous (y) and vertical (z) direction is $15D \times 5D \times 10D$. Figure 1 shows a snapshot of a simulation. The computational domain is resolved with $300 \times 100 \times 200$ grid points. At the inflow boundary the velocity is set to zero outside the nozzle, while the data from the inflow generator is used inside. At the outflow Neumann boundary conditions for the velocity and the pressure are prescribed. Setting the pressure to zero at the top and the bottom boundaries and interpolating the tangential velocities constantly allows mass entrainment.

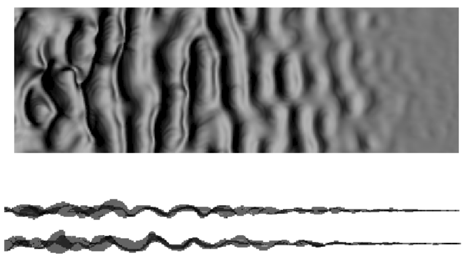

Figure 1: Instantaneous picture of the water film at $Re = 3000$, top and side view (flow is from right to left)

6 Results and Discussion

Our first LES-VOF simulations have been conducted at $Re = 6000$ with 1) a standard Smagorinsky model and 2) the dynamic Germano procedure. In contrast to experimental data of the same configuration [5], breakup was observed and it was concluded that these models do not provide enough dissipation to keep the liquid film interface intact. For this reason we increased the Smagorinsky constant to a value of $C_s = 0.2$ and obtained afterwards reasonable results.

Because the most amplified wavenumber is an important parameter for the prediction of jet breakup, it is informative to compare this quantity (obtained via FFT) in Fig. 2 to experimental data and the predictions from linear stability analysis. In view of some uncertainties concerning the exact inflow conditions, the agreement between experimental and DNS/LES data is very good. The value of λ_{opt} for the highest Reynolds number seems to be slightly to high compared to that one would expect extrapolating the DNS results (taken from [11] and performed with the same code) for $Re = 2000, 3000, 4500$, but nevertheless it lies well in the range reported in the experimental work of Heukelbach et al. [5]. A possible explanation is that the increased effective viscosity leads to an increase of the most amplified wavenumber, that can be concluded from theoretical analysis (see [15]).

Although linear stability analysis is accepted as an important tool, it obviously does not lead in all cases to useful quantitative predictions (see also [17]): For a water film ejected into a gas at rest, the difference between theoretical and numerical/experimental data is of one order of magnitude. The reasons for this difference are probably that linear stability analysis does not account for the influence of the mean velocity profile and the turbulence in the flow and of course that nonlinear terms are neglected.

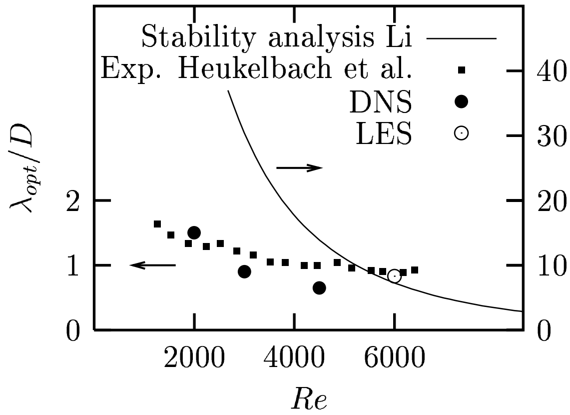

Figure 2: Comparison of the most amplified wavenumber λ_{opt} from DNS results [11], experimental data [5], linear stability theory [15] and LES (present study)

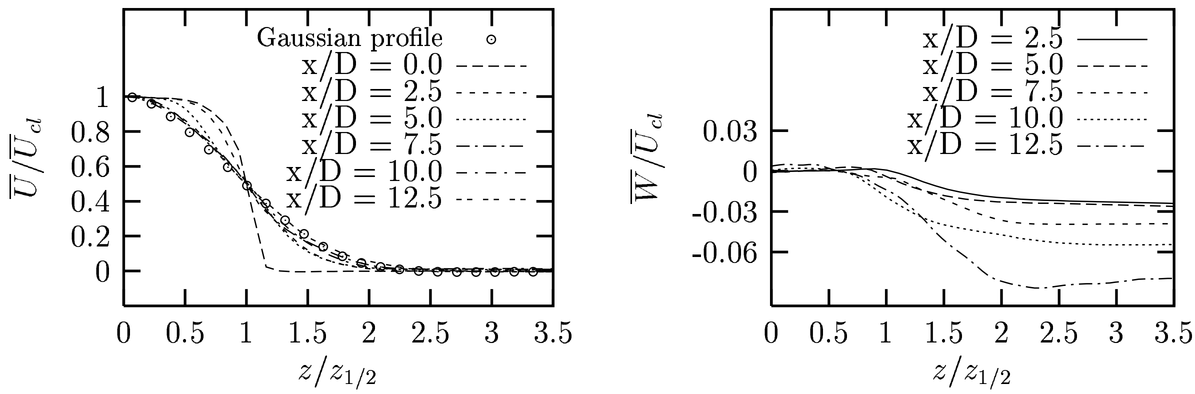

Figure 3: Mean axial velocity (left), mean lateral velocity (right).

For the mono-phasic jet it is generally believed that in the far field the jet reaches a universal self-similar state, that means that all profiles collapse into a single curve when normalized with the local centerline velocity U_{cl} and the jet half width $z_{1/2}$ which is defined through $U(z_{1/2}) = 0.5\, U_{cl}$. Furthermore one knows that a spray behaves in the far field like a mono-phasic jet ([26]). Therefore it seems to be interesting to apply a similar evaluation procedure to the two-phasic jet.

While for the mono-phasic jet there is a huge amount of experimental and even DNS data available where turbulence statistics are presented (see [2],[10]), the authors know of no work where similar measurements for a two-phasic jet have been performed. Therefore we are not able to compare our results in this section with experimental data.

First we turn our attention to the lateral profiles of the mean axial and mean lateral velocity components. As in the mono-phasic case the mean axial velocity is very well represented by the Gaussian profile $U(z)/U_{cl} = \exp[-C(z/z_{1/2})^2]$ with $C \approx \ln 2$. This is in contrast to the DNS of Klein et al. [11] at $Re = 3000$ where an additional inflection point is observed in the mean velocity profile. It is not known if this is a Reynolds number effect or due to the subgrid scale model employed in the present simulations. The lateral mean velocity profiles show that the normalized entrainment velocity is not constant. Therefore the jet cannot yet be in self similar state.

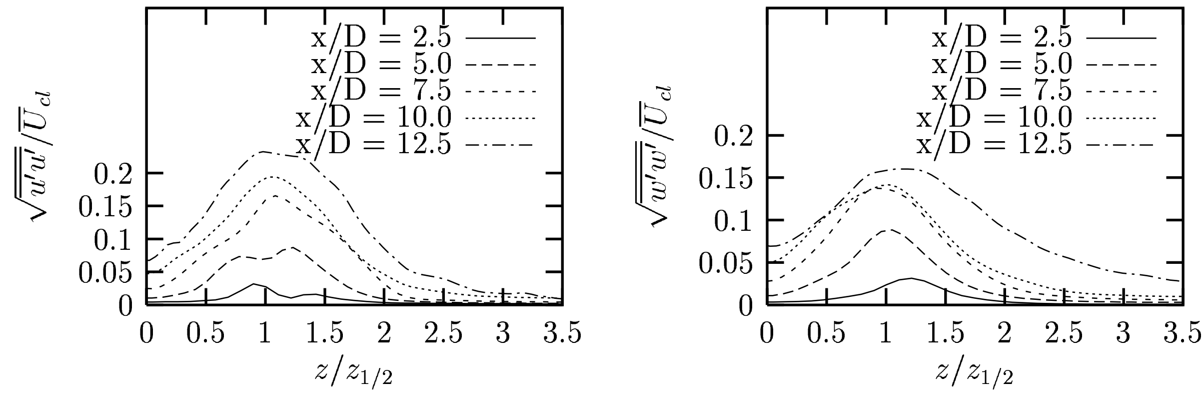

Figure 4: Mean axial velocity fluctuations(left), mean lateral velocity fluctuations (right)

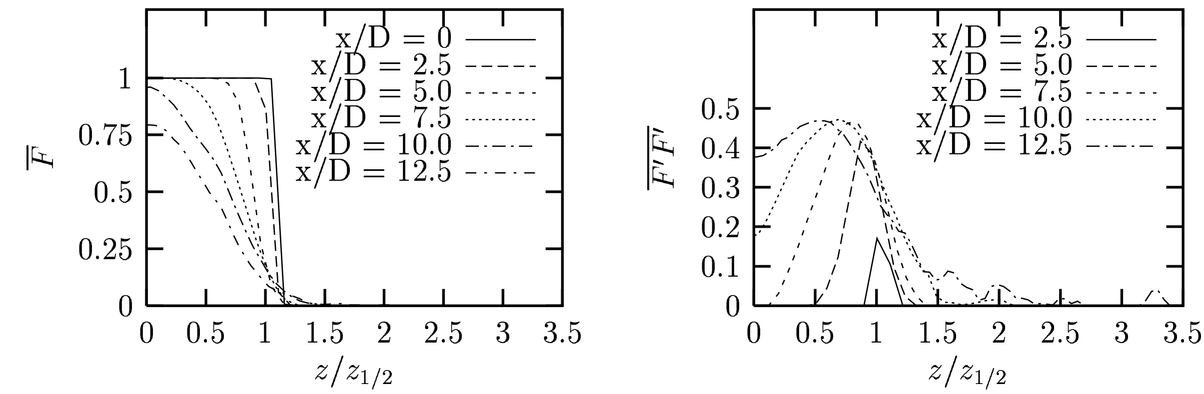

Figure 5: Mean volume concentration (left) and corresponding fluctuations (right)

Figures 4 shows that in contrast to the mono-phasic jet, the intensity of the Reynolds stress components in the shear layer is much higher compared to the centerline value. The same is true for the other tensor components not shown here. Obviously the interface damps the turbulence. Indeed the fluctuation level at the centerline is comparable to the channel flow value, while the peak in the shear layer is close to the fluctuation intensity observed in a free plane jet.

Finally we comment on the statistical evolution of the volume concentration F. From figure 5 it is clear that the oscillations of the water film just reach the centerline at $x/D \approx 10$. Approximately at the same axial distance to the nozzle the fluctuation level has nearly its theoretical maximum of 0.5, at the lateral position of the undisturbed interface.

7 Conclusions

A fully three-dimensional LES of a water film ejected into air has been presented. Assuming that the interfacial topology is well resolved by the grid and that both phases share the same velocity field in the interfacial transition region, from several unclosed terms only the subgrid stresses have to be modeled. It was found that the Smagorinky model yields satisfactory prediciton results when the model constant is increased to a value of $C_s = 0.2$. Quantitative results are presented. In view of turbulence statistics, it has to be mentioned that such data is hard to find in the literature.

References

[1] A. Alajbegovic. Large eddy simulation formalism applied to multiphase flow. In *Proceedings of FEDSM'01*, number FEDSM2001-18192 in ASME 2001 Fluids Engineering Division Summer Meeting, New Orleans, Louisiana, May/June 2001.

[2] J.P. Bonnet, R.D. Moser, and W. Rodi. *AGARD advisory report 345, A Selection of Test Cases for the Validation of Large Eddy Simulations of Turbulent Flows*, chapter 6.3 Jets, page 35. AGARD 1998, 7 Rue Ancelle, 99200 Neuilly-sur Seine, France, 1998.

[3] M. Germano, U. Piomelli, P. Moin, and W. H. Cabot. A dynamic subgrid-scale eddy viscosity model. *Phys. Fluids A*, 3(7):1760–1765, july 1991.

[4] D. Gueyffier, A. Nadim, J. Li, R. Scardovelli, and S. Zaleski. Volume of fluid interface tracking with smoothed surface stress methods for three-dimensional flows. *J. Comp. Phys.*, 152:423–456, 1999.

[5] K. Heukelbach and C. Tropea. Influence of the inner flowfield of flat fan pressure atomizers on the disintegration of the liquid sheet. In *ILASS-Europe 2001, 17. Annual Conference on Liquid Atomization and Spray Systems*, pages 613–618, Zürich, September 2001.

[6] M. Klein. *Direkte Numerische Simulation des primären Strahlzerfalls in Einstoffzerstäuberdüsen.* PhD thesis, Technische Universität Darmstadt, 2002.

[7] M. Klein, A. Sadiki, and J. Janicka. Influence of the inflow conditions on the direct numerical simulation of primary breakup of liquid jets. In *ILASS-Europe 2001, 17. Annual Conference on Liquid Atomization and Spray Systems*, pages 475–480, Zürich, September 2001.

[8] M. Klein, A. Sadiki, and J. Janicka. Effects of the surface stretching or the surface deformation rate on the breakup of a viscous drop in simple shear flow: Numerical simulation. In *5th International Symposium on Engineering Turbulence Modelling and Measurements*, Mallorca, September 2002.

[9] M. Klein, A. Sadiki, and J. Janicka. A digital filter based generation of inflow data for spatially developing direct numerical or large eddy simulations. *J. Comp. Physics*, 186:652–665, 2003.

[10] M. Klein, A. Sadiki, and J. Janicka. Investigation of the influence of the reynoldsnumber on a plane jet using direct numerical simulation. *International Journal of Heat and Fluid Flow, accepted for Publication*, 2003.

[11] M. Klein, A. Sadiki, and J. Janicka. Direct numerical simulation of the primary breakup of a spatially developing liquid jet. In *TSFP3, 3rd International Symposium on Turbulence and Shear Flow Phenomena*, Sendai, Japan, June 2003, accepted for publication.

[12] B. Lafaurie, C. Nardonne, R. Scardovelli, S. Zaleski, and G. Zanetti. Modelling merging and fragmentation in multiphase flows with surfer. *J. Comp. Phys.*, 113:134–147, 1994.

[13] A. Leboissetier and S. Zaleski. Direct numerical simulation of the atomization of a diesel jet. In *ILASS-Europe 2001, 17. Annual Conference on Liquid Atomization and Spray Systems*, Zurich, September 2001.

[14] C.M. Lemos. A simple numerical technique for turbulent flows with free surfaces. *J. Fluid. Mech.*, 15:127–146, 1992.

[15] X. Li. Spatial instability of plane liquid sheets. *Chemical engineering science*, 48:2973–2981, 1993.

[16] D. K. Lilly. A proposed modification of the germano subgrid-scale closure method. *Phys. Fluids A*, 4(3):633–635, march 1992.

[17] S.P. Lin and R.D. Reitz. Drop and spray formation from a liquid jet. *Annual Review of Fluid Mechanics*, 30:85–105, 1998.

[18] T.S. Lund, X. Wu, and D. Squires. Generation of turbulent inflow data for spatially-developing boundary layer simulations. *J. Comp. Phys.*, 140:233–258, 1998.

[19] E.G. Puckett, A.S. Almgren, J.B. Bell, D.L. Marcus, and W. Rider. A high-order projection method for tracking fluid interfaces in variable density incompressible flows. *J. Comp. Phys.*, 130:269–282, 1997.

[20] Muzaferija S., Peric M., Sames P.C., and Schellin T.E. A two-fluid navier-stokes solver to simulate water entry. In *Proc. 22nd Symposium on Naval Hydrodynamics*, Washington D.C., August 1998.

[21] P. Sagaut. *Large Eddy Simulation for Incompressible Flows.* Springer, 1998.

[22] R. Scardovelli and S. Zaleski. Direct numerical simulation of free surface and interfacial flows. *Annual Review of Fluid Mechanics*, 31:567–603, 1999.

[23] J. S. Smagorinsky. General circulation experiments with the primitive equations, 1. the basic experiment. *Monthly Weather Rev.*, 91:99–164, 1963.

[24] G. Tryggvson, B. Bunner, A. Esmaeeli, D. Juric, N. Al-Rawahi, W. Tauber, J. Han, S. Nas, and Y.J. Jan. A front-tracking method for the computations of multiphase flow. *J. Comp. Phys.*, 169:708–759, 2001.

[25] M. Wörner, W. Sabisch, G. Grtzbach, and D.G. Caccuci. Volume-averaged conservation equations for volume-of-fluid interface tracking. In *Proc. 4th International Conference on Multiphase Flow*, New Orleans, Louisiana, USA, May-June 2001.

[26] K.J. Wu, D.A. Santavicca, and F.V. Bracco. Ldv measurements of drop velocity in diesel-type sprays. *AIAA Journal*, 22(9):1263–1270, 1984.