



**HAL**  
open science

# Effect of space charge on the mass resolution of a time of flight mass spectrometer (ToF-MS)

Erick Le Guyadec

► **To cite this version:**

Erick Le Guyadec. Effect of space charge on the mass resolution of a time of flight mass spectrometer (ToF-MS). COMSOL conference 2024, Oct 2024, Florence, Italy. , pp.Comsol2024, 2024, Comsol conf. proc. 2024. cea-04719817

**HAL Id: cea-04719817**

**<https://cea.hal.science/cea-04719817v1>**

Submitted on 3 Oct 2024

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# EFFECT OF SPACE CHARGE ON THE MASS RESOLUTION OF A TIME OF FLIGHT MASS SPECTROMETER (ToF-MS)

*Author : Erick Le Guyadec, ISEC/DPME/SEIP, CEA Marcoule 30207 Bagnols sur Cèze, France*

Introduction: Time-of-flight mass spectrometers (ToF-MS) are instruments of choice for analysing the mass distribution of elements or molecules constituting various samples [1]. They are particularly suitable for isotopic studies of samples in the nuclear industry as well as for research in materials science or pharmaceuticals.

Problem to solve: Typically, a ToF-MS performs ultra-rapid ionization (e.g. photoionization) of a portion of the sample to be analysed and the created ions are extracted and accelerated by instrument electric fields. After that, the ions are released into the free flight section of the instrument where their mass separation occurs. The time of flight is proportional to the ratio  $(Z/M)^{1/2}$  of the molecule where Z is its electric charge number after ionization and M is its mass. At the exit of this zone, the mass-separated ion packets are detected by a fast, high gain ion detector such as microchannel plates. All this, results in a very sensitive instrument, with high mass resolution and capable of covering a wide mass range (from 1 to more than 10,000 mass units). However, when the number of ions created in the ionized volume is too high, this disturbs the local electric field (extraction field) by space charge effect and the extraction of ions is strongly affected. The consequence is a temporal broadening of the ion packet leading to a loss of mass resolution of the instrument.

Presented work: In this study, Comsol Multiphysics software (Version 6.2) is used with the AC/DC Electro-Magnetic module (3D) and the charged Particle Tracing Module. This configuration allows the analysis of space charge effect, the calculation of electric field disturbance and the simulation of the ion trajectory in time and space.

The main equations solved are Maxwell ones in relation with the electric field E:

$$E = -\text{Grad}(V) - dA/dt \text{ and } \text{div}(E) = \rho/\epsilon_0$$

and Lorentz force acting on ions and electrons:  $F = Z \cdot (E + v \times B)$

Where, E is the electric field, B the magnetic field, rho is the space charge,  $\epsilon_0$  is the free space permittivity, V is the electric potential, Z the electric charge of ion and A is the vector potential defined by:  $B = \text{Rot}(A)$ . Afterwards the magnetic field is neglected.

The problem is solved transiently in 3D with the geometry of a standard linear ToF-MS: Extraction length 12 mm, acceleration length 12 mm, free flight length 950 mm (all lengths are along the Z direction chosen for ToF axis), and respective electric potentials of 1730, 1600 and 0 Volt. The chosen ion mass is 100 a.m.u. and the ion charge number is +1. The ionized volume, located in the center of the extraction region, is assumed to be a slice of thickness 2 mm (in Z direction) and lengths 10 mm (in X and Y directions).

The potential & electric field maps and ion packet trajectories are presented in figures 1-2-3 for unperturbed conditions (e.g. 1000 ions are generated in the ionization volume by a laser beam).

The calculation result remains constant until  $2.0E+5$  ions are generated in the volume. Above this limit (corresponding to  $1E+6$  ion/cm<sup>3</sup>), the space charge disturbance becomes active and

consequently the ion packet tends to expand in time and space. We show the calculated electric field in the extraction region when the number of ions is above this limit (Fig. 4). The effect of space charge is illustrated by comparison of the ion pulse time duration at the exit of the free flight region for different levels of space charge (Fig. 5).

The explanation is that the energy distribution of ions relative to their initial position and the time to be extracted from the ionized zone is perturbed. Normally the ion energy in the extraction zone is proportional to the distance to the extraction grid. With this level of space charge this is no longer the case. The consequence is a wider ion packet, which primarily results in lower mass resolution for the instrument. In the worst case calculated where the initial space charge is even higher ( $2.0 \times 10^7$  ions or  $1 \text{E}+8 \text{ ion/cm}^3$ ), the ion packet 'explodes' (Fig. 6), under electrostatic-like repulsion forces. As a result, many ions collide with the walls and have no chance of reaching the detector.

Concluding remarks: The limitation of ToF-MS mass resolution versus space charge has been studied and quantified using Comsol Multiphysics Software.

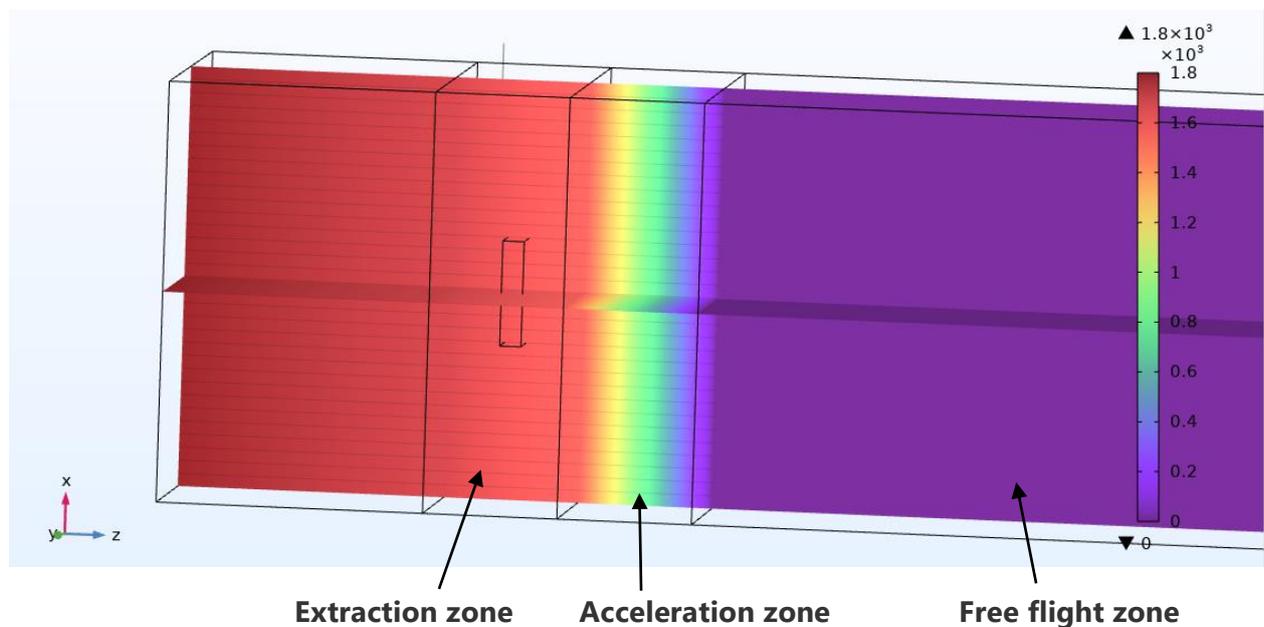
Some ways to mitigate this effect could be studied: Increase the extraction electric field and increase the ionization volume at a constant number of ions.

### Bibliography:

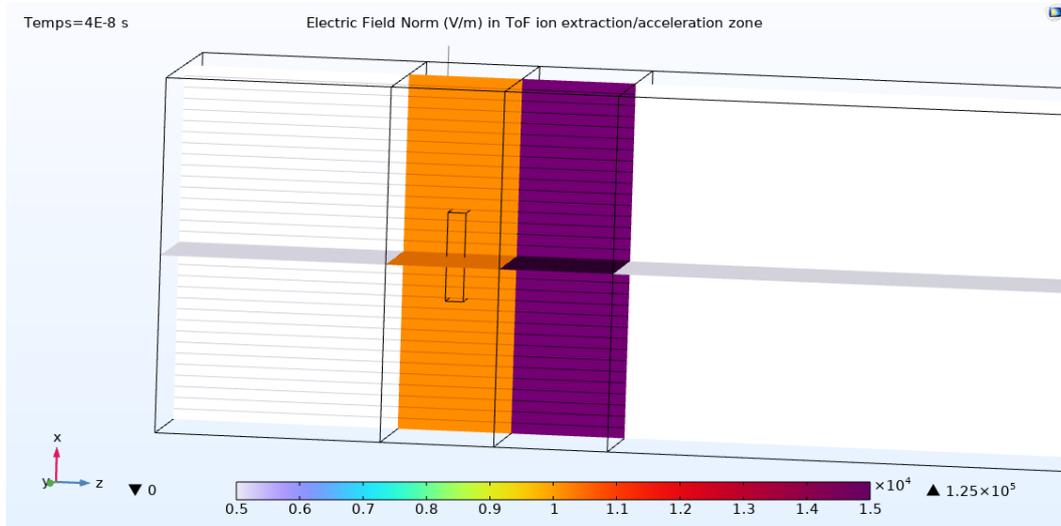
[1] W. C. Wiley,; I. H. MacLaren, *Time-of-Flight Spectrometer with Improved Resolution, Review of Scientific Instruments*, 26, 1150 (1955)

### List of Figures:

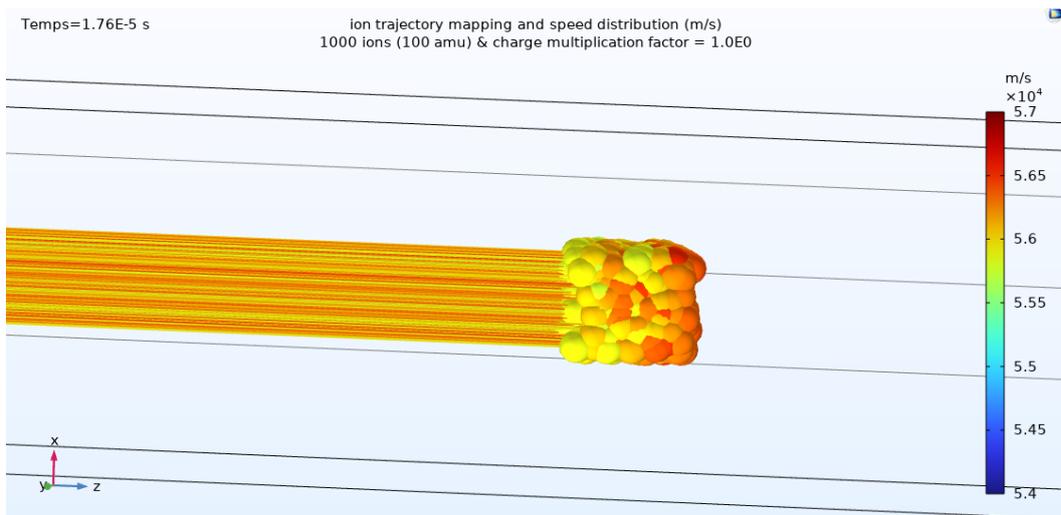
**Fig.1: Electric Potential (V) in extraction/acceleration zone with low space charge conditions (1000 ions)**



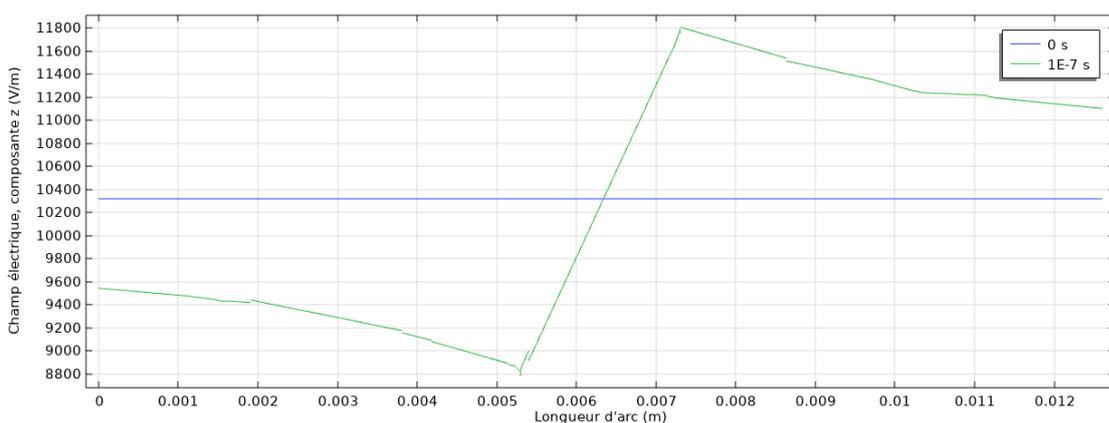
**Fig. 2 : Electric Field (V/m) in extraction/acceleration zone with low space charge conditions (1000 ions)**



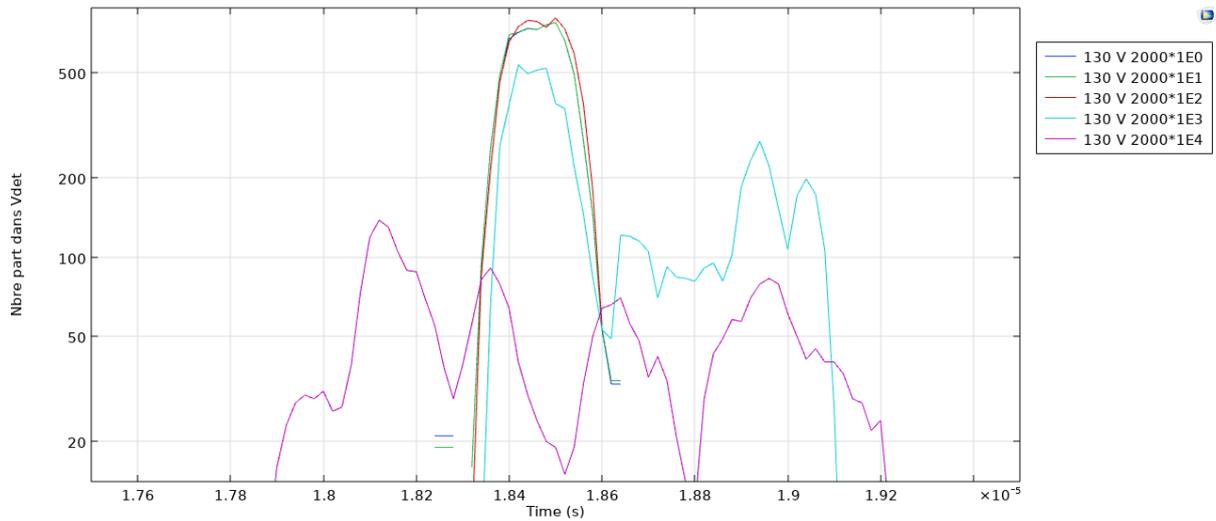
**Fig. 3 : Ion trajectory and speed (m/s) with low space charge conditions (1000 ions)**



**Fig. 4 : Electric Field component  $E_z$  (V/m) along Z axis in extraction zone with high space charge value (2000 E+4 ions) before (0 s) and after (1E-7 s) ionization**



**Fig 5 : Ion packet duration at detector for different levels of space charge (130 V extraction potential and  $2E+3$  to  $2E+7$  ions)**



**Fig 6 : Ion trajectory mapping and speed (global + zoom) with high space charge value ( $2E+7$  ions)**

