Developments on the Toroid Ion Trap Analyzer

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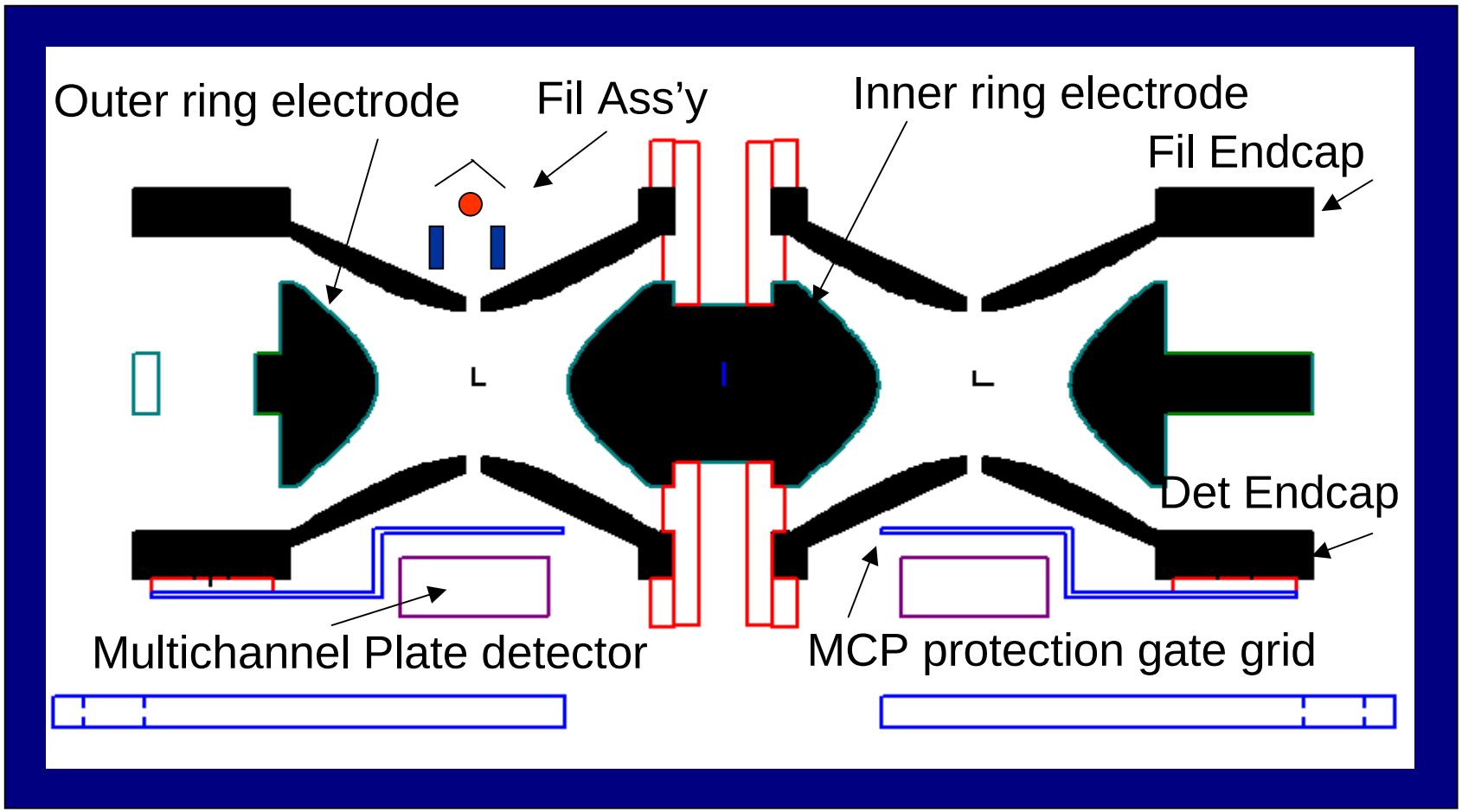
Introduction

- A new (toroidal) geometry for an ion trap mass analyzer has previously been reported.[1] The toroid geometry (Figures 1 and 2) is based on rotating the standard 3D ion trap cross-sectional trapping field around one ring electrode edge (red line in Figure 1) as opposed to around the center of the trapping field (blue line). The resulting trapping field resembles a torus, but has the same operating dimensions (r_0) as a standard commercial 3D ion trap. The potential ion storage volume, however, is significantly increased.

Figure 1: Toroid Ion Trap Analyzer (top inset shows comparison to standard 3D Ion Trap)

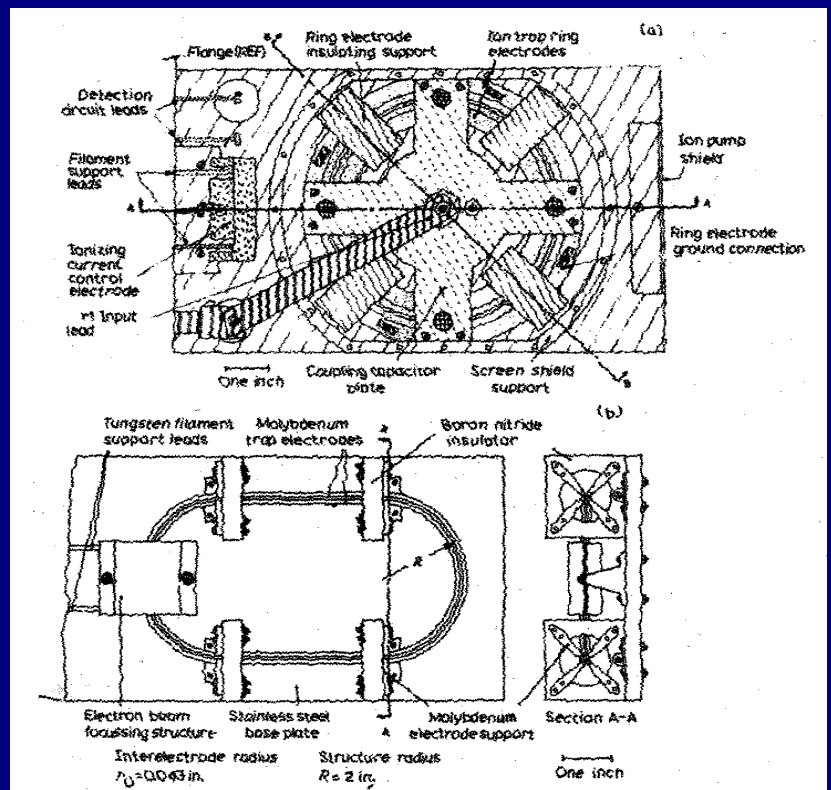
Figure 2: Toroid Ion Trap Schematic

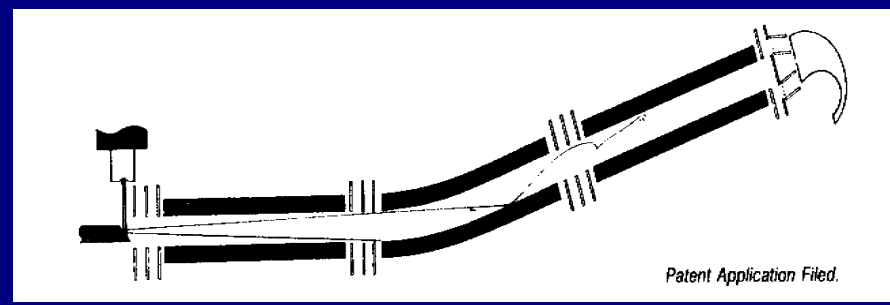


Previous Work

- Curved quadrupolar fields have previously been studied in several forms (Figure 3). Drees and Paul (1964) and Church (1969) studied circular and “racetrack” [2] versions of continuous linear quadrupoles. Brubaker (1968) used curved rf only quadrupole [2] with rf/dc quadrupoles to reduce neutral noise. Syka and Schoen from Finnigan-MAT (1987) employed a curved quadrupole [3] as the collision quadrupole (Q2) and later, octapole for the same purpose. More recently, Bear Instruments have introduced a curved triple quadrupole [4] instrument. In each case, the radius of curvature (R) compared to the radius of the trapping field (r_0) was kept large (R/r_0 >10-50) in order to minimize additional non-linear fields.

Figure 3: Previous Work- Curved Quadrupoles





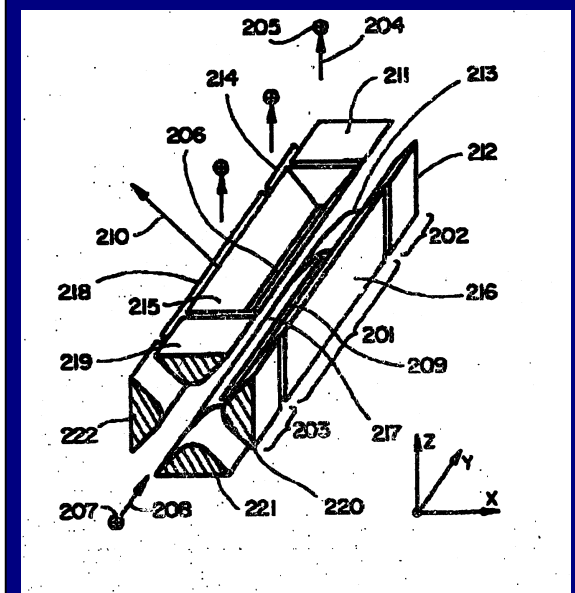
Reference: ***<u>Quadrupole Mass Spectrometry and Its Applications</u>***
Peter Dawson p. 193-4)

<u>Reference: J.E.P. Syka and A.E. Schoen Int. J. Mass Spectrom and Ion Processes 96 (1990) 97-109.</u>

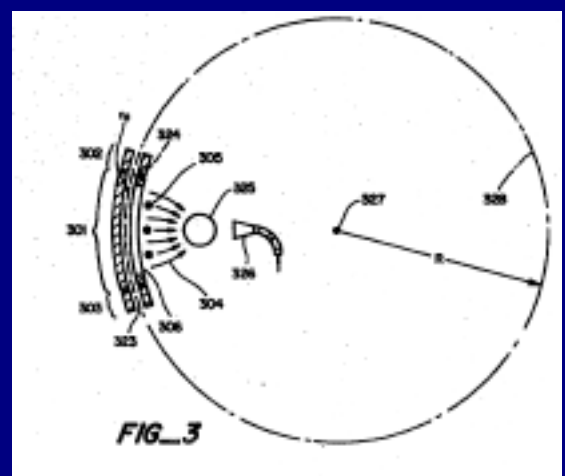
Previous Work (cont'd)

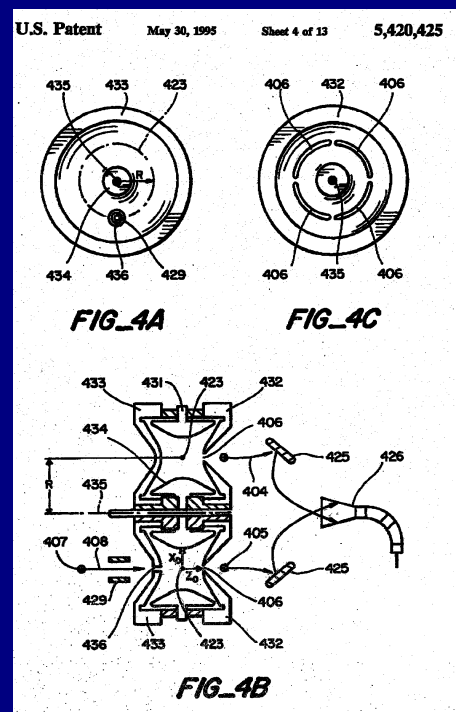
- More recently, Syka and Bier have proposed curved quadrupolar devices as ion traps[5]

LINEAR ION TRAP



CURVED VERSION





Reference: US Patent No. 5,420,525 (30 May 1995)

Physical Characteristics

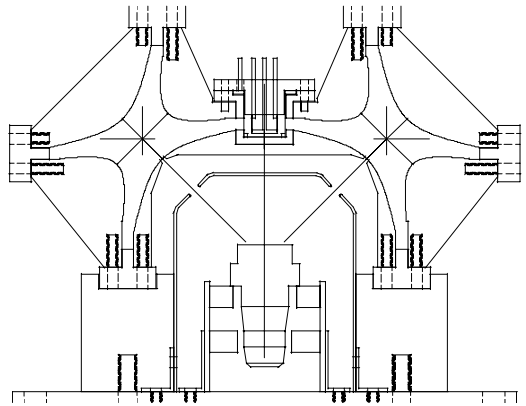
- The toroid ion trap uses a standard Finnigan ITMS electronics chassis with custom electrodes that have the commercial ion trap cross section (r_0=1 cm). The “stretched endcaps” geometry (z_0=0.783 cm) was also translated to the toroid geometry. The center ring electrode has a radius of 1 cm so that the ratio of the radius of curvature to the trapping radius (R/r_0) is equal to 2. This was done intentionally with an eye toward eventually reducing the overall dimensions of the device in order to reduce the size of the required rf drive. The rf drive frequency was reduced to 986 kHz (from 1100 kHz).

Current status - Instrument

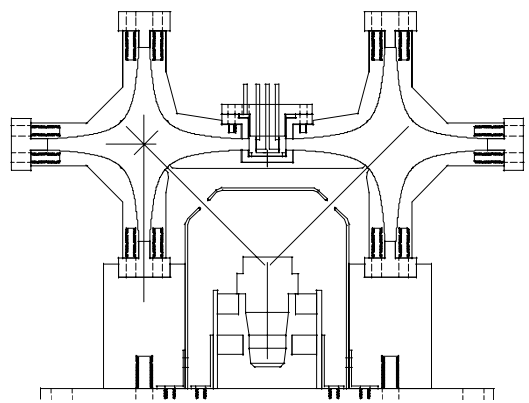
- The current design of the toroid analyzer requires the use of a custom multi-channel plate as the detector. It is desirable from a cost and ruggedness standpoint to be able to replace this costly and fragile detector with a standard CDEM-style electron multiplier. An alternate electrode arrangement geometry for the toroid has been conceived and constructed that allows the use of standard electron multipliers. Figure 4 shows the schematic for both the ion trap cross-section as well as that for the Bier/Syka linear quadrupole cross-section.

Figure 4: Alternate Geometries that Allow Channeltron-style Detector

Ion Trap Cross-section



Quadrupole Cross-section

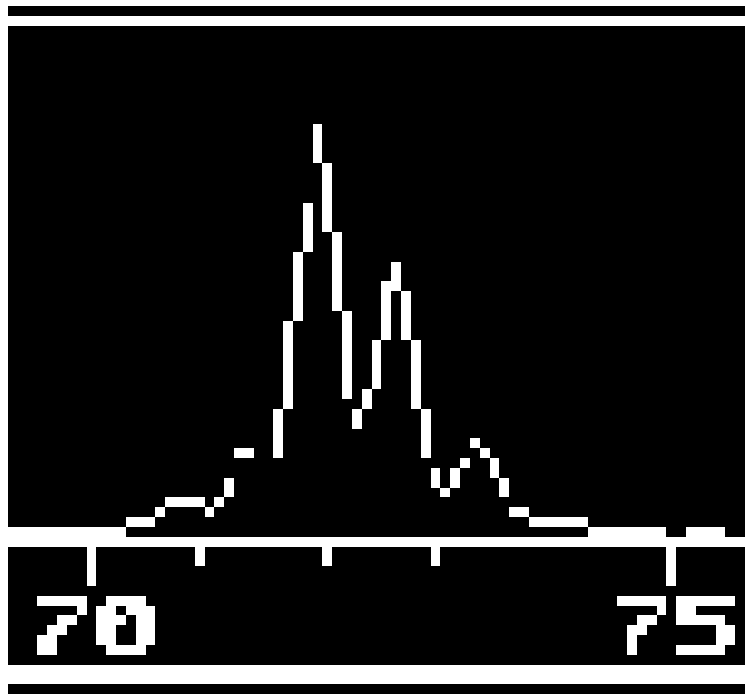


Current Status - Performance

- As previously reported, mass peak widths on the toroid analyzer are ca. 2-3 da (FWHM) wide and <u>very</u> dependent on the value of β_{eject}. In addition, significant peak splitting occurs at discrete values of $\beta_{eject.}$ (see Figure 5) Some minimal improvement in peak width and shape has been observed when fundamental rf frequency increased to ca. 1 MHz (significantly away from the optimum tuned resonant point) but the mass range is subsequently deteriorated. This peak splitting can easily be observed (light blue trace) using a digital storage scope in the “persistence” mode (Figure 6).

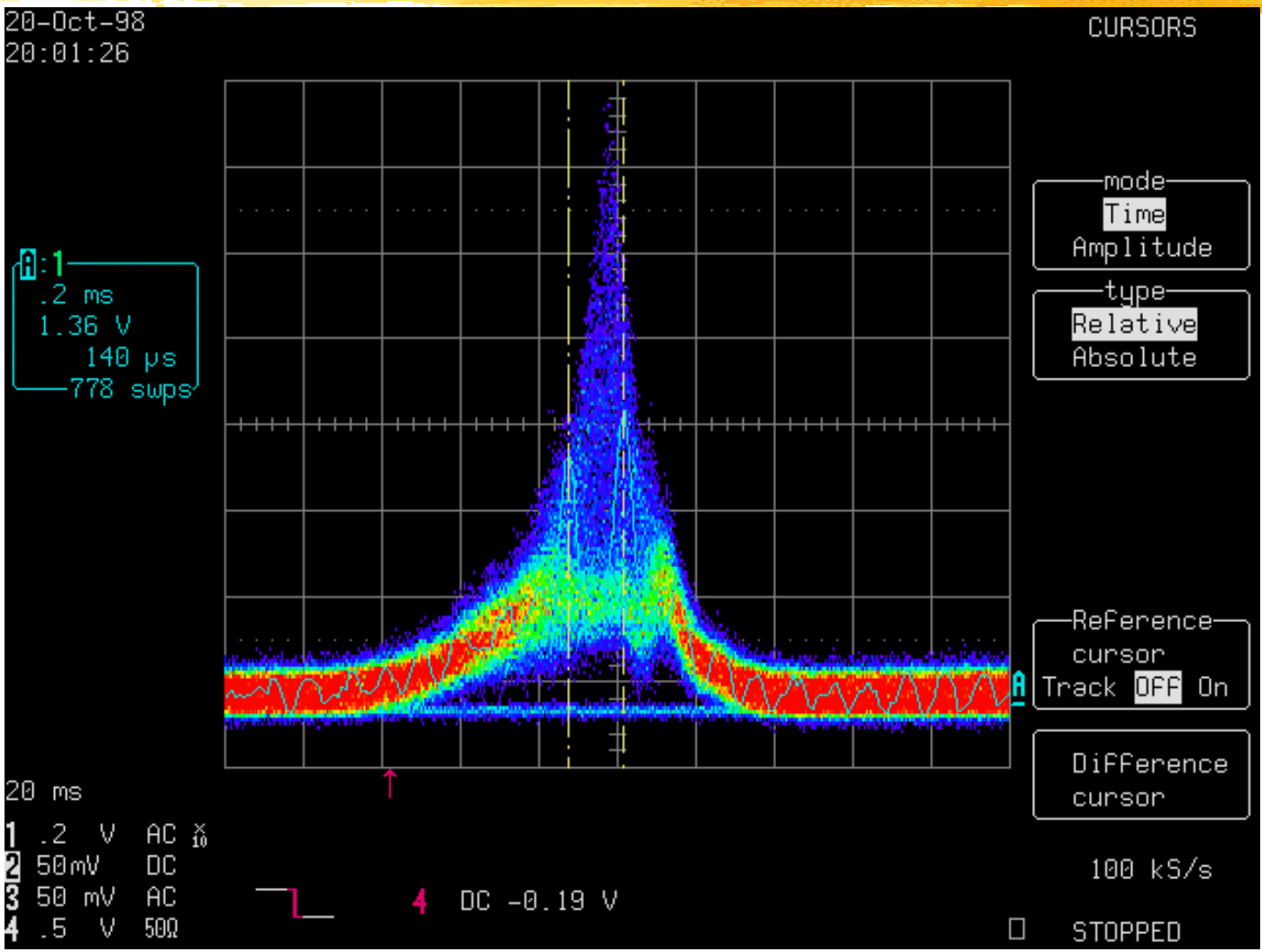
Figure 5: Molecular ion of benzene (m/z 78) at two different β_{eject} values

β_{eject} = 0.399



β_{eject} = 0.388

Figure 6: m/z 78 from benzene - scope “persistence” mode



Peak splitting

- Several possible sources of the observed peak splitting have been considered. These include:
  - Non-linear fields resulting from the curved quadrupolar field geometry.
  - Non-symmetrical trapping field
  - Alignment errors (non-parallel components)
    - component spacing measured
  - Electrode machining imperfections
    - may require tolerances similar to linear quadrupoles
  - Multiple (4) discrete trapping volumes (from the 4 slits on filament and detector endcap

Simulation of Toroid Geometry

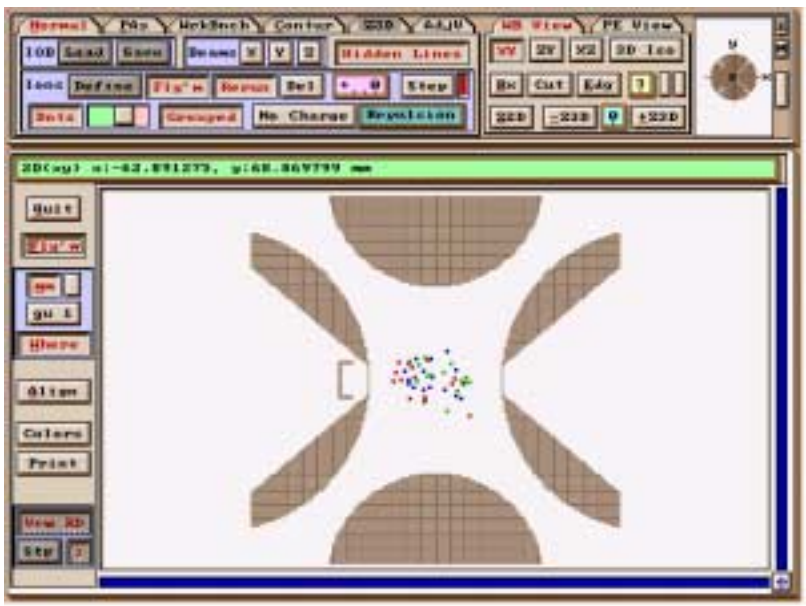
- ***Simion 3D6*** [6] was used to simulate ion motion in a toroid ion trap geometry in order to investigate whether the trapping field for the toroid analyzer was symmetrical.
  - Started with default ion trap potential array provided with the software (it was expected that the circular electrode structure would not significantly alter the <u>comparative</u> results)
  - Modeled the toroid from this cross section (separate rotation) with R/r_0 ratio= 2

Simulation of Toroid Geometry (cont'd)

- Assumed Boltzman distribution of ion energies (ca. 0.04 eV at 300K) formed at a point source of ionization in both cases (not ideal) (Figure 7)
  - In the case of the toroid analyzer, the ions were allowed to migrate around the ion volume (at their Boltzman energies) before simulation of collisional cooling began.
- Collisions (helium) (Figure 8-12) simulated by simple statistical partitioning of energy in an elastic collision using built in ion dampening feature.

Figure 7: 3D and Toroid Ion Trap Ionization Simulation

- Point source ionization simulation of both the 3D ion trap and the toroid ion trap. Figure taken shortly after “birth” of each ion population.



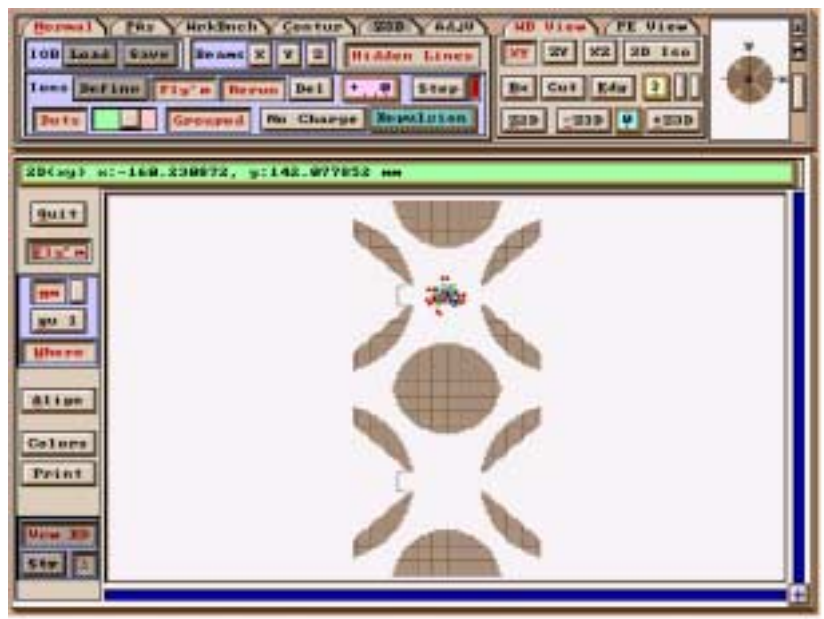
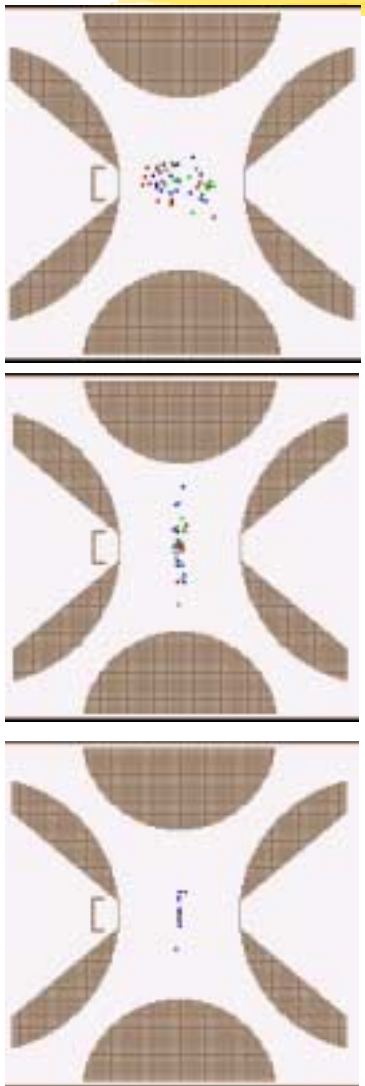


Figure 8: 3-D Ion Trap Simulation



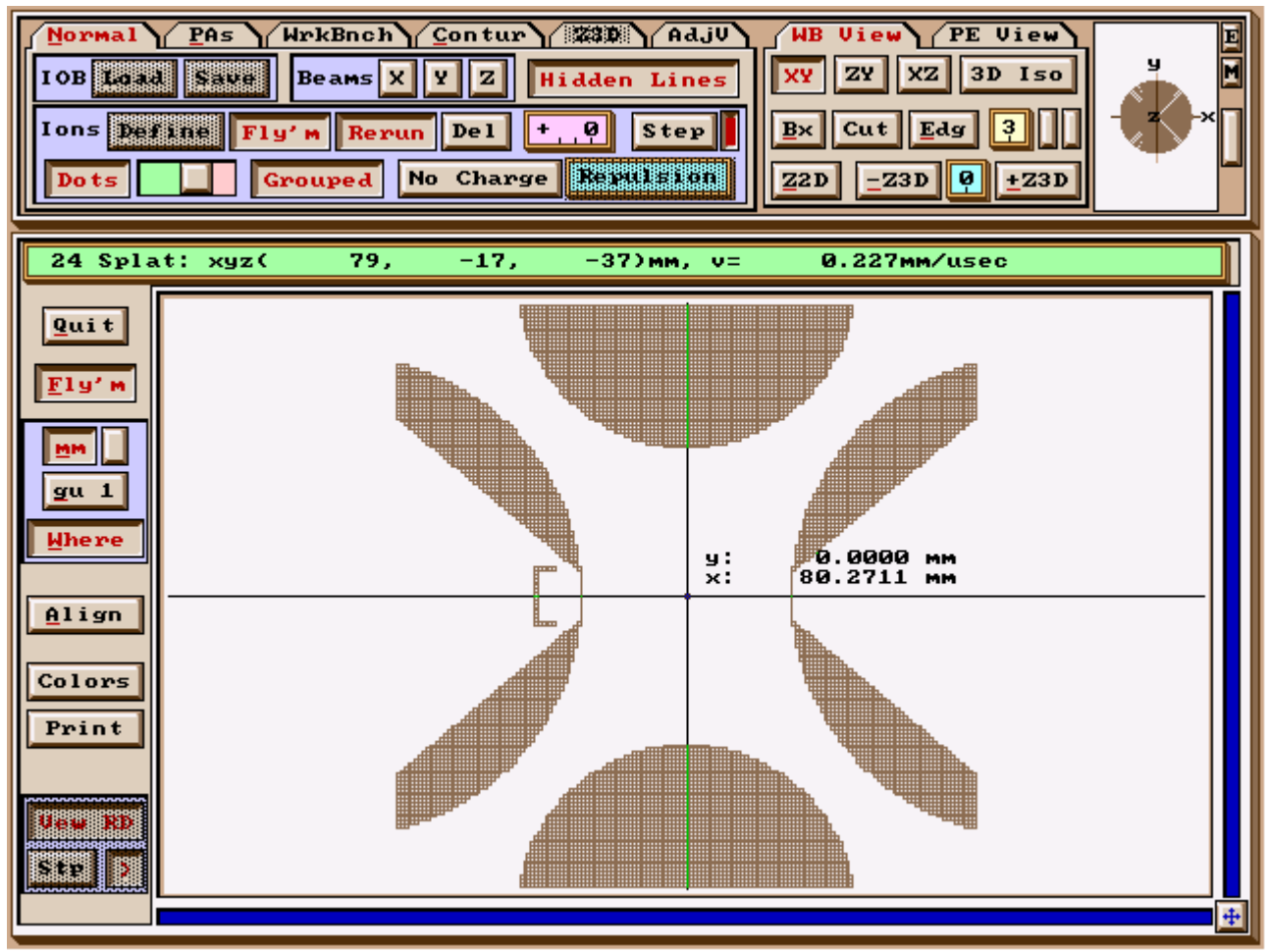


Figure 9: Close up of final ion position on 3D Ion Trap

- In the 3D ion trap, ions settled to bottom of potential well at exactly the center (radial and axial) of the device (crosshair position)

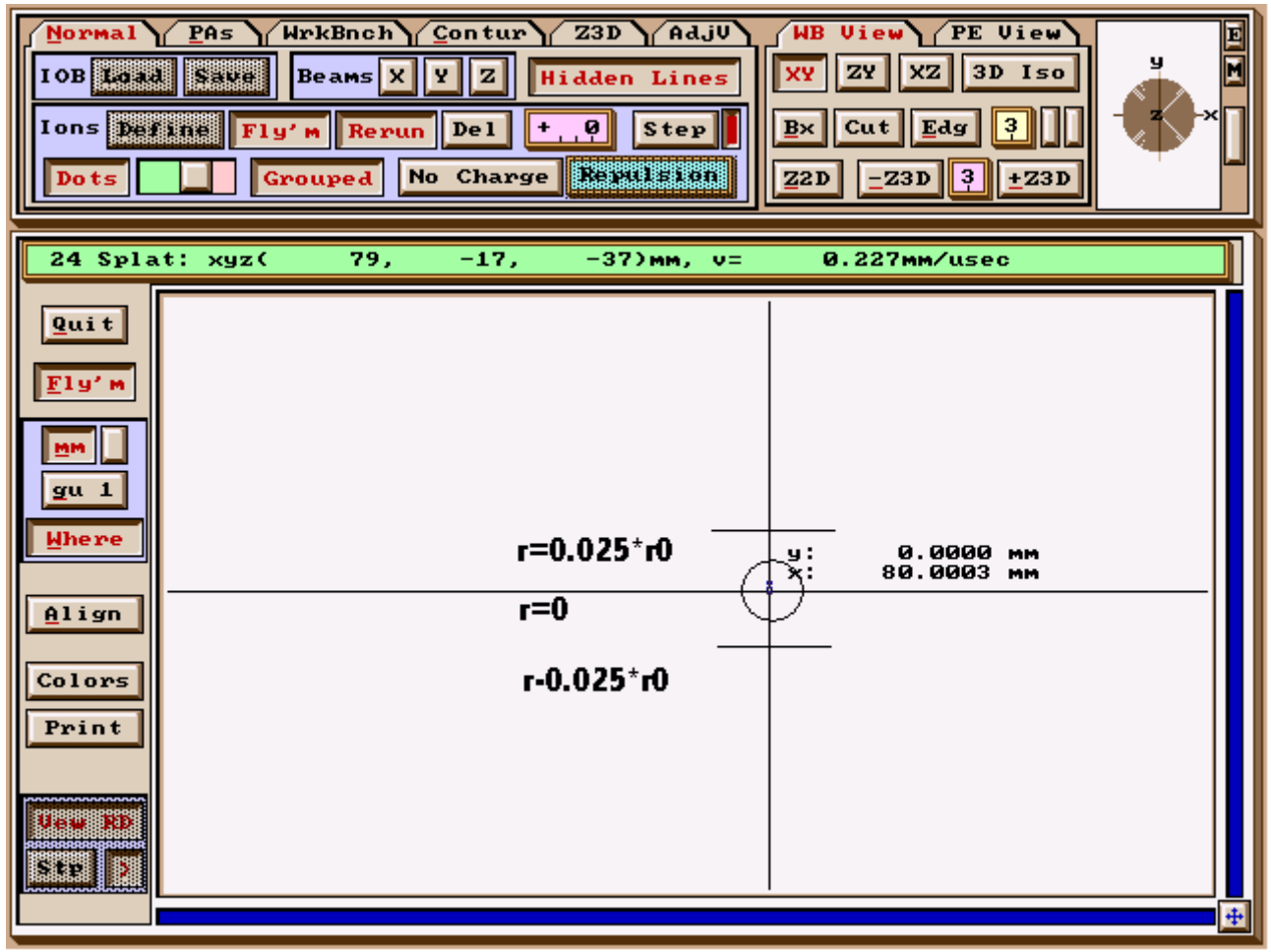
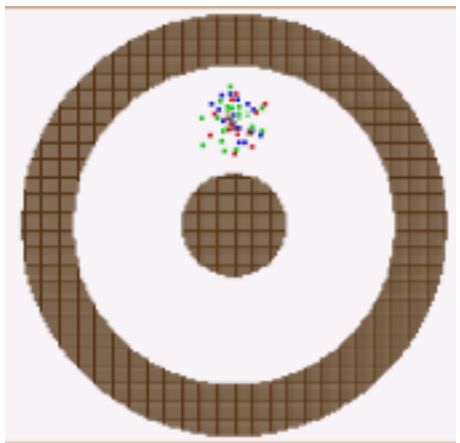
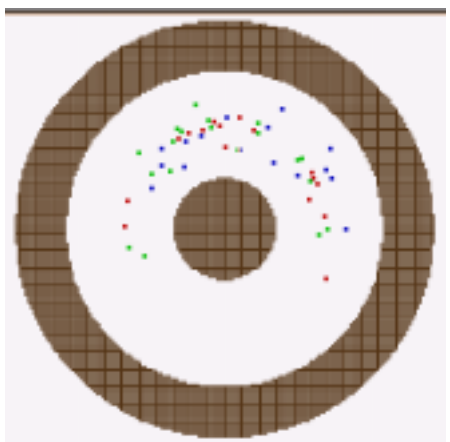


Figure 10: Toroid Ion Trap Simulation





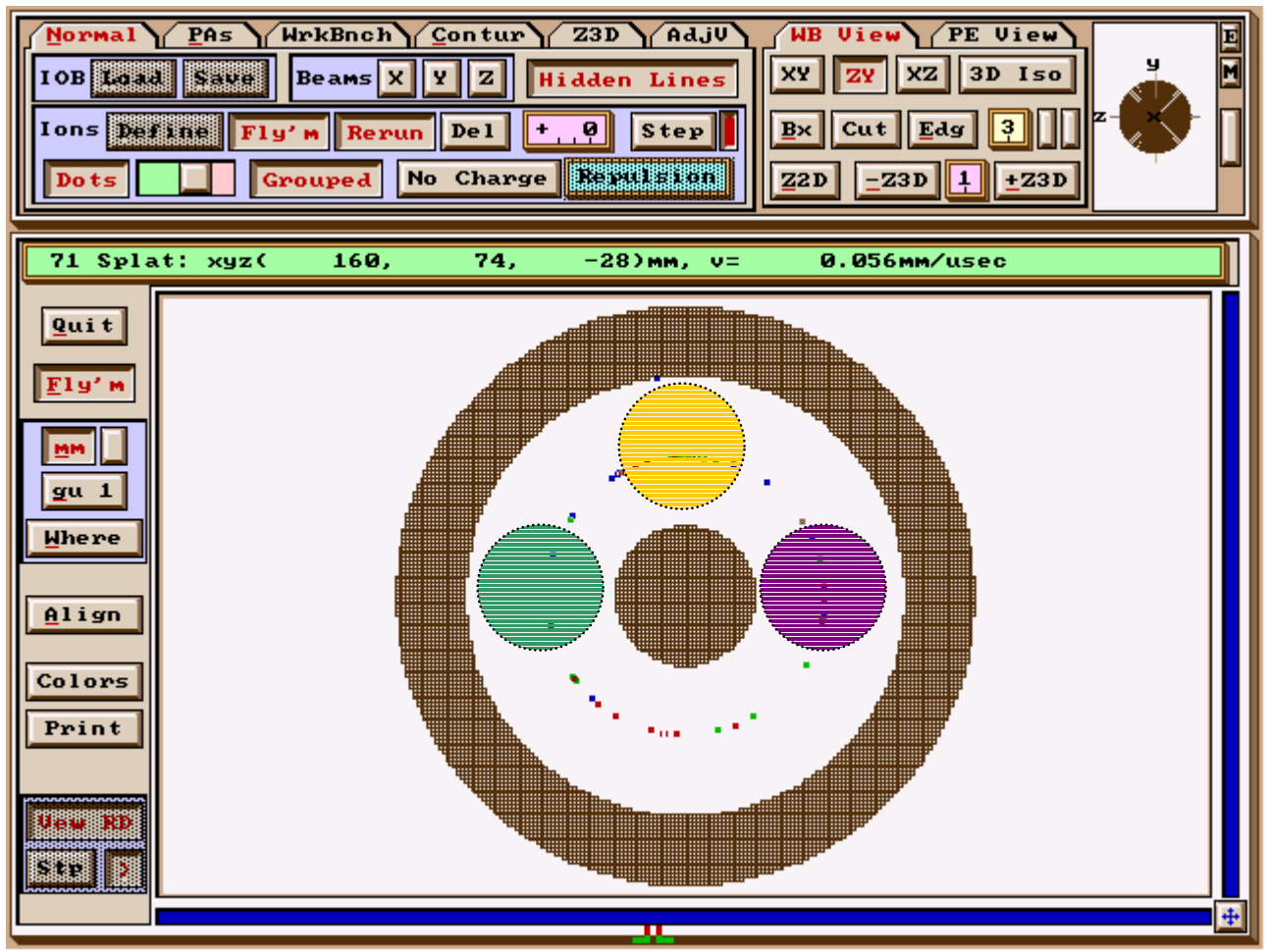
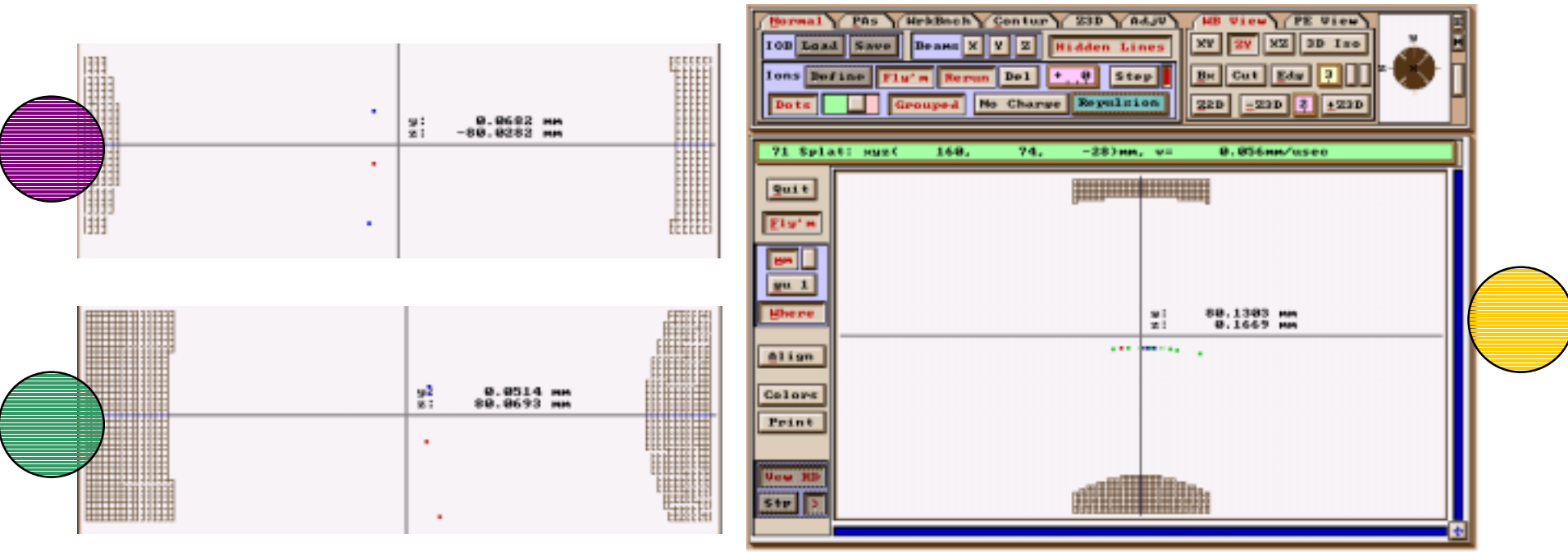


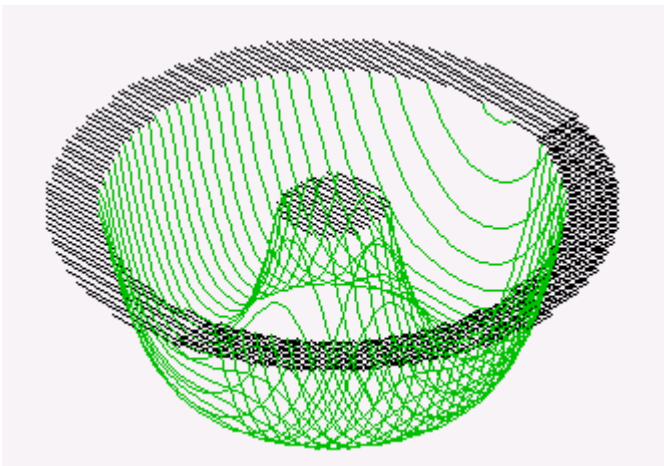
Figure 11: Close up of final ion position on Toroid Ion Trap

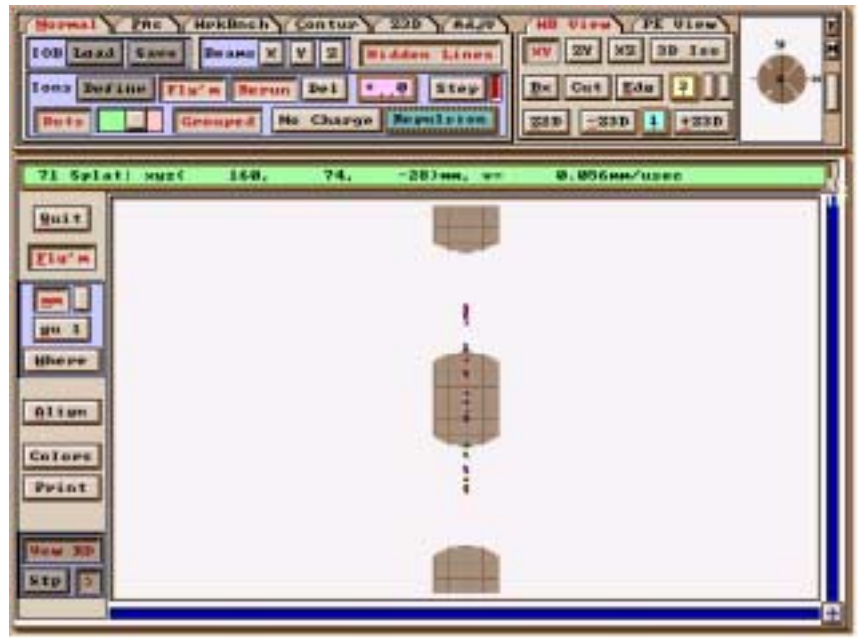


- In each case, the ion population settles to the bottom of the potential well at a radial position that is inside of (closer to the inner ring electrode) the trap physical center (crosshair position) by10% of the r_0 dimension.

Figure 12: Toroid Ion Trap Simulation - Axial Dimension

- In the axial dimension, the ions settle to a point that is in the exact axial center of the device.



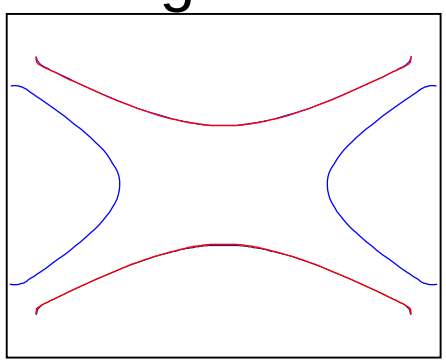


Next Steps

- Investigate whether potential minimum can be relocated to center of the trapping volume.
  - Balance rf between inner and outer electrode
  - (+/- dc offset) between inner and outer electrode
- Electrode and spacer measurements underway
- Multiple exit holes (string of pearls) vs slit exit on endcaps to address issue of 4 discrete trapping regions in current design.

Next Steps (cont'd)

- More likely, a new electrode structure will have to be designed that corrects for the curved trapping field. It would be desirable to simulate a electrode geometry that would approximate the current 3D trapping field by counteracting (correcting for) the non-linear components in the current trapping field by shaping the electrodes (asymmetrically). A program (Poisson/Superfish, Los Alamos National Laboratory) for determining the coefficeints of the various "multi-poles" is available and may provide insight into an optimum design.



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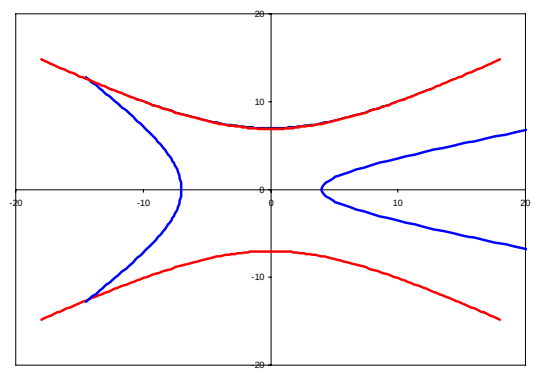

References and Acknowledgements

(1) S.A. Lammert, M.B. Wise, C.V. Thompson, Proceedings of the 46th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, FL, 31 May – 4 June 1998, p. 1174.

(2) Peter Dawson, Quadrupole Mass Spectrometry and Its Applications Elsevier, Amsterdam (1976) p. 193-4)

(3) J.E.P. Syka and A.E. Schoen *Int. J. Mass Spectrom and Ion Processes* **96** (1990) 97-109.

(4) Bear Instruments (http://www.bearinst.com/Default.htm)

(5) Mark Bier and John E.P. Syka; U.S. Patent No. 5,420425 (30 May 1995)

(6) David Dahl, Idaho National Engineering Laboratory

Funding:US Department of Energy - Chemical and Biological Nonproliferation Program (CBNP). Office of Research and Development (NN-20)

Oak Ridge National Laboratory is managed by Lockheed Martin Energy Research Corp. for the U.S. Department of Energy under contract number DE-AC05-96OR22464