ION BEAM OPTIC SIMULATIONS AT THE 1 MV TANDETRON^{TM} FROM IFIN-HH BUCHAREST

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Abstract. The RO-AMS facility was commissioned in 2012 and it has been dedicated to the analysis of several radionuclides, such as: ^{10}Be, ^{14}C, ^{26}Al and ^{129}I. A significant improvement in the operation and setup change of this machine is done by developing an analytical tool for beam diagnostics by using the SIMION® simulation code. Precise ion beam traceability conveys to higher detection sensitivity that is critical in the accelerator mass spectrometry applications. Furthermore, these simulations allow the analysis of various modifications in the ion beam optics of the accelerator by adding, removing or replacing components or changing their relative positions.

Keywords: AMS, Ion-optics, HVE Tandetron^{TM}, SIMION®8.1, CATIA V5

1. INTRODUCTION

The 1 MV HVE Tandetron^{TM} AMS system was commissioned in May 2012, at the National Institute for R&D in Physics and Nuclear Engineering "Horia Hulubei" (IFIN-HH), Bucharest, Romania [1]. This system is the 6th of its kind delivered worldwide by the High Voltage Engineering Europe [2]. Several papers have already described its main constructive features [3, 4, 5, 6] therefore, we will give here only a brief description of the optical elements. The machine acceptance test results were presented in Ref. [7], demonstrating the efficiency of the system in terms of accuracy, precision and background level for measurement of ^{14}C, ^{10}Be, ^{26}Al and ^{129}I radioisotopes ratio [8, 9, 10, 11].

The main goal of the present work is to develop and test a system procedure based on ion-optics simulations, to further extend the range of radioisotopes ratios

measurements. This helps also to decrease the AMS system tuning time by reducing the time required to change the machine setup from an isotope to another.

A short description of the entire system is given in Section 2. For each ion-optical element a 3D view, given by the design code CATIA V5, is presented in Section 3. Detailed presentations of the elements considered in the numerical simulations are included. Comparisons between the obtained parameters values from the simulations and those from the measurements are discussed in Section 4. Finally, conclusions and perspectives are given in Section 5.

Table 1.
Definitions of the acronyms used in the present paper

Acronym	Meaning
EL1	Einzel Lens 1
LE ESA	Low Energy Electrostatic Analyzer
EL2	Einzel Lens 2
LEM	Low Energy Analyzing Electromagnet
LET	Low Energy Tube
HTV	High Terminal voltage
Q-snout	Acc Lens (electrostatic lens)
CEC	Charge Exchange Canal
TEQ	Triple Electrostatic Quadrupole
FC 1	Fixed Faraday Cup
FC 2	Movable Faraday Cup
HET	High Energy Tube
HEM	High Energy Analyzing Magnet
HE ESA	High Energy Electrostatic Analyzer
GIC	Gas Ionization Chamber

2. SYSTEM DESCRIPTION

This electrostatic tandem machine has a compact design as it can be seen in Fig.1. It is equipped with two independently operating Cs-sputter Negative-Ion sources (SO-110 HVE model) [2] capable of high-precision ^{14}C measurements at a ^{12}C injection current, around $100\mu A$ [12]. A rotatable $54°$ low energy electrostatic analyzer (LE ESA) can select for operation one of the two existing ion sources. The first ion beam mass analysis is done on the low energy side by a $90°$ analyzing electromagnet (LEM). Negative ions extraction and $90°$ LEM analysis are followed by a 1MV electrostatic accelerator equipped with a charge exchange (electron stripper) channel with Argon gas at low pressure (10^{-2}mbar range). EL1, EL2, Q-snout and TEQ are electrostatic lens used for beam focusing. Following the charge exchange from negative to positive, the beam passes through the second mass spectrometer, a $90°$ dipole magnet (HEM). A system of Faraday cups (FC1, FC2) placed at the exit of the HEM is used to measure the pilot beam current [13]. One of the cups is movable and can be manually adjusted ensuring the versatility

required to measure different isotope species [4]. For improving the measurements accuracy, the rare isotopes are passing through a 120° high-energy electrostatic analyzer (HE ESA), with a bias voltage up to 120kV. Only the ions with the same energy over charge ratio (E/q) will enter in the detection system. The radioisotopes are counted and identified in a two-anode gas ionization chamber (GIC) equipped with a 75nm silicon nitride (Si_3N_4) entrance window [4,5]. Further on, only the elements of the machine hardware relevant for the present simulations are described in some details.
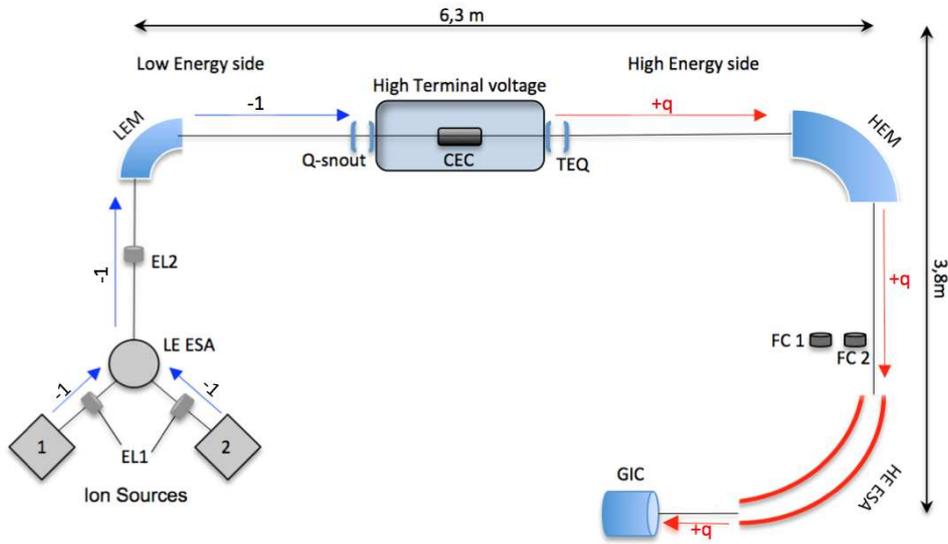

Fig. 1: General layout of the 1 MV HVEE AMS facility at IFIN-HH, Bucharest, Romania. The symbols "-1/+q" are used to indicate the negative/positive sign of the ion beam charge state. The meanings of the acronyms are given in Table 1.

3. ION OPTICS SIMULATIONS OF THE AMS SYSTEM

In the present simulations only the electric and magnetic elements are considered, as they affect the trajectory and energy of the ions in a confined region of space. Each component has been designed in CATIA V5 [14] according to its specifications provided by HVE [2]. The simulation of the ion beam trajectory has been estimated with SIMION® 8.1 computer code [15], and optical elements description files imported directly from CATIA V5. SIMION® 8.1 is a software used primarily to simulate electric fields where the Laplace and Biot Savart equations play a key role. Given a configuration of electrodes, the software calculates trajectories of charged particles in those fields, when particle initial properties are known, including magnetic field and collisional effects. Particle mass, charge, and other parameters can be defined individually or according to

some pattern or distribution. The path of the ions passes through the elements shown in Fig.1, starting from the surface of the sample inside the Cs-sputter ion source and ending in front of the GIC. In the simulations, the voltages and currents of the optical elements are adjusted until the required beam parameters (beam direction, beam energy and beam waist) are obtained, for a given ion specie.

3.1 CS-SPUTTERING ION SOURCE AND THE EXTRACTION SYSTEM

Negative-ion sources based on the sputtering principle have been widely used as injection into tandem electrostatic accelerators employed in basic and applied research [16]. As can be seen in Fig. 2, from the SIMION®8.1 simulations, the main components of a sputtering ion source are: cathode, ionizer, extraction electrode and Einzel lens electrodes [12].
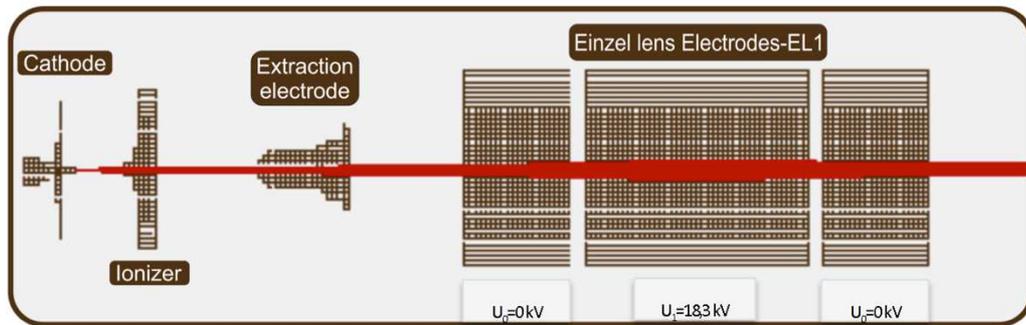

Fig. 2: 2D simulation of the ion source and the first electrostatic lens (EL1) (SIMION® 8.1). The EL1 voltages are obtained from the simulations as given in Table 3.

A systematic study done during the commissioning of the machine and the accumulated operational experiences during the last 4 years (2012-2016), led to the optimal values of the control parameters for the ion source given in Table 2.

The first two voltages from Table 2 were employed in our SIMION®8.1 simulations. The injection energy ($E_{injection}$) of the beam is given by the target (V_{target}) and extraction ($V_{extraction}$) voltages:

$$E_{injection} = (V_{target} + V_{extraction}) \times e \qquad (1)$$

where "e" is the elementary charge.

Table 2.
Ion source parameters for optimal functionality obtained from the commissioning tests and
operational experience. The precision of the values is in the order of 15%.

Target voltage	7 kV
Extraction voltage	28 kV
Ionizer current	18 A
Cs temperature	100°C

The negative ion beam extracted from one of the ion sources is injected in the low energy side of the accelerating system. In order to select the ion beam of interest, on the low energy side the system is equipped with two electric and magnetic filters. The first one is the 54° cylindrical LE ESA (Fig. 3), with a 53,25mm gap between the two electrodes and a 469mm bending radius. Its main role is to switch from one ion source to the other.
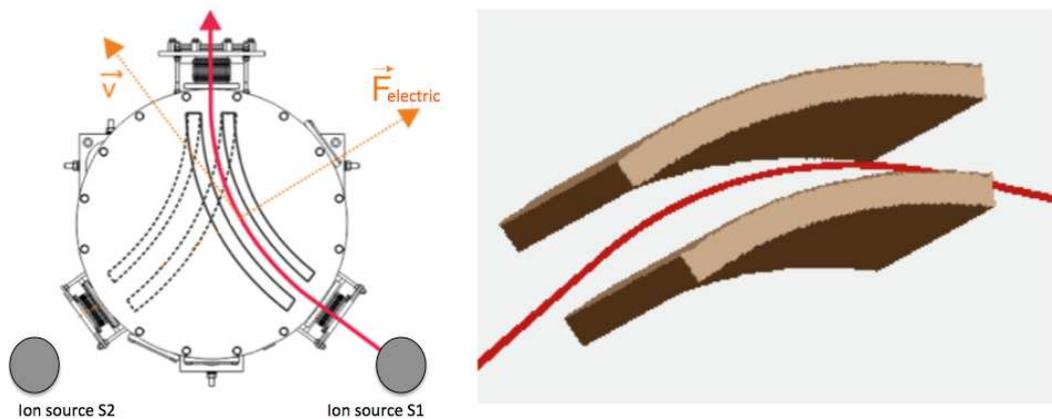

Fig. 3: Technical drawing (left panel) and SIMION® 8.1 representation (right panel) of LE ESA.

The second filter is the LEM (Fig.4). A 90° dipole magnet with a 400mm bending radius and a 40mm gap between the poles. This magnet produces a magnetic field in the range of 0-0.8T making the selection of the ions as a function of their momentum over charge ratio.
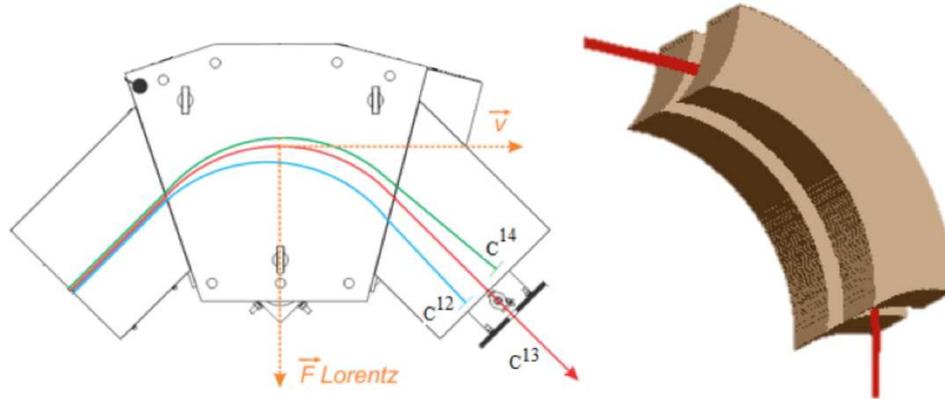
Fig. 4: Technical drawing (left panel) and SIMION® 8.1 representation (right panel) to the low energy sector magnet (LEM); C^{13} is the pilot beam and C^{14} is the "rare isotope" beam.

3.2 ACCELERATION SECTION

The accelerator system is an electrostatic tandem, with the high voltage terminal (HVT) in the range of 100kV to 1MV. The positive high voltage maintained on the HVT is achieved by a Tandetron™ voltage multiplier circuit, consisting of a state of the art parallel fed capacitive coupled Cockcroft-Walton type [2].
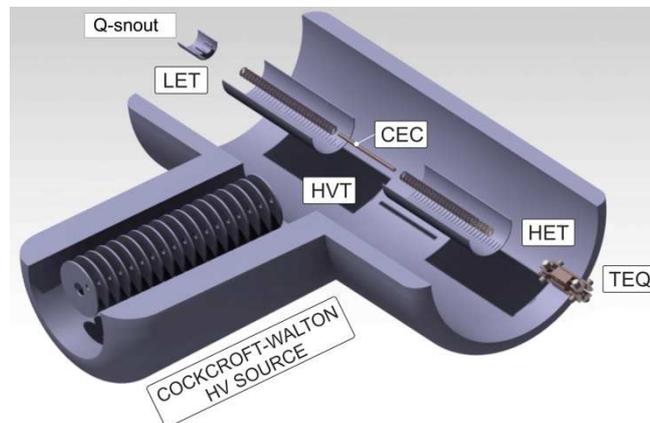

Fig. 5. 3D layout of the ion optical elements of the accelerator system (CATIA V5); the voltage values for Q-snout and TEQ are given in Table 3 and 4.

A pre-accelerating and focusing electrode (Q-snout) is mounted at the tank entrance. This electrode works in parallel to the first stage of the acceleration section in order to collimate and focus the incoming negative particles towards the HVT, in the middle of CEC. A focusing triplet electrostatic quadrupole (TEQ) is installed at the end of the high energy side, which focuses the positive ion beam on both X and Y axis (Fig. 5) [3,17]. In the present simulations, the acceleration tubes are not considered (LET and HET).

3.3   HIGH ENERGY ELECTRIC AND MAGNETIC ANALYZERS

The positive charged ions catching out of the stripper region are further accelerated on the HE side of the system. HEM and HE ESA, two electromagnetic filters, are installed after the accelerating structure. HEM is a 90° double-focusing magnet spectrometer, shown schematically in (Fig. 6). This magnet has a 850mm bending radius and a 40mm gap between the poles and can produce a magnetic field in the range 0-1.5T.
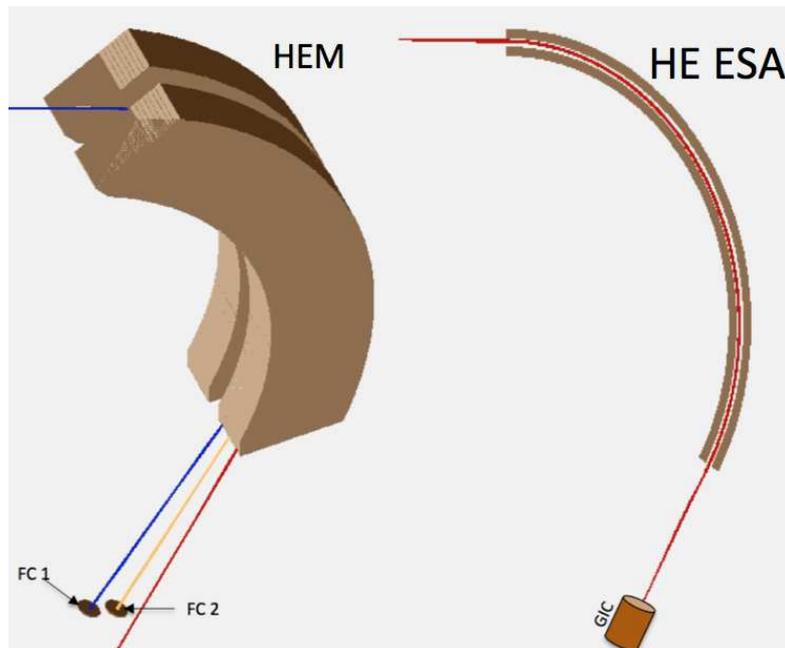

Fig. 6: Ion Optics simulation of HEM (right panel) and HE ESA (left panel) (SIMION®8.1). FC1 and FC2 are Faraday cups used to measure the ion beam currents.

HE ESA is the second electrostatic analyzer filter on the high-energy side with a bias voltage of 120kV, a 2600mm radius, 120° bending angle, and a 32mm gap between the electrodes (Fig.6). The role of the electrostatic analyzer is to separate charged particles according to their energy over charge stage ratio. Finally, the rare isotopes ion detector system is a large gas-filled ionization chamber with two anodes for ΔE and E_{res} measurements and a high detection efficiency close to 100%. As an example details of the detector are given in Ref. [2,7]. This detector is not included in the present ion optical simulations.

4. COMPARISON BETWEEN SIMULATIONS AND EXPERIMENTAL DATA

The operational experience of the 1MV tandem accelerator system shows us that after each shutdown or after any change in the operating conditions, the machine parameters must be optimized again. Effects such as magnetic hysteresis and/or thermal cycling of various subcomponents induce extra uncertainty that propagates to the system operation parameters.

Table 3.
Comparison of the simulated and the experimental values of the parameters on the low energy side.

Name	Isotope	Experimental value	Simulated value	Unit
El 1	$^9Be^{16}O$	16.1 ($\pm$3.0)	17.8	kV
	^{13}C	16.3 ($\pm$2.0)	17.1	
	^{27}Al	16.4 ($\pm$3.0)	17.5	
	^{127}I	15.7 ($\pm$4.0)	16.9	
LE ESA	$^9Be^{16}O$	3.96 ($\pm$0.06)	3.93	kV
	^{13}C	3.91 ($\pm$0.03)	3.89	
	^{27}Al	3.96 ($\pm$0.05)	3.94	
	^{127}I	3.98 ($\pm$0.07)	3.96	
EL 2	$^9Be^{16}O$	17.2 ($\pm$2.0)	16.2	kV
	^{13}C	17.9 ($\pm$1.0)	16.8	
	^{27}Al	17.5 ($\pm$2.0)	16.4	
	^{127}I	15.5 ($\pm$3.0)	15.1	

	Isotope	Experimental value	Simulated value	Unit
LEM	$^9Be^{16}O$	0.19 (±0.05)	0.20	T
	^{13}C	0.13 (±0.07)	0.14	
	^{27}Al	0.23 (±0.08)	0.24	
	^{127}I	0.44 (±0.09)	0.45	
Q-snout	$^9Be^{16}O$	32.4 (±3.0)	33.5	kV
	^{13}C	35.2 (±4.0)	36.8	
	^{27}Al	31.7 (±4.0)	32.5	
	^{127}I	25.7 (±3.0)	27.5	

Table 4.
Comparison of the simulated and the experimental values of the parameters on the high energy side.

Name	Isotope	Experimental value	Simulated value	Unit
TQP	^9Be	16.5 (±3.0)	18.3	kV
	^{13}C	15.9 (±3.0)	17.9	
	^{27}Al	15.1 (±4.0)	17.1	
	^{127}I	13.4 (±5.0)	16.2	
HEM	^9Be	0.62 (±0.05)	0.65	T
	^{13}C	0.56 (±0.04)	0.59	
	^{27}Al	1.05 (±0.07)	1.09	
	^{127}I	1.29 (±0.08)	1.35	
HE ESA	^9Be	49.5 (±0.5)	49.8	kV
	^{13}C	59.5 (±0.4)	59.8	
	^{27}Al	56.6 (±0.6)	56.8	
	^{127}I	51.4 (±0.8)	51.7	

Table 5.
Charge state and terminal voltage values used in the simulation for each isotope.

Isotope	Charge state	Terminal voltage [kV]
^9Be	+1	1000
^{13}C	+2	1000
^{27}Al	+1	700
^{127}I	+3	1000

The summarized data given in Tables 3 and 4 shows a comparison between the experimental values measured during the last five years of accelerator operation and the values coming out from the simulations. Overall a resonable agrement can be observed between the experimental and simulated values.

For practical reasons, the slits and apertures were not taken into account in the present simulation. These were only used as a corrective measure during the actual operation of the machine.

The uncertainties of the experimental values are obtained by calculating weighted average of the parameters determined in time, during the accelerator operation. The simulation input parameters are defined once, at the start of the simulation, after that all the values of the optical elements are kept the same from one simulation to another. This leads to a constant emittance of the ion beam. Two major modifications appear in the ion source during the experimental measurements: i) the surface of the sample differs from a cathode to another, due to the way of producing the sample. ii) the second issue represented by the Cs temperature variation over time $(\pm 5\ C)$, which influences the sputtering process.

All of these leads to changes of the beam emittance, and this is why some corrections have to be made to the ion beam trajectory by modifying the electrostatic and magnetic elements parameters every time a measurement is started.

5.   CONCLUSIONS AND PERSPECTIVES

In the present work, a system procedure to find the main machine parameters for the 1MV electrostatic accelerator has been developed. We present the simulation of C, Be, Al and I radioisotopes with different A/q ratio.

The procedure is based on high accuracy ion-optics simulations performed with SIMION® 8.1. This application allows us rapidly to understand the effect of each ion optics component along the beam path. It can be seen in Tables 3 and 4 that all the values from the simulation are in good agreement with the parameters used in practice. The main reason for the precise correlation of the two sets of parameters resides in the good similarity between the real component geometry. The drawings and the simulations were made in CATIA V5, and in SIMION® 8.1 respectively, in order to calculate the electromagnetic fields that determine the ions trajectory.

Another advantage is given by the fact that the optical parameters can be approximated for different ion species. This is very useful in the context of expanding the capabilities of the AMS machine in the future. While it is impossible to determine absolute values for the physical parameters from a simulation, it provides a good starting point and will greatly reduce the time needed to implement a new kind of measurement. Acceleration tubes and the charge exchange channel, together with the gas ionization chamber will also represent the subject of a future study.

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