

Measurement of the Atmospheric Electricity III

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Procedures of data processing on the measurement with ion mobility spectrometer are described. The electric potential in the interior of capacitor of our mobility spectrometer is numerically calculated with Monte Carlo method. The fringe effect of electrode upon the potential field in the instrument is mainly discussed.

1. Introduction

A cylindrical aspiration capacitor with an electrode subdivided into two segments, recently set up in this institute, which is reported in a series of this subject^{1), 2)}, is commonly used in order to obtain the mobility spectrum of atmospheric ions. The number density of ions in a certain region of the ion mobility is given as the first derivative of observed ion current. Such a technique of the treatment of observational data with ion mobility spectrometer was originated with Misaki³⁾ and improved by Whipple.⁴⁾ This procedure of data processing is briefly described in Section 2, for convenience' sake of our discussion. The electric potential in the interior of instrument has been calculated in two dimensional approximation. We are interested in the confirmation of the appropriateness of this approximation for actual instruments with various sizes. It is the purpose of this paper to show the result of the calculation of electric potential in three dimensional model, i.e. the fringe effect of electrode upon electric field pattern. The electric potential for the case of our instrument is numerically calculated with Monte Carlo method, which is shown in Section 3. However, the motion of atmospheric ions under this field is not yet investigated. Our consideration of the electric potential in actual instruments with various sizes may be significant to a certain extent for usual data analysis, which is under the study.

2. Procedure of Data Analysis

(i) Principle of instrumentation and motion of ions

The actual electrode of our instrument (double-electrode condenser) is shown in Fig. 1. The electric potential between two cylindrical electrodes with the same axis toward z-direction is obtained from solving Laplace equation expressed in the cylindrical coordinate as follows,

$$\nabla^2\phi = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2} = 0. \quad (1)$$

For the case of electrodes with an infinite length, we may take the form of function,

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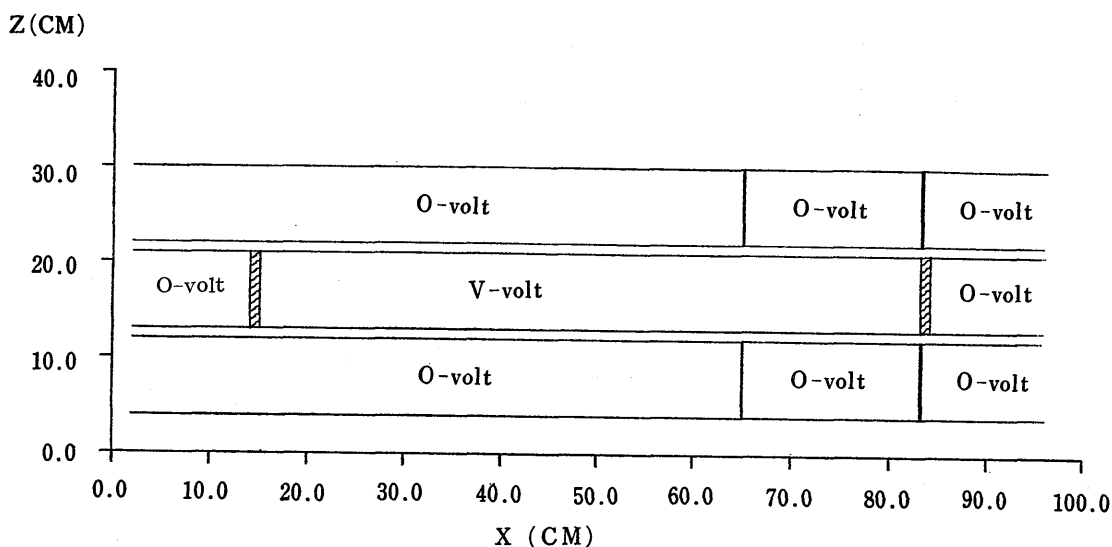


Fig. 1 Schematic diagram of actual electrode of large ion mobility spectrometer in our coordinate system.

ϕ as $\phi = \phi(r)$. The solution of Eq.(1) satisfying boundary conditions is

$$\phi = c \ln r + d, \quad (2)$$

where

$$c = V / \ln(r_i / r_o),$$

$$d = -V \ln(r_o) / \ln(r_i / r_o),$$

r_i and r_o are the radii of inner electrode and outer electrode, respectively. Boundary conditions are taken as $\phi(r_i) = V$ and $\phi(r_o) = 0$. The intensity of electric field is given as,

$$E = -\nabla \phi = -\frac{c}{r}. \quad (3)$$

The motion of charged particles under this electric field attains the equilibrium because of viscosity. The radial component of terminal velocity, v_x of particle at equilibrium is obtained as follows,

$$m \frac{dv_x}{dt} = eE_x - \frac{v_x}{B} = 0, \quad (4)$$

then

$$v_x = eBE_x \equiv kE_x, \quad (5)$$

where m and e are mass and charge of atmospheric ion, respectively. B is the scalar quantity expressing magnitude of the viscosity of air, k is called as electrical mobility⁴ and the motion of ion injected parallel to the axis at the entrance of cylindrical capacitor is in two dimensional plane, which is expressed as $x-z$ plane. Using Eq.(5), the critical mobility, k_c of positive ion injected at the point, $r = r_i$ is given in the following way.

$$l_1 = \int_0^{l_1} dz = v_z \int_{r_i}^{r_0} \frac{dx}{v_x} = \frac{v_z}{k_c} \int_{r_i}^{r_0} \frac{dx}{E_x}, \quad (6)$$

where l_1 is the length of the first electrode of double-electrode condenser. The x and z components of ion velocity are expressed as v_x and v_z , respectively and v_z is a constant. From Eqs.(3) and (6), we obtain

$$k_c = \frac{v_z(r_0^2 - r_i^2)}{2l_1 V} \ln\left(\frac{r_0}{r_i}\right),$$

$$= \frac{\phi}{4\pi a_1 V}, \quad (7)$$

where $\phi = \pi(r_0^2 - r_i^2)v_z$ is the flux of air flow and $a_1 = l_1/2 \ln(r_0/r_i)$ is the normalized length of capacitor (the capacitance of the first electrode condenser divided by $4\pi\epsilon_0$ where ϵ_0 is the dielectric constant of air).

(ii) The mobility spectrum

The critical mobility, k of ion injected at the point of r ($r_i < r < r_0$) is similarly given as,

$$k = \frac{v_z(r^2 - r_i^2)}{2l_1 V} \ln\left(\frac{r_0}{r_i}\right), \quad (8)$$

The number density of ions with the mobility, k which are trapped with capacitor with the same length, l_1 is

$$f(k) \frac{\pi(r^2 - r_i^2)}{\pi(r_0^2 - r_i^2)} = f(k) \frac{k}{k_c}, \quad (9)$$

where $f(k)$ is the mobility density function. Therefore, the ion current to the first electrode of double-electrode condenser, I_1 is

$$I_1 = \phi e \left[\int_{k_c}^{\infty} f(k) dk + \frac{1}{k_c} \int_0^{k_c} k f(k) dk \right]. \quad (10)$$

The current to the second electrode is given as follows,

$$I_2 = \phi e \left[\int_{k_d}^{\infty} f(k) dk + \frac{1}{k_d} \int_0^{k_d} k f(k) dk - \int_{k_c}^{\infty} f(k) dk - \frac{1}{k_c} \int_0^{k_c} k f(k) dk \right], \quad (11)$$

where $k_d = \phi/4\pi(a_1 + a_2)V = a_1 k_c/(a_1 + a_2)$,

$$a_2 = l_2/2 \ln(r_0/r_i),$$

and l_2 is the length of the second electrode. It is the fundamental idea of Misaki²⁾ and Whipple³⁾ that the number density between k_d and k_c is given as the first derivative of observational data. The result is

$$d\left(\frac{I_2}{V}\right)/d\left(\frac{\phi}{V}\right) = e \int_{k_d}^{k_c} f(k) dk, \quad (12)$$

which was deduced from Eq.(11). The resolution of ion mobility spectrum is determined by the ratio, $k_d/k_c = a_1/(a_1 + a_2)$.

3. Calculation of Electric Potential

Monte Carlo method is an effective way to solve three dimensional Laplace equa-

tion, Eq. (1) for arbitrary boundary conditions. The well-known procedure of calculation is as follows. From Eq.(1), we obtain the following difference equation as the second approximation of Taylor expansion.

$$\begin{aligned} &\phi(x+h, y, z) + \phi(x-h, y, z) + \phi(x, y+h, z) + \phi(x, y-h, z) \\ &+ \phi(x, y, z+h) + \phi(x, y, z-h) - 6\phi(x, y, z) = 0, \end{aligned}$$

or

$$\phi(P_0) = \frac{1}{6} \sum_{i=1}^6 \phi(P_i), \quad (13)$$

where the points P_i are six neighbor points of a fixed point P_0 of the cubic lattice and h is an interval between two neighboring points of the cubic lattice (the infinitesimal distance). The boundary conditions are expressed as

$$\phi(Q_j) = V(Q_j), \quad (14)$$

where $V(Q_j)$ is the boundary-value of electrical potential at any boundary, Q_j . Let $V(P_0, Q_j)$ be the value of electrical potential at the point, Q_j on the boundary attained after the random walk to each point of cubic lattice which is started from the point, P_0 . It is a matter of course that $V(Q_j, Q_j)$ comes to be $V(Q_j)$. We can show that the solution, $G(P_0)$ at the point, P_0 of Eqs.(13) and (14) is expressed as,

$$G(P_0) = E\{V(P_0, Q_j)\} \quad (15)$$

when $E\{\}$ denotes the expectation value obtained by many trials of random walk. The result of random walk from the point, P_0 is attributed to the results of random walks from six neighbor points P_i in the probability $1/6$, respectively. Therefore, we get

$$G(P_0) = \frac{1}{6} \sum_{i=1}^6 G(P_i)$$

and $G(Q_j) = V(Q_j)$. Eq.(15) is the solution of Eqs.(13) and (14) by the uniqueness of solution.

For the case of our instrument, we calculate Eq.(15) by using the pseudo random number which is continuatively given by the following iterative formular.

$$x_{n+1} = (2^9 + 1)x_n + 1 \pmod{2^{80}}, \quad (16)$$

where the initial value, x_0 is taken to be 2343. The result of χ -square test of our random number is shown in Fig. 2, where

$$\begin{aligned} \chi_f^2 &= \sum_i \frac{(F_i - f_i)^2}{f_i} \quad (i=1, 2, \dots, 6), \\ \chi_g^2 &= \sum_{ij} \frac{(G_{ij} - g_{ij})^2}{g_{ij}} \quad (i, j=1, 2, \dots, 6), \end{aligned}$$

F_i and f_i are experimental and theoretical frequency, respectively. G_{ij} and g_{ij} (successive correlations) are experimental and theoretical frequency at which the j -th number occurs after the occurrence of the i -th number. The value of χ_f^2 is sufficiently

small but that of χ_g^2 is slightly unfavorable as shown in Fig. 2, the result of which of course induces a slight error to the result of calculation of electric potential.

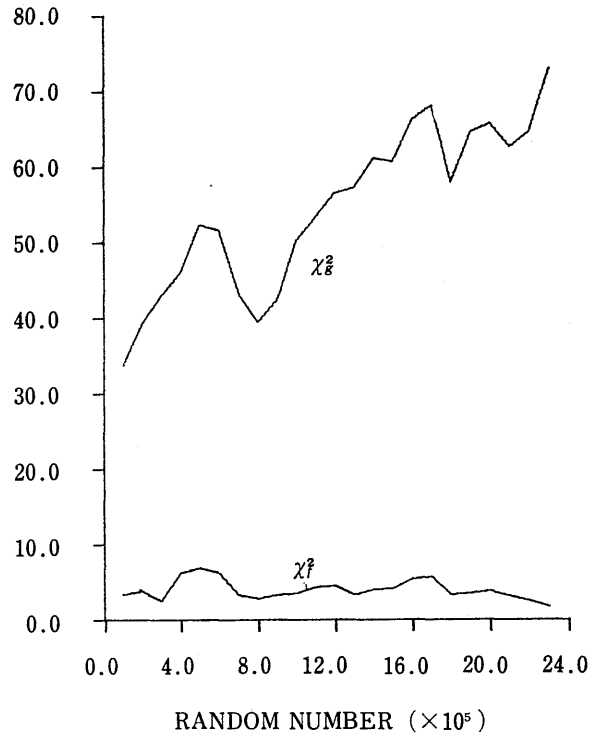


Fig. 2 Result of χ -square test. The values of χ -square, χ_f^2 and χ_g^2 , for the events of random numbers in independent process and simple Markoff process, respectively, are shown for the count of total random numbers.

Table 1 For the case of electrode with an infinite length, the numerical solution by Monte Carlo method is illustrated as compared with the analytical solution, Eq.(2).

$r(\text{cm})$	Analytical Solution	Monte Carlo	Error (%)	Number of Trials	$h(\text{cm})$
4.0(=r _i)	100.0	100.0	—	—	—
4.1	88.93	88.28	0.7	2500	0.02
4.2	78.14	77.96	0.2	2300	0.025
4.3	67.59	67.25	0.5	2800	0.033
4.4	57.29	57.10	0.3	2900	0.033
4.5	47.22	47.07	0.3	2900	0.033
4.6	37.37	37.22	0.4	3200	0.033
4.7	*27.73	*27.77	0.1	3900	0.033
4.8	18.29	18.46	0.9	2800	0.025
4.9	* 9.05	* 9.19	1.5	3100	0.02
5.0(=r _o)	0.0	0.0	—	—	—

However, the error is endurable, which is ascertained by an example of the calculation for the case of electrode with an infinite length. For the comparison with the analytical solution, Eq.(2), the numerical solution by Monte Carlo method is illustrated in Table 1. Some numerical solutions asterisked in Table 1 are shown in Fig. 3 as the function of the number of trials.

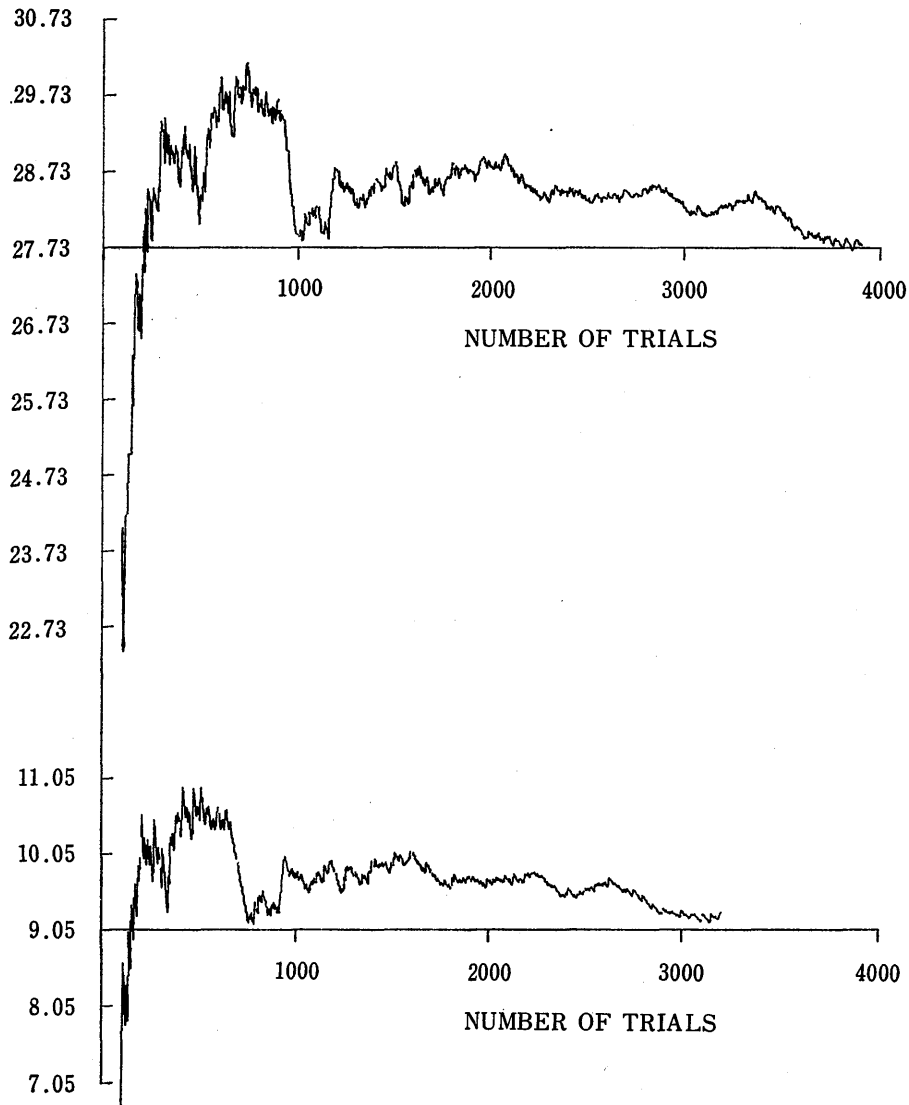


Fig. 3 Asymptotes of some numerical solutions. The solutions asterisked in Table 1 are shown as the functions of the number of trials of random walk.

For the case of actual capacitor of our instrument ($r_i=4.0$ cm and $r_o=5.0$ cm), we show the numerical solutions in Fig. 4, where equipotential lines in a part of the capacitor, i.e. near the fringe of the electrode are drawn, but it should be noted that each potential difference between two neighboring lines is not always identical in

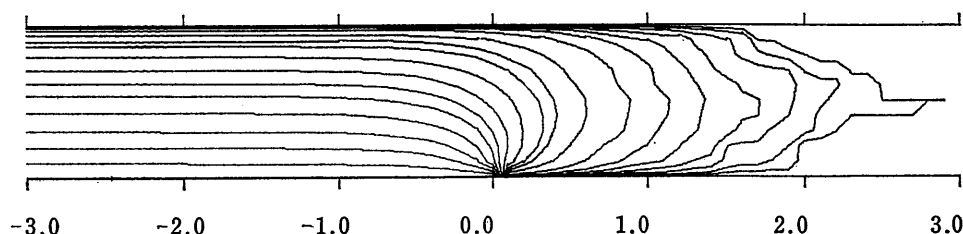


Fig. 4 Equipotential lines in a part of the actual capacitor, i.e. near the fringe of the electrode.

this figure. Equipotential lines become rather rough because of the scantiness of the points at which the potentials are numerically calculated. The appreciable shift of the numerical solution from the analytical one, Eq. (2) for electrode with an infinite length remains within the distance of 3 cm from the fringe for inside and outside of the capacitor. This distance is not so large as compared with the total length of our actual electrode, i.e. 68 cm.

4. Conclusion and Discussion

(1) The solution of Laplace equation in the interior of the cylindrical aspiration capacitor set up in this institute was solved by Monte Carlo method, while the solution in two dimensional approximation is usually used for data analysis on the ion mobility spectrum. It was found that the appreciable difference between the former and the latter remained within no more than the distance of 3 cm from the fringe of electrode in our instrument on large ion mobility spectrum. This difference, however, being conjectured to be more appreciable for small ion mobility spectrometer where the length of r_o fairly differs from that of r_i , the consideration in this paper is necessary to more extent for data analysis on small ion mobility spectrum.

(2) It is the final purpose of our consideration to count the number of ions trapped by the electrode, which is under the study. We must solve the equation of motion of the ion under actual field and consider the removal of ions by the stray field at the entrance of capacitor.

(3) It takes 9 hours on FACOM 270-30 computer to calculate the actual potential field for one instrument in our accuracy. In order to reduce the time of calculation, another method such as relaxation method may be required on the basis of the result of Monte Carlo method.

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