# Determination of mass and thermal accommodation coefficients from evolution of evaporating water droplet

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# ABSTRACT

Evaporation of a droplet of pure water, several micrometers in size, was investigated. The droplet was levitated in an electrodynamic trap placed in a small climatic chamber. The evolution of the droplet and the evolution dynamics was studied, by analyzing the coherent light scattering patterns with the aid of Mie theory. A numerical model of droplet evolution, incorporating the kinetic effects near the droplet surface was constructed. By applying this model to the experimental data, the mass and thermal accommodation coefficients were determined to be  $\alpha_C = 0.12 \pm 0.02$  and  $\alpha_T = 0.65 \pm 0.09$ . This model enabled to find the droplet temperature evolution and the relative humidity in the droplet vicinity with high precision, as well.

Keywords: mass accommodation coefficient, thermal accommodation coefficient, droplet evaporation

## **1. INTRODUCTION**

The processes of evaporation and condensation are in the very heart of various fields of science. Cloud and aerosol microphysics together with construction of climate models,<sup>1</sup> or electrospraying and combustion are just a few examples. In many cases the evolution of a droplet of the size comparable to the mean free path of the gaseous medium molecules must be considered. This in turn requires considering the kinetic effects, taking place near the liquid surface of the evaporating droplet - up to the distance of a mean free path of the vapor molecule in gaseous medium. It is necessary then to supplement diffusion coefficient D with so called evaporation (condensation) or mass accommodation coefficients describe the transport properties of the liquid-gas interface. The mass accommodation coefficient can be perceived as the probability that a molecule (e.g. water) impinging the interface from the gaseous phase side enters into the bulk liquid phase and not rebounds. Analogically, the thermal accommodation coefficient determines the probability that a molecule on impinging the interface from the gaseous phase side enters into the bulk liquid phase and not rebounds. Analogically, the thermal equilibrium with the medium on the opposite side. The coefficients of the transport in opposite directions are considered equal. Both coefficients are phenomenological and should describe solely the properties of the very interface.

# 2. EVAPORATION OF THE WATER DROPLET

A droplet of pure water in the humid (not supersaturated) ambient air evaporates - the droplet is not in equilibrium with its surroundings. The evaporation starts at the cost of the droplet heat. The fastest molecules leave the liquid phase for the vapor and the gradients of temperature and water vapor density near the droplet surface appear. After a fraction of a second the gradients attain some relatively constant value and the evaporation enters its stable phase. The gradients are driving force for further evolution. If the temperature of the droplet  $T_a$  was initially equal to the temperature of the reservoir  $T_{\infty}$  after some time  $T_a < T_a(0) = T_{\infty}$ . Neutral droplets evaporate completely. Charged droplets evaporate until Coulomb explosion occurs. For the droplets of solution a stabilization of the size is possible since the increase of concentration lowers the (equilibrium) vapor pressure over the surface of the solution.

A model of evaporation which was used during the investigation was based on transport equations incorporating the kinetic effects<sup>2-4</sup> and the effect of droplet charge<sup>5,6</sup> The kinetic effects are accounted for by means of the effective diffusion coefficient  $D_k$  and effective thermal conductivity coefficient  $\lambda_K$  which are not constant but are functions of the droplet radius and its temperature. The steady state evaporation of a charged droplet is

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Figure 1. A sample solution of the equation system (1)-(2). The linear approximation of  $T_a(t)$  for  $t \in (t_1, t_2)$ , dashed line.

governed by the mass and heat transport equations supplemented with the Rayleigh's stability condition<sup>7</sup> (see also<sup>8</sup>):

$$\dot{a} = \frac{MD_k(a, T_a)}{Ra\rho_L} \left\{ S\frac{p_s(T_\infty)}{T_\infty} - \frac{p_s(T_a)}{T_a} \exp\left[\frac{M}{RT_a\rho_L} \left(\frac{2\gamma}{a} - \frac{Q^2}{32\pi^2\varepsilon_0 a^4}\right)\right] \right\} , \tag{1}$$

$$\dot{T}_a = \frac{3}{a^2 c_w} \left[ q a \dot{a} - \frac{\lambda_K(a, T_a)}{\rho_L} (T_a - T_\infty) \right] , \qquad (2)$$

$$\frac{E_Q}{2E_\sigma} = \frac{Q^2}{64\pi^2\varepsilon_0\sigma a^3} < 1 , \qquad (3)$$

where  $a, T_a$  and Q are the droplet radius, temperature and charge respectively;  $T_{\infty}$  and S are the temperature and relative humidity far from the droplet (the reservoir volume is  $\sim 10^{64}$  times larger than that of the droplet),  $p_s$  is the saturated vapor pressure at a given temperature,  $\rho_L$  and  $\gamma$  are the liquid water density and surface tension respectively,  $\varepsilon_0$  is the permittivity of vacuum, M is the water molecular mass, R is the universal gas constant,  $E_Q$  is the Coulomb energy of a charged droplet and  $E_{\sigma}$  is the energy associated with the surface tension. The effective diffusion coefficient  $D_k(a, T_a)$  and the effective thermal conductivity  $\lambda_K(a, T_a)$  of the moist air have the forms of:

$$D_k = \frac{D}{\frac{a}{a+\Delta_C} + \frac{D}{a\cdot\alpha}\sqrt{\frac{2\pi M}{RT_a}}},\tag{4}$$

$$\lambda_K = \frac{\lambda}{\frac{a}{a+\Delta_T} + \frac{\lambda}{a \cdot \alpha_T \rho_A c_P} \sqrt{\frac{2\pi M_A}{RT_a}}},$$
(5)

where  $\Delta_C \approx 1.3\lambda_a$  and  $\lambda_a$  is the mean free path of air molecules and  $\Delta_T$  is the 'thermal jump' distance; D is the diffusion constant for water vapor in air,  $c_w$  and q are specific heat capacity and latent heat of evaporation of water respectively,  $\lambda$ ,  $\rho_A$ ,  $c_P$  and  $M_A$  are thermal conductivity, density, specific heat capacity under constant pressure and molecular mass of moist air respectively.



Figure 2. The evolution of radius and temperature of the droplet retrieved from the experiment, compared with the results of numerical calculation from the model utilizing previously determined parameters.

# **3. DETERMINING** $\alpha_C$ **AND** $\alpha_T$

It can be easily noticed (see figure 1), that for steady state evaporation, for some range of time  $(t_1 < t < t_2)$ ,  $T_a(t)$  can be treated as a linear function of time. The influence of the droplet charge and surface tension (as well as feasible in the investigated case solution concentration) upon the solution of equations set (1)-(2) in this region is negligible. For  $t > t_1$  it can be assumed that all the heat flowing to the droplet is used up for evaporation. Then the equation (2) can be much simplified and presented in the following form:

$$Bt + C = T_{\infty} + a\dot{a}\frac{q\rho_L}{\lambda_K} , \qquad (6)$$

where B and C are constants. Utilizing the heat and mass transport equations (6) and (1) (without the charge term) and the function a(t) obtained from the experiment, the values of the coefficients  $\alpha_C$  and  $\alpha_T$  can be determined. They are determined by means of statistical analysis of the solutions of equation sets which are created for any 3 time-points for (6) -  $\alpha_T$  and any 2 time-points for the mass transport equation (1) -  $\alpha_C$  between  $t_1$  and  $t_2$ .

#### 4. EXPERIMENT

An electromagnetic trap kept in a small climatic chamber was in the heart of experimental setup. The detailed description of our experimental setup can be found in.<sup>8</sup>

Temperature in the upper and the lower part of the chamber was controlled separately. Such setup enabled us to get rid of vertical temperature gradients. Horizontal gradients were measured to be negligible. There were also two relative humidity sensors: above and below the trap.

Before the experiment, the chamber was flushed with dry nitrogen (from above LN) in order to get rid of liquid water that accumulates in the chamber during the experiment due to condensation and stray injection. Next, a filtered humid air (obtained by bubbling through the distilled water) was flowed through the chamber from the bottom to the top port. When the required humidity and the satisfactory humidity gradient were reached, the flow was stopped in order to enable uninfluenced trapping. Between the instants of trapping the chamber was flushed with humid air to maintain required humidity conditions.

Applying the method presented in the previous section to five data sets collected under thermodynamic conditions:  $T_{\infty} = 286.3 \pm 0.2$  K and  $286.9 \pm 0.2$ , atmospheric pressure 1006 hPa (public meteorological data) and the relative humidity between 84 and 98% (the approximate values measured with humidity sensors) yielded precisely the same value of  $\alpha_C = 0.12 \pm 0.02$  and an average value of  $\alpha_T = 0.65 \pm 0.09$ . The relative humidity S found simultaneously with  $\alpha_C$  varied from set to set in the range of  $(0.974 \div 0.983) \pm 0.009$ . The evolution of the droplet is extremely sensitive (<  $10^{-3}$ ) to S which makes checking the obtained values with some probe very difficult (accuracy of instruments does not exceed  $(10^{-2})$ .

Values of all parameters pertaining to water, moist air and other properties of the system were taken from literature (e.g.<sup>9</sup>).

The self consistency of the method was verified by comparing the experimental data with the numerical model calculations for the coefficients and humidity previously determined from the experimental data (see figure 2).

## 5. CONCLUSION

We have presented a method of simultaneous determination of  $\alpha_C$  and  $\alpha_T$ . It is based on the analysis of the dynamics of the evolution of radius of the evaporating droplet. The method was applied to a few sets of experimental data and yielded values consistent with other authors' results e.g., <sup>10, 11</sup> Additionally it enabled to find the evolution of the droplet temperature and the relative humidity of the droplet surroundings with a very high precision.

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