EXAMINATION OF A DESIGN AID THAT SIMULATES ION MOBILITY

ABSTRACT

This paper presents a comparison of real IMS hardware devices and their actual data with models of these hardware configurations and their simulated ion trajectories. Two conventional IMS devices and an Ion Well IMS device are presented.

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ABSTRACT

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INTRODUCTION

For the CAM[1] and PCP[2] devices, real signatures are used, along with their physical hardware configurations, to calculate the Ko's of the signatures. The Time Of Flight (TOF) for these signatures are then calculated for 273^0 k and 760 torr. The hardware configurations of these devices are then modeled using LORENTZ,[3] the trajectories launched, and the modeled TOF's found. The hardware TOF's are compared to the modeled TOF's.

Our immediate need is for this simulation is for a design aid to model the ion motion caused by time and position varying electric fields[4] for Ion Wells[5] and other structures.[6,7] This paper also included simplified Ion Well simulation.

First, a look at a new tool for IMS simulation. This tool is a special version of LORENTZ, developed by Dr. Ali Asi of Integrated Engineering Software. This software uses the Boundary Element Method for electric field integration.

A brief word about field integration schemes. Many of you are familiar with SIMION,[8] the old U.S. Dept. of Energy ion motion simulation program that uses the Finite Difference Method. LORENTZ uses the Boundary Element Method. These approaches are distinctly different.

> The Finite Difference Method (used by SIMION) uses several iterations of a truncated Taylor series to define the field value at each rectilinear grid location at which the field exists.
>
> With the Boundary Element Method (used by LORENTZ), the field values are not solved for directly. Instead, an equivalent source that would sustain the field that satisfies the boundary conditions is found. A function describing this source relates

the location and its influence on any point on the boundary. This influence function is called the Green function.

The advantages of LORENTZ are that the software already contains provisions for analysis of slow particles, such as paint drops floating in a gas or liquid, and the developer's willingness to adapt the software package to ion mobility.

To generate and analyze a model using LORENTZ the following steps are performed:

- GEOMETRY setup;
- PHYSICS⇒ BOUNDARY CONDITIONS;
- ANALYSIS⇒ VIEW CONTOURS;
- TRAJECTORY⇒ SETUP and LAUNCH;
- UTILITY, data about the ion motion.

A CAM - LIKE STRUCTURE IS MODELED.

A simplified structure, is presented. The TOF path is 3.6 cm, the voltage across this path is 820 volts, the temperature is 21 ^{o}c. A CAM Output Signal vs. Time signature file is presented in Figure 1. The TOF = 7.6 ms.

The equations for ion mobility are:

Reduced Mobility: Ko = (273/T)(P/760) * K
Mobility: K = V/E = (L^2)/(v * t)

T = temp in Kelvin, P= pressure in torr, V= velocity in cm/sec, E= field in volts/cm
L= TOF length in cm., v= potential in volts, t= TOF time in sec.

For the CAM device, the signature and hardware configurations Ko is calculated.

Ko = (273/(273+21)) * ((3.6^2)/(820 * 7.6E-3))
= 1.93

The TOF is then calculated for 273^{0}c and 760 torr, for comparison with the modeled TOF.

1.93 = (3.6^2)/(820 * t)

t = (3.6^2)/(820 * 1.93)
= 8.185 ms.

The hardware configuration is then modeled using LORENTZ, the trajectories launched, and the modeled TOF found. A quick simulation of the CAM TOF region can be obtained using two plates: the bottom plate for the shutter grid and the top plate for the detector. This structure simulation is shown as Figure 2.

The electric field equipotential lines are shown in Figure 3. At the center, between the plates, the equipotentials are parallel and uniform for the ion trajectory. The ion trajectory is launched from the center of the bottom plate (at Y= 0.5cm.), and the ion traveled to the center of the top plate (Y= 4.1cm), as shown in Figure 4.

The LORENTZ Trajectory Utilities, Figure 5, provided data at each step. The last trajectory value, step 200, is displayed. The ion reached the detector, Y=4.1cm, after a TOF of 8.219 ms.

The LORENTZ trajectory data can be sent to MS Excel for plotting, Figure 6, and the data can then be manipulated using MS Excel to remove the initial Y axis ion launch value of 0.5cm., if this is desired.

Summary: The hardware TOF is compared to the modeled TOF.

Hardware TOF = 8.185 ms.
LORENTZ TOF = 8.219 ms.

The LORENTZ TOF value is 0.42% higher.

A PCP INC. IMS STRUCTURE IS MODELED.

The device, 3M-86, has a 10 cm X 4.12 cm I.D. TOF region, and overall is about 18 cm long. The TOF potential is 2Kv, with 3Kv across the entire structure, and the electric field is 200 v/cm from source to detector.

A PCP 3M86 Signature File,[9] Output Signal vs. Time, is shown in Figure 7. Additional information about the PCP signature and the location of the signature peak is presented below:

This is ripn1.asc file.

IMS Cell Temp	=	28.6^{o}C
Atmos. Pressure	=	762 Torr
Cell Voltage	=	3000 volts
Uo Constant	=	53882
Gas Type	=	AIR
Carrier Flow	=	200 ml/min
Drift Flow	=	500 ml/min
Start Time	=	4 msec
End Time	=	44 msec
Dwell Time	=	40usec for 1011 channels
# Scans	=	1024

Signal amplitude at: 20.52 ms is 1,840,699 units.
20.56 ms is 1,891,225 <<< Taken as signal peak.
20.60 ms is 1,866,360

The signature Ko was calculated for the PCP hardware configuration.

Ko = (273/301.6)(762/760)((10^2)/(2000 * 20.56E-3))
= 2.207

The TOF is then calculated for 273^0 k and 760 torr, and compared to the modeled TOF.

2.207 = (10^2)/(2000 * t)

t = (10^2)/(2000 * 2.207)
= 22.66 ms.

The hardware configuration was then modeled using LORENTZ, the trajectory launched, and the modeled TOF found.

The region around the detector of the PCP device has been simplified for this simulation. Equipotential lines are shown in Figure 8, and detailed equipotentials around the detector are shown in Figure 9.

Output from LORENTZ Trajectory and Utility sub-routines are displayed in Figure 10. The last trajectory value, step 200, is also displayed. The ion reaches the detector, X=0.0, Y=.0.05m, after a TOF of 22.76 ms.
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Summary: The hardware TOF is compared to the modeled TOF.

Hardware TOF = 22.66 ms.
LORENTZ TOF = 22.76 ms.

The LORENTZ TOF value is 0.44% higher.

AN ION WELL IS MODELED.

We are exploring the use of ion wells for the purpose of accumulate ions and as a replacement for the shutter grid commonly found in IMS devices. The use of an ion well has been demonstrated, and hardware is available for evaluation,[5,10] Figure 11.

An ion well can accumulate either positive ions or negative ions at a selected location located between the source and detector in an IMS structure. This is accomplished by combining a Forward Electric (E) Field followed by a Reverse E Field. This E field transition causes all of the ions of the selected polarity that are present in the cell to travel toward the E field transition location. Thus, if the ions of interest are negatively charged, increasing positive voltages are placed on successive electrode rings between the source and the transition location, and the voltages placed on successive electrode rings between the transition location and the detector are decreasing. As the ions move from the source and accumulate in the well. This is shown below.

<table>
<tr><td>Ions of Interest</td><td>Ions of Interest</td></tr>
<tr><td>Forward Electric Field</td><td>Reverse Electric Field</td></tr>
<tr><td></td><td></td></tr>
<tr><td>Positive Ions</td><td>Positive Ions</td></tr>
<tr><td colspan="2">100v 50v 0v 50v 100v</td></tr>
<tr><td></td><td></td></tr>
<tr><td>Negative Ions</td><td>Negative Ions</td></tr>
<tr><td colspan="2">0v 50v 100v 50v 0v</td></tr>
<tr><td></td><td></td></tr>
<tr><td colspan="2">Source E. Field Reversal Detector</td></tr>
</table>

Space charge limits the ion concentration. Excess ions entering the well and long compression times cause ions to move perpendicular to the cell wall, where their charge is removed.

A design for a simplified ION WELL is presented. This design demonstrates that for mobility, the ions travel perpendicular to the equipotential lines. The structure also demonstrates that the ions remain in the well for differing times depending on their initial launch position.

The ion well structure, Figure 12, is 4 cm. on the Y axis and 8 cm. on the X axis. Top and Bottom electrodes are at –400v, both center electrodes are at 0.0v. The center electrodes are spaced 2 cm from the top and bottom electrodes and separated by 2 cm. An ion well is thus created along the X axis at Y=2 cm Equipotential lines are also shown.

Ions are launched every 0.5 cm from the right side of both top and bottom electrodes, Figure 13. Negative ion travel is simulated, in the positive Y direction from the bottom electrode, and in the negative Y direction from the top electrode, toward the center electrode.

An overlay of the equipotential lines, Figure 12, and the trajectories, Figure 13, will yield 90^{o} intersecting lines.

The ion trajectories travel time from the bottom plate to the center electrode for various ion launch locations is shown in Figure 14. Note that ions originating near the center of the ion beam (A) remain in the well for a considerable time, and that ions at the beam edge (D) are initiated much faster.

A typical ion well signature from our Model A IWIMS is shown in Figure 15. Note the sharp leading edge of signature caused by the accumulated ions at the trigger well, also note, the signature tail caused by late arriving ions just prior to the release of the ions into the drift region. This tailing can be improved using an improved ion well design.

CONCLUSION

LORENTZ was able to model real hardware and provided TOF values comparable to data obtained from the real hardware. A minimum of modeling was required to obtain these comparable TOF values.

The TOF values are 0.4% higher than the measured values. This is believed to be related to the relatively small number of calculation steps used and the finite time required by the simulation velocity to reach its terminal value.

This software program was modified to include mobility, and like all modified software, there is a learning curve. This version of LORENTZ has been modified for IMS applications and should prove useful for IMS cell development. Additional features can be refined and added to satisfy the requirements of a specific application.

We will be collaborating with Dr. Ali on his LORENTZ for IMS, particularly pertaining to the inclusion of additional features. Features under consideration include space charge effects and ion dispersion. The use of physical parameters, i.e., ion mass and size, media density, and viscosity to simulate mobility is also possible with LORENTZ and will be explored.

LIST OF FIGURES

Figure 8. PCP structure and equipotential lines are shown.

Figure 9. Simplified PCP detector area detailed equipotentials generated by LORENTZ.

Figure 10. PCP ion trajectory data, LORENTZ Trajectory Utility, end of flight data (Point 200).

Figure 11. Ion Well Ion Mobility Spectrometer, Model A.

Figure 12. Ion Well IMS structure and equipotentials.

Figure 13. Ion Well trajectories.

Figure 14. Ion Well trajectories, displaying ion storage times.

Figure 15. Typical NRI signature for the Model A Ion Well IMS device.

REFERENCES

1 CAM (Chemical Agent Monitor), manufactured by Graseby Dynamics, Environmental Technology Group and Intellitec of Technical Products Group.
2 PCP Inc., 2155 Indian Road, West Palm Beach, FL 33409
3 LORENTZ, supplied by Integrated Engineering Software, Attn. Joanne Morley, 300 Cree Crescent, Winnipeg, Manitoba, Caada. jmorley@integrated.ca
4 Blanchard, W.C., Int. J. Mass Spectrom. Ion Phys., 95(1989)199-210.
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7 Blanchard, W.C., "Focusing and Detection of Trapped Multiply Reflected Ions," 43nd ASMS conf., June 1994.
8 SIMION, Giant Scientific Software, Scientific Instrument Services, Inc. 1027 Old York Road, Ringoes, NJ 08551
9 PCP 3M86 signature file supplied by D.M. Shoff, ERDEC, APG, MD.
10 Blanchard & Co., Inc., 27 Glen Alpine Road, Phoenix, MD 21131

FIGURES

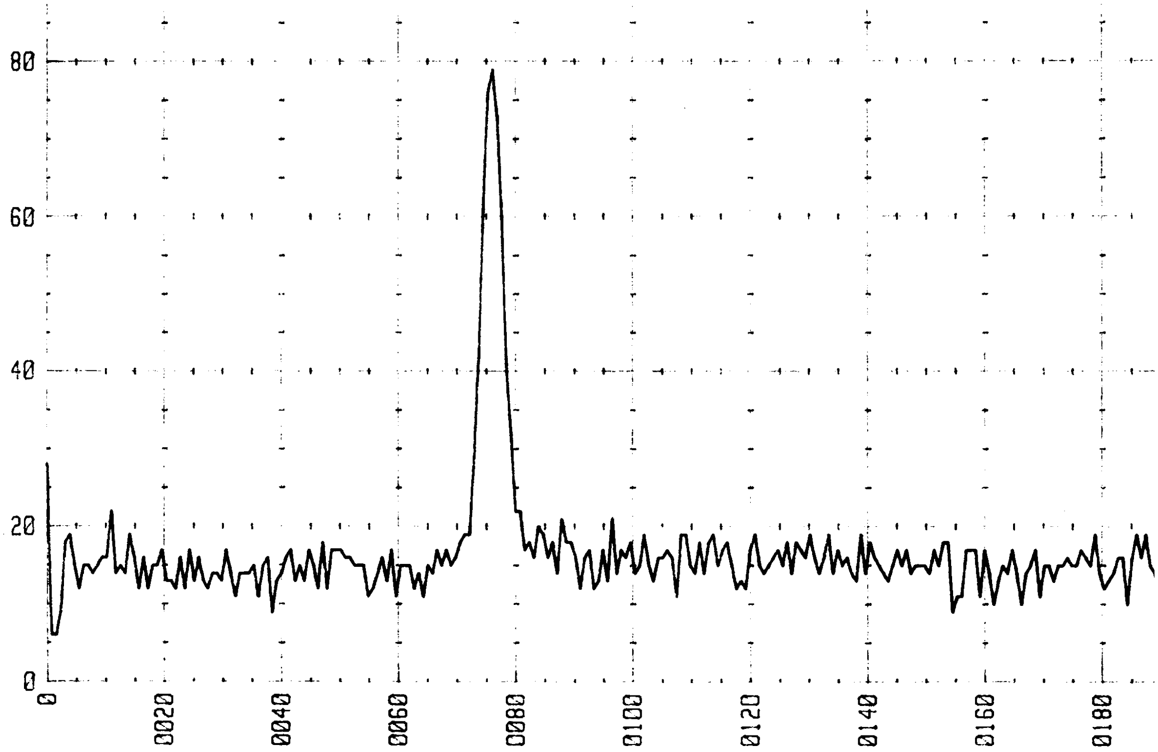


Figure 1. CAM Signature File, Output Signal vs. Time in ms.Temp. ~21^{o}c, TOF=7.6 ms.

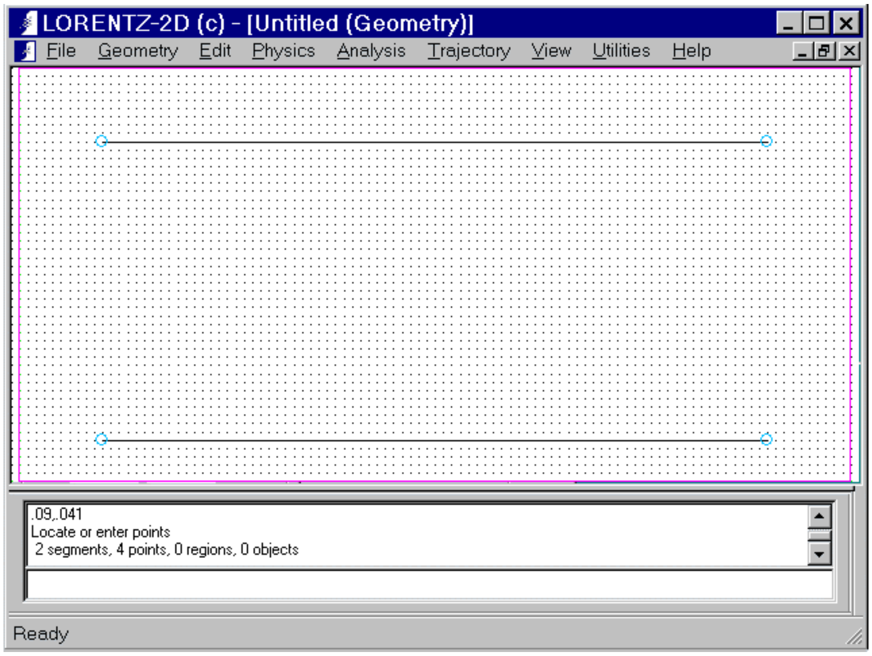


Figure 2. A quick simulation of the CAM TOF region, using two plates: the bottom plate for the shutter grid and the top plate for the detector.

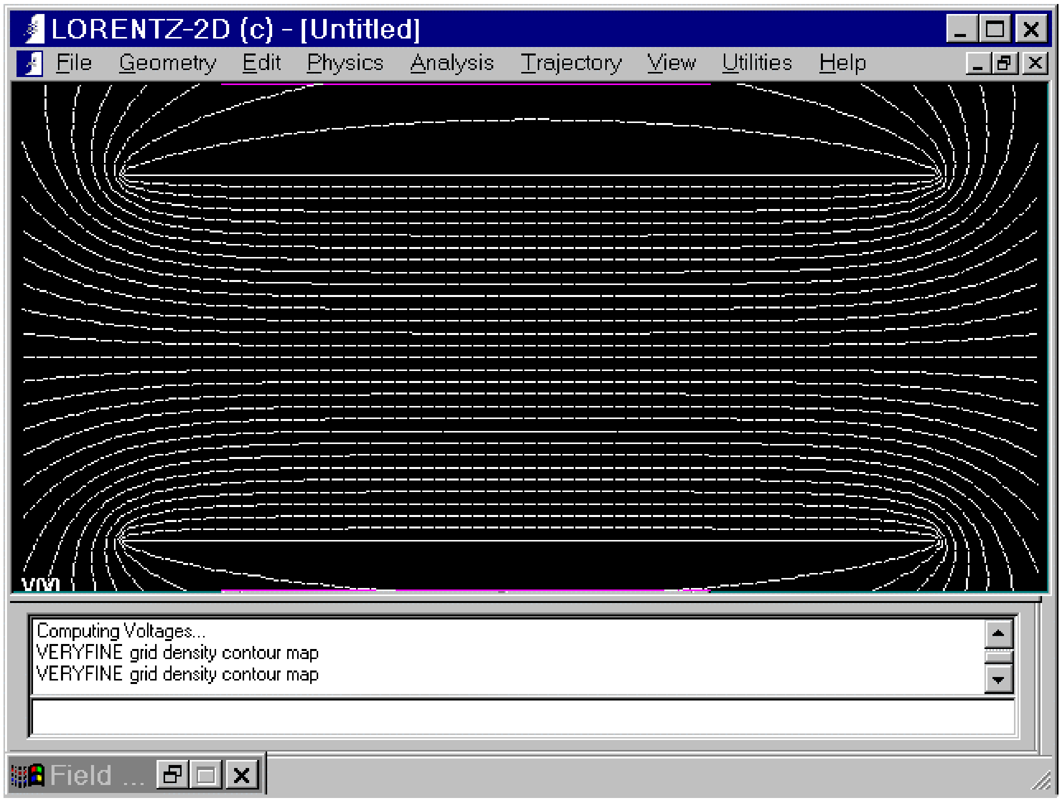


Figure 3. Simplified CAM structure electric field equipotential lines.

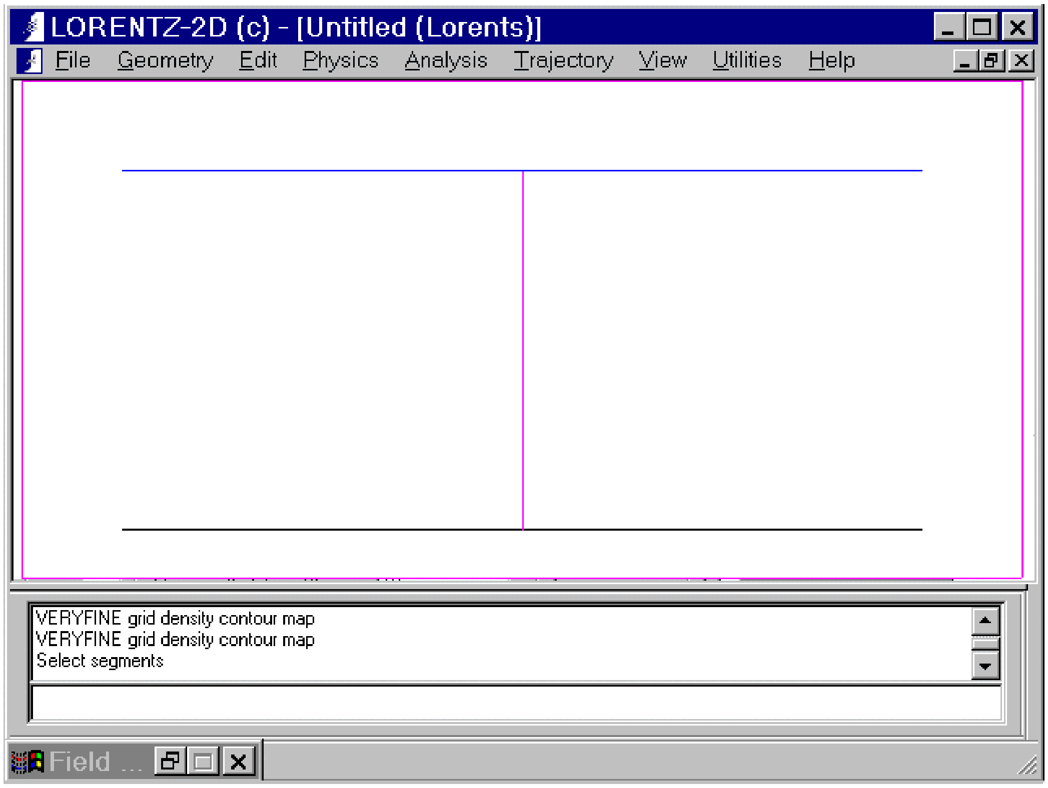


Figure 4. Simplified CAM structure ion trajectory, from the shutter grid (bottom plate) to the detector (top plate).

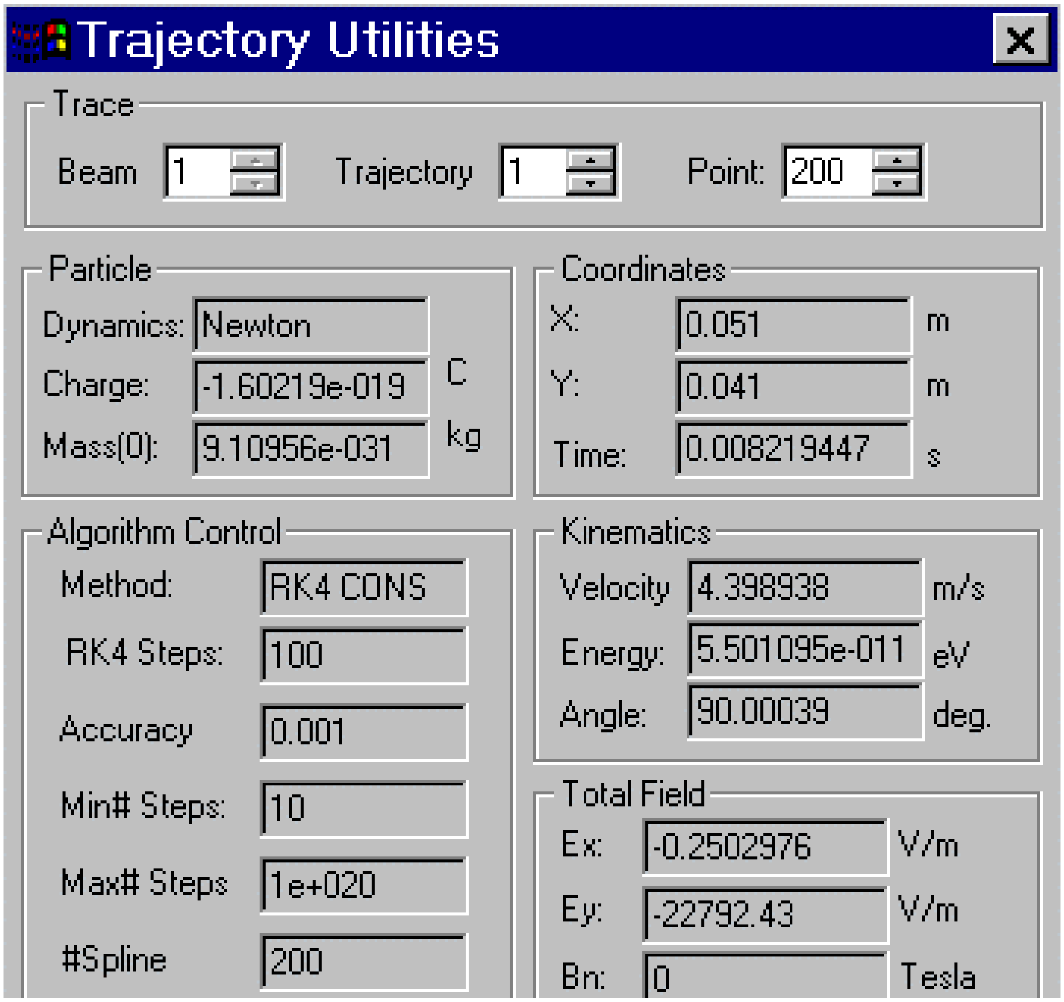


Figure 5. Simplified CAM structure ion trajectory data, LORENTZ Trajectory Utility, end of flight data (Point 200).

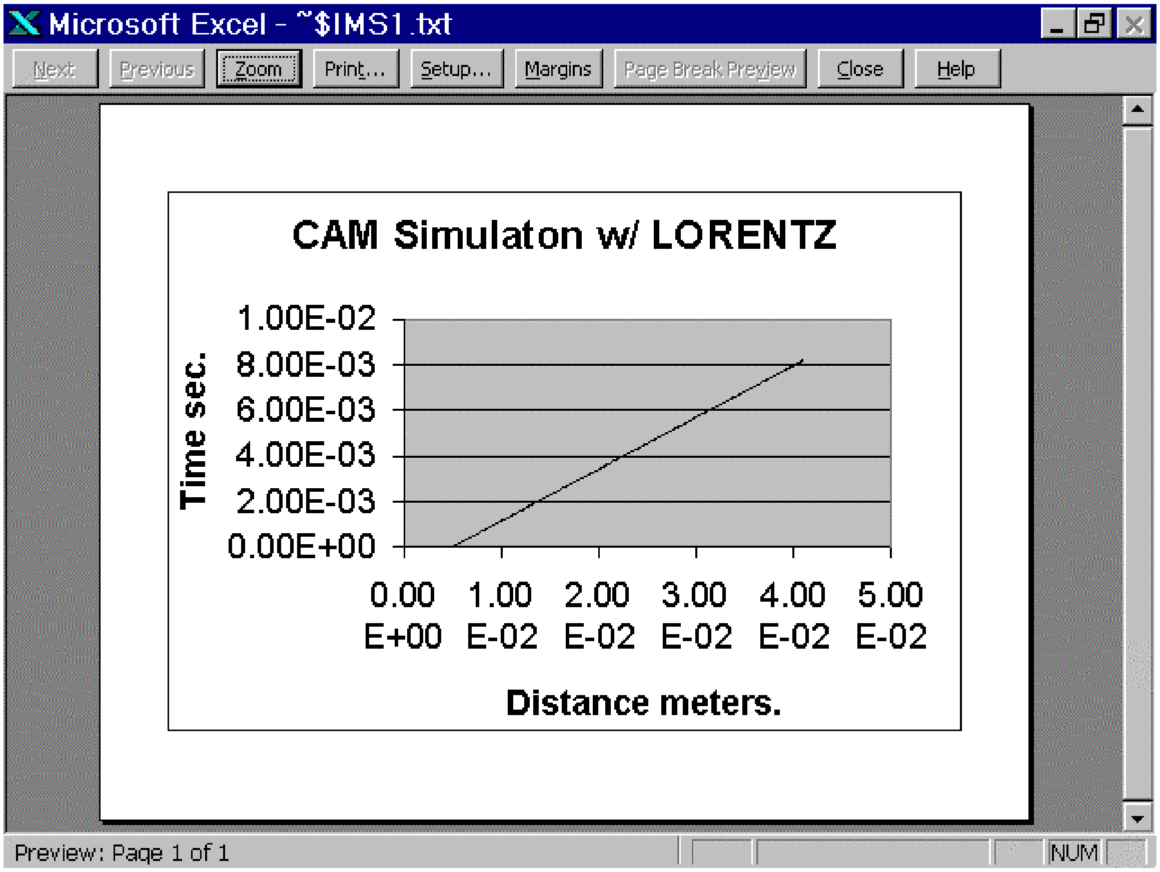


Figure 6. Simplified CAM structure LORENTZ Trajectory Utility data as plotted by MS Excel.

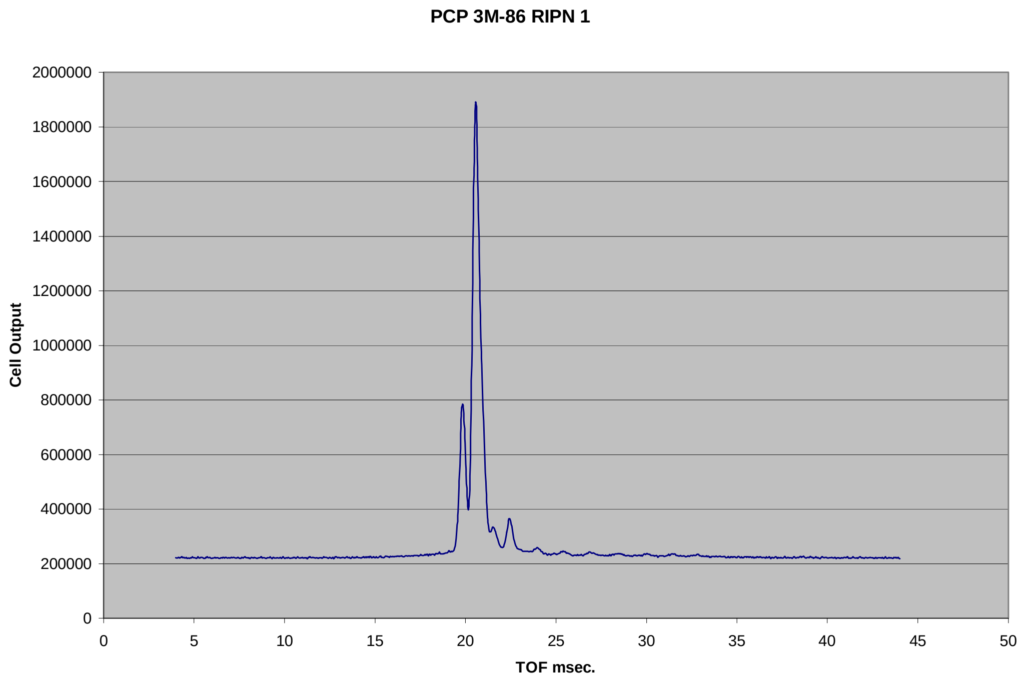
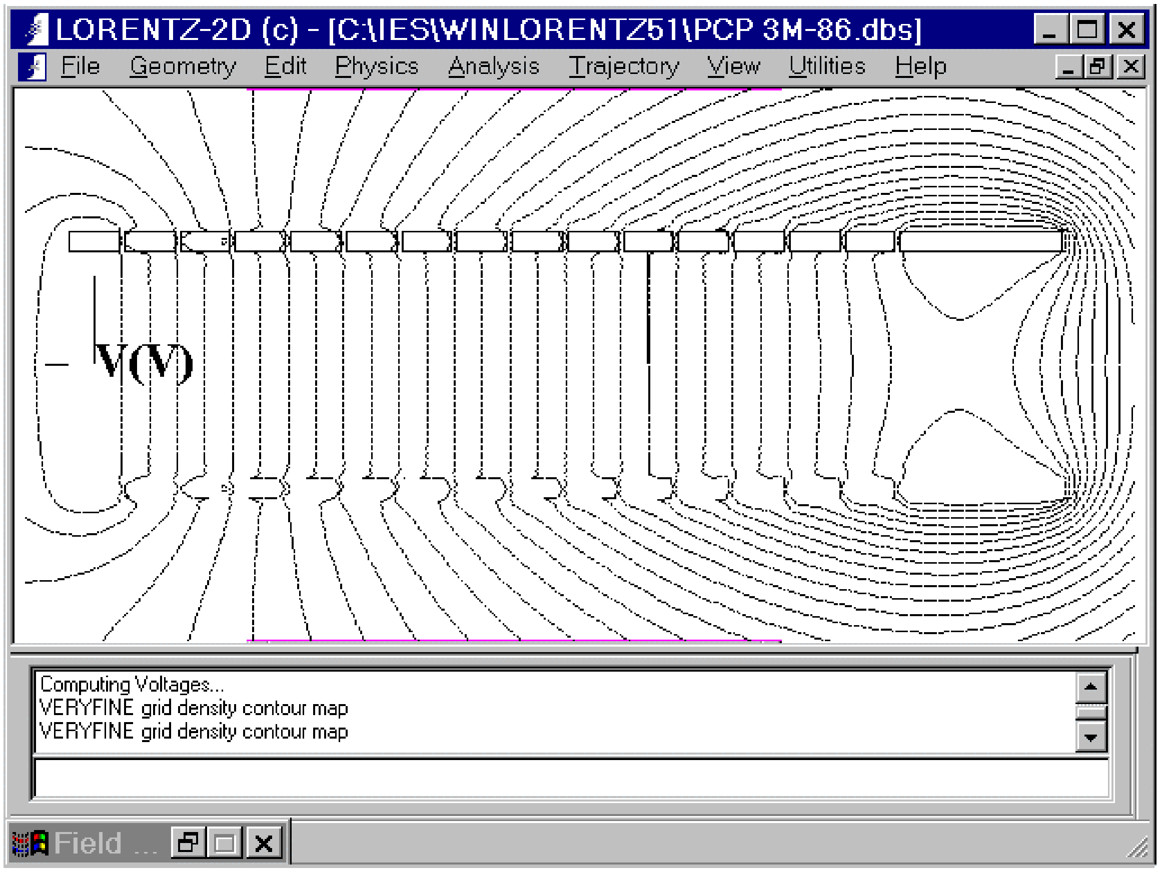


Figure. 7. PCP 3M86 Signature File, Output Signal vs. Time.



The ion source is at the right, under the "HELP" label. The shutter grid is under the 'Trajectory" label, and the detector is under the "File" label. The structure was mirrored around the center X axis as shown by the equipotential lines. Drawing both sides of a mirrored structure is possible but not automatic.

Figure 8. PCP structure and equipotential lines are shown.

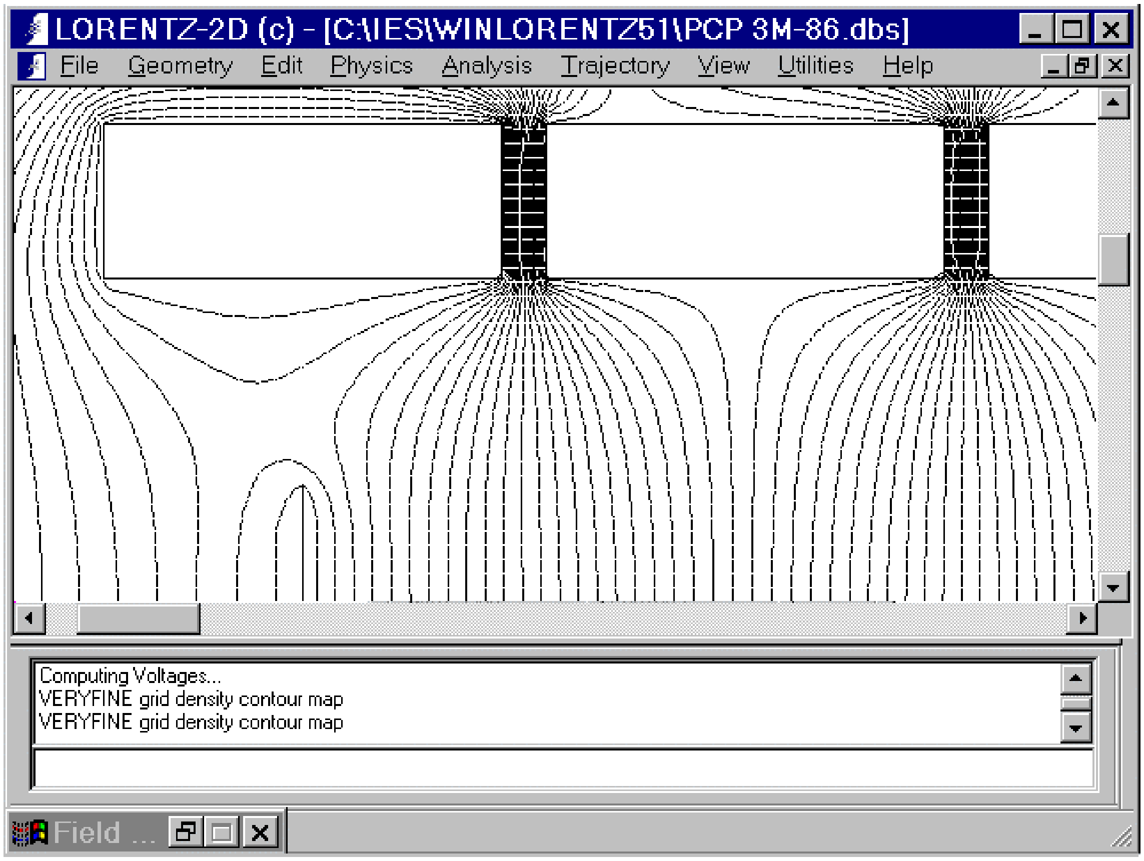


Figure 9. Simplified PCP detector area detailed equipotentials generated by LORENTZ.

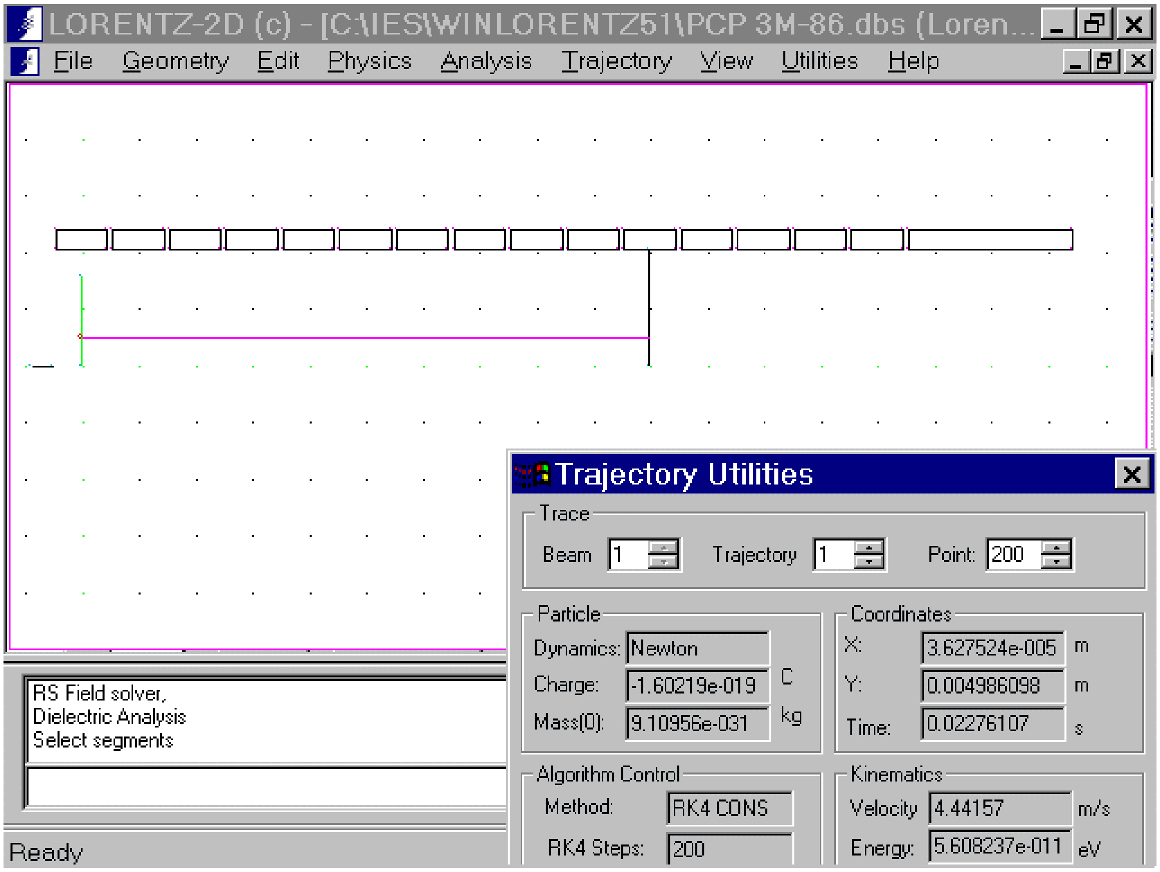


Figure 10. PCP ion trajectory data, LORENTZ Trajectory Utility with end of flight data (Point 200).

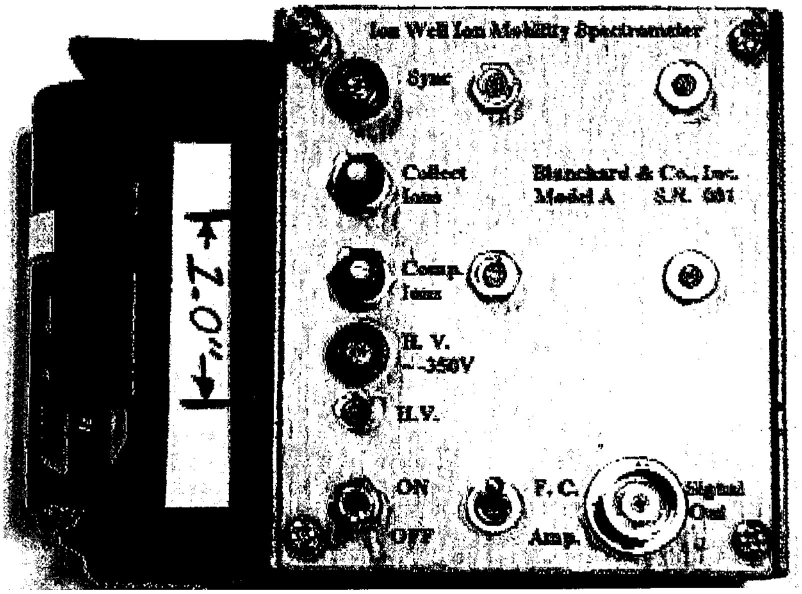
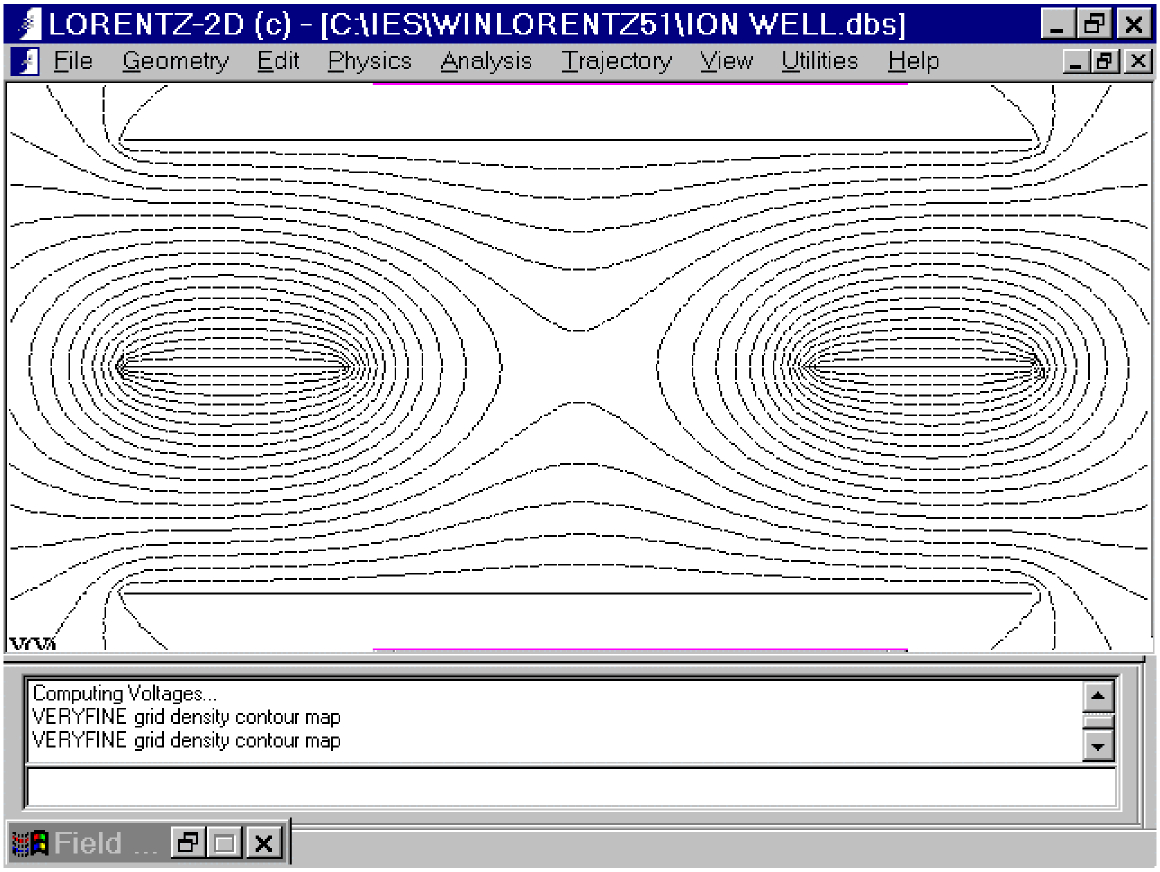
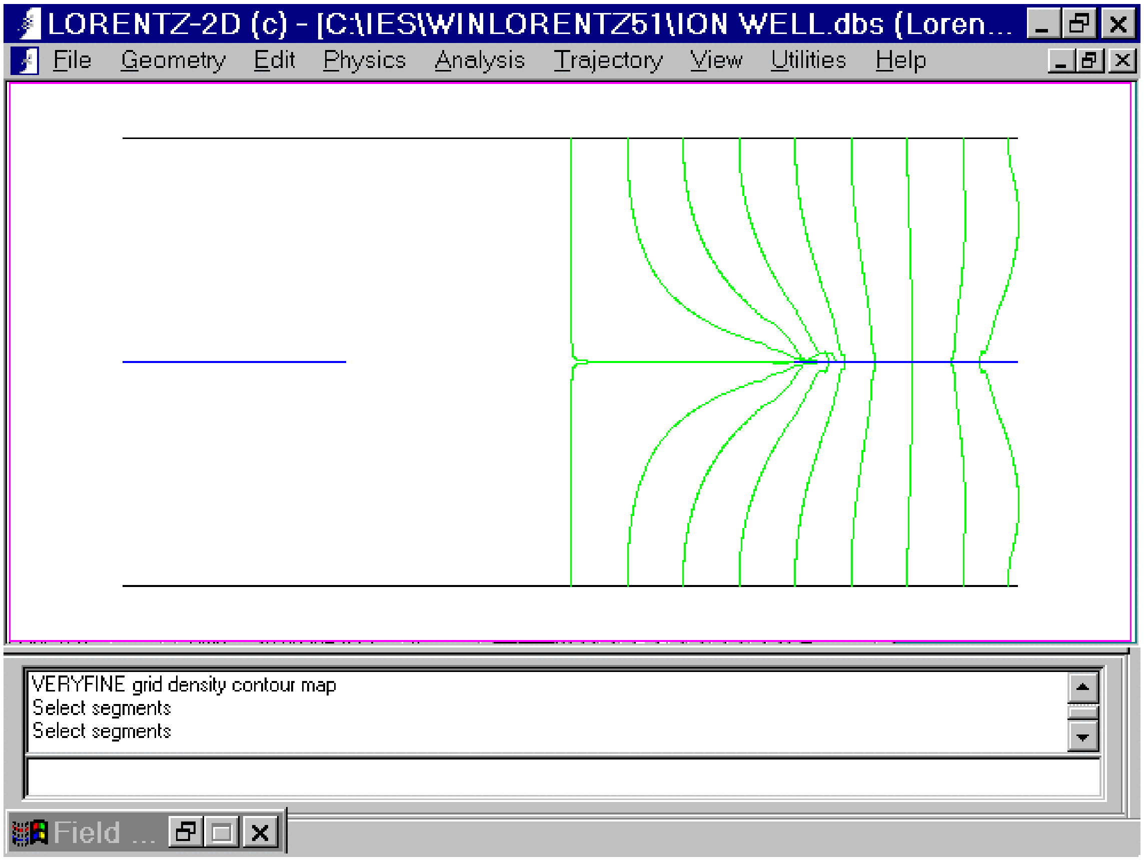


Figure 11. Ion Well Ion Mobility Spectrometer, Model A.



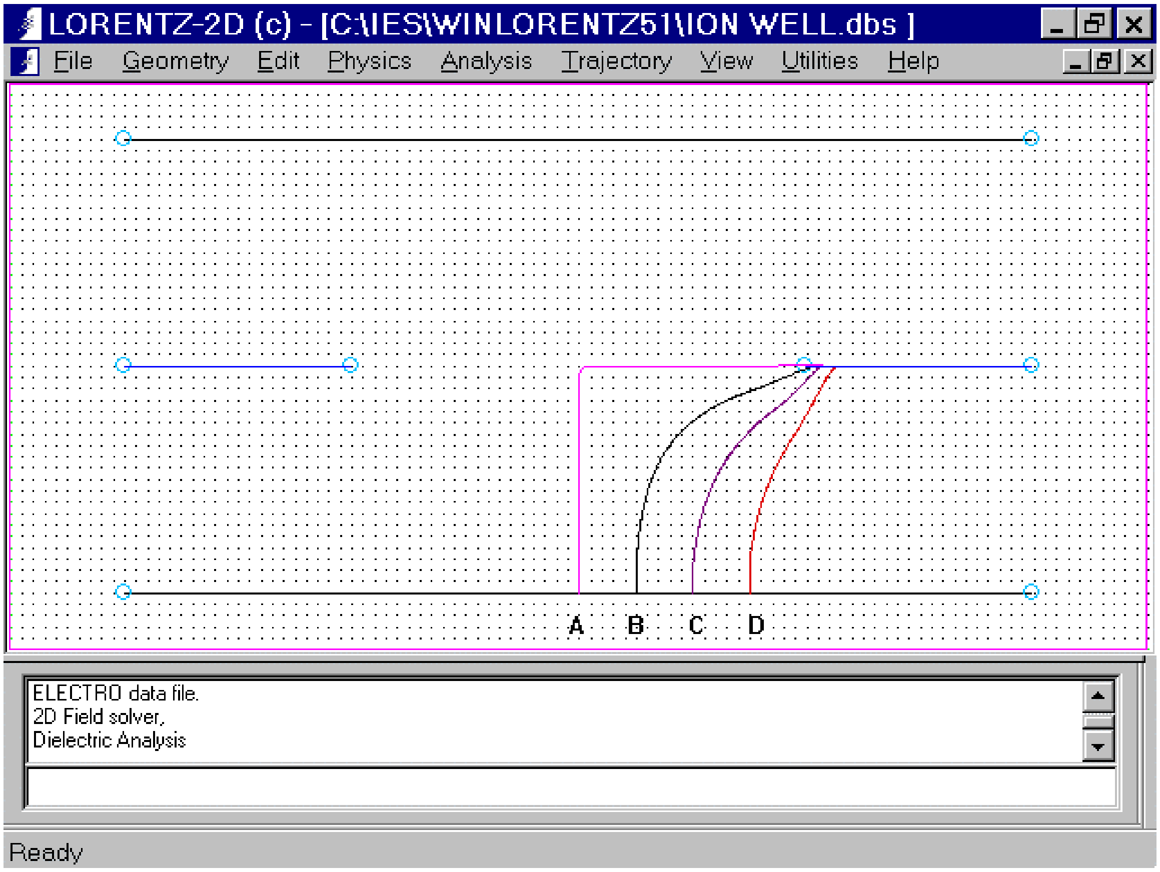
Top and Bottom electrodes are at –400v, both center electrodes are at 0.0v. The center electrodes are spaced 2 cm from the top and bottom electrodes are separated by 2 cm. Equipotentials are incremented by 10 volts.

Figure 12. Ion Well IMS structure and equipotentials.



Ions are launched every 0.5 cm from the right side of both top and bottom electrodes.

Figure 13. Ion Well trajectories.

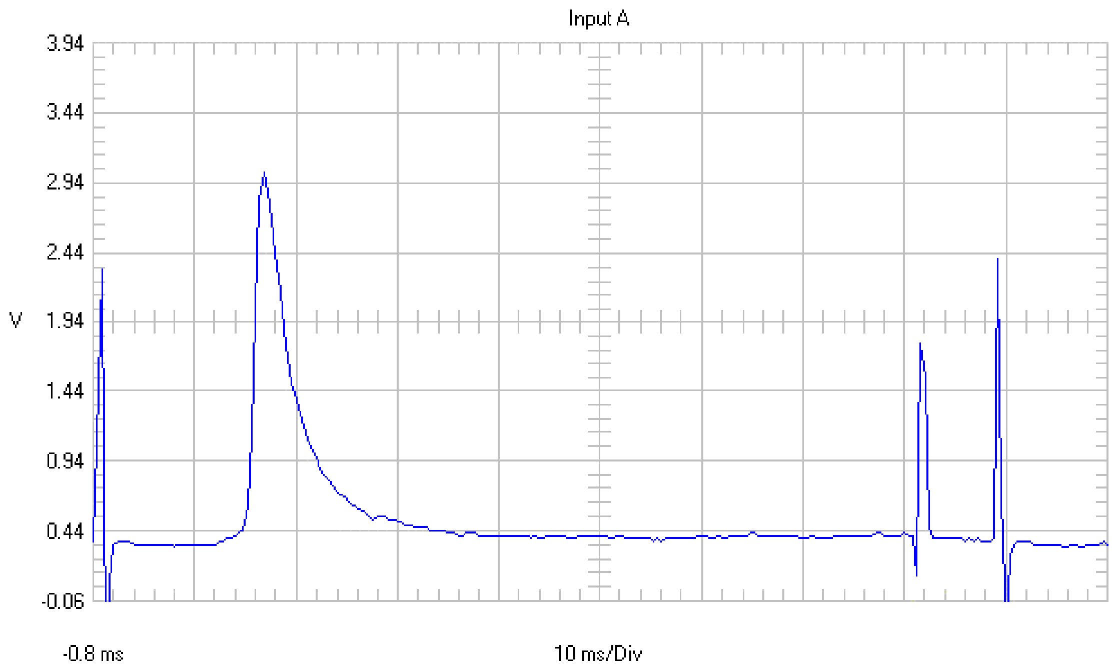


Ion trajectory travel time, from bottom plate to center electrode. Velocity is not constant.

Trajectory	X at Yo	TOF
A	0.0 cm	68.99 ms
B	0.5	14.76
C	1.0	9.58
D	1.5	7.05

Note that ions originating near the center of the ion beam (A) remain in the well for a considerable time, and that ions at the beam edge (D) are initiated much faster.

Figure 14. Ion Well trajectories, displaying ion storage times.



← Start of TOF End of TOF →

Note the sharp leading edge of signature caused by the accumulated ions at the trigger well, also note, the signature tail caused by late arriving ions just prior to the release of the ions into the drift region.

Figure 15. Typical NRI signature for the Model A Ion Well IMS device.