報 文

ORIGINAL PAPERS

Numerical Analysis of Cylindrical Electrostatic Spectrometer

KUNIO YAGI*, HIROSHI MIMA*, YASUO FUJII* AND FUTOSHI KANEMATSU*

(Received 2 June 1976)

The trajectory of the electron injected in the 127° cylindrical electrostatic spectrometer (the main path radius is 90 mm and the slit width is 0.5 mm) is numerically computed in a second order approximation, and the results are compared with the Wollnik theory. His theory is also effective for the inhomogeneous field; but the numerical analysis is necessary to determine the accurate main path conditions. The position of the electron at the exit can be given in an accuracy less than 0.04 percent by a second order solution. With the aid of this solution, the energy distribution of the electron beam coming out through the spectrometer, which has a movable collimator, is computed. The resolution is determined by the main path radius and the beam width at the ideal boundary.

1. Introduction

A theoretical consideration on an effect of fringing field near the slit of an cylindrical electrostatic spectrometer¹⁾ (C. E. S.) has been developed by R. F. Herzog²⁾ and H. Wollnik^{3,4)}. They introduced an conception of an ideal field boundary which lies midway between the slit (which serves for a shielding diaphragm, too.) and the electrodes. See Fig. 1. The electric field produced between the electrodes is assumed to extend constant to the boundary without being disturbed, and not to get beyond the boundary. In other words, one may consider the electrodes to be an ideal condenser with the edges stretched to the plain of the boundary. A charged particle injected toward the slit in reality travels, as shown in Fig. 1, along the solid line which is circular in the deep place between the electrodes, being deviated only near the entrance. If this circular trajectory were

inversely extrapolated toward the entrance according to the idealized field, it would reach the point A on the boundary, from which the path would go out toward the slit along the tangential making an angle $\Delta\alpha$ to the line which the particle was injected along. On the other hand the injected particle would travel straight putting the foot on the point B on the boundary, if the idealized field is taken into account. The discrepancy between A and B is shown as $\Delta\xi$ in Fig. 1. By employing such an imaginary path that has discontinuity on the boundary they succeeded in analyzing the trajectory of a charged particle in the spectrometer, getting out of the troublesome problems which arise from the fringing field effect near the entrance. In this method of analysis it is essential to know the values $\Delta\alpha$ and $\Delta\xi$, which are given by Wollnik as follows for a parallel plate condenser (P. P. C.):

* Faculty of Engineering, Osaka City University, 459 Sugimoto-cho, Sumiyoshi-ku, Osaka 558, Japan

 Fig. 1. Schematic diagram of the ideal and real main paths near the ideal field boundary (η_p^* is given in ref. 2).

$$\Delta\alpha_p \doteq \frac{(0.8b + s + 0.4d)}{6r_0} - \frac{h_0 \cdot \alpha}{r_0} \quad (1)$$

$$\Delta\xi_p \doteq \frac{(0.8b + s + 0.4d)^2}{24r_0} - \frac{h_0^2}{2r_0}$$

An electron injected with an energy E_0 , an inclination α to the real main path and a deviation h_0 from it is ejected with a deviation h_2 from it. If the angle between the two ideal boundaries is 127.28° , the deviation h_2 will be given in a second order approximation as follows⁵⁾.

$$h_0 = r_0 \left(2\beta - \rho - \frac{4}{3} \alpha^2 + \frac{5}{3} \beta^2 - \frac{\rho^2}{3} + \frac{2}{3} \beta\rho \right) - d \left(\alpha + \frac{8}{3} \alpha\beta - \frac{8}{3} \alpha\rho \right), \quad (2)$$

where

$$\rho = (h_0 + d \tan \alpha) / r_0,$$

$$\beta = (\sqrt{E_0} - \sqrt{E}) / \sqrt{E},$$

where the E is the energy for the main path of a radius r_0 .

We computed a real potential distribution and real trajectories for the C. E. S. by a numerical integration method with the aid of a FACOM 270/30, and then determined the values η_c^* , $\Delta\alpha_c$ and $\Delta\xi_c$ which correspond to the parameters η_p^* , $\Delta\alpha_p$ and $\Delta\xi_p$ for the P. P. C..

Using these results we calculated the energy distribution of the ejected electron beam through the C. E. S. which had a movable collimator.

2. Basis of the Method

2.1 Potential distribution

A model is as follows: the sector angle is 127.28° , the radii of curvature for the inner and outer sectors are 80 and 100 mm, respectively, the radius for the main path is 90 mm, the distance between the slit and the sectors is 5 mm, and the width of the slit is 0.5 mm. Potentials of the inner and outer sectors are +114.7 and -102.9 V, respectively, and both the slits are grounded. These values are chosen so that an electron injected with an energy 500 V may travel on the main path and the η_p^* may be approximately equal to zero.

Fig. 2. Arrangement of the C. E. S. for the computation.

An electric potential, since the space charge effect can be neglected in general, has to satisfy the following Laplace equation :

$$\frac{\partial^2 U}{\partial r^2} + \frac{1}{r} \frac{\partial U}{\partial r} + \frac{1}{r^2} \frac{\partial^2 U}{\partial \phi^2} = 0 .$$

If we put $r = I \cdot \Delta r$ and $\phi = J \cdot \Delta \phi$ (I, J : integer), this equation is transformed into the following difference equation in a second order approximation :

$$U_{i,j} = \left\{ \left(1 + \frac{1}{2I} \right) U_{i+1,j} + \left(1 - \frac{1}{2I} \right) U_{i-1,j} + (U_{i,j-1} + U_{i,j+1}) / (\Delta \phi^2 \cdot I^2) \right\} / 2 / \left(1 + \frac{1}{\Delta \phi^2 \cdot I^2} \right) \quad (3)$$

Supposing that the potential distribution between C and D (Fig. 2) on the cylindrical plane extrapolated from the inner surface of the sector electrode is linear, Eq. 3 can be solved by the successive-over-relaxation method. The values used in the calculation are shown as follows:

$$\begin{aligned} \Delta r &= 0.5 \text{ mm}, \\ \Delta \phi &= 5.57 \times 10^{-3} \text{ radian}, \\ \omega &= 1.71124, \\ I &= 161, 162, \dots, 199, \\ J &= 1, 2, 3, \dots, 419, \end{aligned}$$

where ω is an acceleration coefficient, Δr and $\Delta \phi$ are stepsizes, and $r_0 \times \Delta \phi$ is equal to Δr . The flow chart for this computation is shown in Fig. 3.

2.2 Electron trajectory

The equations of motion as follows:

$$\begin{aligned} \ddot{r} - r \cdot \dot{\phi}^2 &= \frac{e}{m} \cdot \frac{\partial U}{\partial r} , \\ 2 \dot{r} \cdot \dot{\phi} + r \cdot \ddot{\phi} &= \frac{e}{m} \cdot \frac{1}{r} \cdot \frac{\partial U}{\partial \phi} . \end{aligned}$$

This system of second order differential equations is transformed into the following system of first order:

Fig. 3. Flow chart for the computation of the potential distribution.

$$\begin{aligned} y_1 &= y_2 , \\ y_2 &= y_1 \cdot y_4^2 + \frac{e}{m} \cdot \frac{\partial U}{\partial r} , \\ y_3 &= y_4 , \\ y_4 &= -\frac{2 y_2 \cdot y_4}{y_1} + \frac{e}{m \cdot y_1^2} \cdot \frac{\partial U}{\partial \phi} \end{aligned} \quad (4)$$

The position r_n , where the electron reaches $n \cdot \Delta t$ sec after the injection into the slit, is expressed by a vector as given below:

$$r_n = r_n (I + \Delta I, J + \Delta J),$$

Fig. 4. Schematic diagram how a trajectory is computed.

where I and J are integers, and ΔI and ΔJ are smaller than value 1. The components of the field strength, interpolated from the potentials of the four points which surround the position r_n , are shown as below:

$$\left(\frac{\partial U}{\partial r}\right)_{I+\Delta I, J+\Delta J} = \frac{U_2 - U_0 + \Delta J \cdot \Delta U}{(I + \Delta I) \cdot I_n ((I + 1)/I) \cdot \Delta r},$$

$$\left(\frac{\partial U}{\partial \phi}\right)_{I+\Delta I, J+\Delta J} = \frac{U_1 - U_0 + \Delta I \cdot \Delta U}{\Delta \phi}, \quad (5)$$

where

$$\begin{aligned} \Delta U &= U_3 - U_2 - U_1 + U_0, \\ U_0 &= U_{I, J}, \\ U_1 &= U_{I, J+1}, \\ U_2 &= U_{I+1, J}, \\ U_3 &= U_{I+1, J+1}. \end{aligned} \quad (6)$$

As U_0 , U_1 , U_2 and U_3 are known, Eqs. 5 and 6 are successively calculated. The results are substituted into Eq. 4 and the next position r_{n+1} can be found by solving Eq. 4 with the 4-th order

Runge-Kutta method. Repeating the process give the real trajectory of an electron. The stepsize Δt is 3.5×10^{-11} sec. and one trajectory was determined by repetitions of 450 times. The flow chart for this computation is shown in Fig. 5.

2.3 Energy distribution

As shown in the following section, the position of the electron at the exit slit can be given by Eq. 2 with a satisfactory accuracy. Therefore the energy distribution of an electron beam coming out through the C. E. S. is easily computed. We consider the spectrometer with a collimator. Incident electrons differ one another in the energy, position and direction. These three quantities are given as:

$$\begin{aligned} E_0 &= 500 \pm 0.1 \times L \text{ V}, \\ h_0 &= \pm s/20 \times M \text{ mm}, \\ \alpha &= \pm \theta/20 \times N \text{ radian}, \end{aligned}$$

where

Numerical Analysis of Cylindrical Electrostatic Spectrometer

Fig. 5. Flow chart for the computation of the real trajectory.

$$\theta = \tan^{-1} (2s/x) ,$$

$$L = 0, 1, 2, \dots, 50 ,$$

$$M = 0, 1, 2, \dots, 20 ,$$

$$N = 0, 1, 2, \dots, 20 .$$

A beam consists of $101 \times 41 \times 41$ electrons; but, the number of electrons which can pass through the entrance slit is $101 \times 41 \times 21$. We rewrite the Eq. 2 as follows:

$$h_1 = h_0 + x \tan \alpha , \quad (7)$$

$$h_2 = r_0 \cdot \left(2\beta - \rho - \frac{4}{3} \alpha^2 + \frac{5}{3} \beta^2 - \frac{\rho^2}{3} + \frac{2}{3} \beta \cdot \rho \right) - d \cdot \left(\alpha + \frac{8}{3} \alpha \cdot \beta - \frac{8}{3} \alpha \cdot \rho^2 \right) , \quad (8)$$

where

$$\rho = (h_1 + d \tan \alpha) / r_0 .$$

The Eq. 7 is computed about each of electrons. If h_1 is smaller than or equal to s , the Eq. 8 is computed. And then, if h_2 is smaller than or

equal to s , we add value 1 to the memory corresponding to this energy. After the end of computations for all electrons, the energy distribution of an ejecting beam is obtained by calling the memories successively.

3. Results

Integrating the electric field on the optical axis over the fringing field region, we evaluated η^* as below:

$$\eta_c^* = 0.0045 \text{ mm}.$$

The trajectory of the electron, started from the mid point of the spectrometer with an energy

500 V along the main path was computed and the conditions (the electron-ejected position and the direction at the exit slit) were determined. These conditions are equal to the main path conditions. These are as follows:

$$\begin{aligned} E &= 500 \text{ V}, \\ \zeta_c &= 0.085553 \text{ mm}, \\ \Delta\alpha_c &= 0.0008405 \text{ radian}, \end{aligned}$$

where ζ is a deviation from the optical axis and $\Delta\alpha$ is an angle to it. The values $\Delta\xi_p$ and $\Delta\alpha_p$ are given by Eq. 1 as follows:

$$\begin{aligned} \Delta\xi_p &= 0.04861 \text{ mm}, \\ \Delta\alpha_p &= 0.0009221 \text{ radian}, \end{aligned}$$

Fig. 6. Relations between the injecting conditions and the electron-ejected position: curve (1) corresponds to the injecting energy, (2) to position, (3) to inclination.

Numerical Analysis of Cylindrical Electrostatic Spectrometer

Table 1. Relations between the injecting conditions and the electron-ejected position: h_2 and h'_2 are the ejecting position calculated by the numerical integration method and by the Eq. 2, respectively.

α (radian)	h_0 (mm)	E_0 (V)	h_2 (mm)	h'_2 (mm)
0.054707	0.5	505	-0.919845	-0.862254
0.054707	0.5	500	-1.467045	-1.402155
0.054707	0.5	495	-2.009898	-1.940985
0.054707	0	505	-0.401598	-0.365373
0.054707	0	500	-0.941499	-0.904275
0.054707	0	495	-1.479843	-1.442106
0.054707	-0.5	505	0.118692	0.129654
0.054707	-0.5	500	-0.414900	-0.408240
0.054707	-0.5	495	-0.949500	-0.945072
0	0.5	505	0.017442	0.040617
0	0.5	500	-0.532584	-0.500922
0	0.5	495	-1.077300	-1.041435
0	0	505	0.543096	0.540540
0	0	500	0.000000	0.000000
0	0	495	-0.542493	-0.539478
0	-0.5	505	1.067895	1.038609
0	-0.5	500	0.530145	0.499068
0	-0.5	495	-0.010098	-0.039402
-0.054707	0.5	505	0.218700	0.229077
-0.054707	0.5	500	-0.328293	-0.314091
-0.054707	0.5	495	-0.873900	-0.856215
-0.054707	0	505	0.746298	0.732042
-0.054707	0	500	0.204750	0.189864
-0.054707	0	495	-0.336798	-0.351252
-0.054707	-0.5	505	1.267443	1.233153
-0.054707	-0.5	500	0.730593	0.691974
-0.054707	-0.5	495	0.191547	0.151857

therefore the main path conditions given by the Wollnik theory are as below:

$$\zeta_p = 0.05322 \text{ mm} .$$

The difference among two main path conditions is relatively small: however, this is important, because main path conditions become the standards to compute h_2 with Eq. 2. Relations between the injecting conditions and the ejecting positions are shown in Fig. 6. and Table 1.

The h_2 was given by the numerical integration method and the h'_2 was given by Eq. 2 with the values ζ_c and $\Delta\alpha_c$. It is clear that h_2 is in satisfactory agreement with h'_2 . Therefore we conclude that the ejecting position can be given in an accuracy less than 0.04 percent by Eq. 2 with accurate main path conditions. An example of the real trajectory, given by the electronic computer and X-Y plotter, is shown in Fig. 7.

Energy distributions are shown in Fig. 8.

Fig. 7. The real trajectory of the electron with the injecting conditions ($E_0 = 500$ V, $\alpha = 0.05472$ radian, $h_0 = -0.08475$ mm) and with the ejecting position $h_2 = -0.77475$ mm.

Fig. 8. Energy distribution of the C. E. S. with a collimator; abscissa is energy and ordinate ejected electron number, length x of the collimator is 14.32 in (a), 28.65 in (b), 57.29 mm in (c).

The resolution R is defined as:

$$R = E / \Delta E,$$

where ΔE is the full width at half maximum. A width Δh of an injected beam at the first ideal boundary is given as follows:

$$\Delta h = 2s(x + d)/x,$$

and we introduce the value R' as below:

$$R' = r_0 / \Delta h.$$

The R and R' are shown in Table 2. It is clear that R almost agree with R' . Therefore, the

Table 2. Effect of the collimator length x for the resolution R , and relation between R and R' .

x (mm)	ΔE (V)	Δh (mm)	R	R'
14.32	4.7	0.8492	106	106
28.65	3.8	0.6745	132	133
57.29	3.4	0.5873	147	153

resolution of the C. E. S. with a collimator is determined by the width Δh at the first ideal boundary.

4. Discussion and Remarks

In order to apply our results to the design

of a C. E. S., the values η^* , $\Delta\xi$ and $\Delta\alpha$ must be accurately determined, though the computation is not easy.

We computed the energy distribution of an electron beam coming out through the C. E. S. the slits of which were not placed on their proper positions. If the slits are positioned within deviations of $\Delta\xi_c - \Delta\xi_p$ from their proper positions, the deviations do not affect the resolution, but shift the peak position in the energy spectrum. The peak shift can be easily corrected. Therefore, if the object of a study is not to investigate the real trajectory of a charged particle but to measure the injected energy, the C. E. S. can be easily designed with the values η_p^* , $\Delta\xi_p$ and $\Delta\alpha_p$ which are determined by the Wollnik theory.

As shown in this paper, we made success in the analysis of the real trajectories in the C. E. S. by the numerical integration method with an electronic computer. This method is also effective to the analysis of a charged particle

motion in electric or magnetic field. However, if the variation in the particle velocity is relatively large, the stepsizes such as Δt , Δr and $\Delta\phi$ must be varied in accordance with its velocity in order to maintain the accuracy of the result. Therefore the program of this analysis is generally complex, but it can be possible with the electronic computer with large capacity and high speed.

Acknowledgement

The authors wish to thank Dr. Y. Tanaka for his valuable discussion.

References

- 1) A. L. Hughes and V. Rojansky, *Phys. Rev.*, **34**, 284 (1929).
- 2) R. F. Herzog, *Phys. Zeits.*, **41**, 18 (1935).
- 3) H. Wollnik and H. Ewald, *Nuclear Inst. and Meth.*, **36**, 93 (1965).
- 4) H. Wollnik, *Nuclear Inst. and Meth.*, **52**, 250 (1967).
- 5) H. Matsuda, *Mass Spectroscopy (Japan)*, **12**, 165 (1964).