PARTEC 2004

Experiment and Simulation of Charged Particle Sprays

Micha-Klaus Müller[1], Tom Winkels[1], Kees B. Geerse[1], Jan C. M. Marijnissen[1], Andreas Schmidt-Ott[1] and Stefan Luding[1]

[1]Particle Technology, DelftChemTech, TUDelft, Julianalaan 136, 2628 BL Delft, The Netherlands

ABSTRACT

In Electro HydroDynamic Atomisation (EHDA) a liquid is dispersed into small, highly charged droplets. This method has applications in medicine, agriculture, pharmacy, among others. The experimental spray is examined with a Phase Doppler Particle Analyser (PDPA) setup and the resulting density and velocity profiles are compared to numerical simulations of a spray in an identical geometry. From the numerical side, the most important result is a scale-up relation that allows to simulate an experimental spray with millions of particles, using only a few thousand model particles. The qualitative agreement between experiment and model is reasonable. For quantitative agreement, further research is required.

1 INTRODUCTION

If a fluid forms a droplet at the end of a capillary tube, the droplet deforms into a cone (Taylor cone) under the action of an electric field. Under suitable conditions a jet is formed at the cone tip. This jet is unstable due to its high charge density and breaks into small, charged droplets. These droplets have a charge that is close to the so-called Rayleigh limit charge, i.e. the highest charge a droplet can have without exploding. This process of Electro Hydro Dynamic Atomization (EHDA) has interesting applications in chemical and biological process technology, including nano-powder production, nano-dosing, nano-reactors and insecticide spraying [1-4]. The last decades have seen efforts to model parts of the system; yet a satisfactory model describing the full spray plume, including all details like liquid flow in the nozzle, evaporation and droplet collision dynamics on the target, has not been developed. Such a model is, among others, necessary for scaling up the process.

The occurrence of droplet evaporation adds considerable complexity to the process, because the droplets exceed the Rayleigh limit by shrinking and thus explode to form smaller droplets. Mono-dispersity is then lost, and thus evaporation is often undesired. In the experiment performed here, we are reasonably sure that evaporation does not occur.

The method described here focuses on the evolution of the spray between the nozzle and the target. It consists in modeling the individual trajectories of the charged droplets in the spray taking into account gravity, drag, external fields, and the self-interaction due to the unipolar charge on the droplets. In addition to the simulations, experimental data have been collected to test the model.

2 EXPERIMENTAL

EHDA is a method of atomising a liquid with the help of an electric field. In the so-called cone-jet mode, very fine, equally sized and highly charged droplets are produced [1]. The experimental set-up is schematically shown in figure 1. Droplet velocity and size measurements are done with a Phase Doppler Particle Analyser (PDPA). The PDPA equipment measures the number, the size and the velocity of the droplets at a single spot [1,2,4]. A 90:10 ethanol/triethylene glycol mixture is sprayed with a flow rate of 7.0 ml/h onto a grounded cylindrical metal target with horizontal symmetry axis. The nozzle is set to an electric potential of 18 kV. The PDPA transceiver and receiver are in front of and behind of the plane, shown in figure 1, respectively. By moving the equipment and thus the point of focus, velocity profiles can be measured. The velocity field in horizontal and vertical direction is shown for a half-plane in figure 3 below.

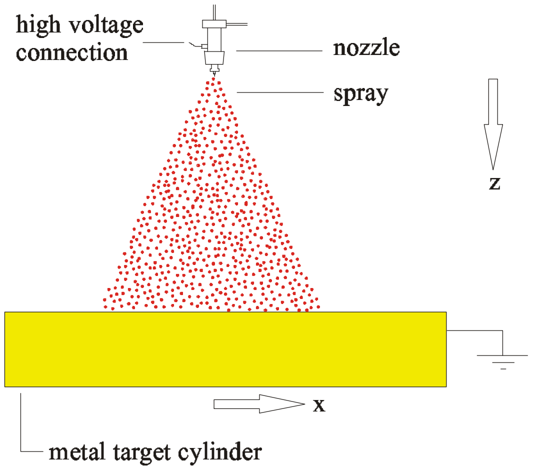

Figure 1: Scheme of the experimental set-up.

In order to resemble the experimental situation as closely as possible, a particle-based modelling approach was used, as detailed in the following section.

3 MODELING

The model developed was used to calculate the spray evolution [1,3,4]. For each droplet produced, the equation of motion

$$m_i \frac{d\vec{v}_i}{dt} = q_i\vec{E} + \vec{f}_D + \sum_{j\neq i} \frac{f_q^2 q_i q_j \vec{r}_{ji}}{4\pi\varepsilon_0 r_{ji}^3} + m_i\vec{g} \ , \qquad (1)$$

with the drag force

$$\vec{f}_D = C_D \frac{\pi}{8} \rho_{air} d_i^2 (\vec{v}_{air} - \vec{v}_i) \left| \vec{v}_{air} - \vec{v}_i \right| \ , \qquad (2)$$

is solved for each time-step dt, for each particle i. The particles are inserted with a certain rate and initial velocity at the tip of the nozzle [4]. The droplet production time (or the inverse production rate) was decreased compared to reality, while the Coulomb interaction charge q was systematically increased. For the numerical solution of the equations of motion for each particle, several assumptions lead to the four terms in Eq. (1):

(i) The first term corresponds to the force on the particles due to the external electric field between the charged nozzle and the target cylinder. For the computation of the electric field MATLAB/FEMLAB was used [3,4].
(ii) The second term is the drag force, where the atmosphere is, here, assumed to be at rest. The drag coefficient leads to Stokes drag in the laminar regime and to turbulent drag for large relative velocities, with a transient regime in between [3,4].
(iii) The third term is the particle-particle self interaction, where the sum extends over all charged particles with charge q and charge correction factor f_q. Image charges are not taken into account here.
(iv) The fourth term is the gravitational force.
(v) All other forces are neglected.

Starting the simulation with single particles being produced one by one, it takes some time until a steady state situation has evolved. The spray shape is shown in figure 2.

Besides the other forces, which are not affected by other particles, the strong Coulomb forces cause every droplet to interact with all other droplets. This leads to a many-body problem with immense effort for large particle numbers. The limits of our computing power (single processor) were reached with about 1000 droplets, for a steady state simulation.

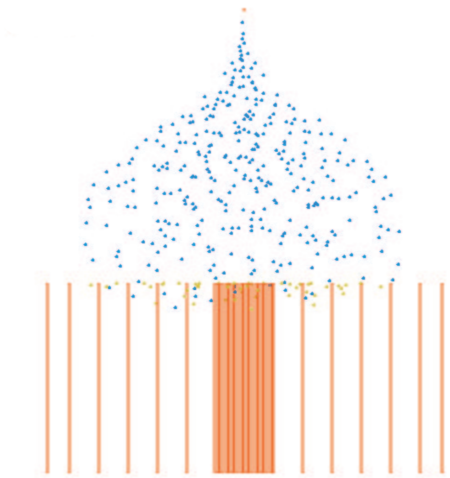

Figure 2: Snapshot from a typical EHDA-simulation. The dots are droplets and the lines indicate cylindrical geometry.

Our approach is therefore to reduce the droplet number (in experiment, typically 100 000 droplets are in the steady-state spray) by reducing the droplet production frequency. To compensate for the resulting reduction in space charge and Coulomb interaction, the particle charge is increased by a factor f_q. The problem is then reduced to finding a scaling relation between charge and concentration/production-rate and verifying its validity.

4 RESULTS

4.1 Self consistent scale-up

In order to find the charge correction factor f_q, as to be used for a realistic simulation, a set of simulations with various production-rates and charge correction factors was performed. The results were examined with respect to the size of the spray cloud/plume, as measured at the target, where the droplets are deposited.
These simulations lead to the following scaling relation between production rates and charge factors for two simulations with identical spray geometry with respect to deposition size:

$$\frac{f_q(1)}{f_q(2)} = \left(\frac{t_{prod}(1)}{t_{prod}(2)} \right)^{(0.54)} \qquad (3)$$

Two simulations were found to lead to identical deposits, if Eq. (3) describes the relation between the varied parameters. Furthermore, it is possible to extrapolate from the range of simulated parameters, which charge factor has to be used for the scaled simulation (with about 1000 droplets) of an experiment (with 100,000 droplets). Assume that for the experiment, $f_q(2) = 1$ is inserted, so that one obtains $f_q(1) \approx 12$ for a ratio of production times of about 100.

4.2 Experiment and simulation

Supplementing the “verification by simulation”, also an experimental verification of the data was performed with reasonable qualitative agreement. The results of experimental and simulation derived velocity profiles are displayed in Figs. 3 and 4, respectively. The unit of velocity is displayed as an arrow in both figures. Note that the velocity in the experiment is systematically larger than the simulation velocity.

The quantitative disagreement is due to the simplifications of the model [4], the most severe of which are: (i) no image charge is used – with an image charge, particles would be accelerated more strongly towards the target, and (ii) the gas is assumed at rest – in reality the gas is accelerated by the particles and moves with them, thus reducing the drag force on the particles and allowing for larger velocities. These points are to be addressed in more detail in a future publication [4].

5 SUMMARY AND OUTLOOK

In summary, a simple modeling approach for charged sprays was presented, taking into account the electric field, the gravity, the drag between droplets and the gas (that is at rest), and the Coulomb interaction of the particles with each other. The simulation model was tested for self-consistency and a scale-up relation was proposed that allows to simulate realistic sprays with much less particles as present in the experiment. Furthermore, comparison with experiments showed a qualitative discrepancy between model and reality, which can be attributed either to missing image charges, the static background gas or the effect of other simplifications.

The next step involves the acceleration of the computation of the particle self-interaction term in Eq. (1), by taking far away particles into account in a mean field way, possibly involving multi-pole expansions. This problem resembles the issue of self-gravity in astrophysical systems like planetary rings [5].

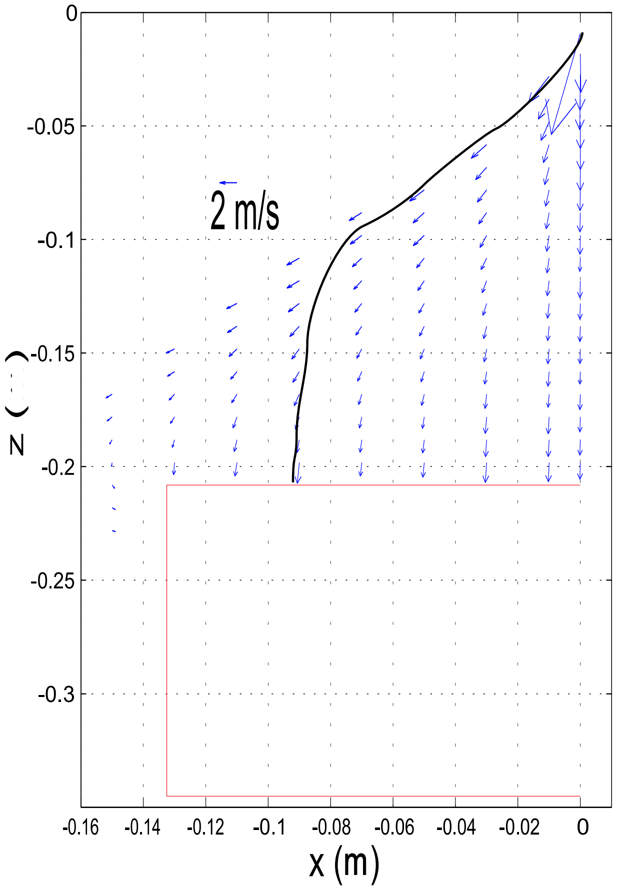

Figure 3: Measured spray velocity profile.

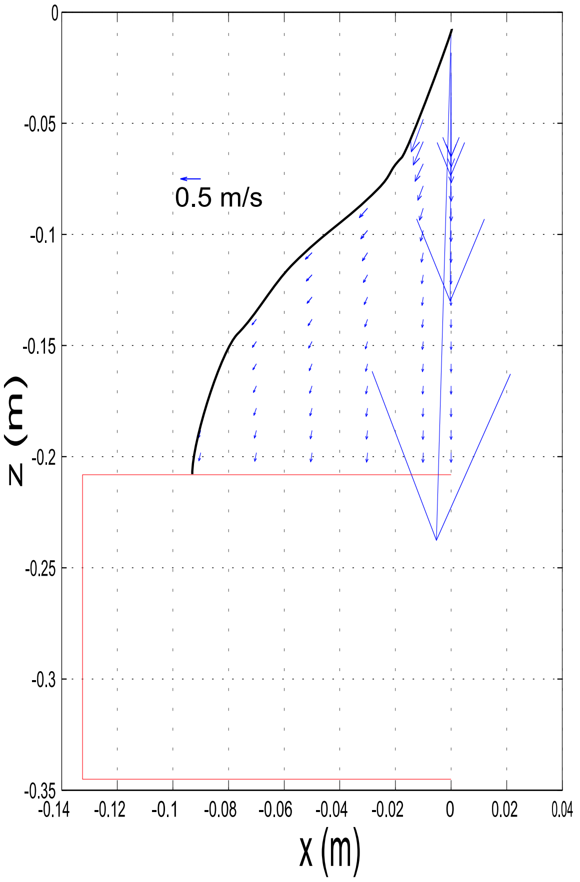

Figure 4: Simulated spray velocity profile.

Considering long-range interactions like those due to gravitational forces between particles in a ring (i.e. self-gravitation) Eq. (1) can then be reformulated to the form:

$$m_i \frac{d\vec{v}_i}{dt} = \sum_{j \neq i} \vec{F}_{ji}^{coll} - G \sum_{j \neq i} \frac{m_i m_j}{r_{ji}^3} \vec{r}_{ji} - \frac{G m_c m_i}{r_{ic}^3} \vec{r}_{ic} \quad (4)$$

where the second term corresponds to self-gravity (paralleling the Coulomb particle-particle interaction term), the last term resembles the central potential of a planet or a star, and the first term accounts for the (typically) short range collisional interaction between the particles.

ACKNOWLEDGEMENTS

This work was partially funded by a research grant of the TUDelft and by NOVEM.

6 REFERENCES

[1] Geerse K.B.: *From people to plants*, PhD Thesis, TU Delft, Faculty of Applied Sciences, Particle Technology, DCT, (2002).

[2] Hartman R.P.A., Borra J.-P., Brunner D. J., Marijnissen J. C. M. and Scarlett B: *The evolution of electrohydrodynamic sprays produced in the cone-jet mode, a physical model*, Journal of Electrostatics, 47 (1999), 143-170.

[3] Winkels T.: *Modeling and Measuring Droplet Trajectories in an EHDA Spray*, Master Thesis, TU Delft, Faculty of Applied Sciences, Particle Technology, DCT (2002)

[4] Winkels T., Geerse K. B., Marijnissen J. C. M., and Luding S.: Modeling Droplet Trajectories in an EHDA Spray, *in preparation* (2004)

[5] Müller M.-K., Luding S.: Ring Structures with dissipative Collisions: MD Simulations and Continuum Theory, *in preparation* (2004)