MODELLING AND SIMULATION OF THE DISINTEGRATION PROCESS IN AN ULTRASONIC STANDING WAVE ATOMIZER

O. Reipschläger, D. Bothe, H.-J. Warnecke, B. Monien*, J. Prüss, B. Weigand*****
mreip1@tc.uni-paderborn.de
Chemical Engineering, University of Paderborn, Warburger Str. 100, D-33098 Paderborn
***Department of Mathematics and Computer Science, University of Paderborn, D-33102 Paderborn**
****Institute for Analysis, University of Halle-Wittenberg, D-06099 Halle (Saale)**
*****Institute of Aerospace Thermodynamics, University of Stuttgart, D-70569 Stuttgart**

Abstract

A numerical approach based on 3D Computational Fluid Dynamics (CFD) for the simulation of the interfacial dynamics during the disintegration process of liquid in a resonant ultrasonic field is presented. Because of different length- and timescales of the nonlinear sound field and droplet dynamics phenomena, a decoupling is necessary for numerical feasibility. In a first step oscillating pressure- and velocity fields of the ultrasonic fields are computed. Direct Numerical Simulations of the disintegration process are then performed with an advanced Volume of Fluid (VOF) – method. The latter is extended by interfacial momentum source terms, taking into account ultrasonic forces, which lead to disintegration of the liquid phase. To resolve the small-sized fluid structures numerically, very fine computational grids are necessary. Therefore, numerical simulations are performed with parallel computing techniques.

Disintegration inside the ultrasonic field is investigated experimentally with high-speed photography. For comparison purposes between numerical and experimental results, an acoustic levitator is used as a less complex system to study the behaviour of single drops in a resonant sound field. Results obtained from numerical computations will serve for optimisation of the ultrasonic standing wave atomization (USWA) technique used for powder coating production and for application of fluid coatings of high viscosity.

Introduction

Powder coatings are used in many different areas and are gaining more and more importance by exceeding other coatings in terms of conservation (nearly no thinner emission, no waste water problems). So far, production of powder coating particles is done by energy-costly milling of polymers. Particles obtained from this process are of sharp-edged irregular shape. With a novel technique some of the disadvantages in current production processes of polymer powder can be avoided. Within this approach, particles are created by disintegration of polymer melt in an ultrasonic standing wave field. Two transducers of about 35 mm in diameter are placed towards in axial direction. Both transducers operate with different fixed frequencies close to 20 kHz. The distance between the transducers is adjusted to an odd number of the acoustic half wavelength $n\lambda/2$ to generate an ultrasonic standing wave field with usually three to five pressure nodes. Due to resonance phenomena, amplitudes of the velocity- and pressure field are very high leading to fields of strongly nonlinear nature.

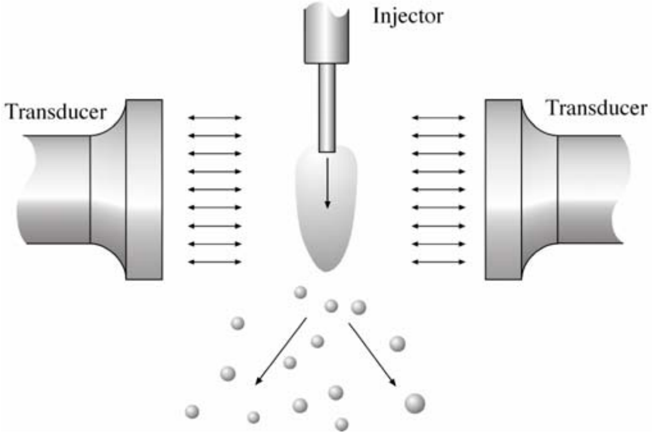

Figure 1. Scheme of the ultrasonic standing wave atomization (USWA) process.

The polymer melt is injected into the ultrasonic field and disintegrates due to the forces acting on it, giving a particle distribution of about 5–100 μm. Resulting particles are of almost spherical shape. This is an advantage over irregular-shaped particles in terms of the ability of maintaining static charge, important for direct application, and the quality of surface smoothness of the coating. Therefore, this process becomes interesting especially for automotive industry.

To gain acceptance in industry, the current USWA technique has to be optimized in terms of energy requirements, product quality, narrow particle distribution and total cost. To gain maximum capacity from this technique, a fundamental understanding of the mechanism of disintegration and a quantitative description of all influencing parameters is required. So far, optimization of the process is done mostly empirically. Measurements of the resulting pressure field between the transducer in dependence of different plate forms are quite time-consuming. Furthermore, variations of frequency and other geometrical parameters are very expensive.

Therefore, a numerical approach based on computational fluid dynamics for simulating the disintegration process caused by the ultrasonic standing wave field is developed. In literature, adequate models can be found for the description of single droplet dynamics in an ultrasonic field, for instance by *Tropea et al.* [1]. *Bauckhage et al.* describes the USWA based on semi-empirical and analytical approaches [2]. Despite of this fact, accurate models describing the disintegration of fluids in a high intensity sound field are still needed. Since the dynamical behavior of the phase boundary is strongly nonlinear with complex topological changes, the free interfacial area has to be taken into account implicitly. A numerical treatment of this problem offers the advantage for variation of geometrical and operational parameters as well as physical properties of the liquid with less effort. On the basis of data obtained from simulations, time- and cost-expensive experimental investigations can be planned, completed or even substituted.

Experimental investigations

When a continuous fluid strand is brought into a pressure node of a resonant sound field with an injector, a quasi-stationary lamella at the nozzle tip develops. Figure 2 shows some shapes of lamellas for differently chosen transducer amplitudes. Photographs are obtained with a digital video camera and a strobe flash (nanolight). The chosen view angle is of about 40 degrees, so the lamella appears to be ellipsoidal. The test substance used is a solution of an alkydale in xylole, which is a common paint raw material with a viscosity of 0.1 Pas, a surface tension of about 0.03 N/m and density of 1.1 kg/m^3. The mass flow rate is set to 100 g/min. At low amplitudes, the cohesive fluid acts like a reflector for the impinging sound waves, which causes a collapse of the resonance conditions. So this mode leads to very insufficient disintegration with a high amount of arising large ligament fragments. At this mass flow rate and for amplitudes above 60 μm, resulting particles have the desired small size with diameters between 5-50 μm.

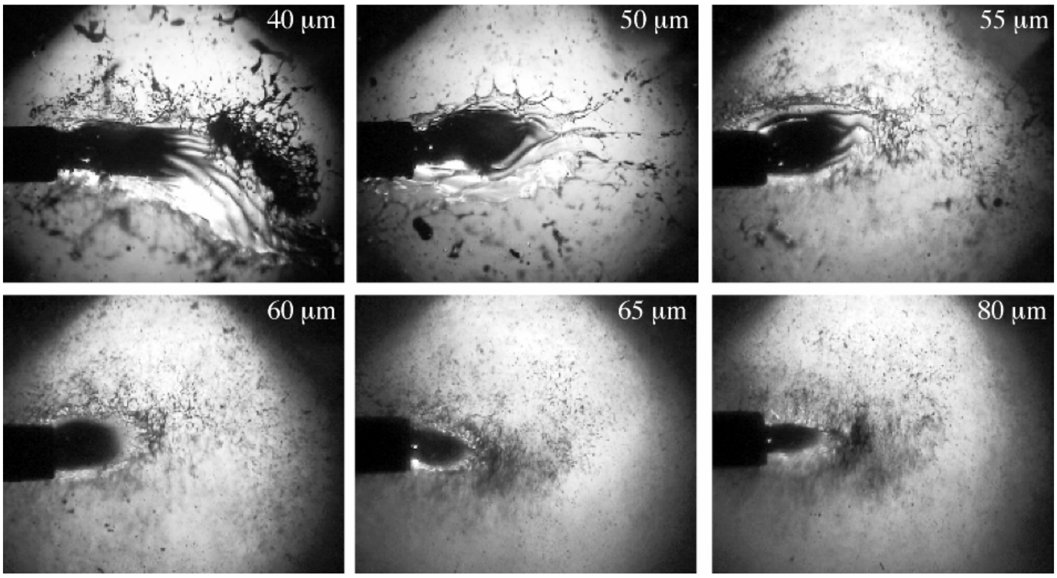

Figure 2. High-speed photographs of the disintegration of a continuous strand of alkydale solution in an USWA with variation of the transducer amplitude.

For a feasible comparison between numerical calculations and experimental investigations, an environment with reduced complexity is needed. For this purpose an acoustic levitator is used to study the dynamics of single drops in a resonant sound field. The levitator is built with a vertically mounted transducer with a fixed frequency of about 20 kHz and a concave front plate also used for the USWA. The reflector is adjusted to a resonance distance of about 22.5 mm, measured from the transducer-plate edge, to obtain stable levitation. With this distance, a sound field with three pressure nodes is obtained. Drops are brought into the central node with a syringe device.

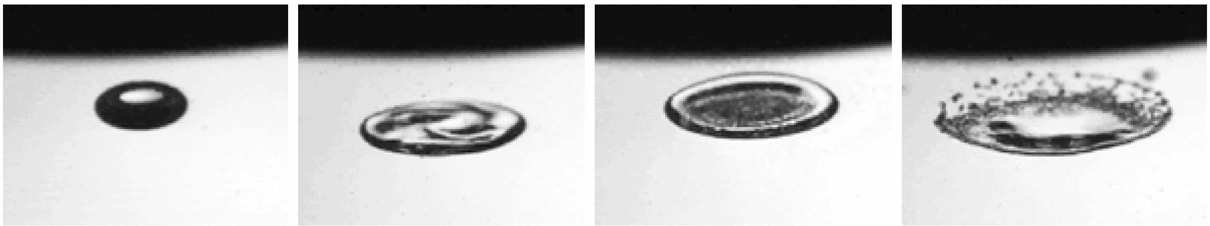

Figure 3. High-speed photographs of the disintegration of an acoustically small drop in a levitator.

For "acoustically small drops", i.e. drops with $kr_s \leq 0.3$, where $k = 2\pi\nu/c_0$ and r_s is the spherical radius of the drop, the mechanism of disintegration is illustrated by Figure 3. When the acoustic amplitude is suddenly increased, the drop drastically flattens to a lamella with a torus-shaped rim. Further flattening leads to disintegration starting from the rim with small droplets flying away horizontally.

Numerical Method

The disintegration of a fluid in an ultrasonic field is a two-phase flow with compressible gas phase. A numerical description of this process has to take into account the nonlinear behavior and dynamics of free interfacial flow topology. Here, physical phenomena take place in different length- and time-scales. Nonlinear oscillations of the sound field happen within a timescale of about 50 μs and a length-scale of 0.1 m, while drop disintegration takes longer time of 5-20 ms but smaller dimensions of less than 0.01 m. A complete description of the flow with a simultaneous treatment of interface dynamics is numerically extremely expensive even on parallel computers and not feasible for calculations with extensive parameter variations. Therefore, a decoupling of gas and liquid phase is done for numerical calculations.

In a first step oscillating velocity- and pressure fields of the ultrasonic fields are computed by solving the Navier-Stokes equations for compressible viscous flows:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\rho\mathbf{u} = 0\,, \qquad \frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = -\nabla p + \nabla\cdot\mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)\cdot \tag{1}$$

This is done with the commercial Finite-Volume CFD – Software *CFX (AEA Technology)*. Computations are performed in cylindrical coordinates for a configuration with two transducers owing concave front plates, which oscillate with a frequency shift of 130 Hz and an average frequency of about 20 kHz. To incorporate the transducer movement, periodic velocity inlet boundary conditions $u = u_0 \sin(\omega t)$ in x-direction and velocity $v = 0$ in radial direction are prescribed. The computational domain encloses additional space up to a radius of 0.0525 m around the transducers with boundary conditions set to constant pressure. Because of different axial and radial gradients, the spatial grid resolution is chosen to a minimum cell length of 0.3 mm in axial and 0.875 mm in radial direction. Each oscillation period is discretised in time with 200 time steps. The software is extended by user routines for the output of temporal averaged velocity- and pressure fields.

In a second step 3D Direct Numerical Simulations of the disintegration process are performed with an advanced VOF (Volume of Fluid) – method [3]. The VOF – method solves a set of Navier-Stokes equations for an incompressible transient two-phase flow. Advection of the dispersed phase is governed by an additional transport equation for the volume fraction *f*:

$$\frac{\partial f}{\partial t} + \nabla\cdot f\mathbf{u} = 0\cdot \tag{2}$$

Here, the dispersed fluid phase corresponds to regions where the *f*-function has the value one, while the interface is located within grid cells for $0 < f < 1$. Surface tension is taken into account based on a conservative approximation of *Lafaurie* [4]. Computations of the disintegration process are performed with the parallelized VOF-code *FS3D*, which has been developed at the *ITLR* Stuttgart [5]. For a good approximation of the free interfacial surface, numerical grids with high resolutions are necessary. Therefore, the numerical simulations are performed on a parallel computer with 96 nodes, owning two 850 MHz -*Pentium III* - processors each.

To take into account ultrasonic forces acting on the surface of the dispersed phase, a coupling of the two numerical methods is required. This coupling is realized by means of interfacial source terms that have been implemented in the VOF – code, which describe the additional momentum flux. Here, retroactions of the dispersed phase on the sound field have been neglected. The following approach is used for the calculations. Regarding the normal relative velocity **u** of the continuous phase in dependence of the surface distance of the liquid phase, the velocity is zero at the interface because of no-slip conditions. Inside a small boundary layer adjacent to the liquid surface a strongly change of relative velocity occurs. Hence, the corresponding force is given by the sum of pressure and viscous stresses. Because of low viscosity, dissipation within the gas phase can be neglected. Then the force can be approximated by the momentum flux through a plane lying parallel to the interface within the gas phase. The corresponding symmetric tensor is commonly named acoustic radiation pressure and is given by

$$\mathbf{P} \;=\; \overline{p}\mathbf{n} + \overline{\rho\mathbf{u}\otimes\mathbf{u}\cdot\mathbf{n}} \;=\; \overline{p}\mathbf{n} + \overline{\rho\mathbf{u}(\mathbf{u}\cdot\mathbf{n})}\,. \tag{3}$$

Since the dispersed fluid phase has a greater inertia than the gas phase, it cannot react on each oscillation of the gas immediately. Hence, pressure and velocity fields obtained from the compressible flow computations are time-averaged. Because of different grid resolutions, the flow fields obtained by *CFX* have to be clipped, interpolated and transformed into Cartesian coordinates before read into the VOF - code.

Simulation of ultrasonic fields

For validation of the numerical method, a circular planar piston in a rigid wall is simulated. Figure 4 shows numerical computations in comparison with an analytical solution [6] for a piston of 35 mm diameter, oscillating with an amplitude of 10 µm at 20 kHz. For a distance of about one transducer radius a maximum in the pressure distribution do to interference of emitted sound waves with waves diffracted at the wall can be found. Good agreement with theory is achieved especially in the near field region.

Figure 5 shows simulated velocity- and pressure distributions along the axis for a concave double transducer arrangement used in the USWA process. The frequencies in this example are set to 19.9 kHz and 20.13 kHz, oscillating with amplitudes of 80 µm. The optimal resonance distance for this configuration is numerically calculated as 37.5 mm in good agreement with the experimental obtained value of about 38 mm. Calculations show the complex effect of nonlinear phenomena resulting from high sound amplitudes. Due to the greater influence of higher harmonics, the velocity distributions become a saw-tooth like shape, which leads to diffuse pressure nodes.

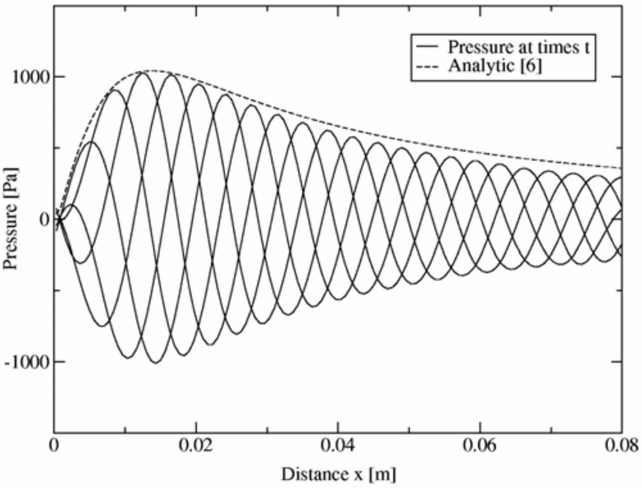

Figure 4. Simulated and analytic pressure distribution along the axis of a planar circular piston

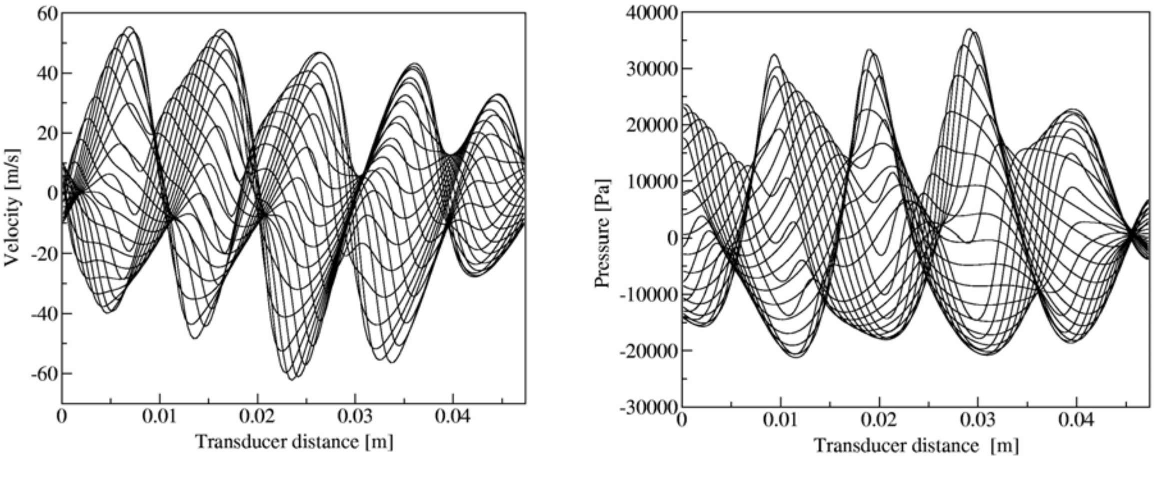

Figure 5. Simulated velocity- and pressure distributions for a configuration with two concave transducers.

Simulation of the disintegration process

In a first step the disintegration of a drop in an ultrasonic field is simulated. For this purpose, numerical simulations of the levitator with geometrical settings used in experiments are performed in *CFX*. Temporal averaged data obtained from these simulations are used to calculate the momentum source terms in *FS3D*. Figure 6 shows numerical simulations for a drop deformation exposed to this levitator sound field assuming two symmetry planes. Here, the isosurface for the *f*-function at $f = 0.5$ is visualized. The drop is exerted an immediate increase of the sound amplitude up to 2 kPa. The computational domain is set to 4 mm with a grid resolution of 64 cells in each direction. The drop has an initial spherical radius of 1.5 mm with physical properties set for water. Computed drop shapes can be compared with the high-speed – photographs in figure 3. Acoustic radiation pressure causes a drastic flattening of the drop, which forms a torus shaped rim and finally disintegrates into finer droplets beginning from the edge. In contrast to experimental observations, results do not show wave structures at the center lamella of the drop. The reason is the absence of high frequent parts of the time-averaged sound fields imported from *CFX*.

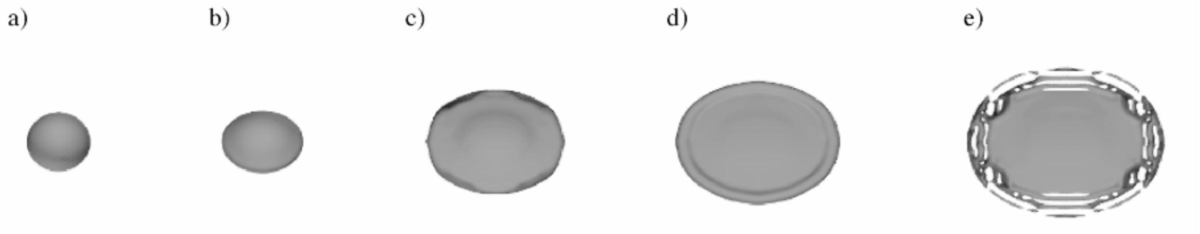

Figure 6. Simulation of a water drop with $r_s = 0.15$ in an ultrasonic levitator field.

Figure 7 shows the same drop exerted to a high-intensity sound field, which is generated with a transducer amplitude of 80 μm. The simulation is done with the assumption of two symmetry planes and a grid resolution of 128 cells in each direction. Disintegration takes place during a short time period of about 6 ms. The size of arising droplets are of about 100 μm in diameter. Droplets smaller than one grid cell cannot be resolved. Comparison with experimental observations concerning the mechanism of disintegration shows good qualitative agreement.

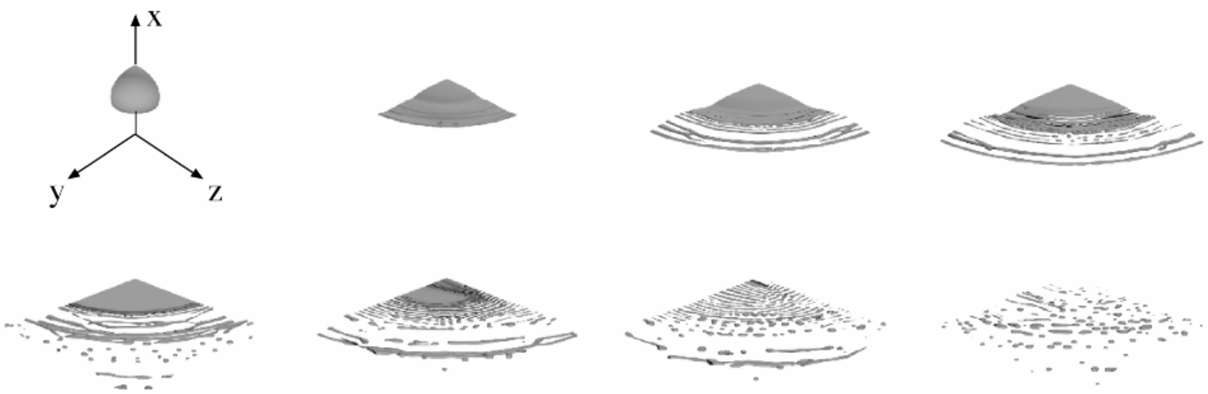

Figure 7. Simulation of a water drop with $r_s = 0.15$ suddenly exposed to a high intense ultrasonic field.

For numerical simulations of the continuous fluid strand disintegration in an ultrasonic field, the nozzle geometry in *FS3D* is set as a circular inlet with a defined length within the computational domain. Ideal tube flow is assumed inside the nozzle, so a parabolic velocity profile is set at the inlet. The strand is calculated under the assumption of symmetry with respect to the *xz*-plane. Figure 8 shows simulations of a continuous strand disintegration of a fluid with physical properties set to an alkydale solution as used in the experiment illustrated by Fig. 2. The length of the nozzle is set to 2 mm, with an inner diameter of 1.5 mm. The nozzle tip lies within the center of the sound field.

After a short time, a quasi-stationary state is reached, where the strand is deformed to a lamella by the ultrasonic forces. It disintegrates into small droplets. The flattened strand surrounds the injector tip, inducing a liquid film, which creeps up the nozzle. A downstream spray occurs. These rather unwanted phenomena can be observed in practice, too.

Conclusions

The developed numerical approach using a decoupling of ultrasonic field- and fluid disintegration simulation is a valuable tool for the optimization of the USWA process. The influence of geometrical parameters and physical properties of the fluid can be examined with feasible numerical effort. Direct Numerical Simulation of the free interfacial flow provides a good insight into the complex flow phenomena. However, further attention has to be paid on retroactions between the dispersed phase and the ultrasonic field.

The authors thankfully acknowledge the Paderborn Center for Parallel Computing (PC^2) for provision of support and computational resources.

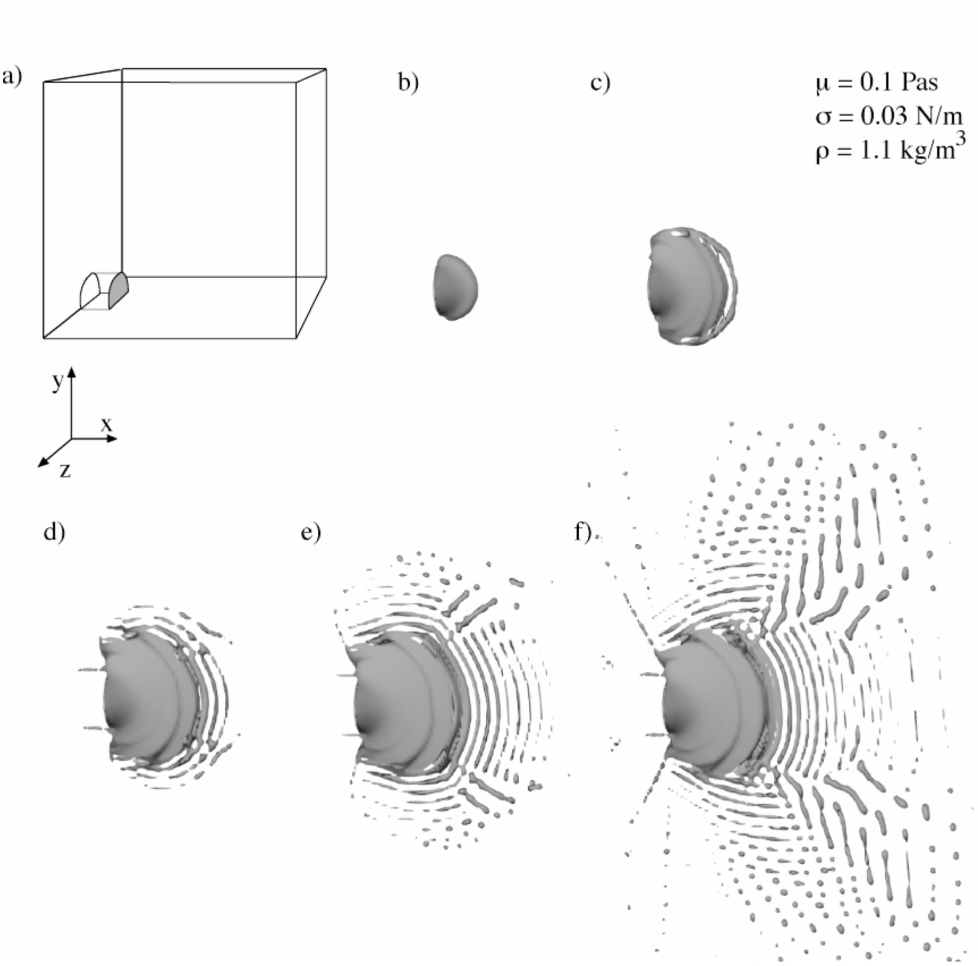

Figure 8. Simulation of a continuous fluid strand with physical parameters of an alkydale solution in a high intense ultrasonic field.

Nomenclature

μ	viscosity
$\mathbf{n}$	normal vector
p	pressure
r_s	spherical radius
ρ	density
σ	surface tension
t	time
$\mathbf{u}$	velocity

References

[1] Yarin, A.L., Pfaffenlehner, M., Tropea, C., “On the acoustic levitation of droplets“, *Journal of Fluid Mechanics* 356, 65-91, (1998).

[2] Bauckhage, K., Andersen, O., Hansmann, W., Reich, W., Schreckenberg, P., “Production of fine powders by ultrasonic standing wave atomization“, *Powder Technology* 86, 77-86, (1996).

[3] Hirt, C.W., Nichols, B.D., “Volume of Fluid (VOF) Method for the Dynamics of Free Boundaries“, *J. Comp. Phys.* 39, 201-225, (1981).

[4] Lafaurie, B., Nardone, C., Scardovelli, R., Zaleski, S. Zanetti, G., “Modelling merge and fragmentation in multiphase flows with SURFER“, *J. Comp. Phys.* 113, 134-147, (1994).

[5] Rieber, M., Frohn, A., “A numerical study on the mechanism of splashing“, *Int. J. Heat and Fluid Flow* 20, 455-461, (1999).

[6] Sutilov, V.A., *Physik des Ultraschalls*, Springer Verlag, 1984, p. 200.