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Electric hexapoles and octopoles with optimized circular section rods

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Abstract

The SIMION 3D Version 6 program has been used to find the potential distributions in various hexapole and octopole assemblies with rods of circular cross section, mounted inside a shield electrode. The deviations of these potentials from the theoretical potentials of an ideal geometry have been computed and plotted. From the study of several geometries, each with different rod to field radius ratios (r_{rod}/r_o), an optimum value for the ratio that gives least deviations has been found for both the hexapole and the octopole geometries. The optimum value of (r_{rod}/r_o) for a hexapole is 0.5375 and that for the octopole is 0.355. (Int J Mass Spectrom 202 (2000) 31–36) © 2000 Elsevier Science B.V.

Keywords: Hexapole; Octopole; Quadrupole; Potential distribution; Ion optics

1. Introduction

Radiofrequency (rf) multipole devices have been used recently to transport ion beams from higher pressure sources into other devices such as mass spectrometers working at lower pressures. In tandem mass spectrometry, quadrupoles working with rf voltages only on the poles have been used as collision induced/activated dissociation cells. In these devices, their ability to confine the charged particles close to the axis as they travel in the axial direction is made use of. Recently, the energy reducing capabilities [1,2] of gas collision cells have been realized and put to practical use. Concurrently, other multipole devices like the electric hexapoles and octopoles, with only the rf voltages applied to them, have found application as ion guides [3]. For example, in inductively coupled plasma (ICP) source mass spectrometer systems, hexapoles have been used to transport ions from an ICP torch to a quadrupole mass spectrometer. Here, they also act as collision cells for modifying the energy characteristics of these ions [4,5]. The ion motion properties in rf multipole fields have been investigated analytically [6,7] and also by computer simulations [8]. Ideal poles whose shape coincides with one of the equipotential surfaces have been assumed in the above simulation studies. However, for ease of construction, cylindrical rods with circular cross section, enclosed in a hollow cylindrical shield, have been utilized in the practical applications listed above [3,4]. Information about the optimum values for the ratio of rod radius (r_{rod}) to field radius (r_o), which can produce nearly the ideal fields, have been generated and reported for the quadrupoles with

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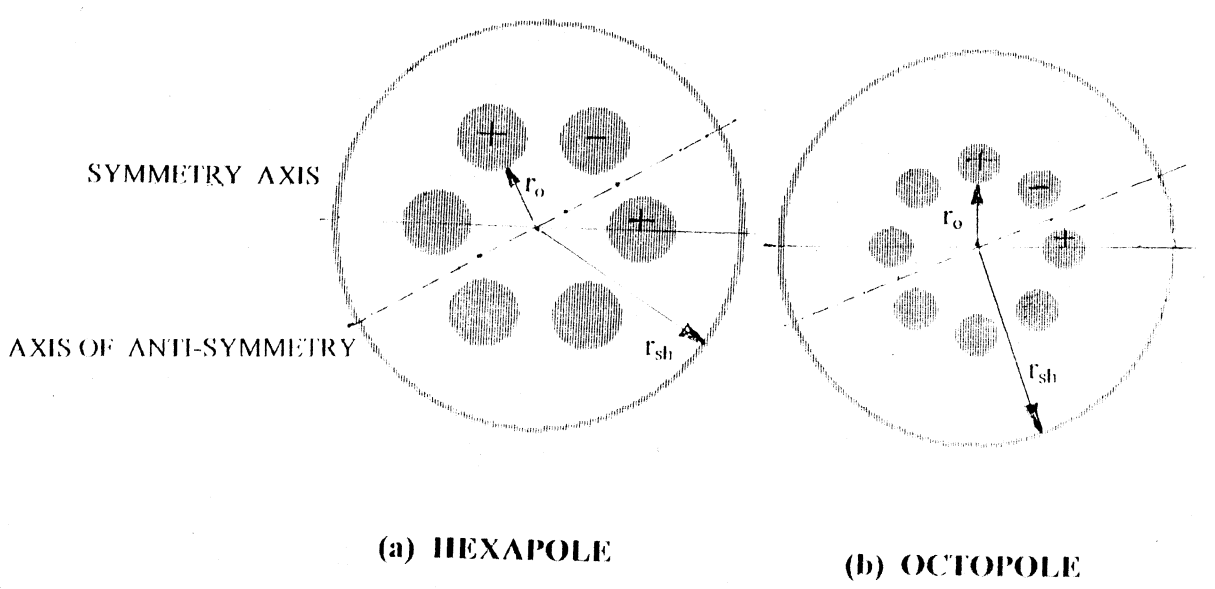

Fig. 1. Cross section of (a) Hexapole and (b) Octopole.

circular cross-section rods [9,10,12]. To the best of our knowledge, this exercise has not been done in the case of hexapoles and octopoles. In this article, we report the details of our study to generate this information both for hexapoles and for octopoles, to be constructed with rods of circular cross section and housed in a hollow cylindrical shield electrode. For this purpose, we have made use of the SIMION 3D Version 6 software package developed and distributed by D.A. Dahl [11].

2. Computer simulation

To generate the required information, it was decided to vary the rod radius for a given field radius, to determine the potential at any desired point in the structure using SIMION, and to compare it with the theoretical value. Fig. 1 shows the hexapole and the octopole geometries used. To determine these potentials in the present study, two-dimensional simulation was used. A field radius of 8 mm has been chosen for both the hexapole and the octopole and these are housed in a hollow shield of inner radius 24 mm that is kept at zero potential. Alternative rods are applied with potentials of equal magnitude but opposite polarities, with respect to the shield electrode. In this study, the rod radius is chosen to vary between 2 and 5 mm for the hexapole, and 2 to 4.8 mm in the case of the octopole. This gives a variation in (r_{rod}/r_o) from 0.25 to 0.625 for the hexapole and 0.25 to 0.6 for the octopole. A ratio (r_{rod}/r_o) value larger than 0.6199 is not possible for the latter case because the neighboring poles touch each other. The value chosen for (r_{sh}/r_o) is 3. Various electrode configurations, each with a different value for (r_{rod}/r_o) within the above range, are simulated by creating "geometry files" (as they are called in SIMION parlance). Mirror symmetry in the Y direction for the hexapole and mirror symmetry in both the X and Y directions for the octopole have been used in the simulation. The potential values at all the nodes or the intersections of grid wires have been calculated by SIMION using the method of finite differences by refining the potential arrays with a convergence limit of 1×10^{-3}. This means that the potential has been determined at every nodal point in the geometry to a value such that the difference in successive iterations is within 0.1% of the electrode voltage. Because of the application of this convergence limit, there is always a finite value of potential assigned to the nodes, even where the theoretical

value is zero. The magnitude of this potential is quite small and is always less than the chosen convergence limit during refining. The SIMION software package allows for refining of the potential arrays down to a convergence limit of 1×10^{-7}, but it takes an impracticably long time to refine an array to this limit. Because the electrodes have been defined in SIMION as a collection of points with predetermined fixed potentials assigned to them, a scaling factor of 50 has been used in the geometry file to minimize errors in the geometrical representation of the curved boundaries of the electrodes. That is, one millimeter is specified as 50 grid units in the simulated geometry, or, the spacing between neighboring grid points in an array represents a linear dimension of 0.02 mm or 20 microns. The SIMION software is configured to directly read the value of the potential at any point in the geometry by taking the cursor to that point, but it cannot be recorded directly into a file for reading and data processing. For the purpose of reading the potential arrays and recording the potentials at the desired points into a readable file, the SIMION manual [11] suggests that one should write and use a special program in C language. We used a different method, which utilizes the ability of SIMION to record the ion voltage at any point on the trajectory of an ion. This ion voltage essentially represents the potential at that point. For this purpose, it is necessary that the chosen point is on the flight path of an ion. Therefore, we chose to start the flight of an ion at the desired point, trace it for a very short duration, and stop it immediately at the end of the selected flight duration. SIMION can plot these short trajectories and can read and process the potential at their starting points and record these values in a file. The trajectories of all the ions starting from various points over the required area have been traced in a similar way by suitably defining their starting coordinates. A "user" program, which can be executed while the ions are being traced, has been written for this purpose. This program allows an ion to be traced for a chosen time interval on the order of 0.1 μs, stop the ion flight, and then recall the ion potential (Φ_{SIM}) at its starting point. It then calculates, at its starting point, the potential in an ideal hexapole (or in an ideal octopole, as the case may be) with the correct pole shape and with the same field radius, r_o. The theoretical potential $\Phi_{th}(x, y)$ at any point, $P(x, y)$, in the ideal hexapole with correct pole shape, is calculated using the expression

$$\{\Phi_{th}(x, y) = (\Phi_o/r_o^3)[x^3 - 3xy^2]\} \quad (1)$$

and that in an ideal octopole is calculated by the equation

$$\{\Phi_{th}(x, y) = (\Phi_o/r_o^4)[x^4 - 6x^2y^2 + y^4]\} \quad (2)$$

Here, Φ_o is the potential applied on the rods with respect to the central point or the ground. Using these values of calculated potential and the SIMION determined potential, the relative deviation σ, with respect to the SIMION potential, defined as

$$\sigma = (\Phi_{SIM} - \Phi_{th})/\Phi_{sim} \quad (3)$$

is also calculated by this user program. The denominator has been chosen to be Φ_{SIM} to avoid the magnitude of the relative error going to values up to infinity at the points where $\Phi_{th} = 0$. For easy visualization of regions of lower errors or deviations, the trajectories of the ions with calculated relative deviations in a particular decade range have been assigned and plotted in a particular colour. Fig. 2(a) and (b), for a hexapole and an octopole, respectively, have been produced in this way. These trajectories are very short and appear as dots in these figures. Table 1 gives the error ranges and the assigned colours for the ion trajectories. In order to compare the geometries with different (r_{rod}/r_o), ions have been traced along three straight lines (spaced equally between the axis of symmetry and the axis of antisymmetry) and inclined with respect to the X axis at 0°, 10°, and 20° for the hexapole and 0°, 7.5°, and 15° for the octopole (Fig. 1). The relative deviations occurring at a given radius have been compared and the geometry with lowest relative errors has been selected as the optimum.

3. Results and discussion

In Fig. 2(a) and (b) the potentials so determined are plotted as relative deviations from the ideal hexapole and octopole fields. These are represented by the

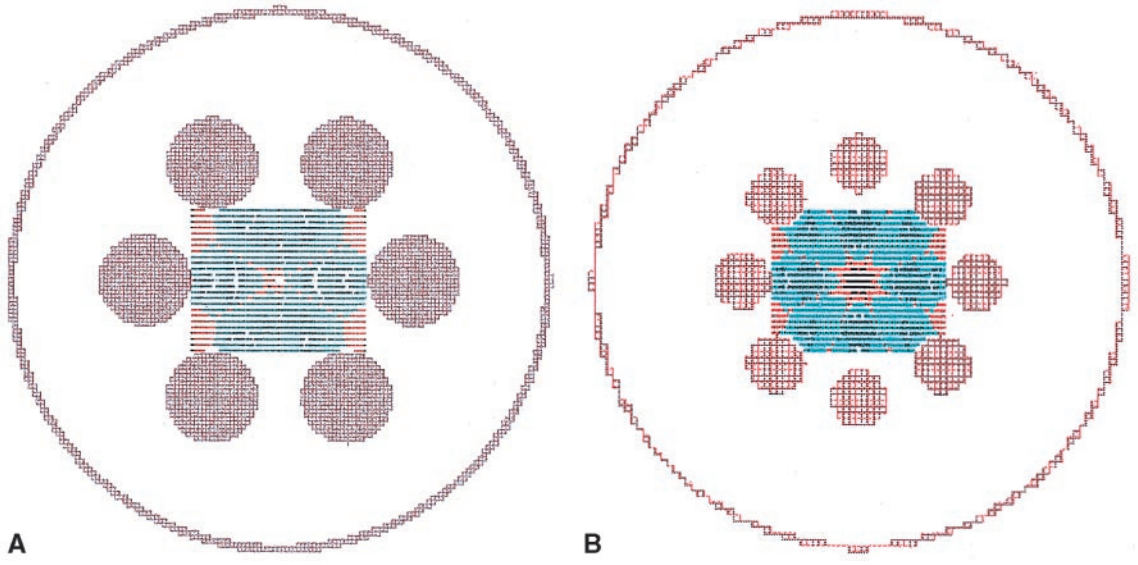

Fig. 2. Relative deviations of potentials from the ideal values for hexapole (a) and octopole (b), represented here as dots of different colours. Table 1 gives the colour code for deviations in different decade ranges.

colours of the dots (very short trajectories) as shown. It is noted that SIMION gives a very small but finite potential at the centre, as well as on the lines of antisymmetry, where the theoretical potential is zero. The magnitude of this SIMION potential is less than the convergence limit applied during the refinement process of the potential arrays. This potential is smaller when the simulation is done with a lower convergence limit or when the size of the array is increased. These changes require an enormously large size for the potential arrays and result in very large computational times for refinement. In the calculation for relative deviations, this value of the SIMION determined potential appears as the denominator. Because of the low magnitude of the potential near the centre, and also at points close to the zero equipotential lines, the relative error is large—100% at the centre and on the zero equipotential lines. This is seen by the colours of trajectories near the centre of the geometry, even though it is expected by intuition that the deviations in potentials near the centre would be lower. Therefore, to assess a given geometry for its ability to produce potentials close to the ideal field, comparison of relative deviations is made only at radii larger than $r/r_o = 0.3$ for various geometries. Relative deviations have been calculated by simulation for the hexapole geometries with a ratio $(r_{\text{rod}}/r_o)_{\text{hexapole}}$ equal to 0.25, 0.375, 0.45, 0.475, 0.4875, 0.5, 0.525, 0.535, 0.5375, 0.54, 0.55, 0.575, and 0.625 (corresponding to rod radii of 2, 3, 3.6, 3.8, 3.9, 4, 4.2, 4.28, 4.3, 4.32, 4.4, 4.6, and 4.8 mm), and for the octopole geometries with a ratio $(r_{\text{rod}}/r_o)_{\text{octopole}}$ equal to 0.25, 0.3125, 0.35, 0.3525, 0.355, 0.3575, 0.375, 0.5, 0.5625, and 0.60; the corresponding r_{rod} values being 2, 2.5, 2.8, 2.82, 2.84, 2.86, 3, 4, 4.5, and 4.8 mm, respectively. Plots of relative deviations against radial distance have been made along the X axis and along straight lines inclined at 10° and 20° for the hexapole and at 7.5° and 15° for the octopole and are compared. The plots for the relative deviations along the X axis are shown in Fig. 3(a) and (b) for the ratios (r_{rod}/r_o)

Table 1
Colour code assigned to different orders of magnitude of σ, the relative error

Range of relative error σ	Colour
$1 > \sigma > 0.1$	Black
$0.1 > \sigma > 0.01$	Red
$0.01 > \sigma > 0.001$	Green
$0.001 > \sigma > 0.0001$	Blue
$0.0001 > \sigma > 0.00001$	White

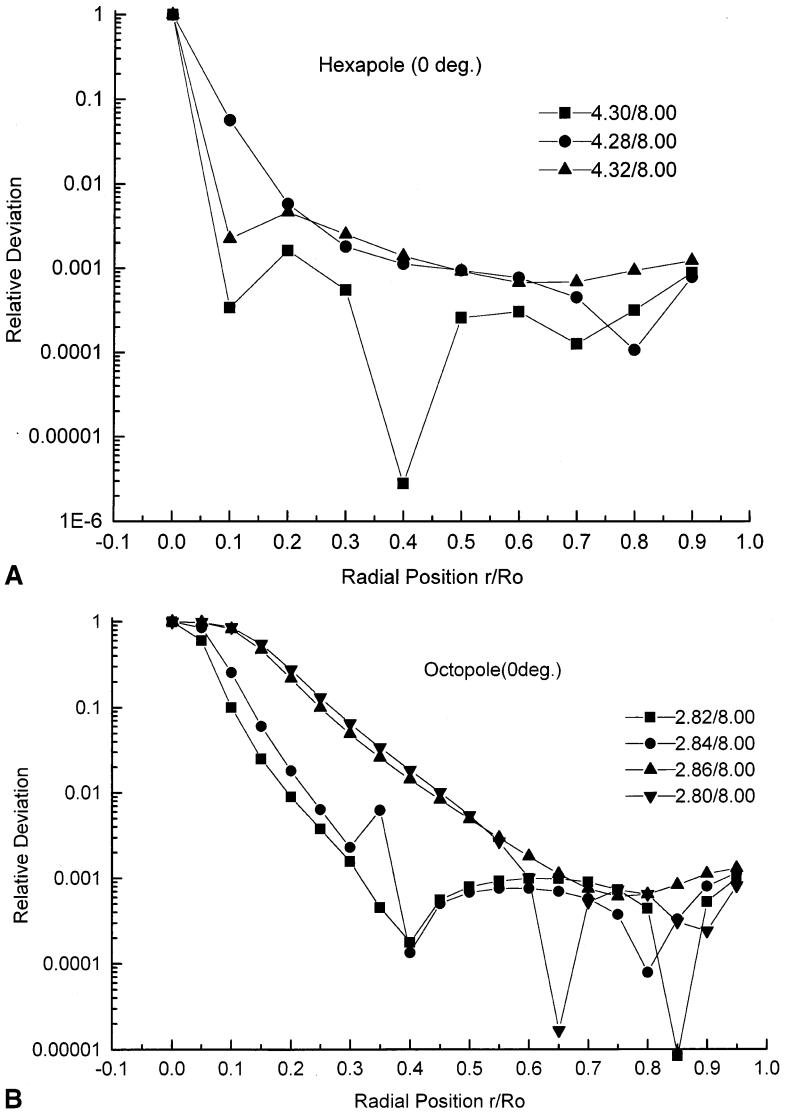

Fig. 3. Plot of relative deviations of potentials from the ideal values for hexapole (a) and octopole (b) with radial distance along a line on the axis of symmetry. Different lines are for different values of the ratio (r_{rod}/r_o).

around the optimum value. From the results of these studies, it is concluded that for a hexapole with a ratio (r_{rod}/r_o) equal to 0.5375, the deviations from the ideal potentials are the lowest. This corresponds to a rod radius of 4.3 mm for the chosen hexapole with a field radius of 8 mm. This optimum value of the ratio $(r_{rod}/r_o)_{hexapole}$ has been further confirmed by simulating additional geometries with field radii of 10 and 5.581 mm. For the octopole geometry with a rod radius of 2.84 mm or a ratio $(r_{rod}/r_o)_{octopole} = 0.355$, the obtained relative deviations are the smallest. Hence it is concluded that this is a good approximation for the ideal octopole field.

To verify the above conclusions, the potentials obtained at different positions from the simulation have been fitted in the multipole expansion series expressions (truncated to "*L*" terms) for both the hexapole and the octopole. The equations fitted are, in polar coordinates,

Table 2
Numerical values of the first five coefficients in the multipole expansion series

Coefficient	$(r_{rod}/r_o)_H$ = 4.28/8	$(r_{rod}/r_o)_H$ = 4.30/8	$(r_{rod}/r_o)_H$ = 4.32/8	$(r_{rod}/r_o)_O$ = 2.80/8	$(r_{rod}/r_o)_O$ = 2.84/8	$(r_{rod}/r_o)_O$ = 2.86/8
A_1	0.99768	1.00111	0.99961	1.012	1.0065	1.04198
A_2	0.00922	0.11754	1.54462	0.0281	−0.0255	−0.07967
A_3	−0.04151	1.54462	0.00007	−0.3008	0.04994	−0.67918
A_4	0.05389	2.6369	0.54384	0.17211	−0.05724	1.23413
A_5	0.00042	−0.98282	0.80653	0.12236	0.03907	−1.285

$$V_H(r, \theta) = {}_H\Phi_0[\Sigma_{1H}^{L} A_L (r/r_o)^{(6j-3)} \cos (6j - 3)\theta]$$

for the hexapole and

$$V_O(r, \theta) = {}_O\Phi_0[\Sigma_{1O}^{L} A_L (r/r_o)^{(8j-4)} \cos (8j - 4)\theta]$$

for the octopole. Here Φ_0 is the potential applied to the electrodes with respect to the shield, with the presubscripts H and O denoting the hexapole and octopole. The maximum number L of the coefficients A_L, has been limited to nine. The values of the first five coefficients in the multipole series expansion are given in Table 2 for the geometries of octopole and hexapole around their optimized values. From this table it is seen that the coefficients A_2, A_3, etc. have quite low values.

4. Conclusions

Simulation studies are done using the SIMION 3D Version 6 software package for electric hexapoles and octopoles using rods of circular cross section housed in a shield at zero potential. The ratio (r_{rod}/r_o) is optimized for the chosen value of $(r_{sh}/r_o) = 3$ to obtain low values of relative deviations from the idealized hexapole and octopole geometries. A ratio of $(r_{rod}/r_o) = 0.5375$ for the hexapole and a ratio $(r_{rod}/r_o) = 0.355$ have been found to offer the lowest deviations from the ideal potentials. The SIMION determined potentials have also been fitted into the appropriate multipole expansion series with a maximum of nine terms and the coefficients of the higher terms are low for the optimized geometries.

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