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Simulation of an off-line ion beam system at ISOLDE

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1 Introduction

On-line isotope separation (ISOL) is a technique in which the ion source of an electromagnetic mass-separator is coupled directly to an accelerator target with high energy protons (1.4 GeV at ISOLDE) so that a continuous beam of unstable nuclei emerges. These isotopes, produced by the driver beam and stopped in the target, are transported into the ion source as atoms by diffusion and effusion processes, where they get ionized and extracted by an applied potential. In order to facilitate testing and development of different ion source types at ISOLDE, a dedicated offline ion source is in development. This includes a standard ISOLDE target geometry directly coupled to a vacuum chamber. However, the initial version of the offline ion source shall be upgraded to accommodate mass separation in form of a quadrupole mass filter. In this work, the first version of the new beamline was defined and ion beam trajectories up to the quadrupole exit were simulated using the SIMION program to get first insights into parameters such as AC and DC voltages, frequency as well as kinetic energy, mass and the charge of the ions as well as finalize the design of the beamline.

2 Quadrupole Mass Analysers

In quadrupole mass analysing devices, electric fields are used to separate ions according to their mass-to-charge ratio (m/z) as they pass along the central axis of four parallel equidistant rods that have fixed (DC) and alternating (RF) voltages applied to them as shown in figure 1. Depending upon the magnitude and frequency of these voltages it can be arranged that only ions of certain masses are allowed to pass the whole length of the quadrupole, and into a detector.

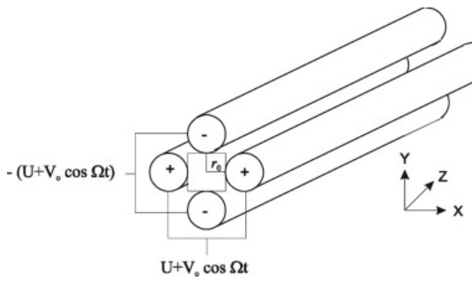

Figure 1: The quadrupole mass filter: the DC and RF voltages (U and V_0 respectively) applied to the rods, r_0 is the minimum distance between the rods.

In figure 1 an quadrupole mass filter is shown where the electric field is produced by cylindrical rods by applying DC and RF voltages, given by $V = -[U - V_0 cos(wt)]$ for the vertical and $V = +[U - V_0 cos(wt)]$ for the horizontal rods. Here, U is the DC potential and V_0 is the amplitude of the RF potential, applied at a fixed frequency in the MHz range. Each rod pair is successively positive and negative, allowing ions to be both attracted and repelled away from the rods or the central axis of the mass analyser leading to a oscillating motion through the quadrupole.

2.1 Equations of Ion Motion

The application of the voltages on the quadrupole rods creates a hyperbolic field given by [1]

$$\phi = \frac{(x^2 - y^2)(U + V \cos \omega t)}{2r_0^2} \tag{1}$$

Where x and y are the distances along the coordinate axes and r_0 is the distance from the z-axis to the quadrupole surfaces.
When $x = y$ and $\phi = 0$, this gives rise to planes of zero field strength within the quadrupole. At all other positions between the poles, the oscillating electric field (ϕ) causes ions to be alternately attracted to and repelled by the pairs of rods. Note that the equation above shows that the field (ϕ) has no effect along the direction of the central (z) axis within the quadrupole. To facilitate the passage of ions through the mass analyser, an accelerating voltage is applied to the mass analyser which is usually in the region of 5 eV to 10 eV for the quadupole used in this work. Hence, the ion will be able to pass through the quadrupole without touching the rods if x and y, which determine the position of an ion from the centre of the rods, remain less than r_0 at all times. When the ion is caused to oscillate with a trajectory whose amplitude exceeds r_0, it will collide with a rod and discharge or exit the mass analyzer and not be detected. So for any particular m/z value the passage of the ion through the quadrupole is dependent upon U, V, ω (radio frequency) and r_0 [4].

2.2 Mathieu Stability Diagrams

When solving the equations of motion for an ion within the quadrupole, the two parameters a and q emerge as crucial parameters in defining regions of stable ion trajectory:

$$a = \frac{8zU}{mr^2w^2}, \quad q = \frac{4zV}{mr^2w^2} \tag{2}$$

In a quadrupole with the radiofrequency ω fixed and ions of a single mass m, only two parameters can be varied, the DC voltage U (to affect the 'a' term) and the RF amplitude V (to affect the 'q' term). By varying these two Voltages in such a way that the spatial X-Y coordinates of the ion never exceeds r_0 the ion is manipulated onto a non-collisional trajectory.
These theoretical values, assuming a perfectly hyperbolical electrode, have to be validated by experiments and simulation to obtain the correct values for the less than perfect real electrodes. The results of varying the voltages can expressed in a plot of a versus q as shown in figure 2. The region within the stability diagram in which all trajectories are stable is roughly shaped like a triangle and may be called the stability triangle. All ions with U and V_0 values lying within the triangle are transmitted; those lying outside the triangle are deflected to one of the rods.
At lower values of V_0, moving inside the stability triangle from outside the Y trajectory changes from being unstable to stable. Likewise, for higher values of V_0, it is the X trajectory which changes from stable to unstable [2].

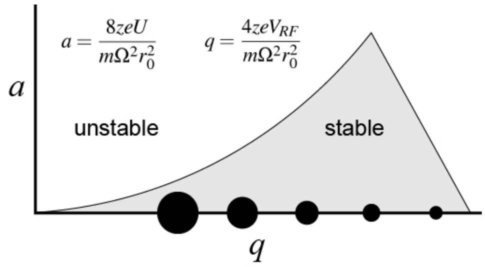

Figure 2: stability diagram

2.3 The Quadrupole Mass Filter

For a quadrupole to function as a mass filter with unit mass resolution, it must be able to separate ions with mass m from its neighbouring masses. That is, we have to be able to tune the quadrupole so that mass m lies within the stability triangle but neighbouring masses are not. The appropriate values for the DC and RF amplitudes (U and V_0) can be derived from the parameters a and q for a given mass. For lower masses we substitute the value of mass m by $m \pm 1$ to ensure that these are located outside of the stability triangle. The straight scan line line of stable trajectories for all masses is given by the constant ratio of U/V.

3 Simulation of the beamline

3.1 SIMION 8.1

SIMION is a software program for charged particle tracking and ion optical simulations. Mainly, it calculates 2D/3D electrostatic and certain magnetic fields and determines the trajectories of charged particles passing through those fields, thereby determining the ion beam characteristics. SIMIONs methods are direct via finite difference methods Runge-Kutta for solving the required partial differential equations (PDEs), particularly the Laplace Equation for solving potential array for non electrode, and ordinary differential equations (ODEs) [2]. The user defines electrodes or magnets within a 2 or 3D space and the program calculates the respective fields of non-electrode or non-magnet points. Each potential array, or "instance", is placed in an "ion optics bench" along with other arrays that may represent other parts of an instrument. This approach allows each section of a system to be modeled independently. Charged particles can be flown through the ion optics bench and their trajectories calculated. The user programming aspects of the system allow users to define time dependent fields and manipulate the properties of the charged particles. [3]

3.2 Simulation of a quadrupole mass filter

In order to examine the characteristics of a quadrupole in SIMION, an example quadrupole with four rods with half minimum distance of r =0.4 cm was investigated. In addition to the quadrupole, this simulation included entrance and exit structures. Using

SIMION's user programming features, ions with initial positions and energies were introduced, as discussed in the following. An image of this initial example with particles of mass m =100 amu passing through is shown in figure 3. The applied potentials are 27 V for the DC part and 166 V for the RF part.

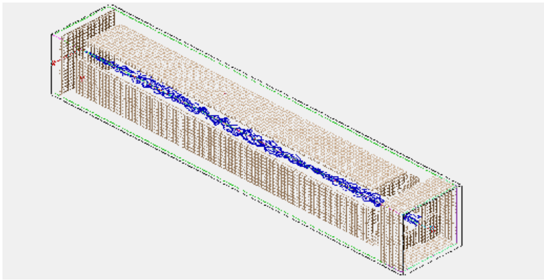

Figure 3: Quadrupole with entrance aperture, 4 hyperbolic rods and particle detector after exit. Ions with an energy of 10 eV and 100 amu are shown to pass through.

3.3 Simulation of the QMF to be implemented into the beamline

After these initial tests to get familiar with the SIMION software and its lua language, the geometry of the actual quadrupole to be used was imported into SIMION, shown in a cut view in figure 4. In addition to the four quadrupole rods, there are 4 smaller rods to accommodate the changes in the field made by the cylindrical shape instead of the hyperbolic one assumed by theory.

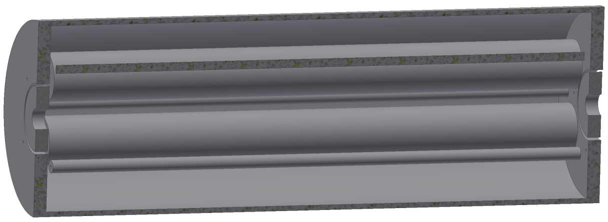

Figure 4: 3D view of Extrel 150 quadrupole.

The frequency is fixed to 1.2 MHz and the mass of the ions to 100 amu with positive charge and a kinetic energy from 5 ev to 10 ev to account for the geometry of the quadrupole and its resolution. The cylindrical quadrupole has a half minimum distance between the opposite rods of r = 0.8331 cm Then the DC and RF voltages calculated from a and q parameters are applied in order to to make the beam pass through the quadrupole with a stable trajectory. The resulting voltages for a particle with mass m = 100 are 117.7 V for the DC part and 583 V for the RF part. After initial tests, it became clear that the resolution of the mesh as well as the quality of the coonversion from .stl to potential array files had to be increased in order to properly represent the quadrupole. Furthermore, there was the need of boundaries around the quadrupole rods to shield the particles from the electric field before entering the quadrupole rods. After the addition of the cylindrical boundary and by adjusting the most accurate conversion from stl to potential array, the QMF was successfully run as shown in figure 5.

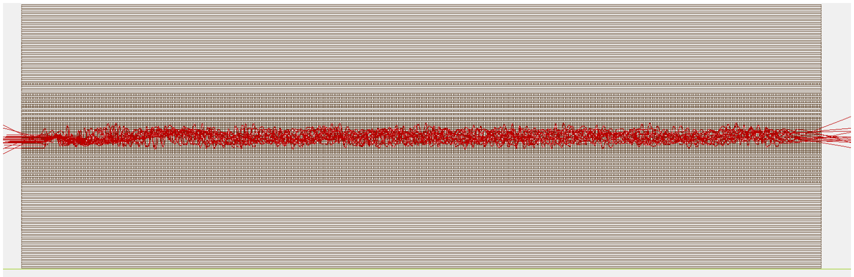

Figure 5: simulation of quadrupole with a box

3.4 Ion injection and extraction

Finally, the quadrupole was implemented in a first version of the complete beamline starting with the extraction electrode and the injection into as well as the transmission through the QMF. The injection and extraction part is composed of an extraction electrode, which extracts the ions from an ion source into the beamline. This is followed by an Einzel lens.
The Einzel lens consists of three cylindrical electrodes and it is used in ion optics to focus the an ion beam without changing in the energy of the ions. The voltage of the first and third electrodes is equal to zero but the voltage of the second electrode is equal to 320 v in order to create a focus for the beam, resulting from the potential difference between the three electrodes.

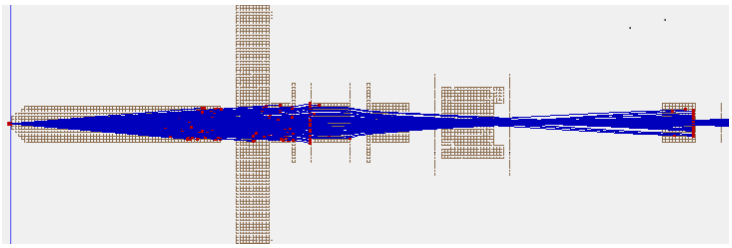

Figure 6: Extraction and injection of ions into the quadrupole.

Subsequent to the Einzel lens there is a bending box enabling to steer the ions vertically and horizontally with adjustable voltages for every side, which here are equal to 15 V. After a free region where a Faraday cup will be implemented, the ions are decelerated as they enter a field of -400 v to pass through the quadrupole with kinetic energy equal to 10 eV. This deceleration is necessary due to the resolution of the QMF being antiproportional to the kinetic energy of the ions.
Finally the whole beamline, combining the injection part and the quadrupole with an extraction energy of 500.5 eV was simulated, shown in figure 7.

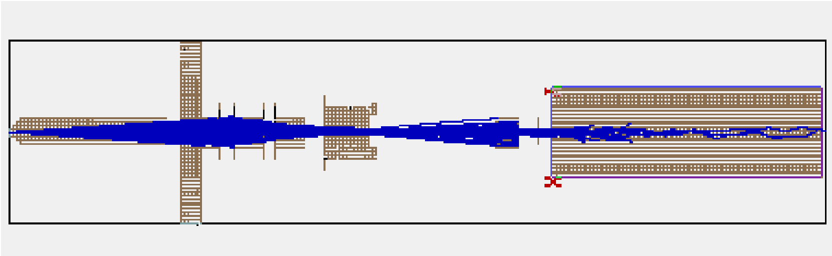

Figure 7: Simulation of the entire beamline including mass separation through the quadrupole.

4 Outlook

The goal of this report was to simulate the ion optics and ion transmission into the quadrupole as well as validate its parameters for mass separation so the design and upgrade of the beamline can be concluded.
One of the most critical parts is the efficient injection of ions into the quadrupole. Based on the work in this report, the geometry and ion optics of the beamline can be further optimized, concluding in the manufacturing and building of the setup.

5 Acknowledgements

Thank you David Leimbach for your effort and supporting me.

References

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