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Installation and Operation of the Ion Optical Program SIMION

P. J. Todd
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D. H. Smith

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P. J. Todd, H. S. McKown, and D. H. Smith

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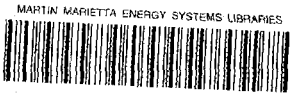

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ABSTRACT

SIMION is a Fortran program that helps design electrostatic lenses. Both equipotential and ion path plots can be obtained. The program has proven extremely useful in numerous applications, ranging from mass spectrometer ion sources to setting up primary beam optics for organic SIMS. This report is a tutorial on its use, leading the user step-by-step through the various options. Examples are given, and a sample lens is analyzed and refined. Anyone with an interest in design of ion optics will benefit from acquiring and applying SIMION, either in its Fortran or its IBM-PC form. It is the former that is described here.

I. DEVELOPMENT AND USE OF THE ION OPTICAL PROGRAM SIMION

Introduction

The ion optical program SIMION was written in its original form by D. C. McGilvery as part of his undergraduate honors work and was subsequently published as part of McGilvery's Ph.D. Thesis (Latrobe, 1978). It was the good fortune of one of us (PJT) to have worked with McGilvery while he occupied a postdoctoral position at Cornell. During this time, a tape copy of the original program was obtained which eventually found its way to ORNL. Extensive use has been made of the original program here[1-4] and elsewhere since then, primarily in the design of mass spectrometer ion sources. We have made a few changes to the original program, mostly to facilitate data input and output, not necessarily to make the program more user-friendly, just a little less user-tedious. It is a tribute to McGilvery's efforts that these changes have been largely superficial. Our main contribution to the development of the program is expanded documentation contained in this report. For the record, we request that any published reports on the use of SIMION include reference to McGilvery's thesis.

By and large, the requests for the program that we have received have been from chemists involved in mass spectrometry, and who have what might be called a passable knowledge of ion optics. In this regard, SIMION can serve as an excellent tutorial device as well as a tool for calculating surprisingly accurate ion trajectories. In the hands of the novitiate, SIMION makes possible development of highly sophisticated ion optical devices. As a tool for the more experienced, the same result is achieved, but in a much shorter period of time. In this report, we detail the installation procedure required for use of the program and provide an example of the use of the program to develop a simple-minded ion source.

Program Structure

A main program (SIMION) is used via which various subroutines are called. The information which is passed from subroutine to subroutine is

a matrix consisting of 5000 points which represents a potential distribution. Subroutine NEW is used to define the name and limiting parameters (e.g. voltage and dimensions) of a potential array to be developed. BILD is to assign values to the ion optical elements of the array. REFINE is employed to calculate the potential distribution of the array. SAVE is used to store the array on disk, and OLD is used to recall a saved array. TRAGIC and CONTUR use the calculated potential distributions to calculate and plot trajectories of charged particles and to plot potential curves for the array respectively. Subroutine END provides a convenient exit.

As a separate option, the program READPT (run independently from SIMION) is included which allows a potential array to be retrieved from disk and printed out on standard computer paper. This is particularly useful in ascertaining that an array has been entered correctly.

Program Limitations

SIMION is only useful for the calculation of charged particle trajectories under the influence of electrostatic potentials, and these trajectories can be estimated only to within 10%.[5] Our experience with SIMION is that 10% is an upper limit to the uncertainty, and, more commonly, the accuracy of voltage applied to electrodes calculated to bring about focus is better than 5%. However, to obtain such accuracy requires that long periods of time be dedicated to calculating the potential distribution of ion optical elements. Furthermore, space-charge effects are not computed by the program so that, at low ion voltages and with high currents, substantial differences would exist between calculated and observed focusing conditions.

Most importantly, SIMION is not capable of generating a potential array necessary to bring about a specific ion trajectory. (Electrode configurations are generated by the user; SIMION merely makes it possible to ascertain what final ion trajectories such a configuration of electrodes will cause ions with the specified initial trajectories to have.)

As a consequence, if a serious study is not made of what approximate ion optical properties are required and what system of ion optical elements is likely to generate such trajectories before SIMION is used, a great deal of time is wasted. Numerous texts exist regarding charged particle optics.[6,7] These should be used in conjunction with the program.

II. SIMION INSTALLATION

1.0 System Requirements

1.1 PDP-11 with at least 24K usable memory.
    1. RT-11 V3 or subsequent versions OPERATING SYSTEM.
1.2 TRANSFER MEDIUM
1.2.1 Preferably DOUBLE DENSITY, SINGLE SIDE FLOPPY.
1.3 FILE STORAGE MEDIUM may be same as 1.2.1, but preferably system disk.
1.4 TEKTRONIX 4010 or 4012 keyboard display.
1.4.1 HARD COPY UNIT is desirable.
1.5 PRINTER
1.5.1 The keyboard on the printer is used for data input.
1.6 WARNING: SIMION as written on the transfer medium is configured for a single user system. For multiuser systems, the program MUST be modified to avoid system crash. READ ALL THE INSTALLATION INSTRUCTIONS BEFORE RUNNING THE PROGRAM.

2.0 Procedure

2.1 Loading

If the system in use has a hard disk unit, copy the entire floppy onto the hard disk, e.g., (See System Documentation for details).

```
.COPY  DY0:  DL0:
```

N.B.: The program received is the SIMION source program as written. Since systems vary from lab to lab, some modifications of the source program will be necessary. These are easily accomplished by reasonably experienced programmers (e.g., graduate student).

2.2 Editing

2.2.1 PLOT.MAC This program contains the addresses of the Tektronix status register and data buffer in lines 5 and 6. It must be configured to the particular system using the text editor to change the existing statement:

```
        VTPRS = 176524 ; address of 4010 STATUS REGISTER
to:     VTPRS = ------ ; address of 4010 STATUS REGISTER
```

and the existing statement:

```
        VTPRB = 176526 ; address of 4010 DATA BUFFER
to:     VTPRB = ------ ; address of 4010 DATA BUFFER
```

2.3 After Exiting the editor, enter:
@SIMC to execute the command file SIMC

4 When the computer finishes the necessary compilation and assembly, enter:
@SIM

3.0 IF YOU ARE USING A MULTIUSER SYSTEM, THE FOLLOWING MUST BE DONE BEFORE SIMION IS RUN. FAILURE TO DO SO WILL CAUSE A SYSTEM CRASH. If you are using a single user facility, no problem will occur.

3.1 EDIT REFINE.FOR

3.2 Delete statements 7, 8, 9, 901, 999, 1001 and 1002.

3.3 Change statement C902 to 902.

3.4 Optional: Line 12 may be changed to type every Nth line of the Refine operation. For very fast computers, e.g., VAX, the printing portion is the slowest step. Since generally between 100 and 1000 interactions are used in refining the potential contours of an ion lens, it is advantageous to print only every tenth line or so.

3.5 Exit the editor

3.6 Enter @SIMC

3.7 Enter @SIM

4.0 Now you are ready to use SIMION.

III. CASE STUDY: DESIGN OF A MASS SPECTROMETER ION SOURCE

1.0 Setting up an Electrode Array

Lay out on a piece of graph paper a cross section of the ion lens system to be employed. Figure 1 shows how this is done for the example, an experimental ion source design. The graph can have up to 5000 points, e.g., 50 x 100. The longer axis will generally be the X axis. If the system has rotational symmetry about the X axis, lay out only one side with respect to the X axis. The same is true if the ion axis lies within a central plane of symmetry. If the lens system has neither symmetry, both sides must be drawn. Examples of the three types of symmetry are shown in Fig. 2.

The rationale for assigning the matrix to be one of three symmetries is two-fold. For circular symmetry, the calculation of trajectories is done using (R,Z,Ø), i.e., cylindrical coordinates, whereas when no circular symmetry is present, (X,Y,Z) coordinates are used. Since determination of potential contours involves solution of the Laplace equation, by iterative approximation, e.g.,

$$\frac{\partial V}{\partial X^2} + \frac{\partial^2 V}{\partial Y^2} + \frac{\partial^2 V}{\partial Z^2} = 0$$

the approximating equations are different depending upon coordinate systems. Secondly, when potentials on either side of the X axis are equal, only one-half as many potential points need be calculated. This means that effectively 10,000 potential points may be calculated instead of 5,000. The greater the number of points/element, the greater will be the accuracy of the calculations.

Two points are worth mentioning regarding choice of the matrix dimension. First, ion trajectories are generally important between one slit and another. (Note that slit here is defined as an aperture, through which ions are transmitted.) A slit is not a lens element and is usually at ground and almost always in an area where no field $(\partial V/\partial q) = 0$ is present. The position of slits should be included in the diagram.

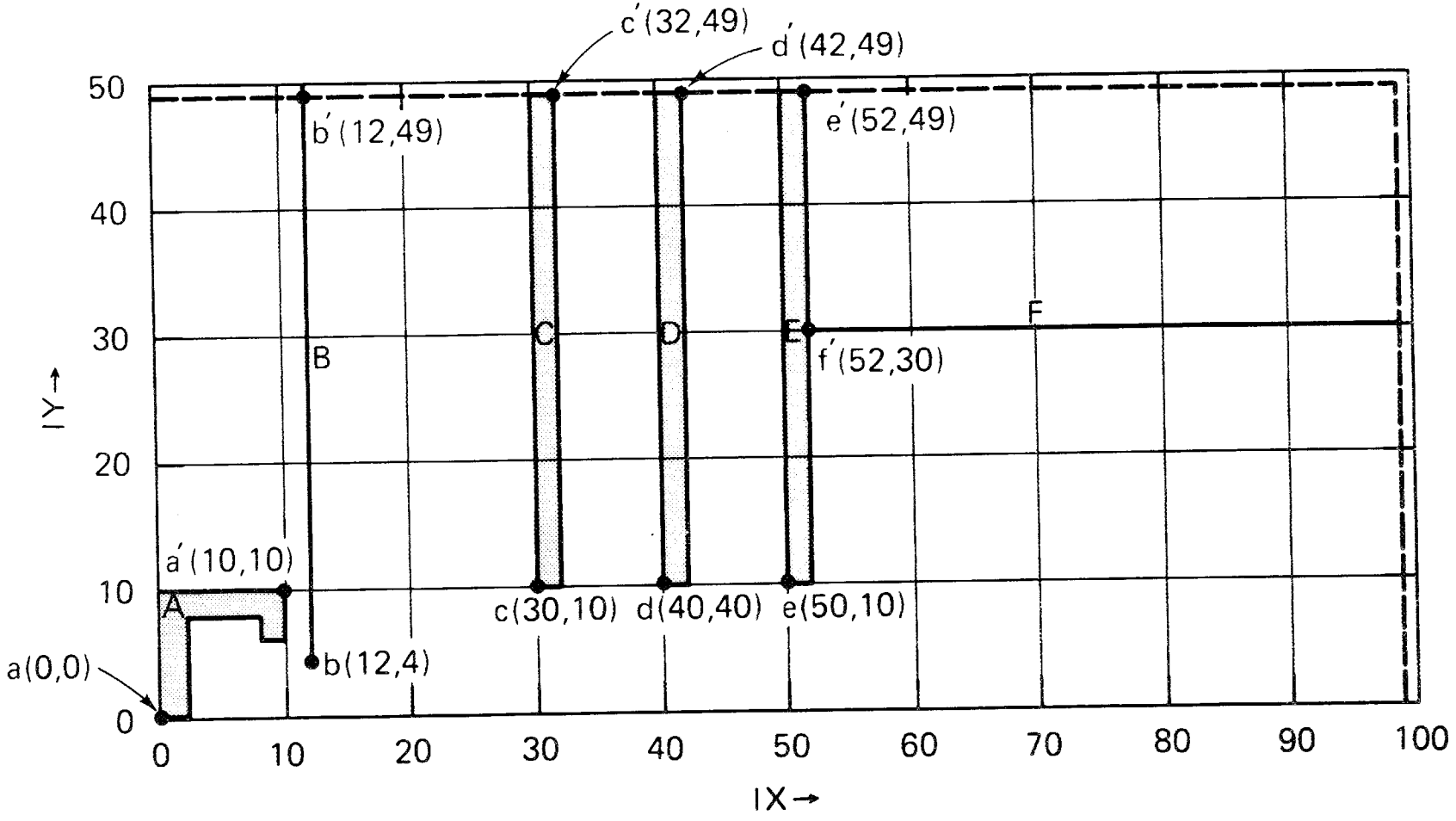

Fig. 1. Layout of electrode array

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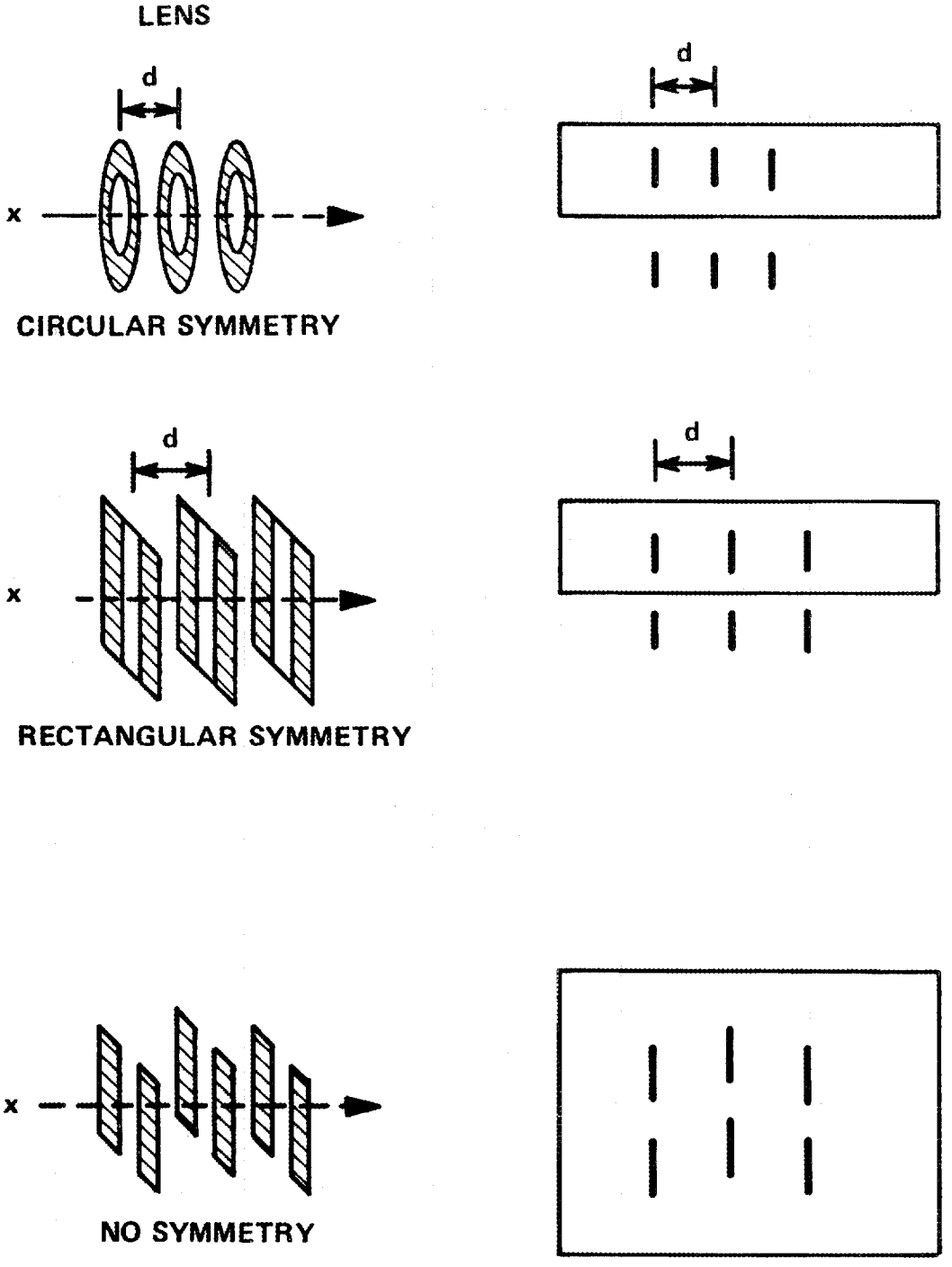

Fig. 2. Symmetry in lenses

Secondly, the boundary of the graph must represent regions where (a) there is no field or (b) the field is shielded from the ion beam. The latter case is particularly useful when ion sources are being studied, because 10,000 volts are often applied.

A sample layout, with applied voltages, is shown in Fig. 1. Note that the coordinates of the grid go from 0 to 99 and 0 to 49. This is a 5000 point grid because 0,0 is a point. Arbitrarily, we have assumed that the system has circular symmetry about the X axis, and as a result only graphed half of the system. Note that we have included the lower left and upper right coordinates of each electrode. Such information is required by the program.

An important factor in graphing the system is scaling. It does not matter what actual size the lens is, but you do want to keep things to scale. The temporal scale used in SIMION assumes the matrix points are 1 mm apart. If on your grid you wish to have a 10 mm distance between points, no effect is observed in trajectory calculations unless you want to know the time elapsed for the transit of an ion through the lens.

1.1 Setting Applied Voltages to the Electrodes. Assign potentials to the electrodes. This is done rather arbitrarily unless you know something about ion optics. For example, a sector mass spectrometer uses about an 8 keV source. Hence, electrode A is at +8000V. Furthermore, electrode E must be at ground; i.e., it has zero potential. We will also make the potential on electrodes B and C zero. This makes the lens subsystem, C,D,E, what is called an Einzel or unipotential lens. To element D we will assign a potential of 5000V.

SIMION can handle both positive and negative potentials. The maximum potential that would be entered would be the most positive. If all potentials were negative, then the most positive potential would be 0.

To many people the voltage reference system used for ion lenses causes confusion. For ion sources, lens potentials are actual applied potentials. For other lenses, the potential listed in texts and references is referenced to the potential at which the ions' kinetic energy would be zero; this would, in general, be different from the applied potential. For example, a two-element lens with respective potentials listed as 2000 and 3000 V in the text actually has applied potentials of 0 and 1000 V, respectively, and is meant to operate on 2000 eV ions. SIMION uses actual applied voltages and actual initial ion kinetic energies.

1.2 Entering the Data. The following is applicable to the design shown in Fig. 1. In the following description, we will use the designation CTRL/X to indicate simultaneous pressing of the CONTROL and X keys; this is the convention followed in most manuals.

1.2.1 Key in:

R SIMION [Carriage Return, CR]

1.2.1.1 The system responds:

OPTIONS AVAILABLE, SPECIFY BY TYPING FIRST LETTER OLD, NEW, END, SAVE, MODIFY REFINE, TRAJECTORIES, CONTOURS, AREA

1.2.1.2 Enter N [CR] (for new).

1.2.1.3 The system responds:

PLANAR GEOMETRY, TYPE-1, CYLINDRICAL SYMMETRY, 0, PLANAR SYMMETRY, +1.

1.2.1.4 Enter 0 [CR], since we are doing the example.

1.2.1.5 The system responds:

MAX ELECTRODE POTENTIAL?

1.2.1.6 Enter 12000 [CR]. We generally add 1000 volts to the highest potential we expect to use or, say, 10V for low energy systems, but it is often useful to use up to twice the maximum expected voltage.

1.2.1.7 The system responds:

ARRAY DIMENSIONS (IX,IY)

1.2.1.8 Enter 100,50 [CR] (See Step 1.0)

1.2.1.9 The system responds:

SPECIFIC SCALE FOR MULTIPLE PLOTS? USE 0 (zero) IF OKAY.

This query is used for determining trajectories for a number of successive, independent lenses which are joined by field-free regions ($\partial V/\partial q = 0$) and for which SIMION calculations are done independently. For example, if you have a series of independent lenses, you do the potential and trajectory calculation for the first lens, then use the final trajectories of the first lens as the initial trajectories in the design of the second lens, etc. Each lens would be entered and evaluated using a different run of the program and each array would be stored on disk as a separate file. By using a constant scale, calculations for each independent lens may be done and the hard copies of the plots all connected to make an impressive figure. The largest element is used to determine the scale factor by the use of:

$$SF \quad \frac{443}{IY-1} =$$

and

$$SF = \frac{1023}{IX-1}$$

where IX and IY are the array dimensions for the particular element. Whichever SF is smallest is the one to use. Once the scale factor is chosen, it can be used to make each successive plot on the Tektronix to the same scale (the same distance between points from lens to lens). For a single plot, just type a 0 (zero) as we do, to let the computer do the graphic scaling.

1.2.1.10 Enter 0 (zero) [CR].

1.2.1.11 The system responds:

For X+Y SCALES EQUAL TYPE E, OR TOTAL SCREEN, T. This particular command is necessary because, in general, the matrix dimensions will not have the same relative X and Y dimensions as the Tektronix display. If you use E, a portion of the screen will be unused, but the X and Y dimensions of the computer plotted diagram will be the same, e.g. 1 mm between dots in vertical and 1 mm between dots in the horizontal. If you use T, the computer will fill the screen with your matrix, but the spacing between dots will be different along the vertical and horizontal axes.

1.2.1.12 Enter E [CR].

1.2.1.13 The system responds.
M FOR MIRROR DISPLAY.

1.2.1.14 Enter M [CR]. This option is merely for graphic purposes. Since most ion optical systems are symmetric, graphics typically only show one-half of the system. For convenience, SIMION plots this one-half and its mirror image. If you don't want it, simply hit [CR], but M looks better.

1.2.1.15 The system responds:
FUNCTION DATA PLEASE?

1.2.1.16 Now comes the fun part. Take a look at the elements shown in Fig. 1. They are all rectangles. They represent but one of four possible electrode configurations.

1.2.1.16.1 To describe a rectangle, enter:
R, lower left coordinates, upper right coordinates, e.g. for electrode C in Fig. 1:
R, 30, 10, 32, 49

1.2.1.16.2 To enter a right triangle, enter:
T, coordinates of acute angle vertex, the x length (which is negative if moving toward X = 0) and the angle (degree) with respect to the X axis. If the hypotenuse is between the base and the X axis, the angle is negative. (This goes against convention, but is the system employed here.)

1.2.1.16.3 To enter a circle, enter:
C, coordinate of the center, radius.

1.2.1.16.4 To enter a point, enter:
P, coordinate of point.

1.2.1.17 For the problem at hand, enter:
R, 0,0, 10,10 [CR]
E, 8000 [CR] (See Note 1 below)
E, 30, 10, 32, 49 [CR]
E, 0 [CR]
R, 40, 10, 42, 49 [CR]
E, 5000 [CR]

R, 50,10,52,49 [CR]
E, 0 [CR]
R, 52, 30, 99, 30 [CR]
E, 0 [CR]
R, 99, 0, 99, 50 [CR] This last entry ensures that the ions are
E, 0 [CR] passing into a field-free region with V=0.
X [CR]

Note 1. After entering the coordinates of an electrode, and hitting the [CR] key, the system will "echo" E, 0. or the last entered value for an electrode. If that particular potential is suitable, hit [CR] and it will be entered; if not, enter E, potential, as indicated.

1.3 Saving the File

1.3.1 The X[CR] command causes the entries to be plotted on the Tektronix terminal. If you have entered the coordinates properly, the screen will appear as in Fig. 3 and the printer will echo OPTION? Compare the screen with your graph; you will note that the rectangle bounded by (0,0) and (10,10) is completely enclosed. This is not what the graph in Fig. 1 shows. Hence, the screen must be modified. However, before doing that we recommend that you "save" the present plot in its own file.

1.3.2 Accomplish this by entering:
S [CR]

1.3.3 The system echoes:
POTENTIAL ARRAY, OUTPUT FILNAM.EXT

1.3.4 You can then name the array as you choose. Typically, you will use the abbreviated name of the subject electrode system and the three initials of the designer.

1.3.5 The "SAVE" option is a very important command. It not only stores on disk the electrode configuration, but also the calculated potential contours. These contours are calculated using an option "REFINE," which has not been executed so far in this exercise, but for accurate determination of the contours, anywhere between 30 minutes and 12 hours are required. Files can always be deleted as progressive steps are taken, but if there is no backup made between

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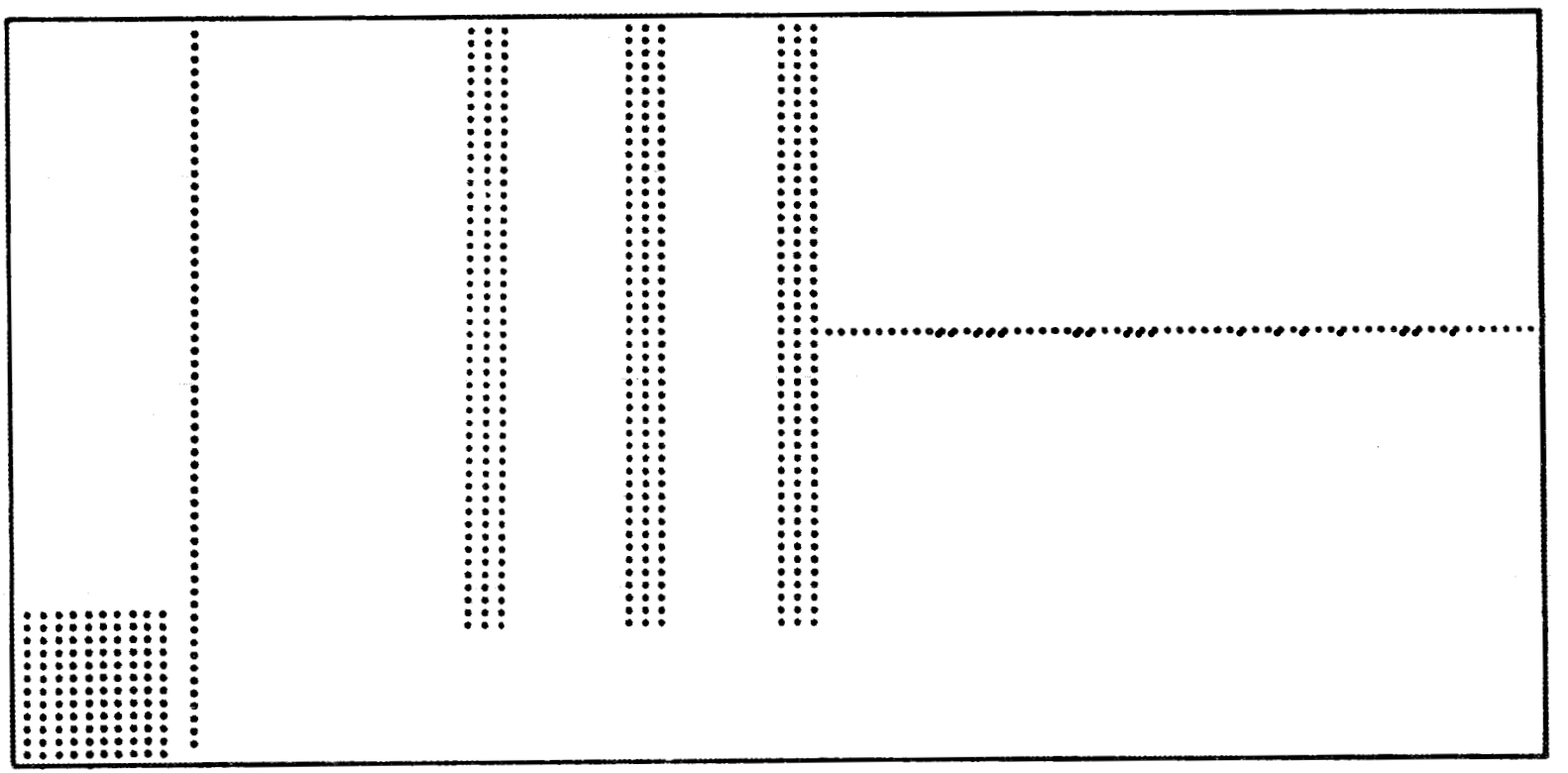

Fig. 3. Terminal display of electrodes

successive option commands in running SIMION, data can be lost if there is a system failure during operation. Hence, we recommend in the initial steps of setting up an electrode system that the file be saved between each major option command.

1.3.6 The system echoes
"OPTION?"

1.3.7 Enter E [CR]

1.3.8 This returns the console to RT11, which echoes with: .

1.4 Printing the Electrode Array. Before modifying the electrode array, we recommend that the potential array coordinates be printed out on the printer. This is accomplished by the program READPT.
Hence, enter:

1.4.1 RUN READPT [CR]

1.4.1.1 The system responds:
ENTER POTENTIAL ARRAY, FILNAM.EXT

1.4.1.2 Enter the FILNAM.EXT you saved from 1.3. The system responds:
KCYL = 0 ELECT = 12000.00 IX = IY = 50
DATA OR ELECTRODE PLOT?

1.4.1.3 The KCYL = 0 is symmetry employed in 1.2.
ELECT = 12000.00 is the maximum electrode potential, and IP and IY are the array dimension. The query can be answered by entering E or D. Enter E to get a printout of the electrode array as follows: E [CR]

1.4.1.4 The system responds:
ENTER 6 FOR OUTPUT ON LINE PRINTER.
ENTER 7 FOR OUTPUT ON CONSOLE TERMINAL.
Generally, you will enter: 7 [CR]

1.4.1.5 The system responds with a printout of the electrode array, with points on the axes numbered. When modifying the electrode array, these coordinates are very handy. Note that there is a difference in distance between points on the X and Y axes. This is a printer function. Occasionally, depending on the operating system, carriage return on the printer will cause the printed electrode array to be confusing. If this happens, enter CTRL C and, when back to the monitor, enter: SET TT: NOCRLF [CR] to suppress

carriage return. Then begin again at 1.4.1. When the printout has been completed, the system will print:
DATA or ELECTRODE PLOT?

1.4.1.6 Hit CTRL/C to interrupt READPT and get back to the program monitor. The printout for points entered so far is shown in Fig. 4. Compare it to Fig. 3.

1.5 Modifying the Electrode Array. Two points are worth mentioning here. First, commands used in entering data [1.2] are essentially the same commands used in modifying the system. Secondly, if you detect an error during the actual entering of data, simply re-enter the electrode coordinate and potential and everything will be fine, presuming of courtse that you don't make the same mistake again, or a new one. This presumes a great deal, as our experience indicatees.

1.5.1 To begin the modification, enter

1.5.1.1 RUN SIMION [CR]

1.5.1.2 When queried as to OPTION?, enter
O [CR] (for OLD)

1.5.1.3 When queried, enter the FILNAM.EXT selected in 1.3.

1.5.1.4 When queried as to OPTION?, enter
M [CR]

1.5.1.5 The system responds:
FUNCTION DATA PLEASE?

1.5.1.6 We have a new operation to enter here, the "NONELECTRODE." The point of this operation is to "remove" electrode material; it converts an existing electrode or space into a new space. It can be thought of as an electrode eraser, but it does more, because it has a potential that must be associated with it. Remember that in the design of ion optical systems, each point in matrix space has an actual potential associated with it. The calculation of these potentials is what is performed by the program. You can help the program do this by assigning potentials to nonelectrodes which are roughly what the potentials should be. This reduces the number of iterations required for convergence. For example, you can see that electrode A needs to be hollowed out. This is accomplished by entering:

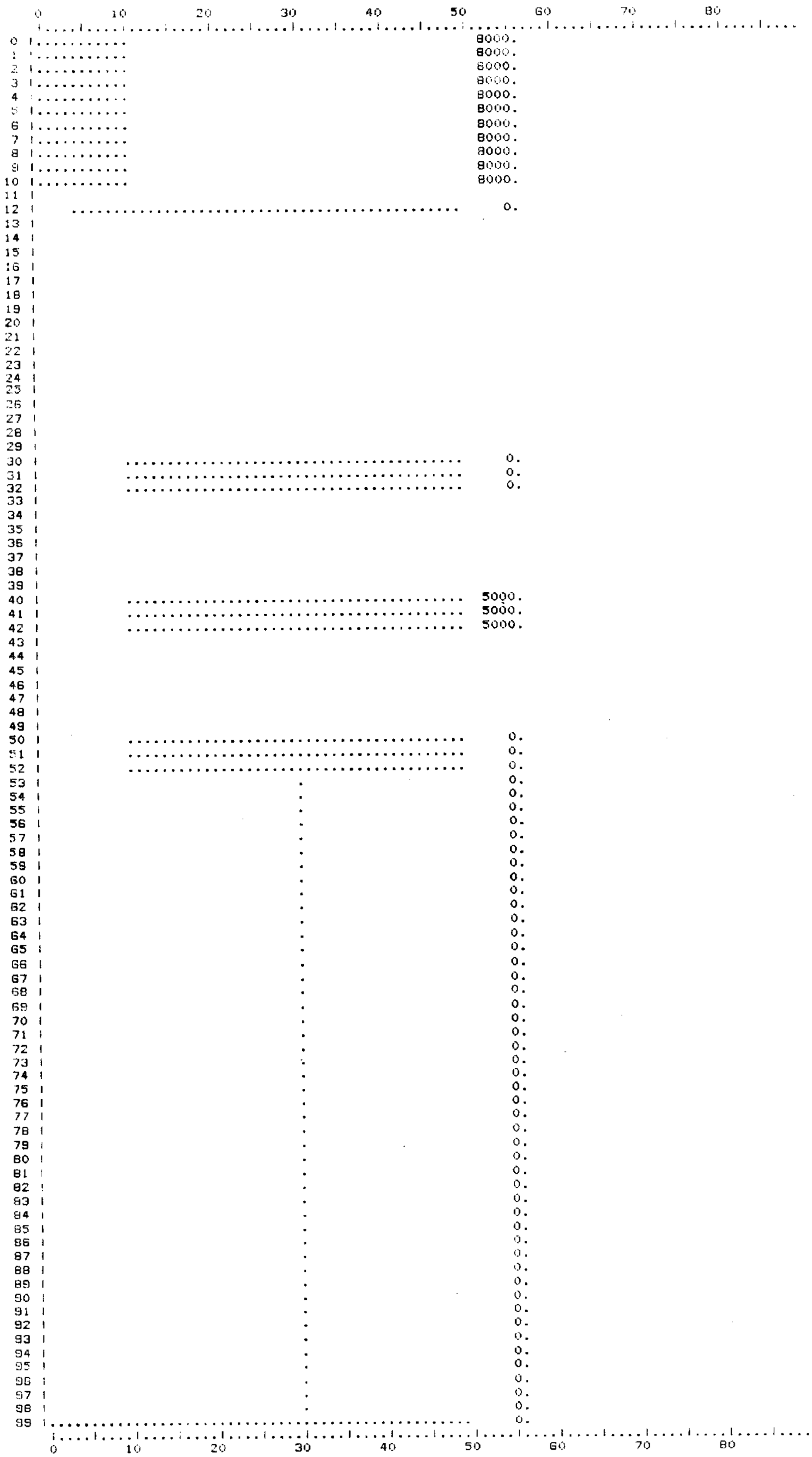

Fig. 4. READPT display of electrodes

R,3,0,7,7 [CR]
N,8000 [CR]
R,8,0,10,5 [CR]
N,4000 [CR]
R,12,0,12,3 [CR] (Used to correct electrode B aperture.)
N,0. [CR]
X [CR]

The first R and N entries indicate that the potential in the region hollowed out is 8000V, which is approximately what it will be. Similar approximations are used for the subsequent entries.

You will note that when electrodes are hollowed out that the extreme coordinates are one less than where we wish the final electrode to remain. This is because electrodes are indicated as points on the matrix, as are nonelectrodes. A point cannot be both an electrode and a nonelectrode at the same time, and the last command has precedence.

1.5.2 After the display on the Tektronix is as shown in Fig. 5, respond to the OPTION? query with a SAVE command again (See 1.3). Note that files created and stored by SAVE cannot be changed. If an electrode array file is called, and subsequently modified as above, a new file must be created or the original data will be lost. If your modifications consist merely in correcting input errors, you may choose not to change file names to reduce clutter in your disk directory. Print out on the line-printer using the program READPT, as shown in Fig. 6. Compare the output to the original graph shown in Fig. 4

2.0 Calculation of Potential Distribution. The heart of this program is the calculation of the potential distribution. Depending upon the desired accuracy, the time required for calculation varies from about one-half hour (100 successive approximations to solution) to days. Generally, between 100 and 1000 approximate solutions will be required to obtain satisfactory results. Entry is as follows:

2.1 R SIMION [CR]

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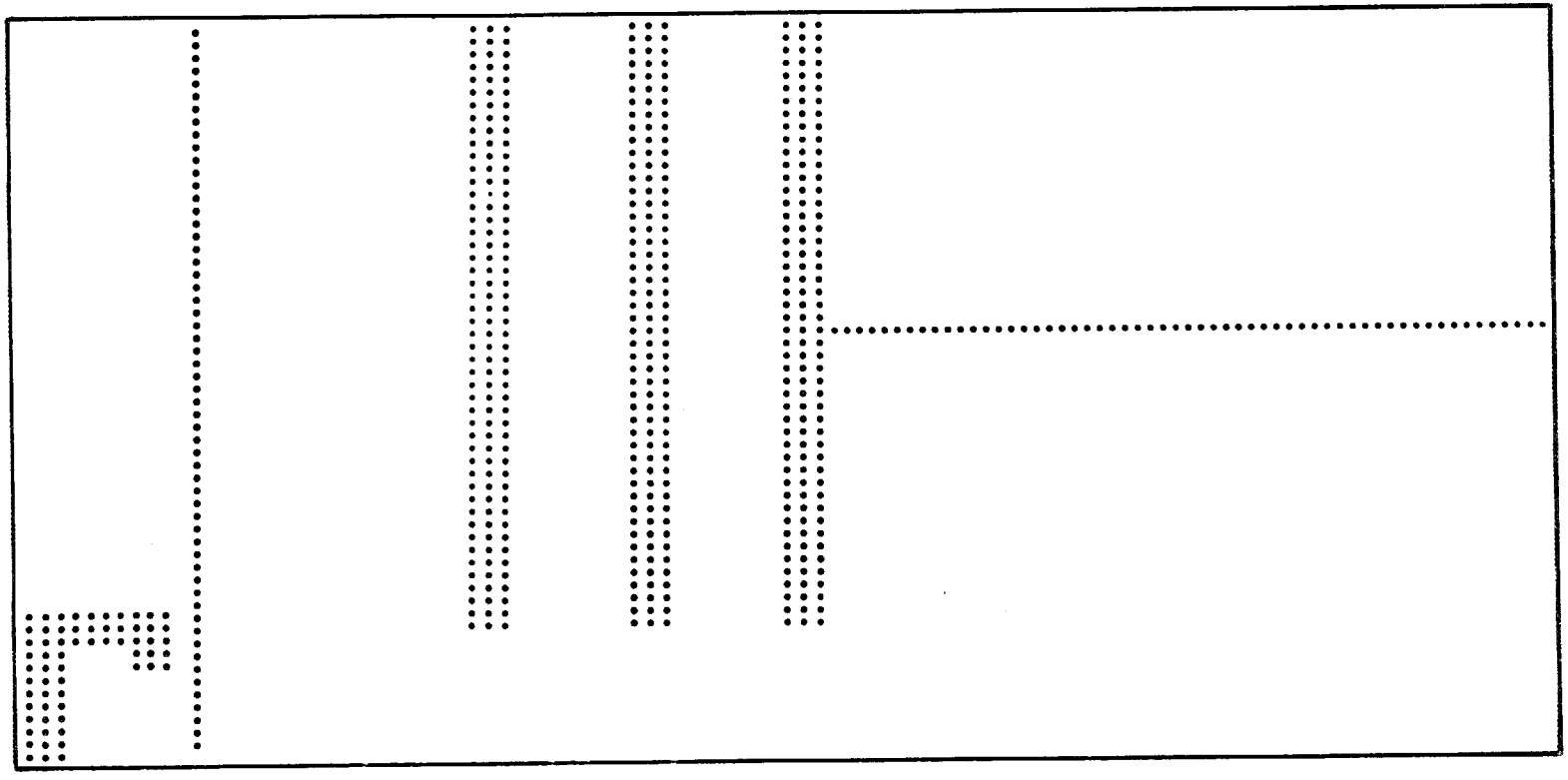

Fig. 5. Modified terminal display of electrodes

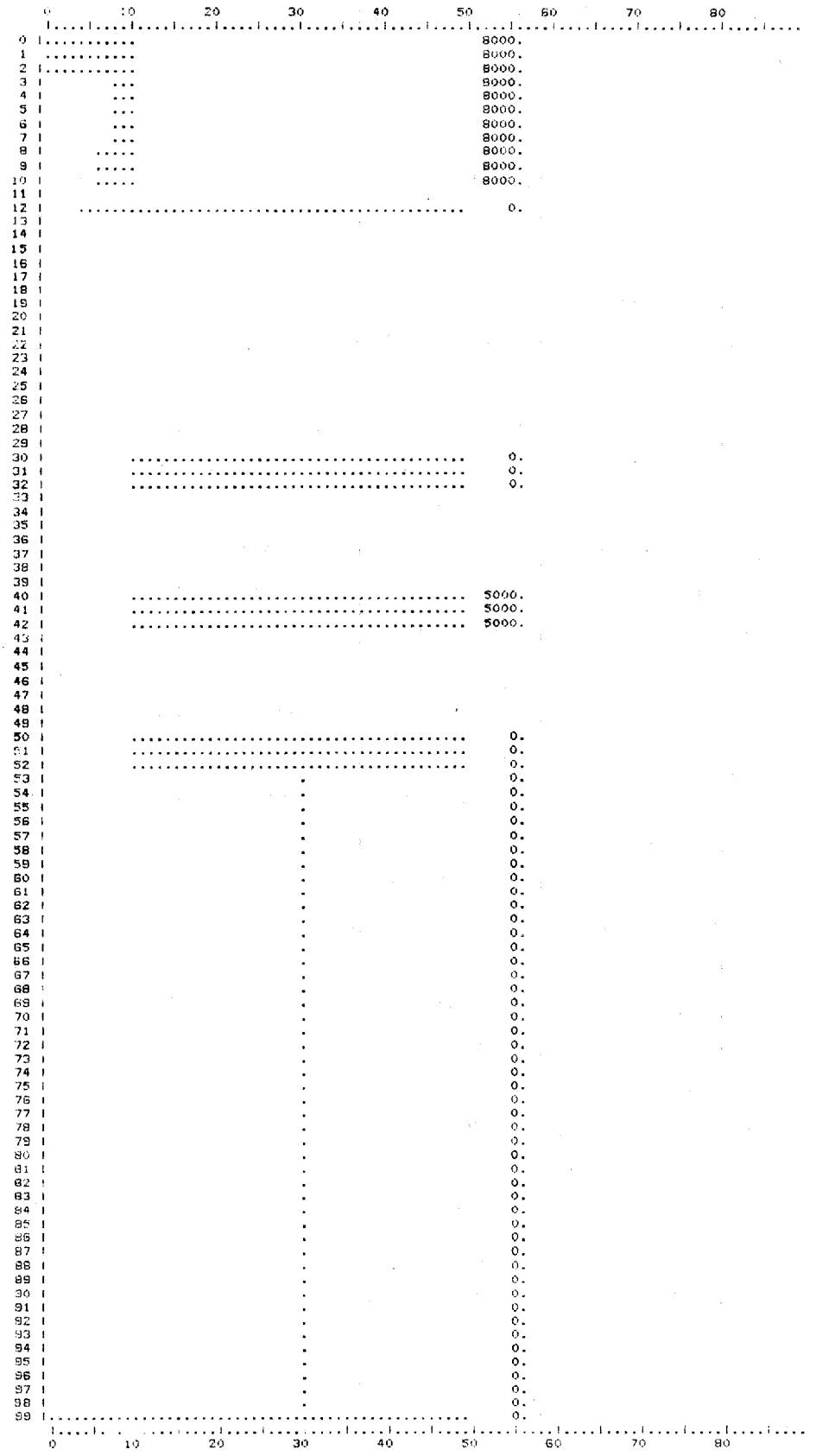

Fig. 6. Modified READPT display of electrodes

2.2 In answer to the "OPTION?" query, enter the alphabetic:
O [CR]

2.3 In answer to the query FILENAME.EXT, enter the name assigned to the file in Step 1.5.2.

2.4 Answer the usual queries which follow, as you choose, but they are largely irrelevant until the OPTION? query, which is answered by:
R [CR]

2.5 The system responds:
NO. OF ITEREATIONS, OVER-RELAXATION FACTOR, LOWER LIMIT 30,000,
.4, 10.

2.5.1 No. of Iterations: This is the number of successive approximation solutions which will be completed before the computer stops, unless the system reaches a specified accuracy (See Lower Limit, below).

2.5.2 Over-Relaxation Factor: This factor ranges from 0.6 to 0.4, with 0.4 being the default value. When solutions to potential distributions are determined by relaxation techniques, differences between the (n-1)th solution and the nth solution are multiplied by over-relaxation factor and added to the nth to generate the n+1 solution. The over-relaxation factor should be large (.6) at first when there is a vast difference between the potential of the n and n+1 solution. As successive solutions become closer, and if too large an over-relaxation factor is used, the solution will oscillate about the correct one but never reach it. We generally recommend using an over relaxation factor of 0.6 for the first 50 to 100 solutions, then reducing to 0.4 as the solutions approach desired degree of accuracy.

2.5.3 Lower Limit: This term specifies the desired degree of accuracy in the following way. The absolute difference between each potential calculated for the (n-1)th solution and the potential of each point calculated in the nth solution is summed and is a measure of how far away from the final solution the current solution is. Suppose the nth solution were the exact solution. Then the (n+1)th solution would be the same, and the total difference between potentials in the nth and (n+1)th solution would be zero. At this point, which, by the way, is generally well on the way to

Doomsday, the computer can do no more. Generally, using a value of between 1. and 100. will yield an adequate solution. When the specified accuracy is reached, the computer will exit REFINE and you can move on.

2.5.4 If no entries are made, just hit [CR] and the printed numbers will be used as default values for REFINE. If you want to use different values, enter the number of iterations, relaxation factor, and lower limit in that order, as, for example, 100, .6, 10 [CR].

2.5.5 The terminal responds:*

```
^C, ^O & ^P
1   125.5   0.4
2   120.8   0.4
.     .     .
.     .     .
.     .     .
```

2.5.6 The ^C, ^O, ^P indicate options which you can enter to effect either the refinement or printing of (a) the iteration number (b) the error between it and the previous solution, and (c) the over-relaxation factor, which are printed by default in the respective three columns above. These options are amplified below.

2.5.6.1 C (CTRL/C). This terminates the running of REFINE, leaving the program in SIMION so that the SAVE option may be utilized. You should hit this key ONLY ONCE to terminate the refine option without losing the calculated potentials. We recommend periodic saving of the array during operation of REFINE to avoid loss of too much computing time in case of (gasp!) power failure. This key is particularly useful for leaving the computer work overnight. You will note that the default value for the number of interactions is 30,000, which would require 10-20 days, so it will just keep running and refining in your absence. When you come back, hit CTRL/C and get onto more exciting things.

2.5.6.2 ^O (CTRL/O). This suppresses printing the results of each iteration--a decidedly useful option for long runs (30,000 iterations would take up about 500 pages of paper).

*This feature only applies to single user systems. It is the feature deleted in Part II.3.0. of SIMION INSTALLATION on multiuser facilities.

2.5.6.3 P (CTRL/P). This command restarts printing. When you have run over a night or weekend, etc., and wish to see what was accomplished in your absence, hit CTRL/P to view the ongoing calculations before you decide whether or not to terminate the subroutine.

2.5.7 Whether you terminate the run with a CTRL/C or REFINE terminates itself, it ends with the OPTION? query. Almost always, you should enter

S [CR]

for SAVE and store the determined potential distribution. You can subsequently delete, using RT-11, earlier files relating to the same electrode assembly and keep only the latest refinement. However, if you do not SAVE, in a new file the results obtained by REFINE, all the refined potentials will be lost if the system goes down or you inadvertently erase a portion of it. Furthermore, after refinement, changes can be made using the MODIFY routine discussed earlier, but any new potentials and electrode configurations added or deleted will require going through REFINE again. Changes made to potentials/electrodes will not be written into the file from which the working array was retrieved unless you keep the same file name and thus destroy the original values.

2.7 Step 7. Obtaining the Potential Distribution. This is obtained by first entering the R SIMION command, taking the OLD option, specifying the particular file and answering the OPTION? query with:

C [CR]

2.7.1 The system responds with:

1 FOR AUTOMATIC, 2 FOR MANUAL ENTRY, 3 FOR PREVIOUS CONTOURS

These three options make it possible to enter the potential contours you wish to see in a way which is most convenient to the user.

Automatic. Entering a 1 [CR] results in the query

2.7.1.1 STARTING POTENTIAL:

The response is to enter the lowest potential whose curve is desired; for example for 1000 V, the entry is:

1000 [CR]

The system responds with:

2.7.1.2 NO. OF INCREMENTS, SIZE OF INCREMENT (I2,F10.0)

The number of increments is the number of potential curves you wish plotted (up to 20), and the difference in voltage between successive potential contours. For example, we have entered

6, 1000 [CR]

to obtain six contours, to wit: 1000 V, 2000 V, 3000 V, 4000 V, 5000 V and 6000 V.

The system responds with:

2.7.1.3 ENTER CONTOUR NUMBER FOR LIST

If you wish to have the X and Y coordinates of a particular potential contour, say 3000 V, you enter:

3 [CR]

This simply means that the (X,Y) coordinates will be printed on the printer for the THIRD potential contour you requested above, i.e., the three here is coincidental to the 3000 V contour.

The value of this option is apparent if you wish to look at contours in a small region of the entire system. The potential contour coordinates can be multiplied by a factor of ten, treated as electrodes, and used to generate a new file. The new system could then be used to obtain the residence time of ions in the particular region of interest, such as, say, a source block.

2.7.1.4 To suppress the listing option, simply enter: [CR]

The system responds by displaying on the Tektronix the potential contours as shown in Fig. 7.

2.7.2 Manual Entry. This option is effected by entering:

2 [CR]

This system responds with:

2.7.2.1 CONTOUR POTENTIALS, LEAST TO LARGEST, X ENDS LIST

This option is different in both the way contour potentials are entered and the requirements of the entries. First, the voltage difference between contours need not be the same for all contours, but the lowest potential must be entered first, and each successive entry must be greater than its predecessor. Second, each contour is entered independently, followed by a [CR] as follows:

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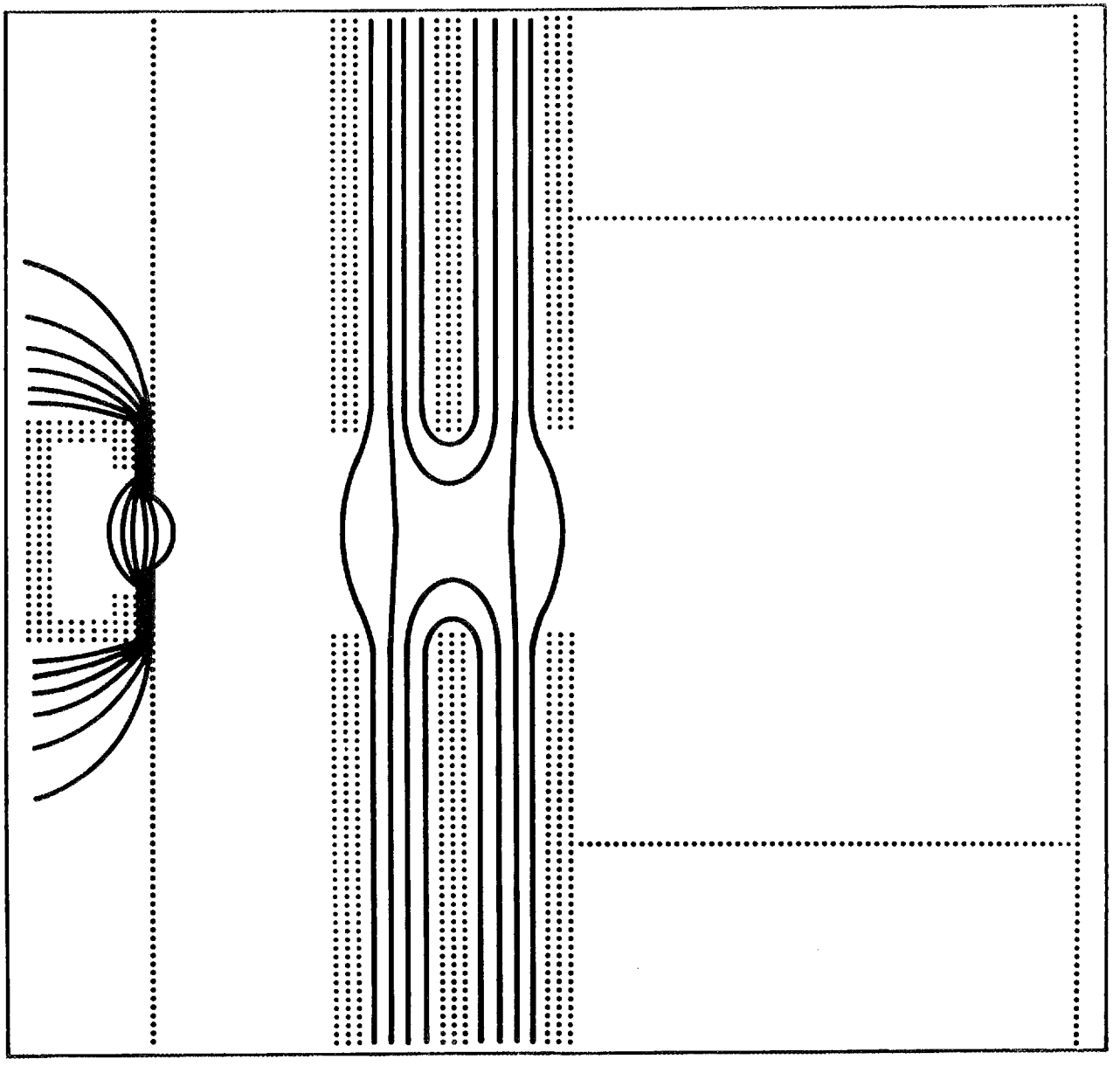

Fig. 7. Terminal display of potential contours

6000 [CR]
6500 [CR]
7000 [CR]
7500 [CR]
X [CR]

2.7.2.2 The X [CR] causes the system to respond with the CONTROL NUMBER FOR LIST prompt, which can be answered as described above to start plotting the desired contours on the Tektronix as shown in Fig. 8. Note that, although the contour potentials are all separated by 500 V, this simply is coincidence.

2.7.3 Previous Contours. Entering 3 [CR] accesses a time-saving option that allows you to use a set of contours already plotted for a previous configuration. This eliminates the need to re-enter contour values for each iteration in the approach to a final design.

3.0 Plotting Trajectories. Trajectories are determined, plotted, and printed by the subroutine TRAGIC. It may be entered via the query OPTION? after the execution of any of the previously mentioned subroutines, by responding with:

T [CR]

The system responds with:

3.1 1 TO USE PREVIOUS TRAJECTORY PARAMETERS,
0 OTHERWISE:

3.1.1 Generally, this query is answered with 1[CR] only if you want a new plot of recently plotted trajectories on the screen; otherwise [CR] should be entered.

The system responds to a [CR] with:

3.2 GRID SPACING (MM), VOLTAGE SCALING, TIME INT.

3.2.1 GRID SPACING. This refers to the distance between grid points and depends on how big the actual system would be. For example, if in the example shown the length of the assembled lens along the X axis were to be 20 cm = 200 mm, the response to GRID SPACING would be 2. Generally, for roughing out an ion optical system, scaling is irrelevant and any number (such as 1) can be entered.

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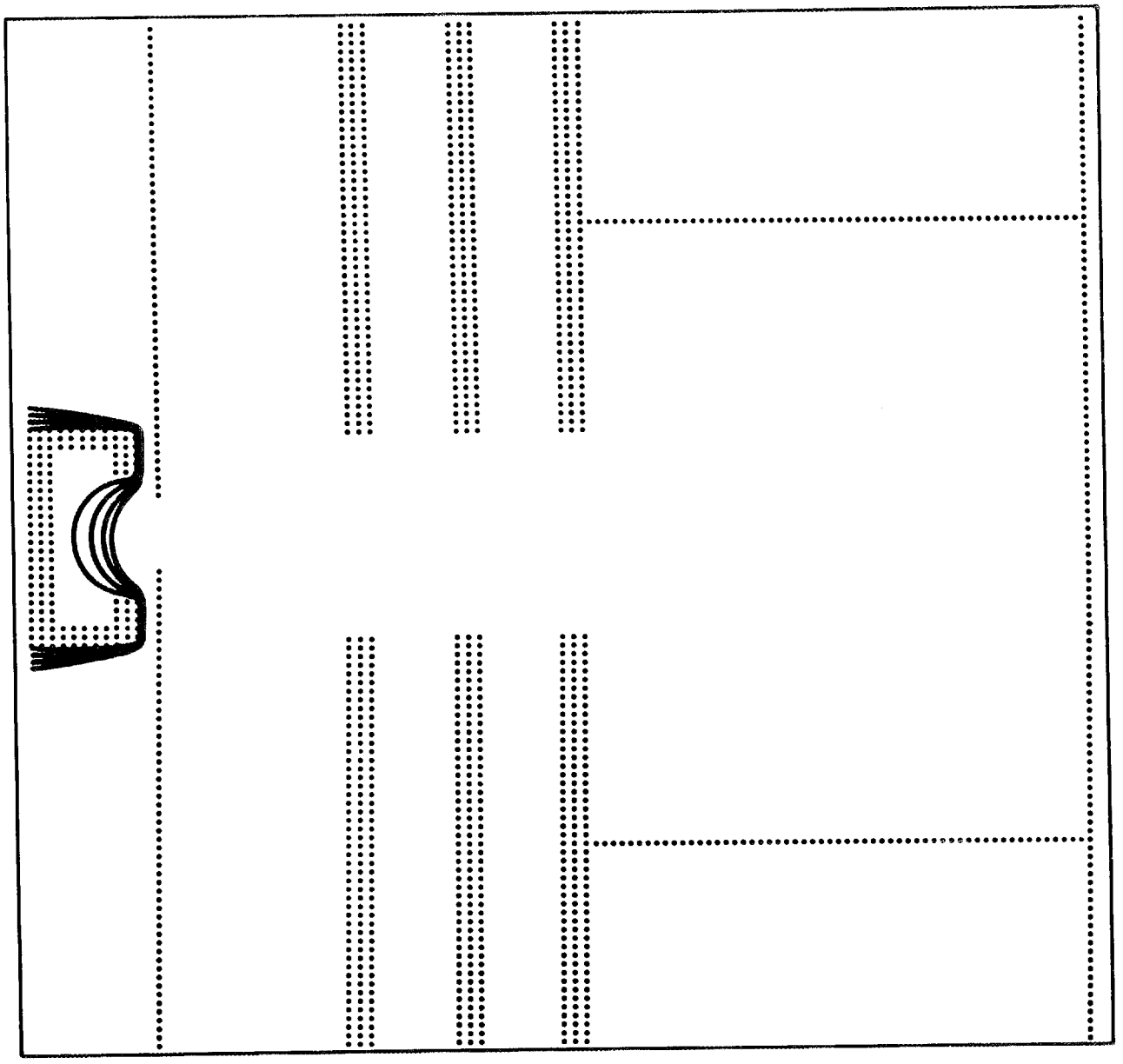

Fig. 8. Example of a contour "close-up"

3.2.2 VOLTAGE SCALING. To convert, say, all the potentials to one-half their previous values as entered in Steps 1-5, enter 0.5 and so on. Again, this option is largely irrelevant in ion optical design, but does affect ion residence time in any particular location on the grid, and, unless a study of residence times is underway, a 1 may be entered.

3.2 TIME INTERVAL. This variable yields the time interval between successive force calculations. This is primarily a plotting tool, which specifies how long a delay is desired between successive calculations of ion trajectory. Generally, a 1 is entered. A small number such as .01 will result in a less accurate plot and a large number will result in taking forever to plot a trajectory.

3.2.3.1 For the example in progress, the entry is

2,1,1 [CR]

to which the system responds

3.3 M/E Of Ion, M/E of Fragment

3.3.1 M/E of Ion. The mass-to-charge ratio of ions does not have any effect at all on trajectories in electrostatic potentials except as discussed below. However, the m/z value of an ion does affect the residence time in any particular element and the total flight time. If this is of interest, enter the appropriate m/z value. If not, enter 1. Note that m/e implies a + or - sign. + is the default value, but negative m/e values can be used for negatively charged particles.

3.3.2 M/E of Fragment. If an ion fragments during transit of the ion optical system, the ion fragment's kinetic energy will be a fraction of the kinetic energy of the parent; hence the trajectory of the daughter ion will be different from the parent's if the ion traverses an electrostatic field.

If the fragmentation is of interest, enter both parent and fragment ion M/z values, such as 100, 50 [CR].

If the fragmentation is not of interest, simply enter the m/z value of the parent, e.g., 100 [CR]

The system responds:

3.4 STARTING COORDS X, Y, INCREMENTS DX, DY

Starting coordinates are the starting coordinates in units of your array of points of any ion, either where the ions are formed or where they enter the ion optical system under consideration. The increments DX, DY are the starting coordinates for the first calculated trajectory plus the increments for the next successive trajectory calculation. For example, the entry

3,0,0,1 [CR]

would start the first calculated trajectory at point (3,0) and the second trajectory calculation at point (3,1) and so on.

The system responds:

3.5 ION ENERGY, ANGLE WRT X AXIS (DEG), INCRS DE, DTHET

Since all ions generally have a kinetic energy, be it thermal (.1 eV) or otherwise, they must have a trajectory which is specified by the angle with respect to the X axis. The increments DE, DTHET are similar to the incremental additions made to initial positions described above. For example, in the case at hand, the entry is

1,0 [CR]

to which the system responds:

3.6 HOW MANY TRAJECTORIES, FOR NEW PLOT TYPE N

This is self-explanatory, but it is worth mentioning that if incremental values, DE, DTHET, DX, DY are used, all are incremented at each successive plot. The typing an N, preceded by a comma after the number of trajectories, redraws on the Tektronix a new display of the electrodes as well as plotting trajectories. The entry for three trajectories shown in Fig. 9 is

3,N [CR]

at which point the trajectories are plotted on the screen and various characteristics of the trajectories are printed out as shown below along with input entries for the problem at hand.

4.0 Results

It is clear that the ion optical system shown in Fig. 9 does not focus particles emitted from the surface of the source. However, we do note that there is a cross-over at X = 18. From Fig. 7, we can see this point lies in a field-free region (dV/dx = 0). Furthermore, it appears that the lens system of elements C, D, E is too weak to focus these ions. We need to know what voltage need be applied to the center element, electrode D, to make this lens system focus.

Now the focusing capabilities of an Einzel lens are determined, in part, by the ratio of the mid-element voltage to the kinetic energy of the ion. For example, the kinetic energy of the ion at the crossover (18,0) is 8000 eV. The mid-element voltage is 5000 V. Hence, the ratio is 8/5. Suppose we started with an ion at the crossover point, and varied its kinetic energy until focusing occurred. Such trajectories are plotted in Fig. 10 where (after some trial and error) we entered into TRAGIC parameters the initial coordinates 18,0, initial kinetic energy 3500 eV, theta as 7° and an incremental energy of 500. Hence, the trajectories plotted are for ions of 3500 eV and 4000 eV. Clearly, the 3500 electron volt ions are focussed by the 5000 V potential of the midelement. This ratio 3500/5000 brings about focus for ions that are either formed at (18,0) or arrive there with a divergence angle < 7°. For 8000 eV ions, the applied potential required for focus would be

$$8000 \times \frac{5000}{3500} = 11{,}400 \text{ volts.}$$

Using the subroutine MODIFY, electrode D was given the potential 11,400 V. The new electrode assembly potential distributions were then calculated using the program REFINE. Last, the trajectories were plotted on the Tektronix and are shown in Fig. 11. As can be seen, the ions formed at position (3,0) and (3,1) are brought to a focus, but that ions formed at position (3,2) are not quite focussed. It is clear, overall, that only a modest success was achieved. To use the given electrode

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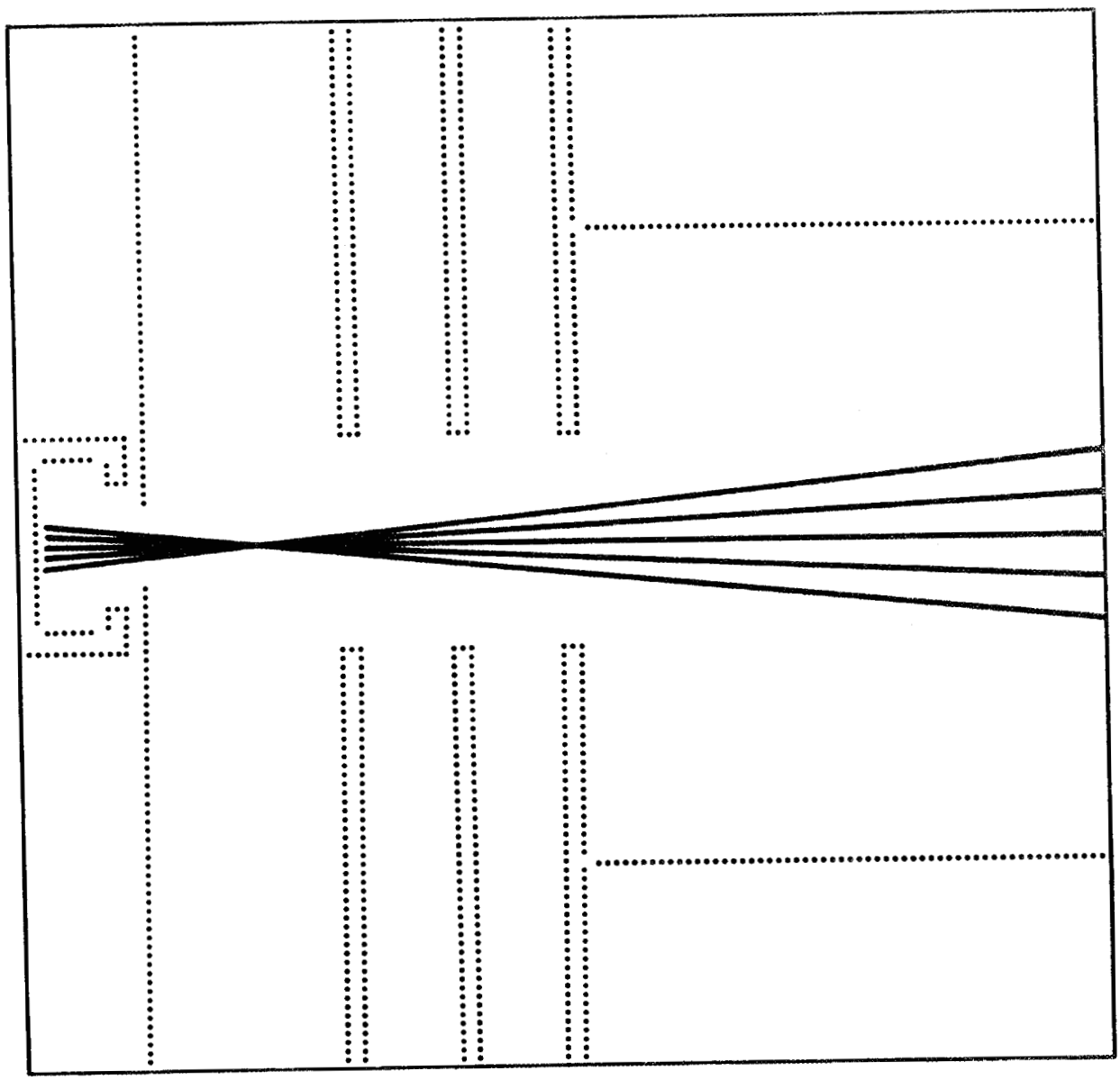

Fig. 9. Original ion trajectories

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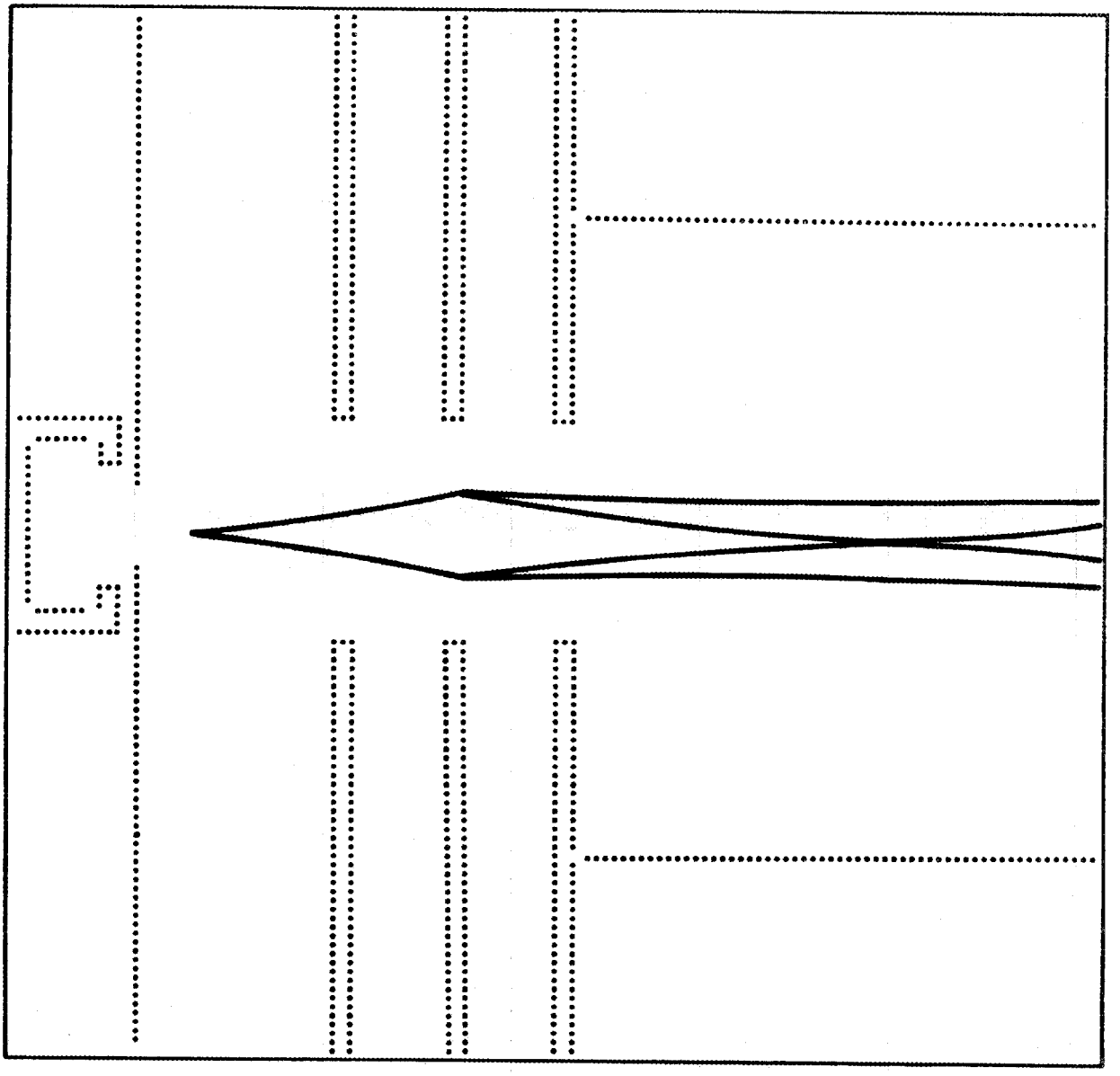

Fig. 10. Modified ion trajectories

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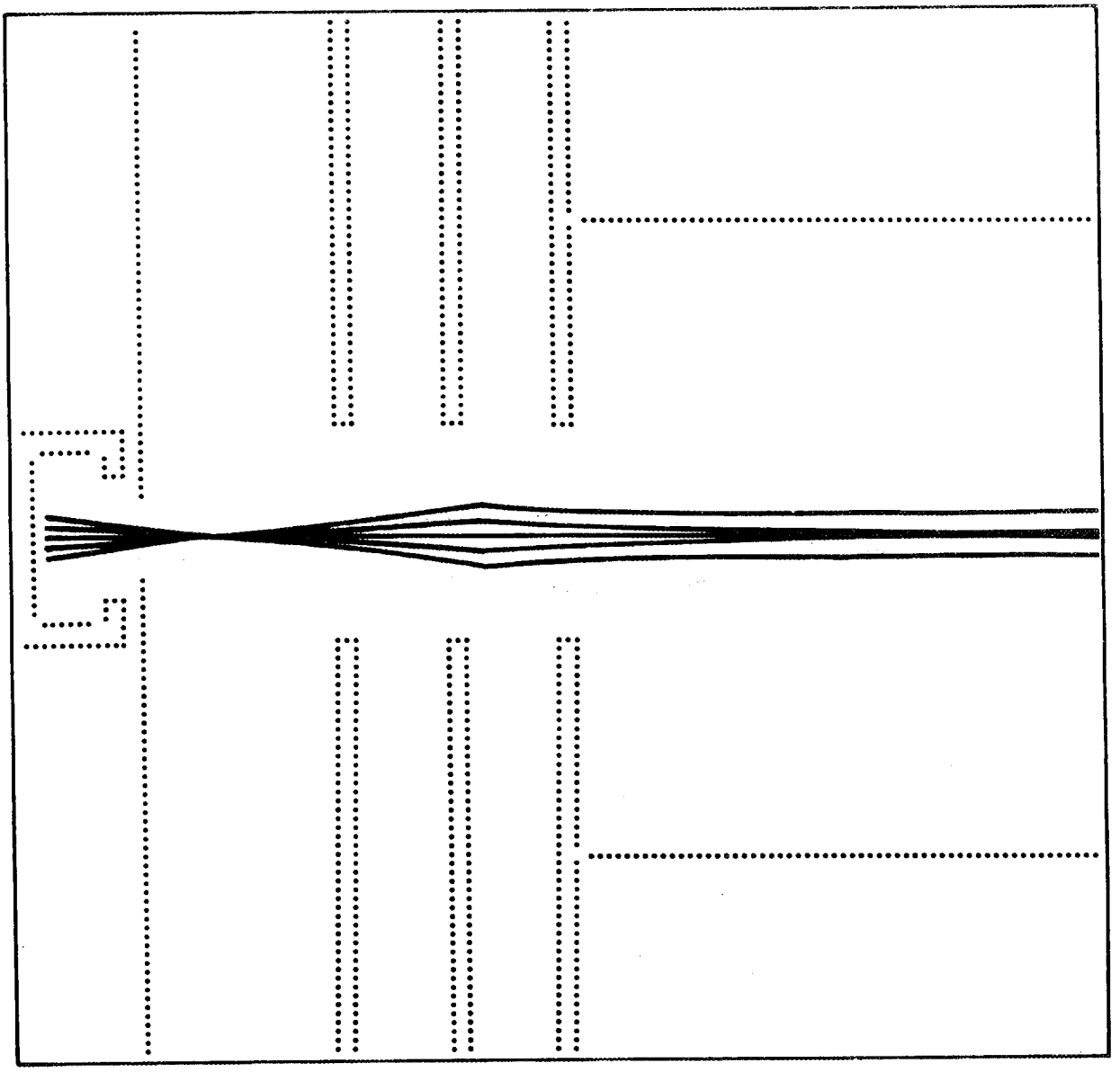

Fig. 11. Final ion trajectories

assembly as an ion source, only those ions formed within a spot size diameter of 2 mm would be effectively transmitted into the mass spectrometer. Actually, this compares favorably with most commercial instruments, but could be improved. We leave that exercise to the reader.

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Internal Distribution

1. M. V. Buchanan
2. W. H. Christie
3. J. M. Dale
4. G. L. Glish
5. D. E. Goeringer
6. L. D. Hulett
7. C. P. Leibman
8. M. P. May
9-13. H. S. McKown
14. S. A. McLuckey
15. C. A. Pritchard
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17. R. W. Shaw
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