Improved Performance Obtained On The Toroid Ion Trap Mass Analyzer Using Asymmetric Electrodes

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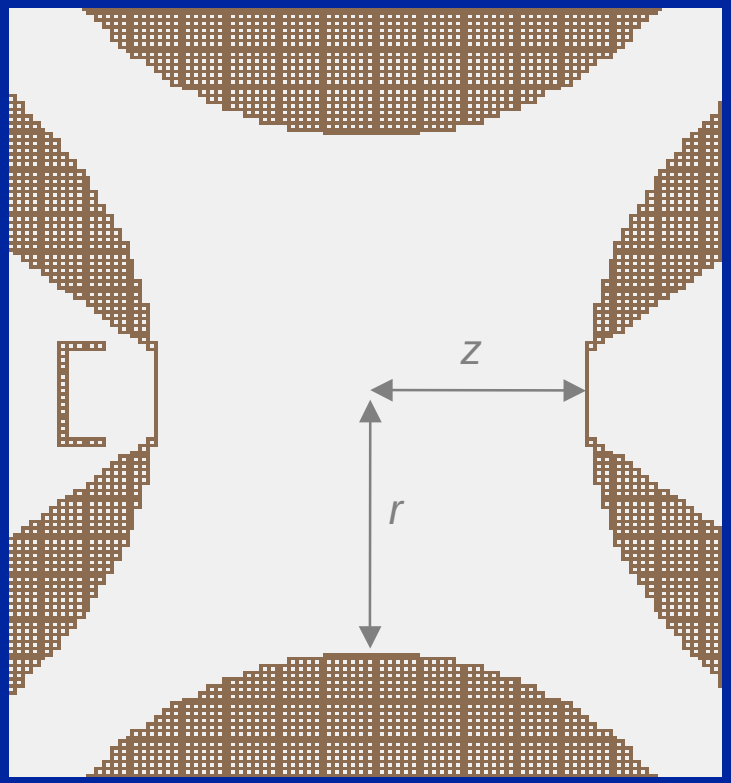
Ion Trap Parameter Constraints

- 3-D Ion trap is an "Ion Bottle" with somewhat fixed <u>relative</u> dimensions (r_0 vs. z_0)
- Space charge still a primary limitation of ion traps
- Optimized at

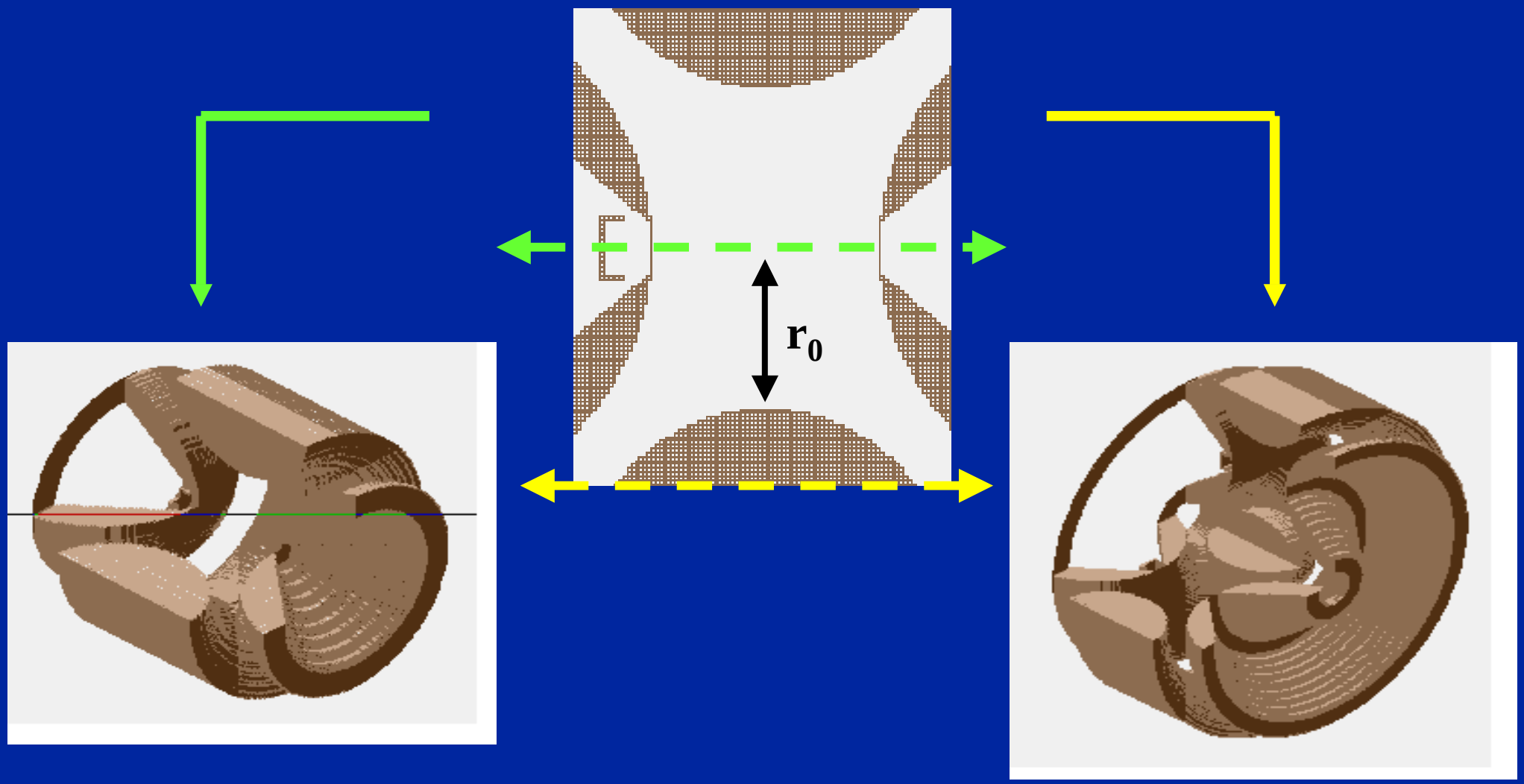
  r_0 =1cm, ~8.1kV$_{0\text{-}p}$

  - large increase in r_0 not practical due to arcing of rf high voltage
  - reduction in r_0 will lead to early space charge

$$q = \frac{-8 * e * V}{m * (r_0^2 + 2z_0^2) * \Omega^2}$$



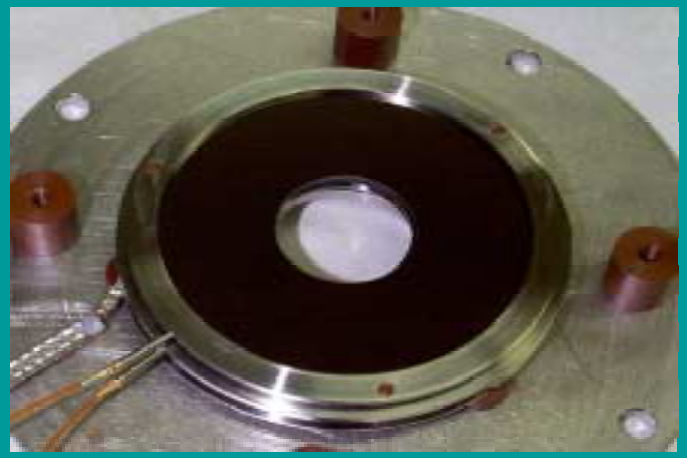
Rotations of Ion Trap Field Cross-section



Toroid Ion Trap Enabling Features

- Significant increase in ion storage capacity for given device radius
  - For 1 cm r_0 cells, 400-1000 fold increase
- New degree of freedom for ion motion
  - potential for increased internal energy deposition in MS/MS experiments
- Possible new mode for ion injection
  - tangential “orbital capture”
- Reduced r_0 devices with large ion storage capacity
  - Reduced size analyzers with similar ion storage capacities as commercial ion traps
  - Significantly reduced operating rf voltages leads to direct drive rf circuits instead of tuned resonant “tank” circuit

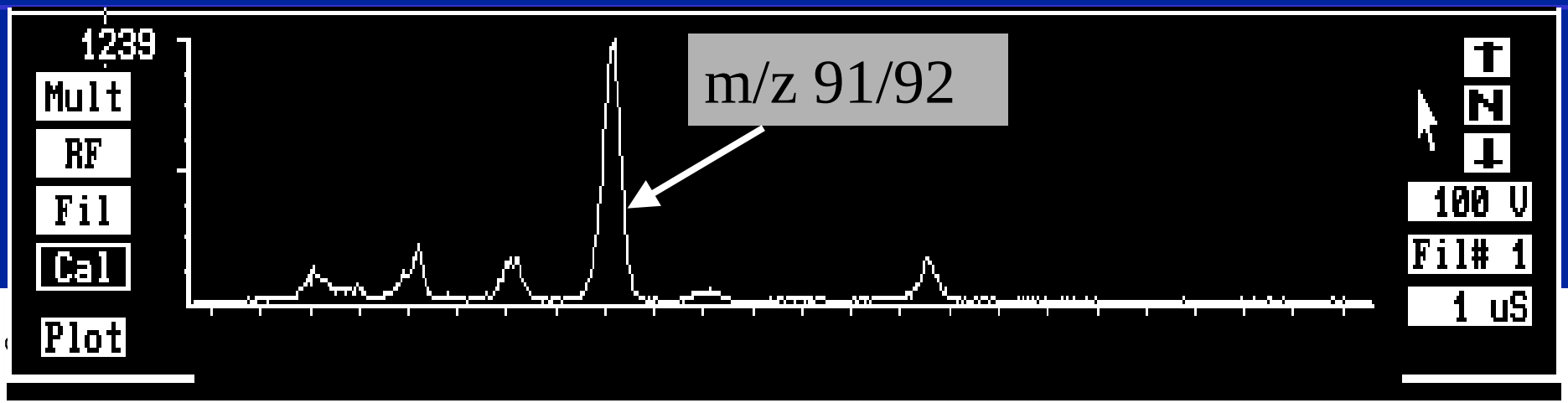
Symmetric Toroid Ion Trap Analyzer



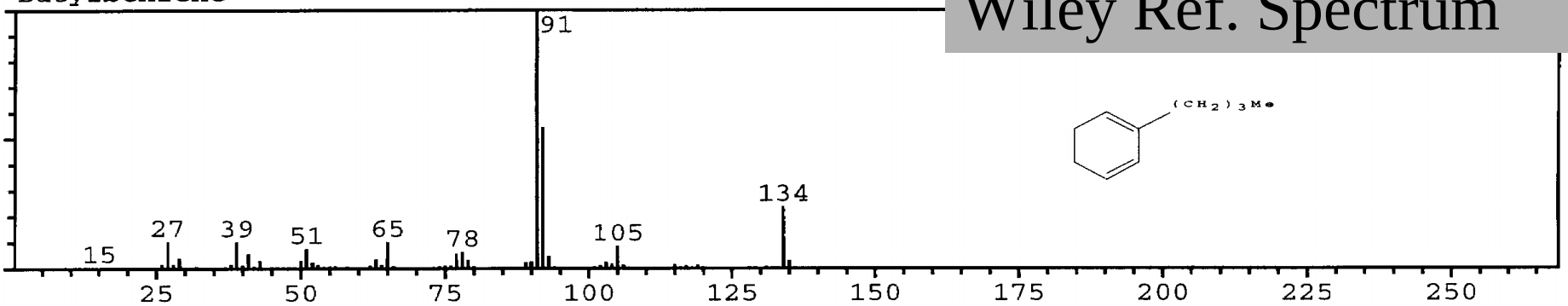
Physical Characteristics of Toroid Analyzer

- Standard r_0 (1 cm); $R/r_0 = 2$
- Uses ITMS Electronics with few modifications
  - r_0 = 1 cm allows standard operating parameters
  - filament and resonance ejection circuitry directly compatible
- Increased capacitance of cell (~34 pf compared to ~25 pf for std. Ion trap cell) which requires:
  - re-tapping coil (down 10 turns from previous setting)
  - modification of rf drive frequency to 990 kHz (from 1100 kHz)
- Requires annular detector (currently using custom multi-channel plate detector)
  - other designs conceived which may allow use of standard channeltron-style detectors

n-Butylbenzene on Symmetrical Toroid Analyzer

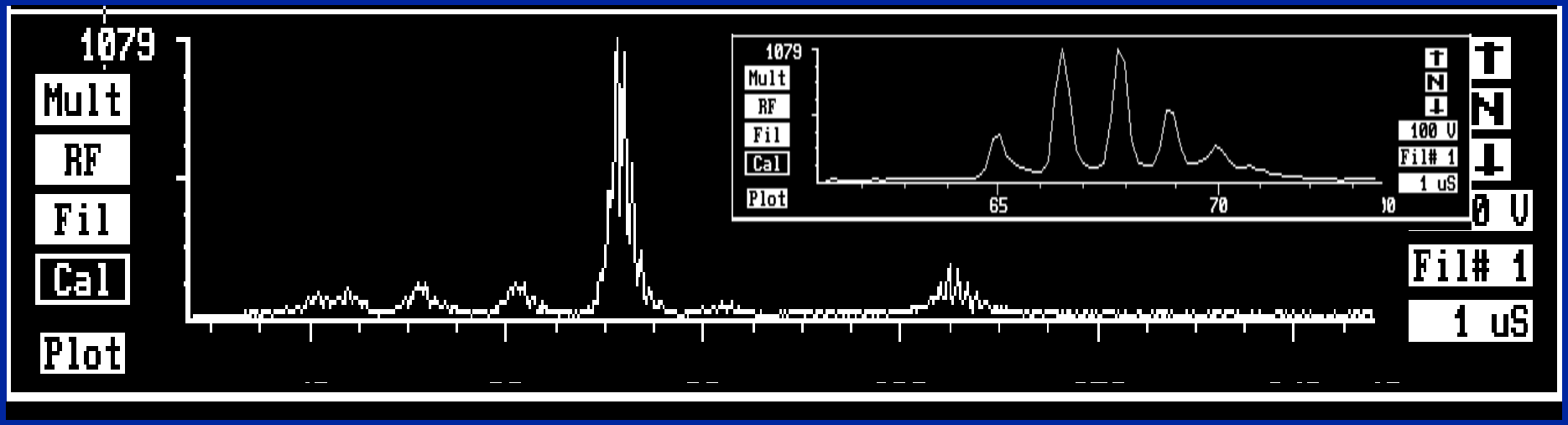


Id: 71038 CAS Reg No: 104-51-8 MW: 134 Form: C10 H14
Benzene, butyl- (CAS)
n-Butylbenzene
Butylbenzene



Effect of Ejection q-value

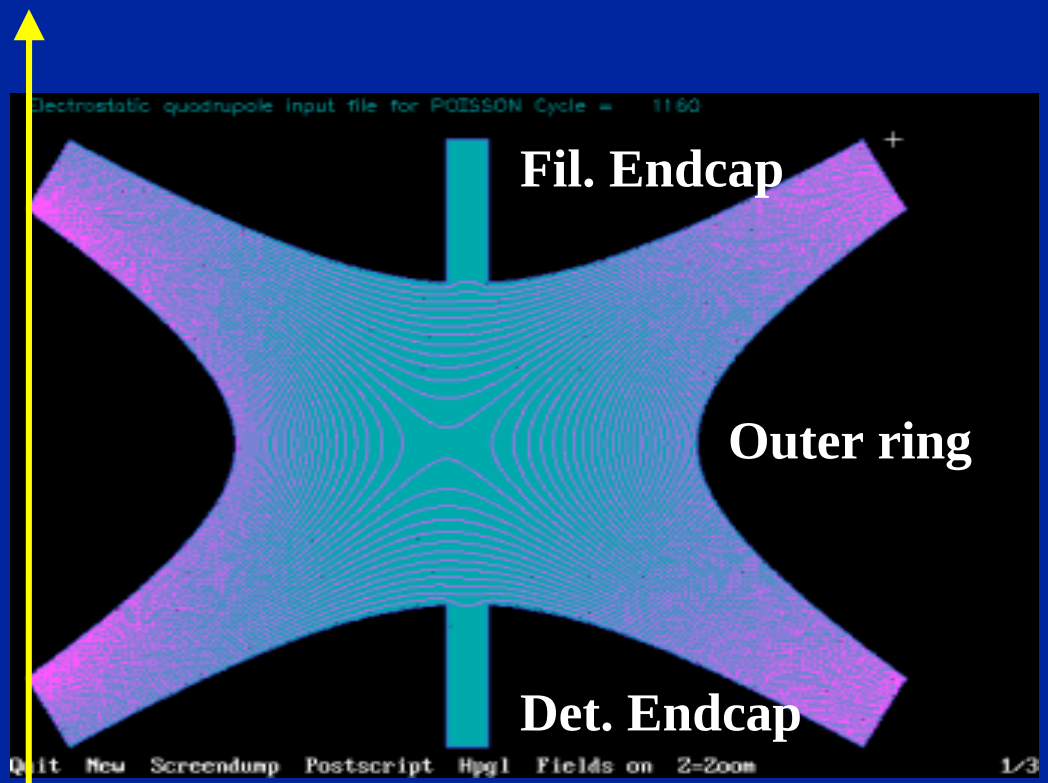
- Peak Splitting encountered with small changes in ejection frequency.
- Spectra disappear/reappear as ejection q-value is scanned.



Trapping Field Evaluation

- **Trapping Field for the Toroid Ion Trap examined using POISSON (Los Alamos National Labs)**
  - Commercial ion traps have:
    - essentially <u>linear</u> field growth with position (quadrupolar field)
    - superposition of small, <u>positive</u> non-linear (mostly octapole) field - intentionally added by stretching endcap distance or asymptote angle
- **Ion Trajectory Simulations Performed using ITSIM (Purdue University)**
  - Latest version allows importing output files directly from POISSON
    - Critical, since there is no mathematical solution to Laplace equation for the toroid geometry

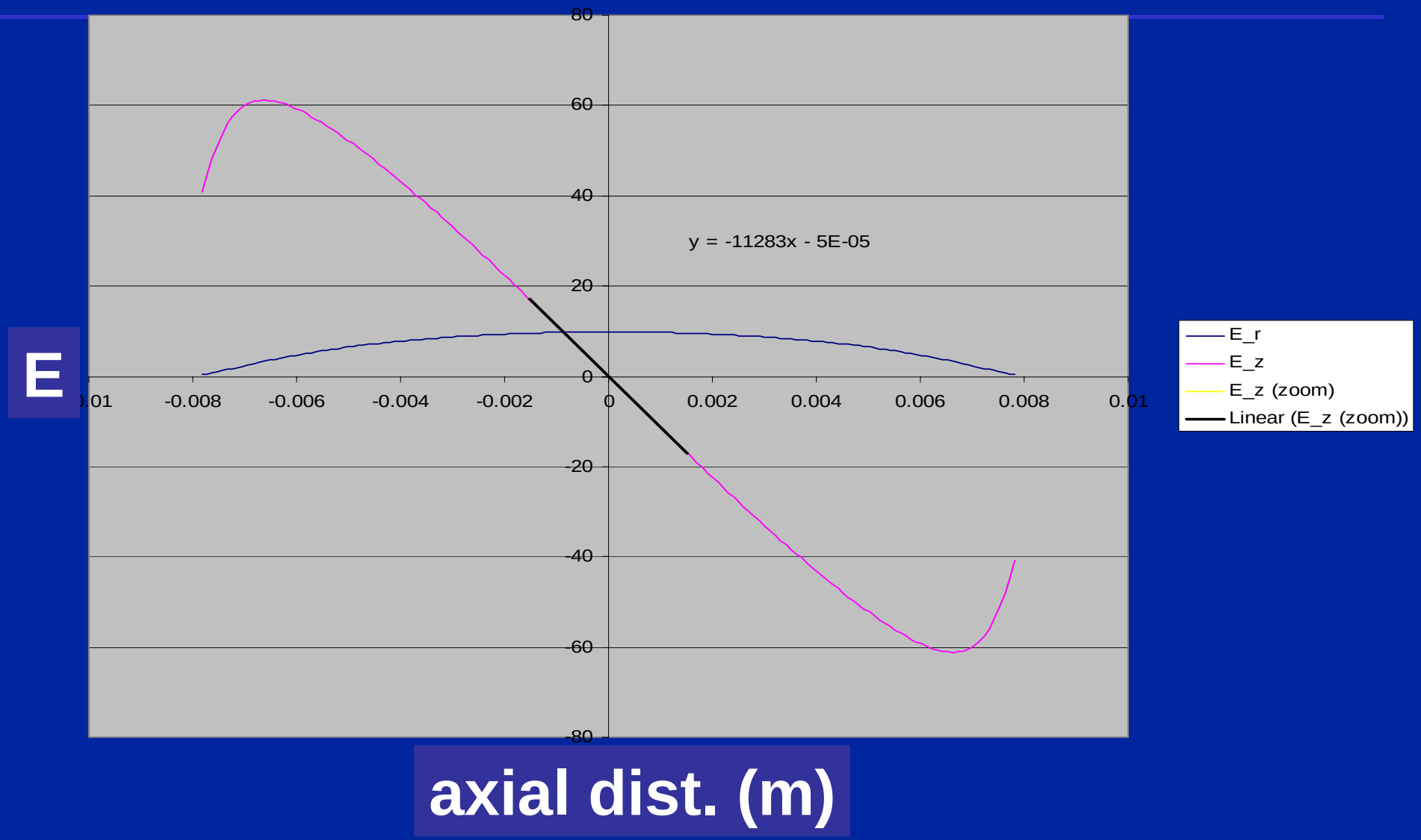
Symmetric Toroid Geometry



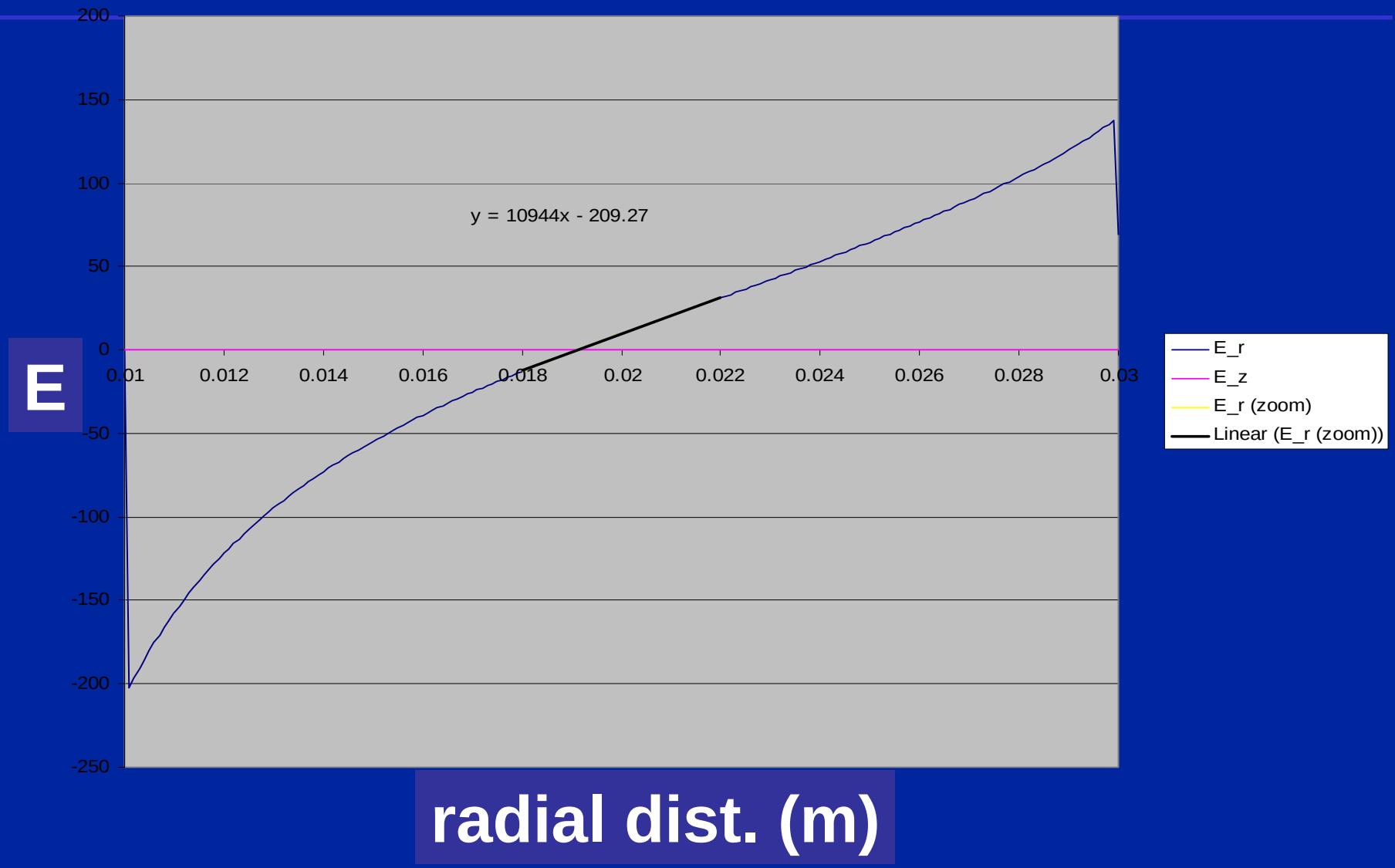
Rotation axis

- Inner ring asymptote = 0.707
- Outer ring asymptote= 0.707
- Endcap (z_0) = 0.783 cm (11% stretch)
- Inner ring r_0 = 1 cm
- Outer ring r_0 = 1 cm
- Asymptote truncation at 2.2 * r_0
- Entrance/Exit slits= 1.78 mm dia.

Axial Trapping Field Analysis: Symmetric Toroid Analyzer

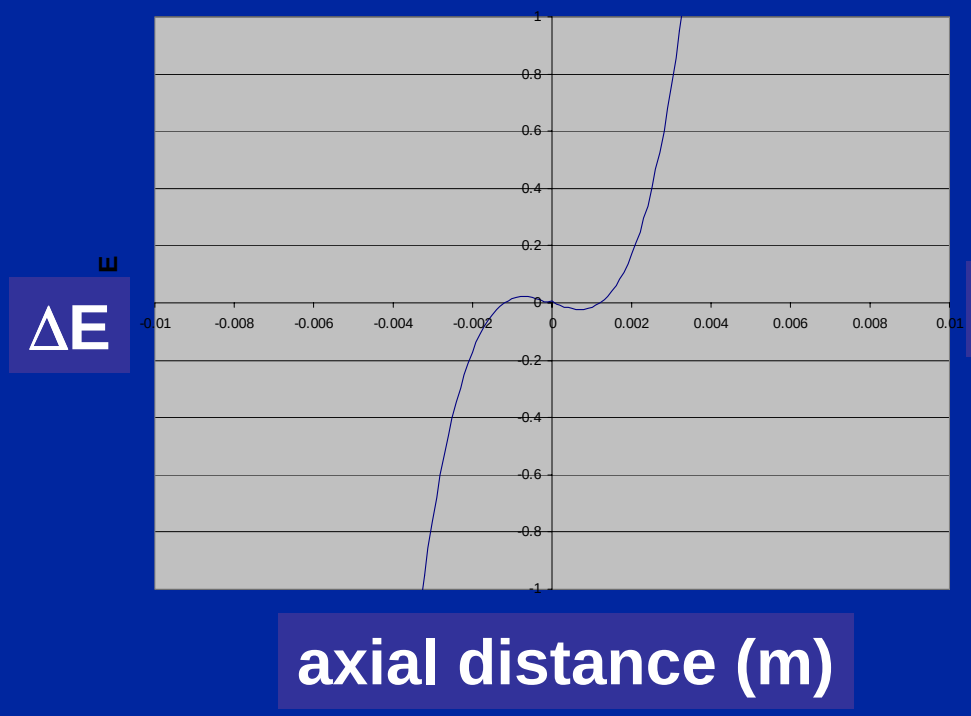


Radial Trapping Field Analysis: Symmetric Toroid Analyzer

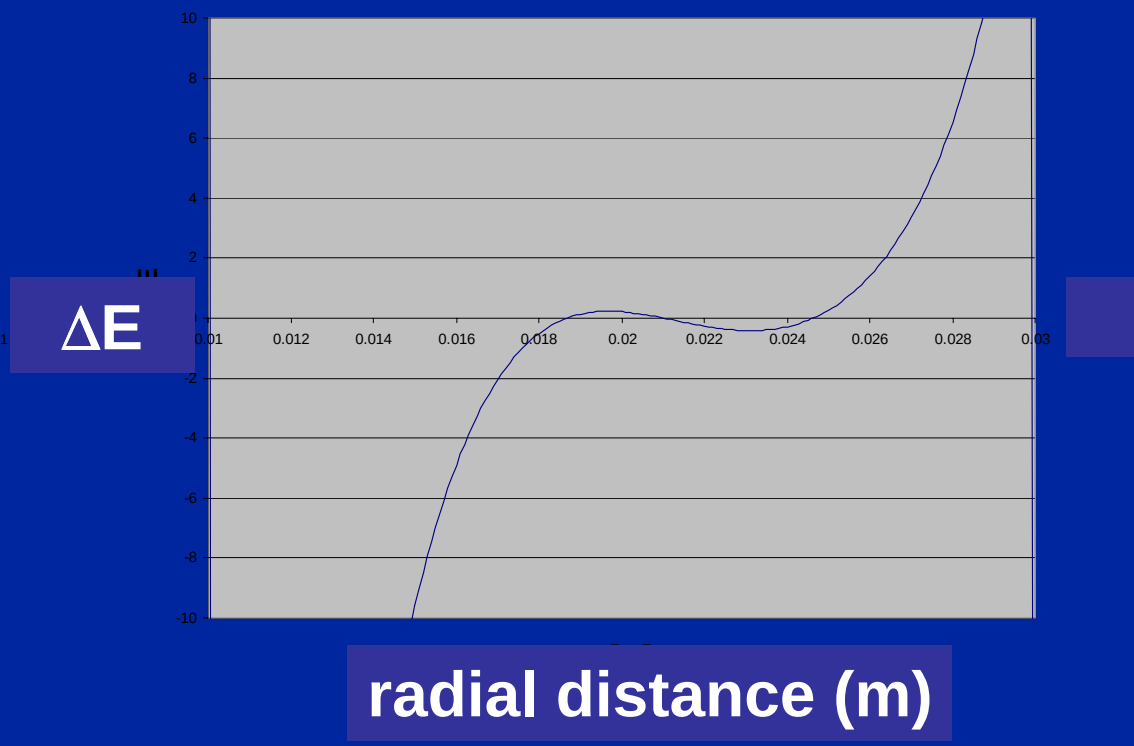


Symmetric Toroid Analyzer

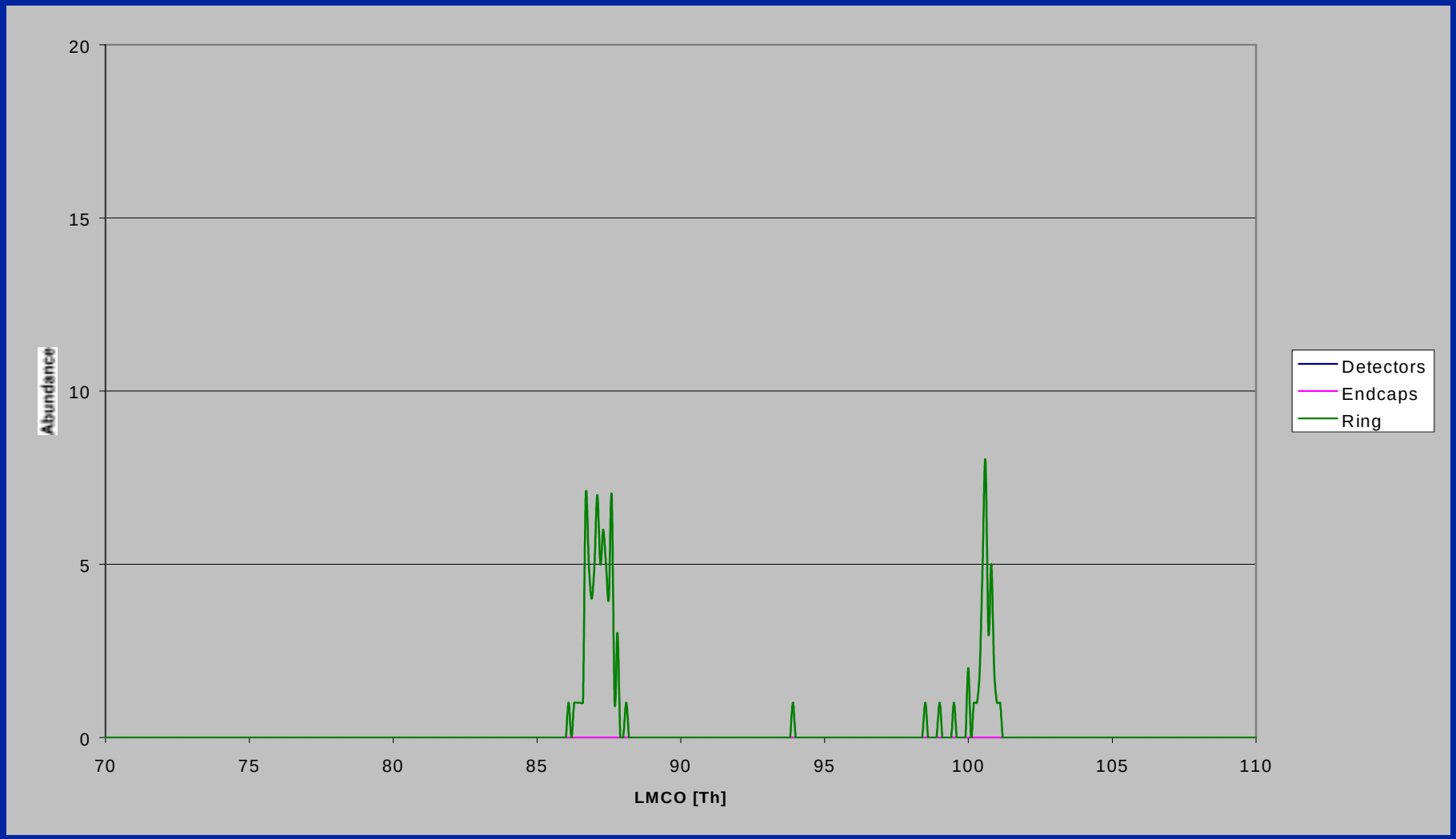
Axial Deviation from Linearity



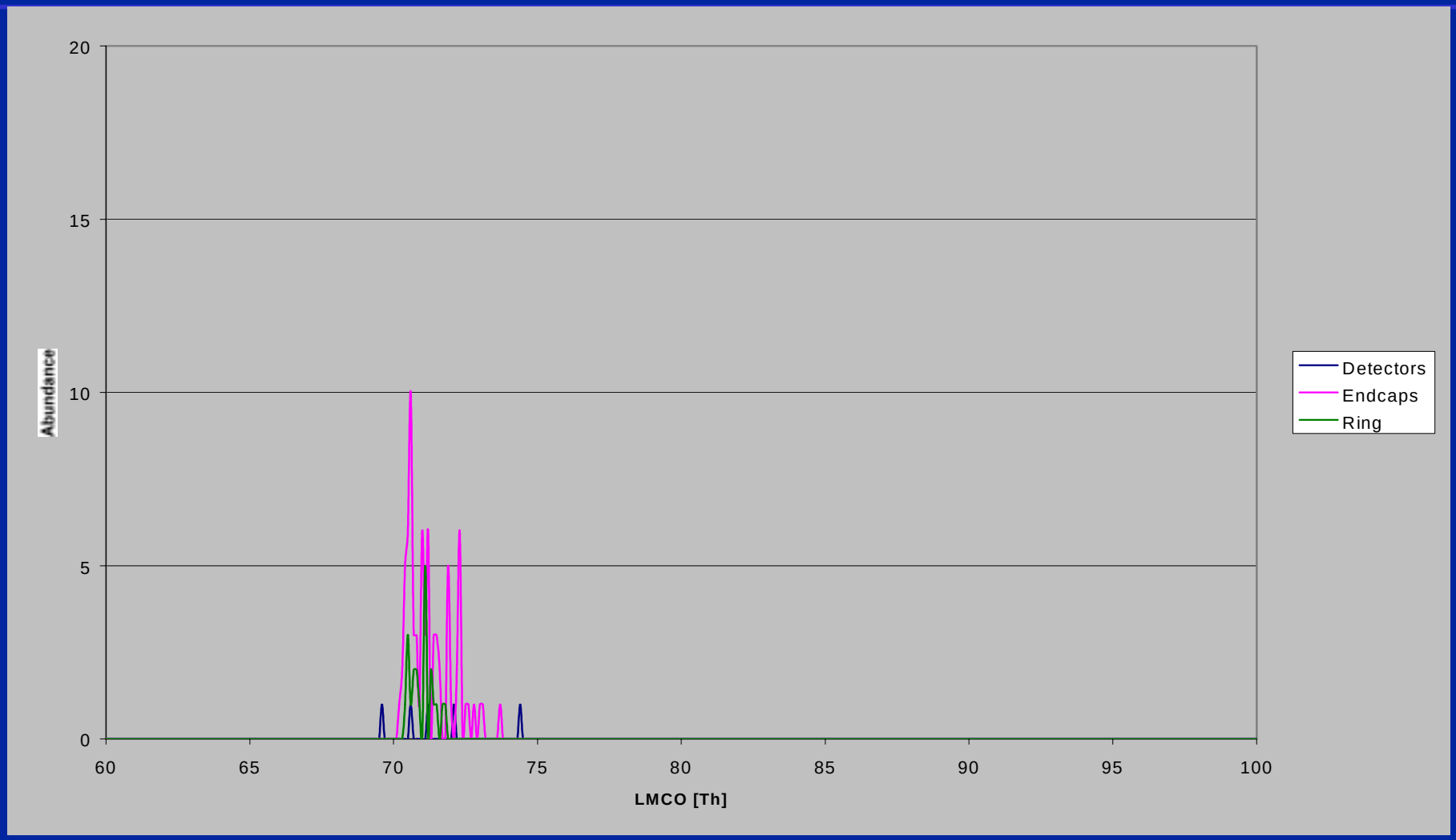
Radial Deviation from Linearity



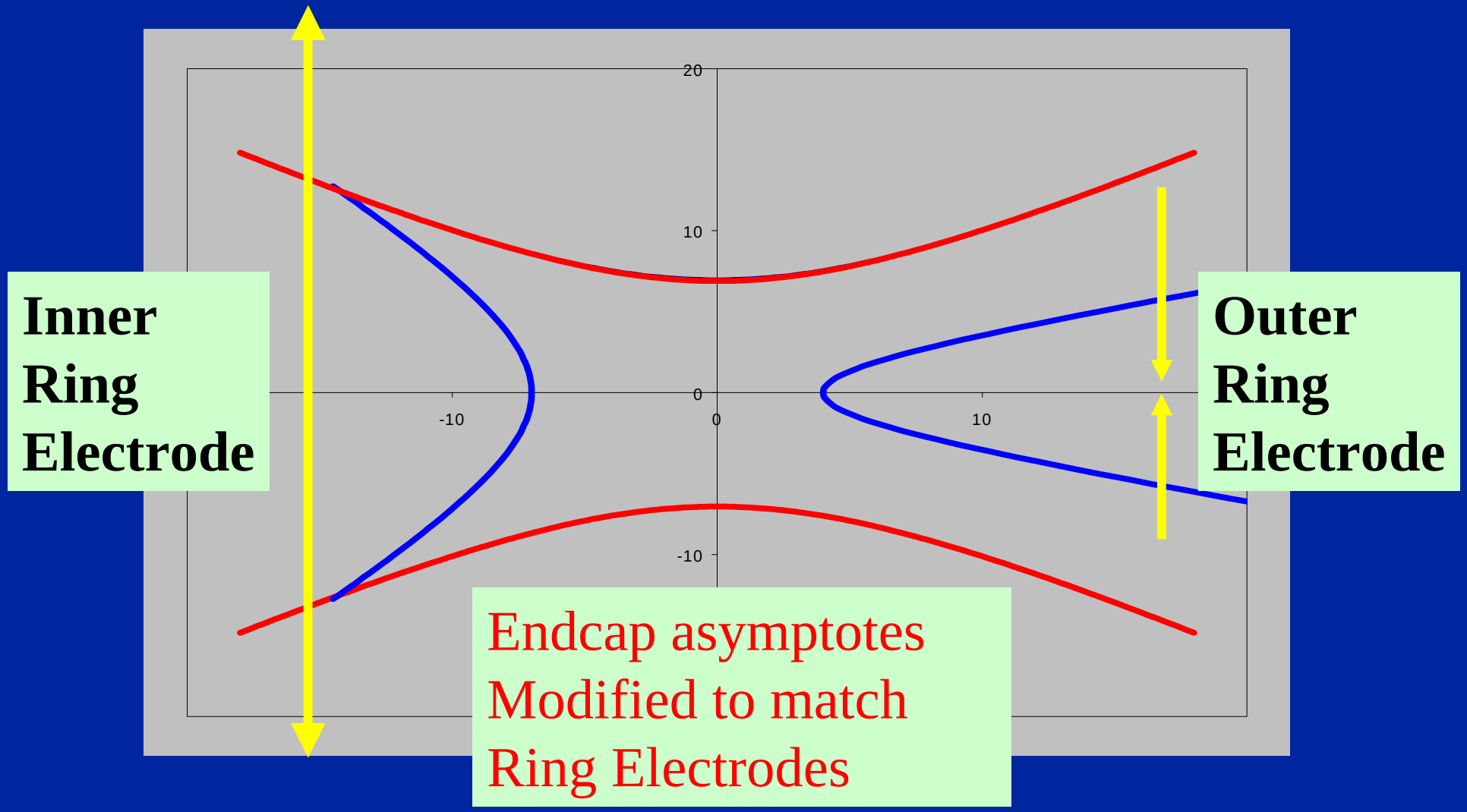
Symmetric Toroid Simulation - Boundary Ejection



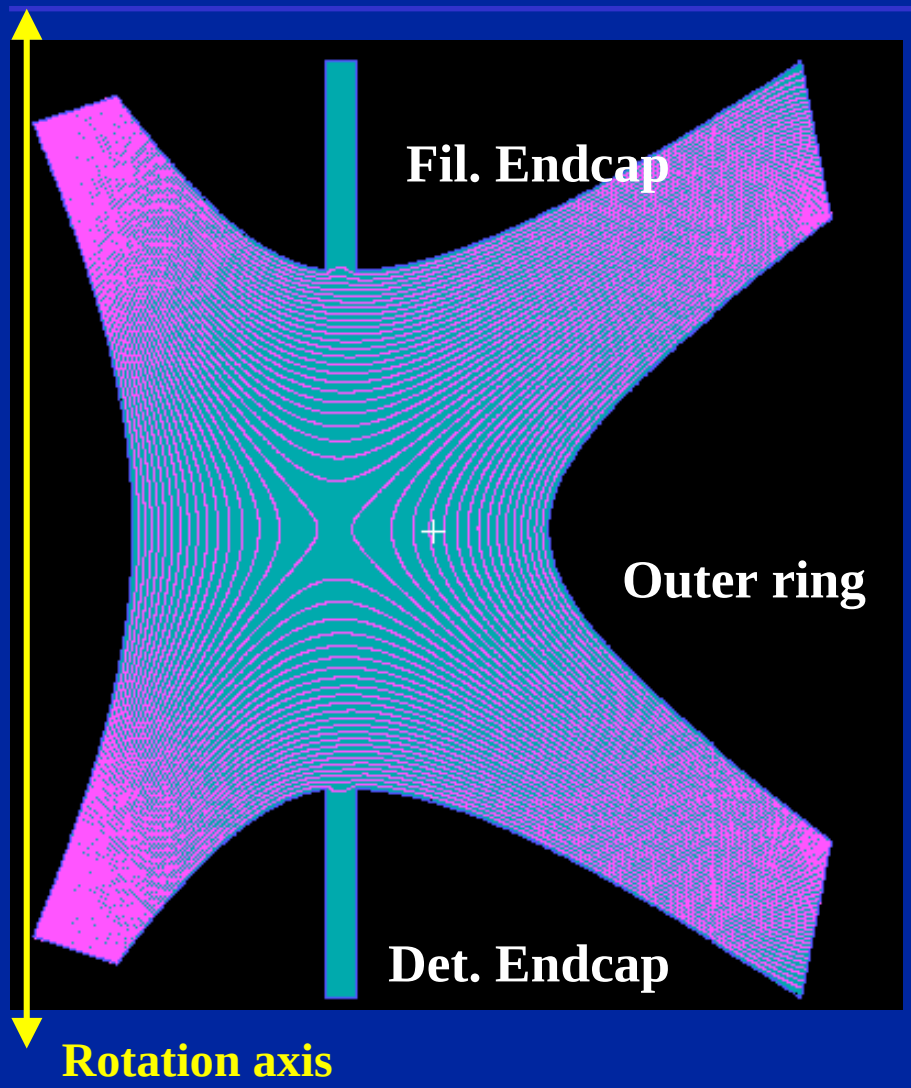
Symmetric Toroid Simulation - Ejection @ β = 0.55



Correction of Non-linear Fields

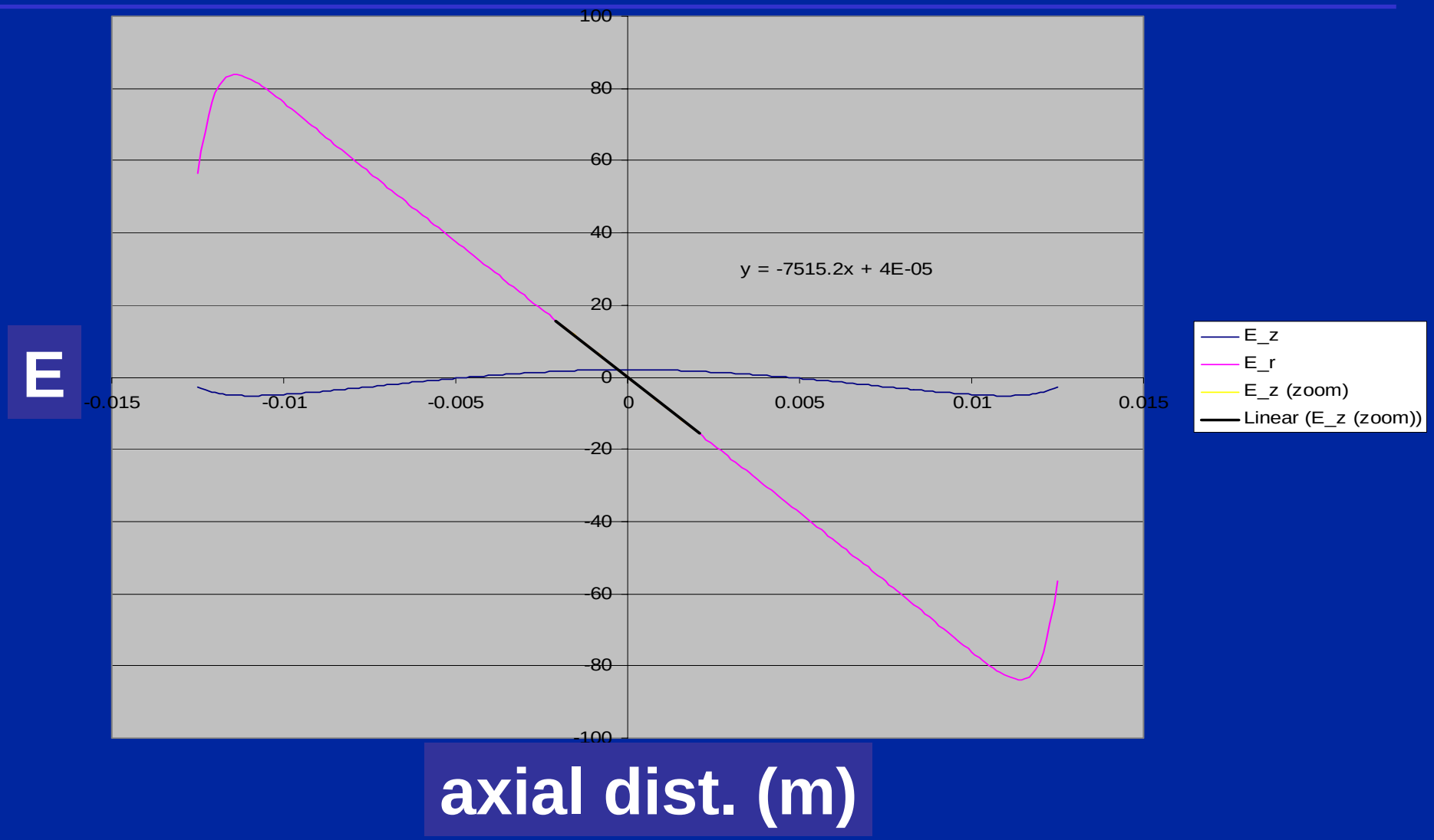


Asymmetric Toroid Geometry

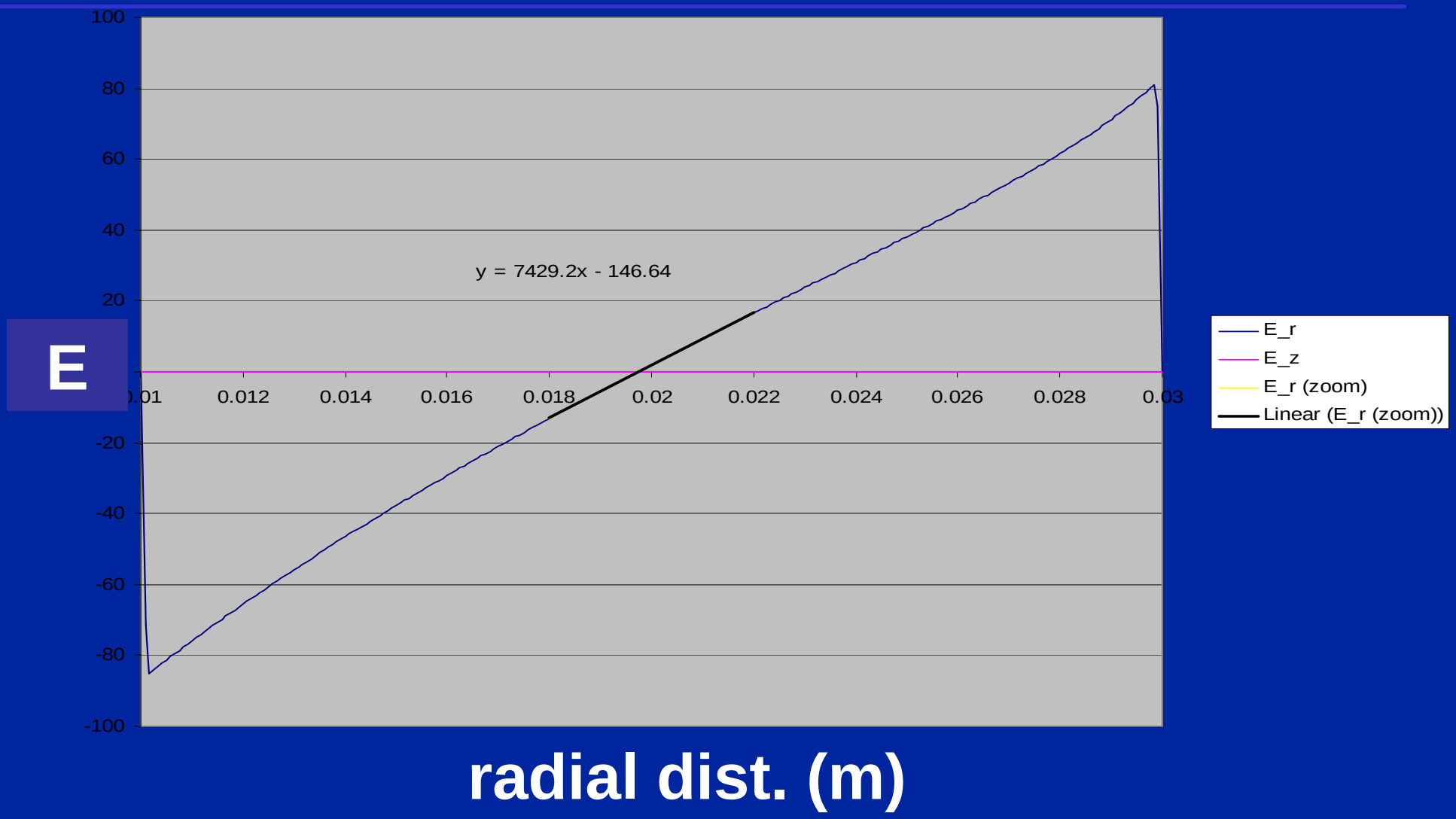


- Inner ring asymptote = 1.8
- Outer ring asymptote= 0.7
  (+/- 0.55 from symmetric)
- Endcap (z_0) = 1.25 cm (no stretch)
- Inner ring r_0 = 1 cm
- Outer ring r_0 = 1 cm
- Asymptote truncation =2.2*r_0
- Entrance/Exit slits= 1.5 mm dia.

Axial Trapping Field Analysis: Asymmetric Toroid Analyzer

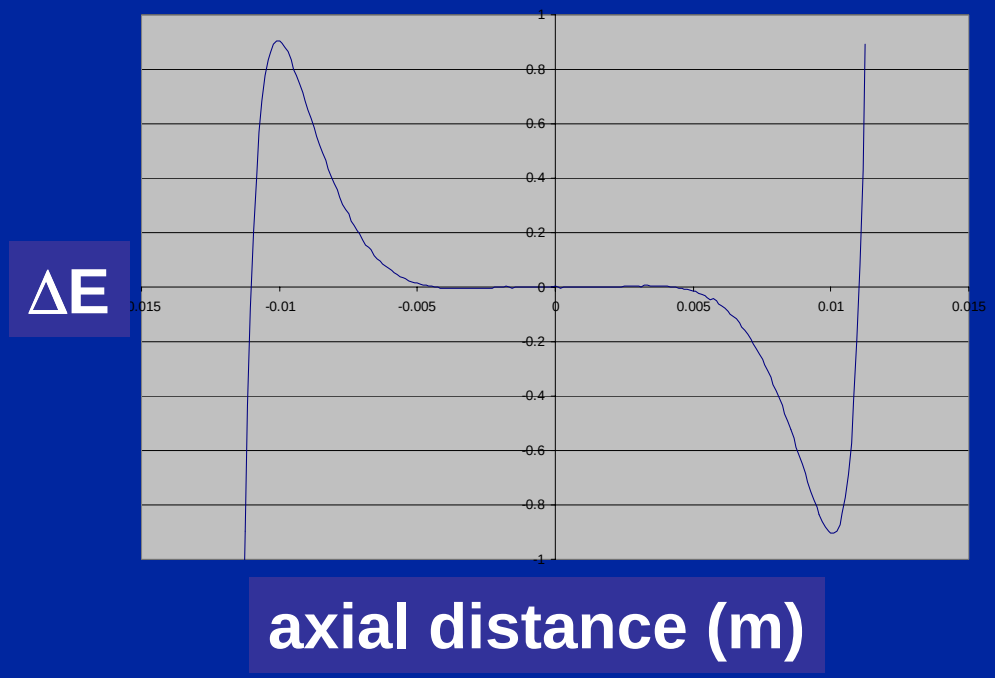


Radial Trapping Field Analysis: Asymmetric Toroid Analyzer

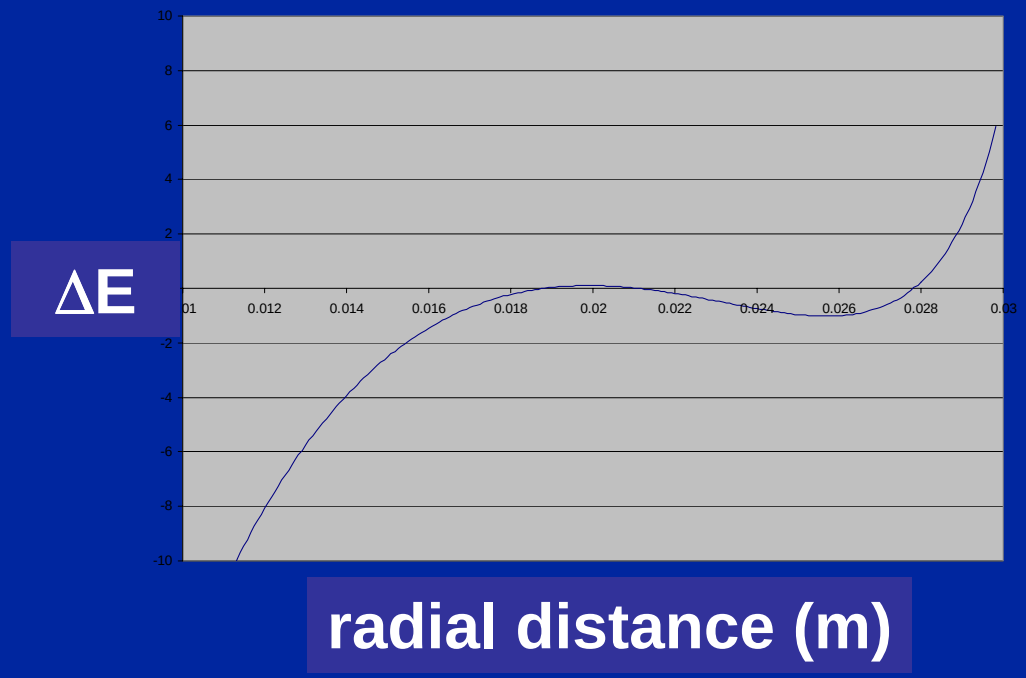


Asymmetric Toroid Analyzer

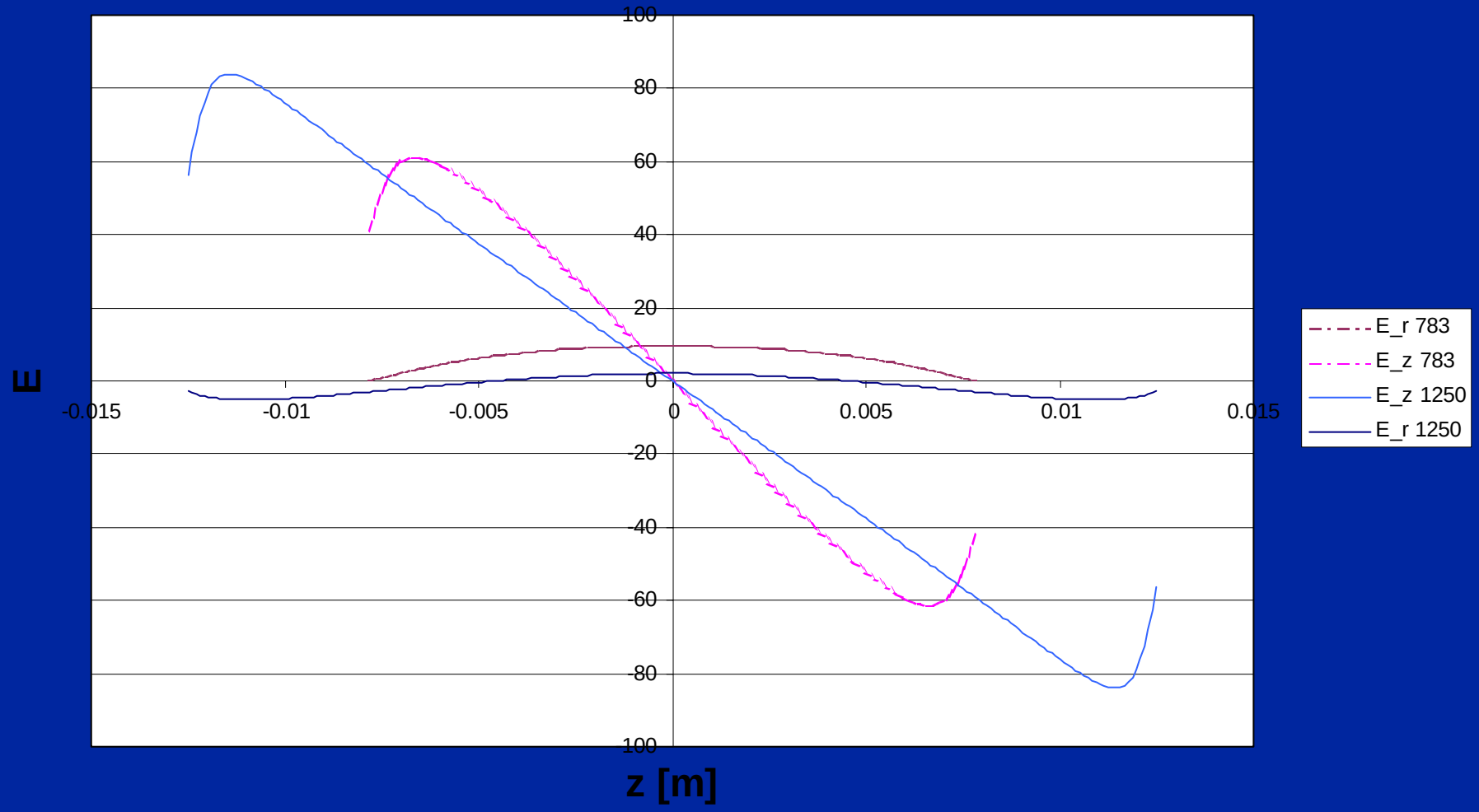
Axial Deviation from Linearity



Radial Deviation from Linearity



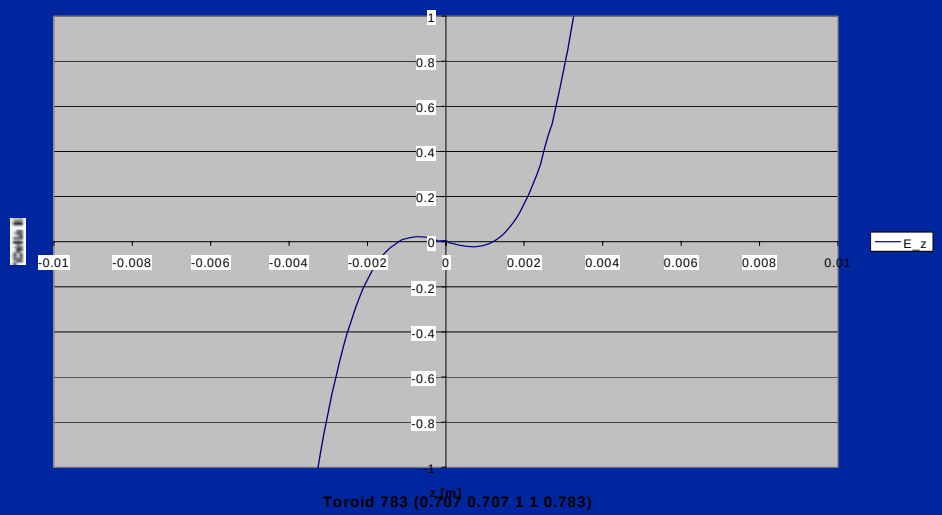
Comparison of Trapping fields for Symmetric and Asymmetric Toroid Analyzers

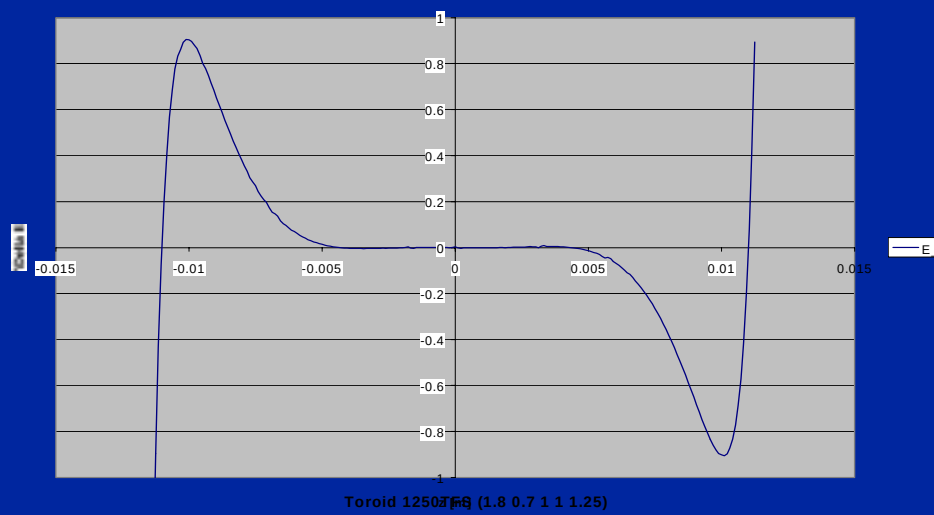


Deviations from Linear Field Strength Symmetric vs. Asymmetric Toroid

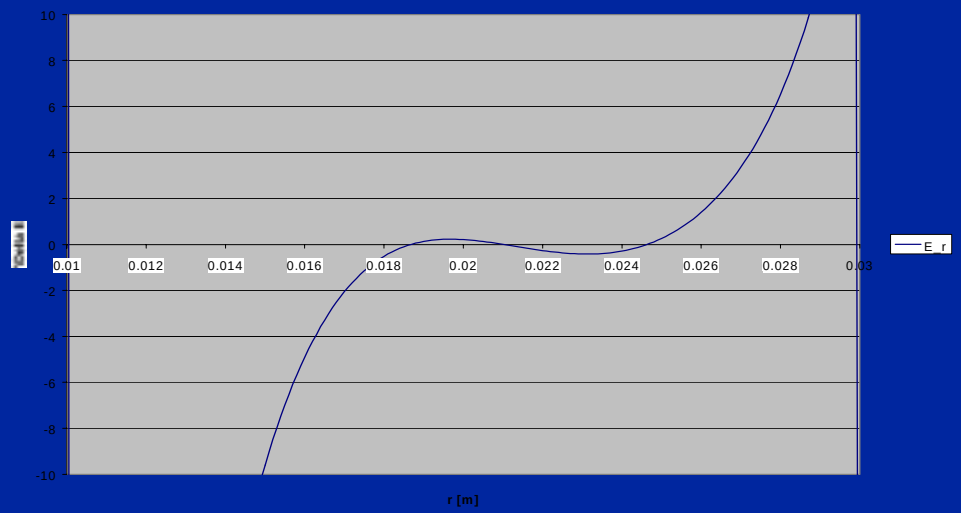
SYMMETRIC TOROID | **ASYMMETRIC TOROID**

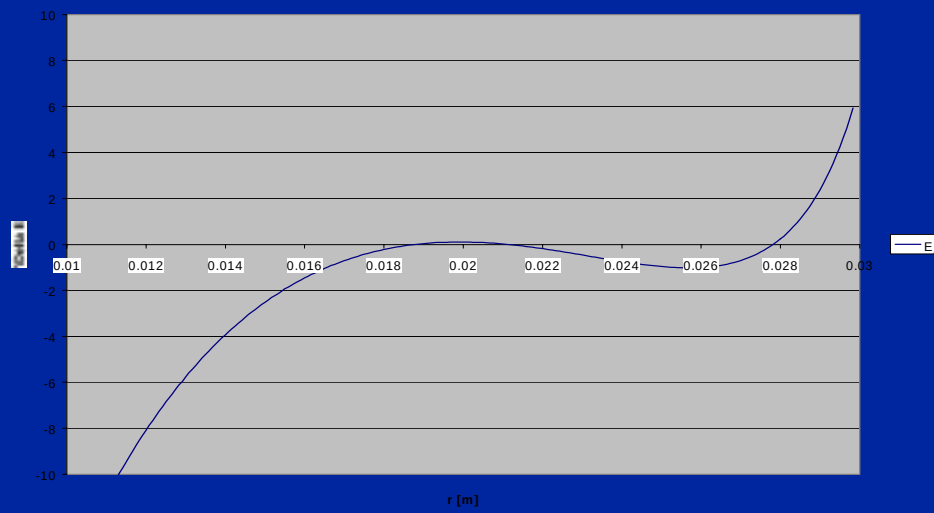
AXIAL FIELD ΔE



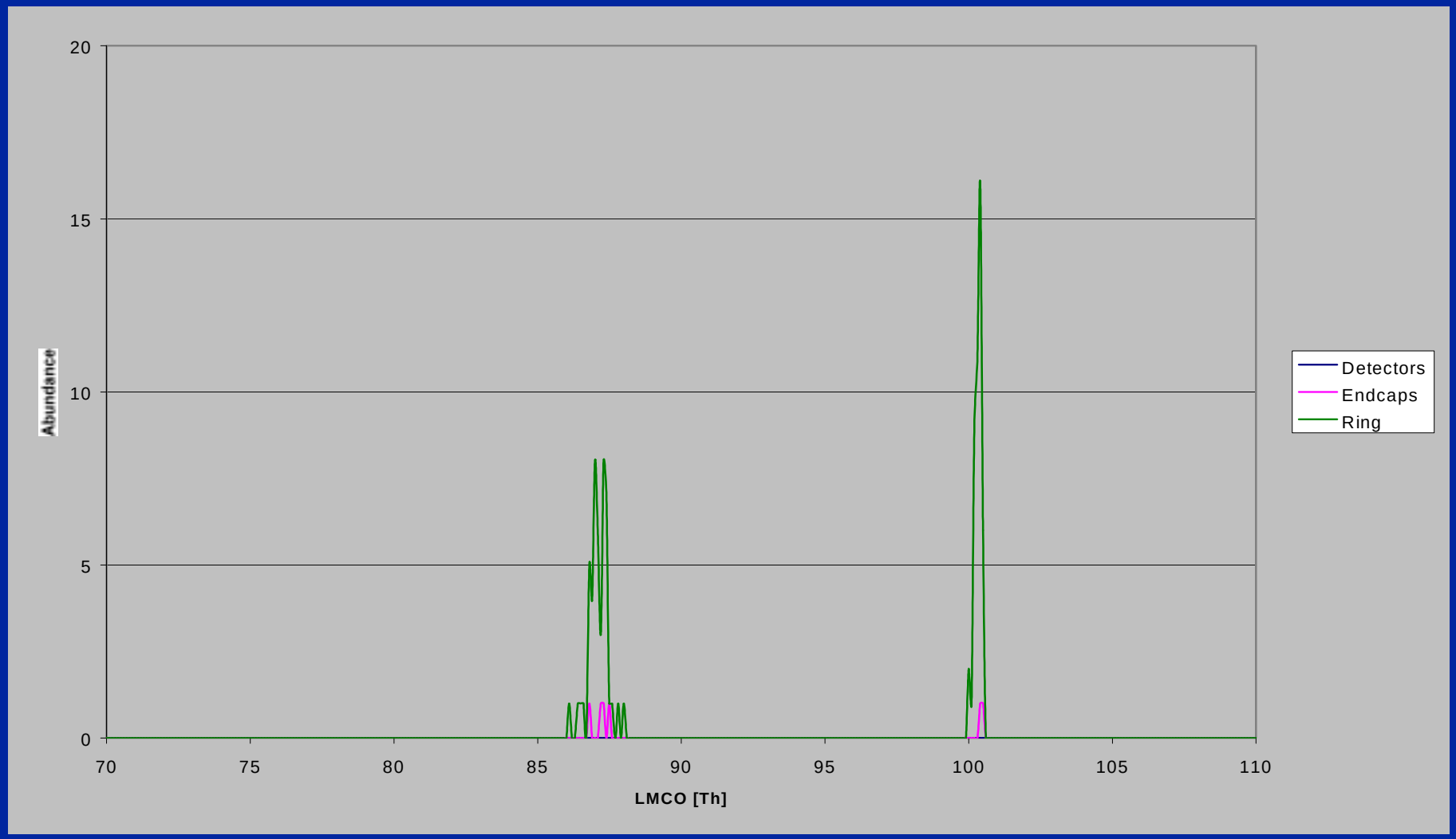


RADIAL FIELD ΔE





Asymmetric Toroid Simulation - Boundary Ejection



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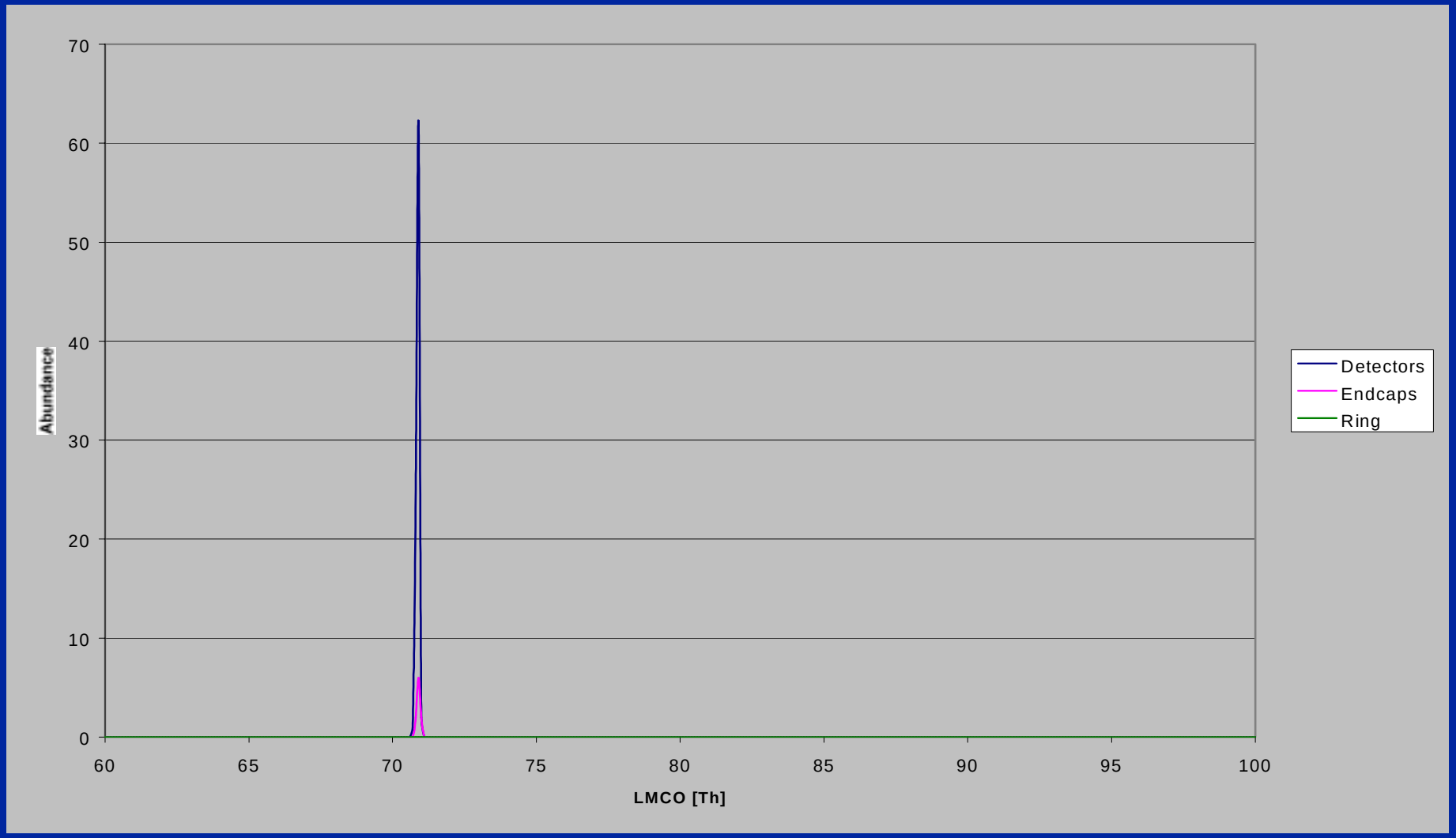
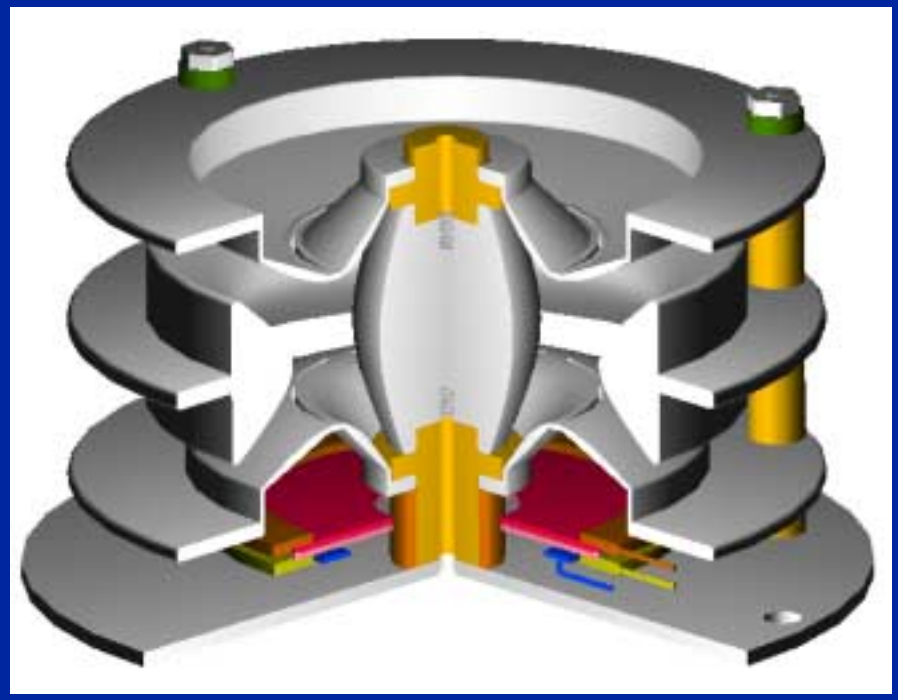


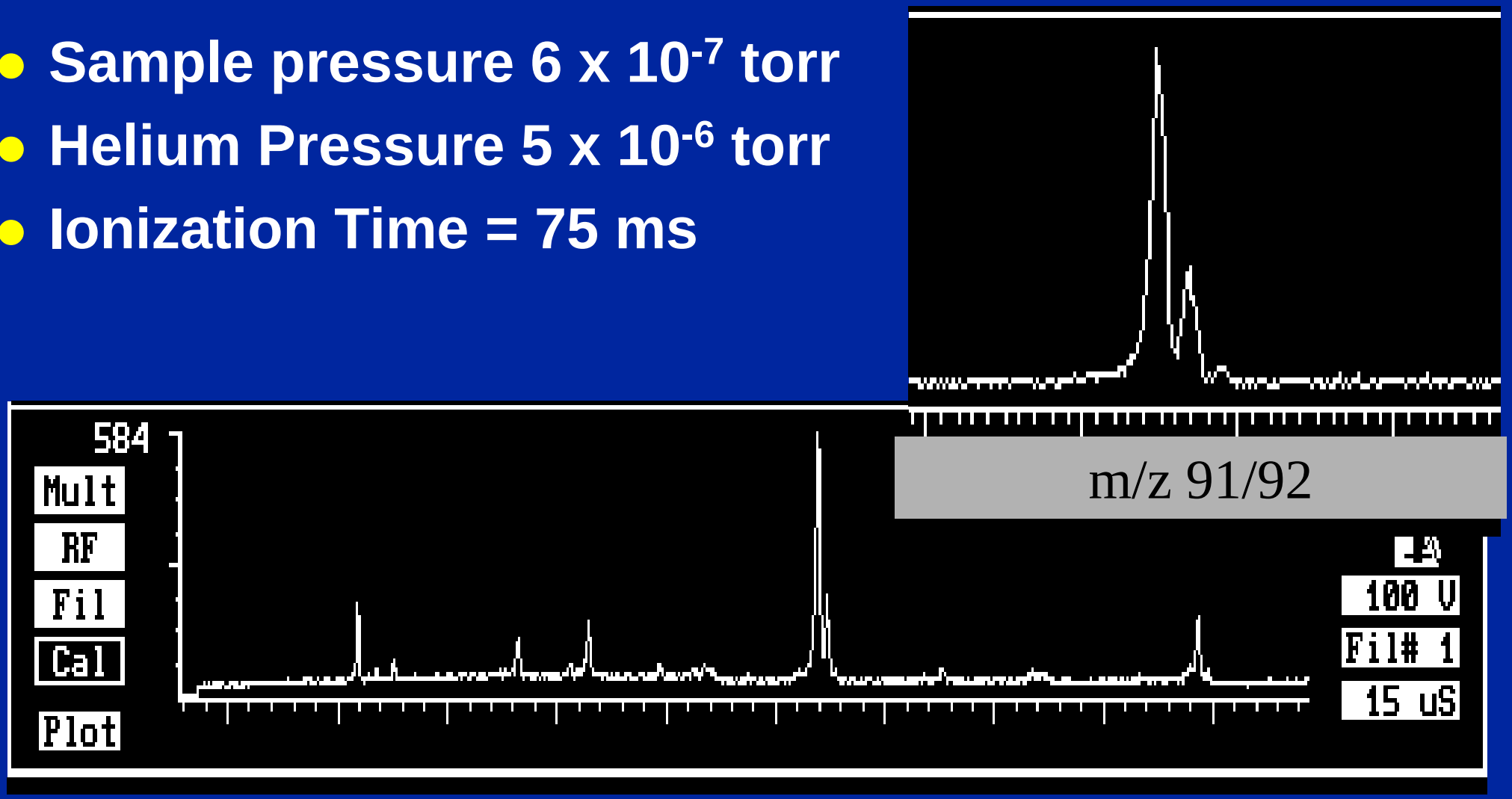
Asymmetric Toroid Analyzer Geometry

- **RF Frequency moved from 990 kHz (symmetrical) to 1040 kHz (asymmetrical)**
  - close enough to electronics design frequency to allow full rf scan



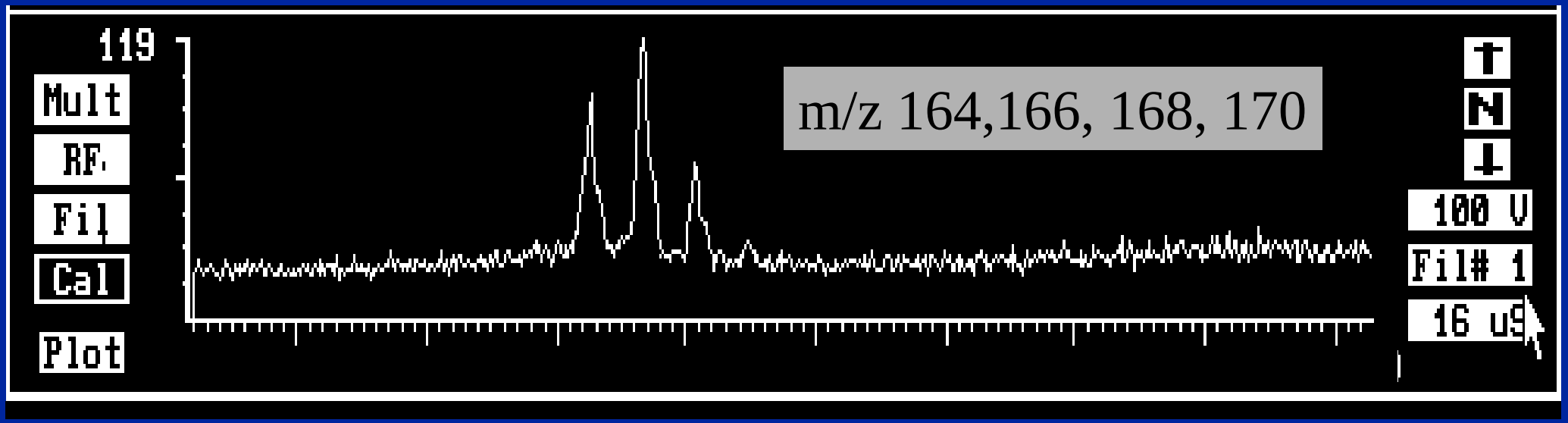
n-Butylbenzene

- Sample pressure 6 x 10^{-7} torr
- Helium Pressure 5 x 10^{-6} torr
- Ionization Time = 75 ms



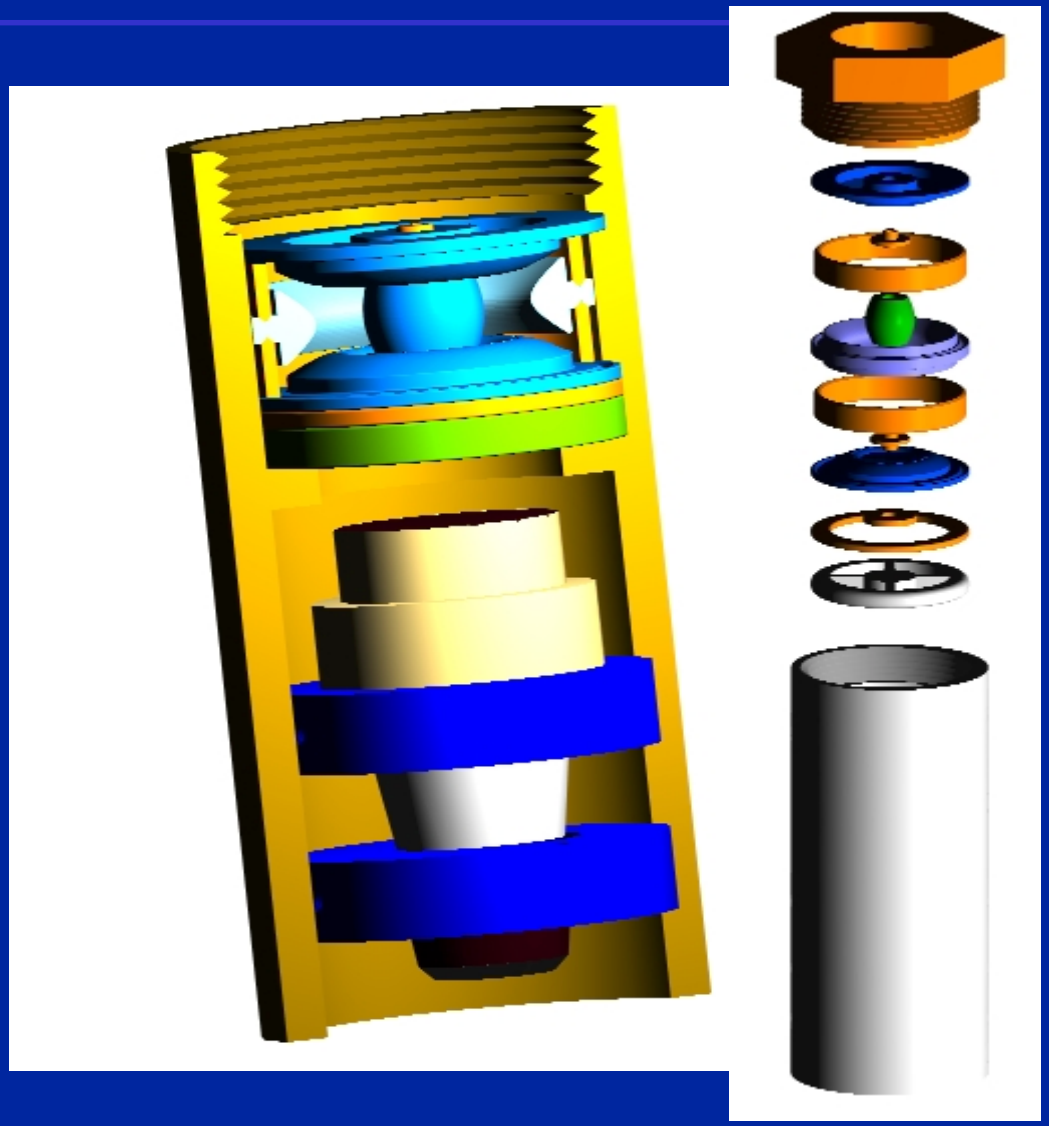
Perchloroethylene

- Sample pressure 5 x 10^{-7} torr
- Helium pressure 5 x 10^{-6} torr
- Ionization time 100 ms

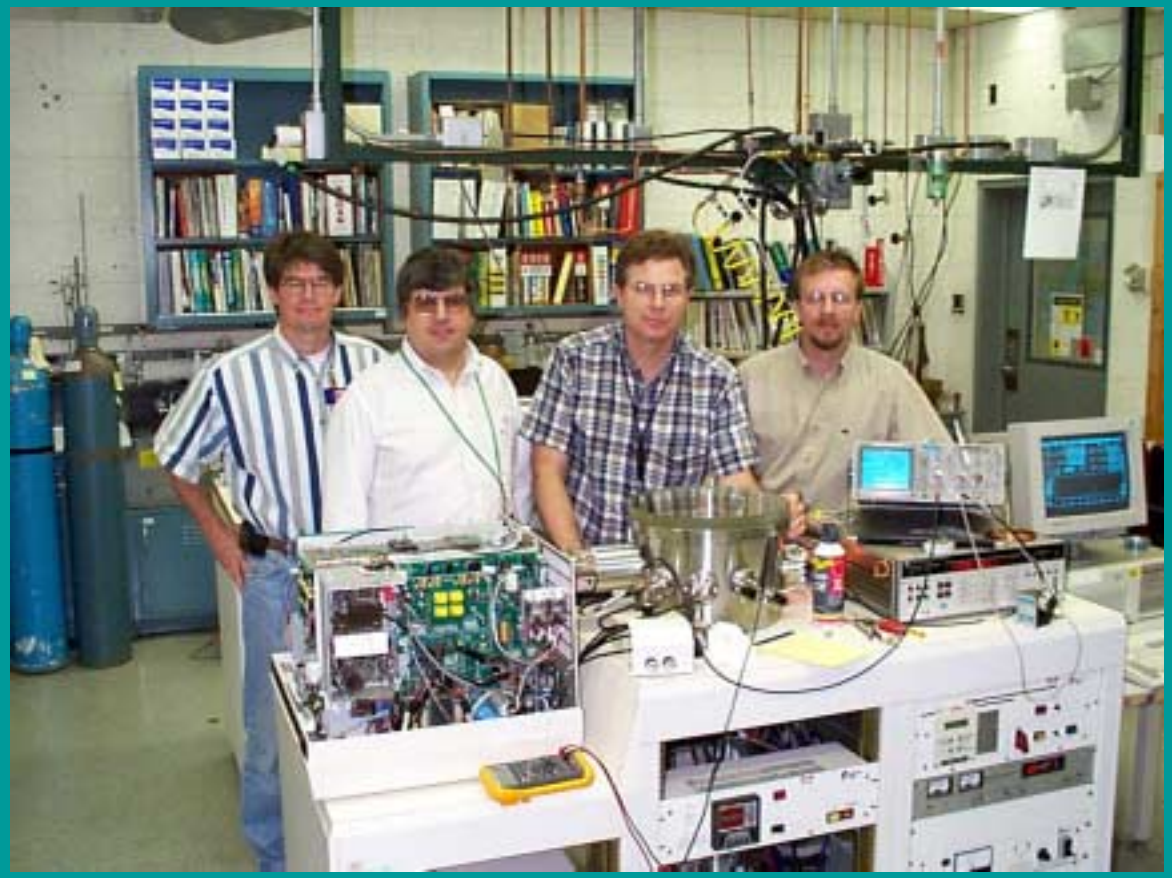


Next steps

- **Construction of 1/5 size Toroid (r_0 = 0.2 cm)**
  - Low voltage direct drive rf
  - Ejection slits < diameter of K&M electron multiplier
  - Issues with level of machining tolerances
  - Machining of slits presents a special problem.



Acknowledgements



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