



Charge of water droplets during evaporation and condensation

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ABSTRACT

A mechanism of water (ice) electrification during evaporation or condensation is proposed, based on non-linear equations of electrodiffusion in a moving medium. The electrification is caused by the difference in coefficients of the diffusion of intrinsic charge carriers in water (ice), i.e., protons and hydroxide ions, as well as their accumulation and depletion at the evaporation and condensation front accordingly. The accumulation (depletion) of the carriers is contingent on the existence of a potential barrier for the transition from water (ice) to vapor. The electrification intensity is affected by a double electric layer created by orientational defects at the surface of water (ice). Dependencies are calculated between the electric field intensity at a flat surface of water and ice, and the phase transformation rate. The electric charge of spherical water droplets is evaluated for various droplet radii.

1. Introduction

Interest in the origin of electric charge in water particles in clouds and atmospheric precipitation has developed for many reasons. First of all, this interest is connected to the traditional craving for a deeper understanding of the nature of atmospheric electricity (Harrison, Aplin, & Rycroft, 2010; Kuznetsov, 2004; Rakov & Uman, 2003; Shimogawa & Holzworth, 2009; Williams, Markson, & Heckman, 2005). Secondly, it is connected with solving the mystery of the fast growth of water droplets to raindrop size in clouds (Elperin, Kleeorin, Liberman, & Rogachevskii, 2013), where a mechanism of electric coagulation may play an important role (Shavlov & Dzhumandzhi, 2016). Thirdly, this interest is associated with the ability of charged particles to become ordered in space, to influence the viscosity of airborne droplet media and the processes of heat and mass transfer in the atmosphere (Shavlov, Sokolov, Hazan, & Romanyuk, 2014). A known issue of clear air turbulence may also be related to the electrical interaction between water particles (Shavlov & Sokolov, & Dzhumandzhi, 2016).

In earlier works (Frenkel, 1949; Sedunov, 1972; Voyeykov, 1904), the selective adsorption of air ions at water surfaces was indicated as the reason for water droplets being charged in the atmosphere. The adsorption was controlled by the electric double layer existing at the water surface. The field of this layer hampered the adsorption of positive ions, facilitating the adsorption of the negative ones. At present, many works have been published on the molecular simulation of adsorption at the water-gas interfaces of halide anions, including F⁻, Cl⁻, Br⁻ and I⁻, and alkaline cations, such as Li⁺, Na⁺, K⁺, Rb⁺ and Cs⁺, which are widespread in natural water environments (Jungwirth & Tobias, 2000; Consta & Kapral, 1999; Yang & Li, 2005; Caleman, Hub, Maaren, & Spoel, 2011; Otten, Shaffer, Geissler, & Saykally, 2012; Saykally, 2017). In these works, the water drops were on the whole electrically neutral, but due to polarization forces, anions and cations could be irregularly redistributed between a drop volume and its surface. It was shown that halide anions have minimum free energy at the water-gas interface, while alkaline cations have minimum free energy in the water volume. In the work of (Jungwirth & Winter, 2008), research was carried out into the adsorption of the proper ions, protons

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and hydroxide ions, of water. It was established that the pH index of the water surface layer is shifted to the acidic values of $\text{pH} < 4.8$ due to the surface adsorption of protons. The obtained results are important for understanding the chemical interaction of water droplets with atmospheric gases, which can cause ozone layer depletion. It should be noted that the quoted modern works considered ion adsorption in the presence of water and gas phase equilibrium. There is no phase equilibrium in clouds. The water droplets continuously exchange matter with gas, they either evaporate or grow due to condensation. Simultaneously, the conditions of ion adsorption may alter appreciably. In addition, water droplets may lose their electrical neutrality. The charge acquired by the droplets may depend on the direction and rate of phase transformation. Indeed, the experiments of (Dong & Hallett, 1992) showed that the water phase is charged negatively in relation to vapor in the case of water evaporation and charged positively in the case of condensation. In the processes of evaporation and condensation, ice could be charged in opposition to water. It is obvious that molecular simulation of selective adsorption of ions at the water-gas interface is not sufficient for mathematical simulation of water droplet electrification processes during evaporation and condensation. The equation of continuous media (Landau & Lifshitz, 1960) has to be used, which takes into consideration the ionic diffusion, electric drift and transfer of matter through the interphase boundary.

The types of ions that control the charge of water droplets in clouds are indicated by a known fact that the electrical conductivity of the mist environment in a cloud is ten times higher than the electrical conductivity of pure air with no water droplets (Imyanitov & Chubarina, 1965). The ions that appear in gas in the presence of water droplets are apparently the proper ions, protons and hydroxide ions, of water. These ions move from the water into gas phase during the evaporation and condensation of droplets.

In our previous work (Shavlov, 2009), we proposed an electrodiffusion model of water electrification during its evaporation (condensation) with the participation of the proper charge carriers of water, namely, protons, hydroxide ions and orientational defects. The non-equilibrium quantity of these carriers was generated in the process of phase transformation. An electric field was calculated at the water-gas boundary. The influence of phase transformation rate on the field value and polarity was studied. There were several drawbacks in this work: a) the possibilities of charge separation in the conditions of phase equilibrium of water (ice) and vapor were not considered; b) the difference in H_2O molecule condensation coefficients for water and ice was not taken into account; c) non-linear variants of the problem which are, as a rule, more realistic, were not calculated.

The current work is dedicated to the simulation of the inter-phase separation of protons, hydroxide ions and orientational defects during evaporation and condensation of water and ice. The calculations are free from the drawbacks of our previous work (Shavlov, 2009). Non-linear macroscopic equations of electrodiffusion in a moving medium are used. We consider the difference in proton and hydroxide ion diffusion coefficients, and their accumulation and depletion at the evaporation and condensation fronts, accordingly. The accumulation (depletion) of carriers is caused by the existence of a potential barrier during the transition from water to gas. The value of the potential barrier is a reflection of the microscopic properties of charge carriers in various phases. In this work, we calculate the electric field at the water (ice) surface during evaporation and condensation. We then evaluate the efficient electrical charge of spherical water droplets at various phase transformation rates.

2. Problem formulation

Let us consider a flat contact of water or ice with a vapor-air mixture at the standard atmospheric pressure and temperatures at which water and ice may exist. Charge carriers in water and ice are represented by protons, hydroxide ions and orientational L - and D -defects. The equilibrium concentrations of the protons and hydroxide ions are many orders of magnitude less than the equilibrium concentrations of the orientational defects. On this basis, the process of charge carrier transport in water or ice can be divided into two: 1) the process of diffusion of orientational L - and D -defects in a self-consistent electric field and 2) the process of diffusion of protons and hydroxide ions in the absence of a self-consistent electric field destroyed by orientational defects, and in the presence of a self-consistent electric field of orientational defects as an external one. This approach is similar to the separate consideration of the diffusion of majority and minority charge carriers in semiconductors (Bonch-Bruyevich & Kalashnikov, 1977).

It is to be recalled that the orientational defects appear and disappear when water molecules in a condensed phase turn. They appear in pairs, one L - and one D -defect, and disappear (recombine), also in pairs. An L -defect, which carries a negative charge, corresponds to such an orientation of two closest water molecules, where there are no protons on the line connecting oxygen atoms. A D -defect (positive charge) corresponds to two protons on the line; defect-free condition (no charge) – one proton on the line. Protons and hydroxide ions are also born in pairs when water molecules dissociate, and disappear (recombine), again in pairs.

In a vapor-air mixture, a charge is carried by protons and hydroxide ions. Orientational defects do not exist in this medium, as water molecules rotate at a high rate and do not interact with each other, except for encounter processes. We consider air to be sufficiently transparent for vapor, so that the vapor concentration slightly depends on the distance from the evaporation or condensation front. For this purpose, the phase transformation rate must be low. In a vapor-air mixture, protons and hydroxide ions diffuse in a self-consistent electric field.

The calculation method is as follows. At first, we formulate and solve the problem of the diffusion of orientational defects in water and ice, and calculate the self-consistent field, which we call *an electric double layer field of orientational defects*. Then, we formulate and solve the problem of inter-phase separation of protons and hydroxide ions in the electric double layer field and calculate the electric field in vapor near the water or ice surface. Finally, with the help of this field, we estimate the effective electric charge value of spherical water droplets with various droplets radii and at various evaporation and condensation rates.

2.1. Orientational defect problem

Let us assume that water or ice takes half-space area $x > 0$. The majority charge carriers in these systems are orientational

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