Journal of Aerosol Science 118 (2018) 82–99

Contents lists available at ScienceDirect

Journal of Aerosol Science

journal homepage: www.elsevier.com/locate/jaerosci

Analysis of the space charge singularity near the Taylor cone apex via simplified Eulerian model for electrospray beams in vacuum

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ARTICLE INFO

Keywords:
Electrospray
Eulerian model
Space charge
Taylor cone

ABSTRACT

A simplified Eulerian model for the description of steady state electric charge dispersion in vacuum, including space-charge effects, is introduced. The model is based on a potential velocity field for the charged particles, which is valid if all the particles are emitted with the same kinetic plus potential energy. Despite the high simplicity of the present model, the mathematical system still encompasses several types of singularities, which are analyzed here in full detail, thus enabling the numerical solution of the system. The model is applied to the description of electrospray emission in vacuum, in the limit of high electric conductivity liquids, assuming that all particles are emitted with zero initial velocity. Our main result in this regard is a relation existing between the cone semiangle α and the electrospray beam angular width. In particular, we show that the cone semiangle can only take values between a minimum angle ca. 21.89 deg, and a maximum value given by Taylor's angle (ca. 49.29 deg), with lower values of α corresponding to wider beams, while higher values of α correspond to narrower beams.

1. Introduction

When the interface between an electrically conducting liquid and an insulator (air or vacuum) is charged beyond a certain value a conical structure is formed (Zeleny, 1914, 1915, 1917). As explained by Taylor's analysis, the formation of this conical structure, known as the Taylor cone, is due to the balance between the electrical pressure and the opposing surface tension (Taylor, 1964). One of the most relevant results derived from Taylor's analysis (Taylor, 1964) is the value of the cone semiangle, 49.29 (deg), which is known as Taylor's angle. A remarkable aspect of the Taylor cone is that its apex is the source of a spray of submicron charged droplets, usually known as *electrospray* (Fernández de la Mora, 2007). Since the initial observations on droplet disintegration by Zeleny and later explanation of the phenomenon by Taylor, loc. cit., the type of electrohydrodynamic atomization known as electrospray has become of great relevance owed to its applications in several fields (see, e.g., Lozano & Martínez-Sánchez, 2005; Perez-Martinez & Lozano, 2012; Perez-Martinez, Guilet, Gierak, & Lozano, 2011 and references therein). This explains the considerable literature available on the properties and structure of electrospray beams (see, e.g., Driesel, Dietzsch, & Mühle, 1996; Driesel, Dietzsch, Hesse et al., 1996; Fernández de la Mora & Loscertales, 1994; Gamero-Castaño & Fernandez de la Mora, 2000; Gamero-Castaño, 2008; Romero-Sanz & Fernández de la Mora, 2004; Tang & Gomez, 1994). From the theoretical point of view, Taylor's analysis (Taylor, 1964) is based on neglecting the corrections owed to the space charge distribution around the cone. Space charge effects are also neglected in the numerical analysis of Pantano, Gañán-Calvo, and Barrero (1994), where the shape of tip-ended, axisymmetric, electrified menisci is analyzed. On the other hand, Fernández de la Mora (1992) formulated an approximated conical model, valid for atmospheric electrosprays with negligible inertia including space charge effects, while inertia effects were analyzed by the

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https://doi.org/10.1016/j.jaerosci.2018.02.002
Received 2 August 2017; Received in revised form 26 January 2018; Accepted 2 February 2018
Available online 06 February 2018
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Lagrangian model by Gañán-Calvo, Lasheras, Dávila, and Barrero (1994) for atmospheric electrosprays with significant inertia.

Electrospray experiments in air (Fernández de la Mora, 1992) show that small flow rates lead to cone semiangles close to Taylor's angle. Nevertheless, smaller values of the cone semiangle are observed as the flow rate increases. A similar behavior is also found in electrospray experiments in vacuum. In this regard, the experiments of Driesel, Dietzsch, Hesse et al. (1996), Driesel et al. (1996) show the influence of the space charge on the tip shape of Taylor cones with jet-like protrusion in vacuum. In particular, the cone semiangle and the jet-like protrusion's length and diameter are measured as a function of the ion emission current. The qualitative explanation for this phenomenon is based on the fact that the emitted spray contains charge of the same sign as the liquid cone and, hence, the repulsion produces smaller cone semiangles than Taylor's angle. The aforementioned theoretical model by Fernández de la Mora (1992) provides an analytical explanation to the space charge effects on the cone semiangle for the case of a conical atmospheric electrospray of identical droplets with negligible inertia, which is originated at the apex of a conductor liquid cone. According to this model the cone semiangle can only take values below Taylor's angle and, in addition, mathematical relations between the spray semiangle, the cone semiangle and the emitted electric current are derived, showing that as the spray current is increased higher values of the spray semiangle and lower values of the cone semiangle are obtained (Fernández de la Mora, 1992).

In this work a simplified Eulerian model (SEM) is introduced to describe the dispersion of identical charged particles in vacuo. The mathematical model assumes axial symmetry and steady state. The present SEM is based on the fundamental hypothesis of considering an irrotational velocity field for the emitted particles. Thus, the velocity field is given by the gradient of a scalar function called the velocity potential. We show that, under the present symmetry assumptions, this result is to be expected when all particles are emitted with the same potential plus kinetic energy. Hence, knowledge of three real scalar fields: charged particles number density function, electric potential and velocity potential, allow for the complete Eulerian description of the system. The three equations that determine the former scalar fields are given by the energy conservation equation, Poisson's equation and the continuity equation. Self-similar solutions in spherical coordinates (or conical solutions) are investigated in detail. In particular, the model is applied to analyze the electrospray in a small neighborhood around the cone apex, where the space charge effects are dominant (Fernández de la Mora, 2012). On the other hand, provided the aforementioned simplifying assumptions apply, the mathematical analysis of the present SEM shown below is fully general, and it will be also of interest for the modelization of electric charge dispersion in vacuum in other systems of interest (e.g., conical metallic cathodes, Finn, Antonsen, & Manheimer, 1988).

The paper is organized as follows. In Section 2 we introduce the present Simplified Eulerian Model (SEM), along with its underlying assumptions, conservation equations and boundary conditions. This section concludes with the dimensionless formulation of the SEM, based on the characteristic scales in the space charge region, which are derived from dimensional considerations. The solution of the former SEM, based on separation of variables, is shown in Section 3. This leads to the formulation of the corresponding angular system, which is also shown in this section. The aforementioned angular system is a nonlinear boundary value problem in terms of the angular variable. The numerical solution of this system requires previous knowledge of its asymptotic behavior near its corresponding singular points, which is the subject of Section 4. Based on the results found in Section 4, in Section 5 we introduce, and successfully apply, a strategy for the numerical integration of the angular system. The main results derived from the aforementioned numerical solution are analyzed in Section 6. Finally, we conclude in Section 7 with a summary of the main conclusions derived from the present work.

2. Problem formulation

Fig. 1 shows a schematic of the ideal problem geometry considered in the present work. An infinitely conducting electrified liquid

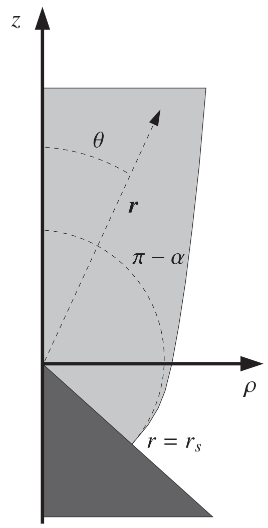

Fig. 1. Sketch of the problem geometry and notation ($\rho \equiv$ distance to symmetry axis).

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