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Modeling simple-jet mode electrohydrodynamic-atomization droplets' trajectories and spray pattern for a single nozzle system

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ABSTRACT

Electrohydrodynamic atomization (EHDA), or simply Electrospraying is the process of influencing the breakup of a liquid into droplets by using a strong electric field. There can be different modes of Electrospraying depending, basically, on the created electric field strength and the liquid flowrate, for a specified liquid. Among these modes, the so-called cone-jet mode is the most explored one. This is due to its ability to produce highly charged monodisperse droplets in the nano- to micro-meter size range. Another mode of interest, which can also produce monodisperse droplets is the simple-jet mode. This mode is less explored when compared to the former. Within the papers that were explored by the authors, Agostinho et al. (2012) were the first authors to carefully investigate and characterize this mode. In their work, the authors reported about the influence of the electric field and the liquid flowrate on the droplets' size and spray dispersion. They also pointed out that the charge on these droplets can be expressed as a certain percentage of their Rayleigh limit.

So far, there has been no model proposed to describe the droplets' trajectories in the simple-jet mode. This paper describes the design and the implementation of a physical model for determining the droplet trajectories in this mode. The model is done, specifically, for a single nozzle/ring-up configuration. It is a two-dimensional model, which solves the force balance equation for each droplet breaking up from the jet. It takes into consideration; the initial droplet velocity, the force of gravity, the electric field force, the inter-droplet coulombic force and the drag force. The droplets' deformation and reorientation were hypothesized, from observations, to play a major role in initiating the droplets' dispersion. They were simulated by implementing periodic displacements on the droplets' center of charge from its center of mass. The calculated droplets' trajectories' envelope angle was fitted to the experimental envelope angle by adjusting the droplet charge around the values that were reported by Agostinho et al. (2012). The model was validated by comparing the shapes of the theoretical and experimental sprays.

The model offers new possibilities of modeling the droplets' trajectories in complex geometries, and of introducing additional forces to manipulate their trajectories in the simple-jet mode.

1. Introduction

Electrohydrodynamic Atomization (EHDA), or simply Electrospraying, is the process of influencing the breakup of a liquid into droplets by using a strong electric field (kV.cm^{-1}) [1]. William Gilbert (1600) is the first author to report the effect of a strong electric field on a liquid surface. In his work "*De Magnete*", he noted that when a piece of charged amber is brought close to a liquid droplet standing on a dry surface, it changes its shape from spherical into conical [2]. Since then, many authors have made a lot of contribution into the study of this phenomenon and implemented it in electrospraying [1,3].

In electrospraying, the strong electric field is produced by applying a potential difference between a nozzle and a conductive surface positioned close to it (counter electrode). This is usually performed in three different configurations, i.e. nozzle/ring-up, nozzle/ringdown and nozzle/plate [4]. For each of these

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configurations, there are different modes of electrospray, which can be created depending, basically, on the liquid flowrate, electric field intensity, and liquid properties, such as surface tension, electrical conductivity, electric permittivity, viscosity and density [5,6]. Cloupeau and Prunet-Foch (1990) were, probably, the first authors to classify the different electrospraying modes, relying on the morphology of the meniscus and the formed jet [7]. Later on, the same authors, and Grace and Marijnissen (1994) extended the classification further into dripping, spindle, intermittent cone-jet, cone-jet, and the multiple-jet modes; for low flowrates, and the simple-jet mode; for higher flowrates [8,9]. Among all these modes, the cone-jet mode is, so far, the most explored because of its capability of producing highly charged monodispersed droplets in the nano- to micro-meter size range. More information about this mode can be found in the literature [3,10,11].

Many theoretical investigations have also been conducted to predict some of the electrospray characteristics, such as the droplets' movement, the spray pattern, the liquid breakup process, etc. Most of these investigations, however, are done only for the cone-jet mode. Gañán-Calvo et al. (1994) proposed an electrospray model using the Lagrangian model of particle motion [12]. The author used the momentum equation given by Tchen (1947) and Maxey (1983), taking into account four types of forces, namely: gravitational force, electric field force, coulombic force and drag force [13]. Tang and Gomez (1994) modified this model further by calculating the electric field using the measured droplets' velocities [14]. Grace and Dunn (1996) presented a two-dimensional mathematical model to describe the droplet behavior within an electrodynamic fine spray [10]. Later on, Hartman et al. (1999) modeled the Taylor cone and calculated the spray dispersion. Unlike Gañán-Calvo and Tang, Hartman calculated the background electric field using Gauss Law and assumed a smaller radial displacement of the droplets at their region of formation. The author also assumed a bimodal droplet size distribution instead of the lognormal droplet size distribution used by Gañán-Calvo [3]. Later on, Geerse (2003) described a three-dimensional model for predicting the droplet dispersion and the deposition region. He calculated the background electric field using FEMLAB® software package [4]. Grifoll-Taverna, J. and Rosell-Llompart, J. (2009) described a numerical model that predicts the spray characteristics in the same mode, using a nozzle/plate configuration [15].

The simple-jet mode has not been so much explored as the cone-jet mode, both, experimentally and theoretically. However, it is the recommended mode for applications that depend on electrospraying at high throughputs, such as spray drying, and desalination systems [1]. Agostinho et al. (2012) are, probably, the first authors to experimentally analyze and characterize this mode. In their work, the authors defined an operational window for this mode in relation to the electric potential and the liquid flowrate for deionized water. They further investigated the effect of liquid electric conductivity on the spray diagram and found out that it only plays a very small role, concerning whipping and dispersion limits. Additionally, they pointed out that the droplet charge can be expressed as a certain percentage of their Rayleigh limit [1]. The authors, further, presented a simple-jet multi-nozzle system and reported its influence on liquid evaporation [16].

In this work the authors are proposing a physical model which can be used to describe the droplet trajectories in the simple-jet mode. The specified input parameters include: background electric field, droplet initial velocity, droplet size distribution, jet breakup length and droplet charge. These parameters were specified for a given set of liquid flowrate and applied electric potential. The background electric field is calculated using COMSOL Multiphysics® software package. The droplets' trajectories are calculated by solving the force balance equation for each droplet using MATLAB®. The input parameters of the model, as well as the real spray pattern used to validate the model, were obtained by analyzing images taken with a high-speed imaging system.

The model was qualitatively validated by comparing equivalent theoretical and experimental spray shapes, and quantitatively by comparing their axial cross-sectional areas. After validating the model, different components of the forces acting on the droplets were analyzed. This analysis indicated that the coulombic force was the major component contributing to the droplets' dispersion.

The model introduces new possibilities of modeling in more complex geometries and of predicting the kind of extra forces, such as secondary electric field and an airflow, necessary to manipulate the droplets' trajectories in the simple-jet mode.

2. Methodology

The adopted method for constructing and validating the model can be resumed in three steps: data acquisition, calculation of the droplets' trajectories, and validation. Data acquisition was done by both calculating the background electric field with COMSOL Multiphysics® software, as well as by experimentally obtaining other input parameters, such as the droplets' initial velocity, droplets' average Feret diameter, droplets' size distribution and the jet breakup length. Sequentially, these input parameters were used to calculate the droplet trajectories and consequently, the spray patterns using MATLAB®. Finally, the model was validated by comparing the theoretical spray patterns to their equivalent experimental spray patterns. This process was done for different values of the liquid flowrate and electric field intensity. In the validation phase, whenever a deviation of more than 10% between the theoretical and experimental spray patterns was found, the droplets' charge was adjusted in the model and their trajectories were calculated again. A more illustrative view of the followed steps is as shown by the fluxogram presented in Fig. 1. A detailed explanation for each step is given in the next section.

2.1. Input parameters

The data input part of the model was based on two main steps, i.e. calculation of the background electric field using COMSOL Multiphysics® software, and obtaining the spray/droplets characteristics.

2.1.1. Calculation of the background electric field

The process of calculating the background electric field as a function of the setup geometry, using COMSOL Multiphysics® software package, started by defining the geometry for a single nozzle/ring-up configuration (Fig. 2). This geometry was similar to the one which was used for all the experiments. It is known that the best environment in this case would be a 2D axisymmetric or a 3D. However, as will be also further commented, to take advantage of the known symmetry of EHDA sprays and make the model simpler, the authors decided to opt for a 2D environment. Additionally, the validation technique which was to be used to verify the final trajectories of the droplets was also a two dimensional technique. Therefore, the definition was done using the 2D space dimension package in the electrostatics interface of the software's AC/DC module, for a stationary study scenario. The geometry was defined with a nozzle of outer diameter (OD) of 0.51 mm and an inner diameter (ID) of 0.25 mm. The distance between the nozzle tip and the counter electrode ring was set to 17 mm. Materials were defined using the in-built COMSOL Multiphysics® Material library in the following way: copper was used for the counter electrode ring, stainless steel 405 annealed for the nozzle, FR4 (circuit board) for the counter electrode support, and finally, air was used for the