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Numerical modeling of the Linac4 negative ion source extraction region by 3D PIC-MCC code ONIX

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At CERN, a high performance negative ion (NI) source is required for the 160 MeV H- linear accelerator Linac4. The source is planned to produce 80 mA of H- with an emittance of 0.25 mm mradN-RMS which is technically and scientifically very challenging. The optimization of the NI source requires a deep understanding of the underling physics concerning the production and extraction of the negative ions. The extraction mechanism from the negative ion source is complex involving a magnetic filter in order to cool down electrons' temperature. The ONIX (Orsay Negative Ion eXtraction) code is used to address this problem. The ONIX is a selfconsistent 3D electrostatic code using Particles-in-Cell Monte Carlo Collisions (PIC-MCC) approach. It was written to handle the complex boundary conditions between plasma, source walls, and beam formation at the extraction hole. Both, the positive extraction potential (25kV) and the magnetic field map are taken from the experimental set-up, in construction at CERN.
This contribution focuses on the modeling of two different extractors (IS01, IS02) of the Linac4 ion sources. The most efficient extraction system is analyzed via numerical parametric studies.
The influence of aperture's geometry and the strength of the magnetic filter field on the extracted electron and NI current will be discussed. The NI production of sources based on volume extraction and cesiated surface are also compared.

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Abstract. At CERN, a high performance negative ion (NI) source is required for the 160 MeV H^- linear accelerator Linac4. The source is planned to produce 80 mA of H^- with an emittance of 0.25 mm $mrad_{N\text{-}RMS}$ which is technically and scientifically very challenging. The optimization of the NI source requires a deep understanding of the underling physics concerning the production and extraction of the negative ions. The extraction mechanism from the negative ion source is complex involving a magnetic filter in order to cool down electrons' temperature. The ONIX (Orsay Negative Ion eXtraction) code is used to address this problem. The ONIX is a self-consistent 3D electrostatic code using Particles-in-Cell Monte Carlo Collisions (PIC-MCC) approach. It was written to handle the complex boundary conditions between plasma, source walls, and beam formation at the extraction hole. Both, the positive extraction potential (25kV) and the magnetic field map are taken from the experimental set-up, in construction at CERN. This contribution focuses on the modeling of two different extractors (IS01, IS02) of the Linac4 ion sources. The most efficient extraction system is analyzed via numerical parametric studies. The influence of aperture's geometry and the strength of the magnetic filter field on the extracted electron and NI current will be discussed. The NI production of sources based on volume extraction and cesiated surface are also compared.

Keywords: Negative ion source, PIC MCC modeling, Linac4
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INTRODUCTION

At CERN, H^- ion sources based on volume and cesiated surface production mechanisms are developed in the framework of the 160 MeV linear accelerator Linac4 project [1]. The source has to supply 80 mA beam intensity within an emittance of 0.25 mm $mrad_{N\text{-}RMS}$ that is technically very challenging and requires a deep understanding of the extraction mechanism from the negatively charged plasma sheath.

In the source hydrogen plasma is generated by the up to 100 kW ~2 MHz external radio-frequency (rf) system [2] via a solenoidal rf antenna inductive coupling. A permanent magnet octupole in Halbach configuration is installed around the plasma chamber and generates a magnetic field cusp structure [3]. Plasma diffuses in the expansion chamber made of Aluminum Oxide or Nitride (Al_2O_3, A1N) ceramic with inner diameter of 48 mm and outer diameter of 64 mm [1]. In the extractor, negative ions are dragged out by a 25 kV bias potential applied to the puller electrode against the plasma chamber.

In the plasma volume, negative hydrogen ions are mainly produced by collisions of low energy electrons (~1eV) with exited $H_2(v)$ molecules in high vibrational states (v>5). However, due to the numerous NI destruction processes (induced by high energy electrons), only a small amount of the negative ions are effectively extracted from the plasma. To enhance NI yields, Cs atoms, that act as electron donors, are used in most H^- sources [4]. Negative hydrogen ions are created at the Cs covered surface via thermo energetic neutral gas or positive ions impact [5].

Another important issue of the source is to minimize the co-extraction of undesirable electron beam. These electrons cause short but very intense heat loads on the electron dumping system and increase the beam emittance.

At present, two extraction systems are proposed: for the volume source, a cylindrical aperture shape (already in commissioning); and for the surface source a double chamfered conical structure is planned to start operation in the middle of 2013. The sketch of both extractors is depicted in Fig. 1 (left). Both extractors consist of one aperture of 6.5 mm diameter and are positioned at the same distance with respect to the puller. The aperture wall could be biased against the plasma in order to affect the co-extracted electron current.

ONIX code has been used to model the negative ion extractions and the plasma behavior in the vicinity to the extraction aperture in its modified version based on the original self-consistent 3D PIC-MCC [6]. The present work is focused on the general description of both extraction systems. The self-consistent positive ions meniscus formation is shown together with the screened potential distributions. The extracted NI and co-extracted electron currents are analyzed for different configurations of the magnetic filter. Finally, the possibility of increasing the NI extracted current from the ions produced at the Cs covered surface is analyzed and compared to the one extracted from the volume.

SIMULATION MODEL

ONIX was initially developed to model the radio-frequency negative ion source for ITER Neutral Beam Injector [7]. The code is fully 3D self-consistent electrostatic code based on the PIC-MCC approach. It is able to deal with complex boundaries geometries, which is the case of the extraction aperture. The code includes full 3D magnetic field map taken from the experimental source designed to reduce the co-extraction of the electron beam as well as the high extraction potential but preserving the NI extracted current. To reach the steady state of the simulated system in a reasonable computation time, ONIX code is parallelized via the Message Passing Interface approach using spatial domains and particles decomposition techniques. One typical program run performed on 20 CPUs takes about 12 days.

Each simulation domain has been successively implemented in the code corresponding to the extraction systems IS01 and IS02, respectively. Hence the simulation volumes include the extraction aperture of 6.5 mm diameter spatially extending 30mm*20mm*20mm in x, y, z directions respectively (Fig.1 right, x – is the symmetry axis). The main difference between these two simulation domains is the aperture's shape: in the IS01 system it is represented by the 1 mm cylinder length(see Fig. 1 bottom IS01), whereas in IS02 it is double chamfered as two cones with joint bases with smaller radius of r=3.25mm and larger radius R=10 mm (see Fig. 1 top IS02). The boundary conditions assume perfect metal walls surrounding the box in y and z directions. The plasma (given parameters, density, temperature) is assumed in the left side of the box (0<x<12.5 mm).

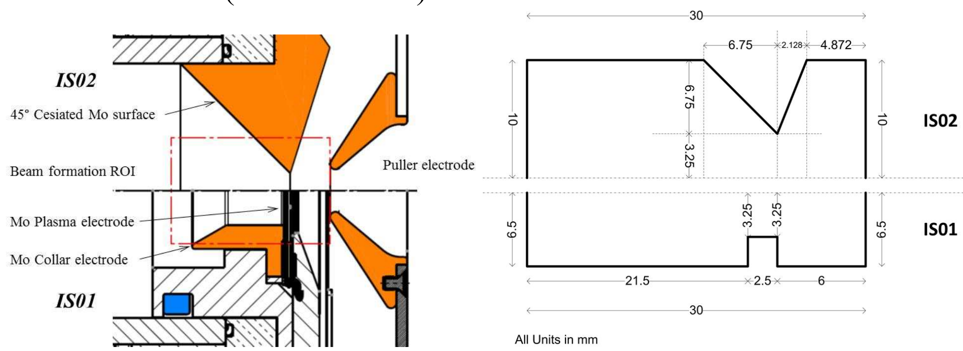

FIGURE 1. Left – sketch of the Linac4 beam formation region for H^- volume production (IS01 bottom) and cesiated surface production (IS02 top). The extraction aperture is 6.5 mm diameter and the distance from the centre of the aperture to the 25 kV puller electrode is 7mm. The simulated beam formation region of interest (ROI) is indicated with a dot-dashed line. Right - schematic view of the simulation domains used in the ONIX code (x-y mid plane) for modeling IS01 – at the bottom and IS02 extraction system – at the top.

The potential distribution along the volume is calculated as the solution of the Poisson's equation:

$$\nabla^2\varphi = -\rho/\varepsilon_0 \tag{1}$$

The iterative Preconditioned Conjugate Gradient method [8] is used to solve Eq. 1. To get the realistic potential distribution in the vicinity to the extraction aperture, which has a circular cross section; special techniques are implemented in the Poisson solver to deal with domain boundaries lying between mesh nodes [7, 9]. The Dirichlet condition is referred to all solid wall boundaries of the simulation domain with constant potential value. The input potential profile applied to the right box boundary of the simulation domain (after the extraction aperture) is calculated using the real puller geometry by the commercial OPERA 3D code. In most of the simulations the rest of the domain boundaries are assumed to be grounded (V=0). Very good agreement has been found for the potential distribution inside the simulation volume between OPERA calculations and the ONIX code results.

The electric field is calculated weighting the potential distribution surrounding the second mesh neighbors (18 nearest PIC nodes):

$$\mathrm{E} = -\nabla\varphi \tag{2}$$

The full 3D magnetic and electrical field maps of the cusp system and the extraction gap has been calculated by using the TOSCA module of the OPERA software package, which uses finite element methods to solve electro- and magneto-static problems in a scalar potential formulation. Resulting field distributions were used as input profiles in the ONIX code. The field firstly is interpolated on the PIC grid nodes and after on each current particle position.

The plasma density and temperature far from the extraction aperture are assumed constant and where taken from the experiments [10]. The initial plasma is composed of H^+, H_2^+, H_3^+, H^- and electrons. The density was set to $n_0=10^{18}$ m^{-3} for the positive and negative species with the source ratio: $S_{H}^+/S_{H2}^+/S_{H3}^+=0.7/0.2/0.1$; $S_e/S_H^-=0.5/0.5$. The initial electron temperature is T_e=5eV, whereas the ions temperature was set to 1.5 eV. ONIX code assume a uniform neutral gas background, that is reasonable for relative small ionization degree (<5%) with constant density $n_H=10^{20}m^{-3}$.

The Monte Carlo Collision module includes the self-consistent NI production in the volume via electron dissociative attachment to the vibrationally exited molecules $H_2(v)$ and list of the most important NI destruction processes as detailed in Ref. [6]. Electron elastic collision ($e+H \rightarrow e+H$) has been added to the module due to the importance of the electron energy transfer that could reduce co-extracted electron current.

At the beginning of the simulation (t = 0), the spatial distributions of the positive and negative species are the same, i.e. the plasma is neutral. For a stable plasma simulation the chosen time step should be smaller than the inverse plasma frequency and the size of the PIC cell should be smaller than the Debye length. In addition to these basic criteria the most important condition, know as the CFL (Currant Friedrichs Lewy) [11] condition, must be fulfilled. In current simulations, the typical runs performed using ~20 millions macro particles (~50 particles per cell) with the mesh 110*100*100 nodes. The code performance is ~0.1μs per day on 20 CPUs with the time step $\Delta t = 3*10^{-12}$s $<1/\omega_p \sim 1.77*10^{-11}$ s. Let us note that simulation deals with the extraction (sheath) region, so even if the cell size is few times larger than Debye length the CFL criteria is always satisfied.

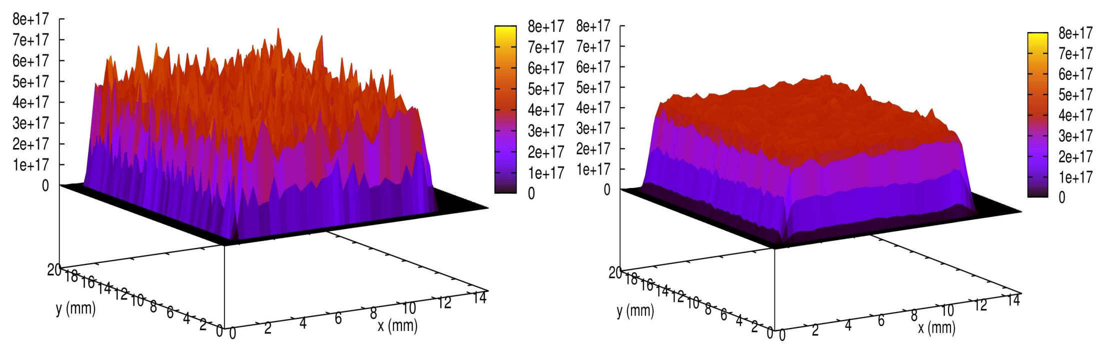

FIGURE 2. Initial electron density distribution using 8 (left) and 64 (right) points charge assignment routine.

In order to decrease the numerical heating that could arise from high plasma density, the second order charge assignment routine has been developed. The advantage of this procedure is visible in Fig. 2 where the initial electron density distribution is shown a) for first order projection procedure using 8 nearest PIC nodes and b) for the second order projection procedure using 64 PIC nodes. One can clearly see that the spikes present on Fig. 2 left have disappeared (Fig. 2 right), reducing the numerical heating. Moreover, test simulations with different number of macro particles per cell have been done to prove the absence of the significant influence of the numerical noise. It was found that simulations with 50 particles per cell give the extracted current, potential and charge density distribution similar to the one obtained with 150 particles per cell. Therefore, realistic 3D simulations with a plasma density as high as $n=10^{18}$ m^{-3} can be performed with the improved version of the ONIX code.

RESULTS AND DISCUSSION

General system behavior

The simulations were performed with an initial plasma density filling the first 12 mm of the simulation domain. With time, the plasma expands and the negative ions together with the electrons are extracted through the aperture. When the fluctuations of the extracted currents reach its minimum and the potential map does not change (~3 %) steady state regime is considered.

The very high positive bias potential (25 KV) applied to the puller electrode attracts negative ions out of the plasma source, but it simultaneously repels positive particles towards the plasma chamber. Positive ions will stay along the potential isolines forming a specific semi-spherical structure called "meniscus". Fig. 3 shows the positive ion spatial density distribution: a) H^+ initial position for IS01, b) H^+ steady state distribution for IS01, c) H^+ initial position for IS02, d) H^+ steady state distribution for IS02. The self-consistent positive ion organization in the "meniscus" structure close to the extraction aperture is visible in Fig. 3. The "meniscus" position and its width strongly depend of the shape of the extraction aperture (especially its diameter) and the applied potential to the puller [5]. The similar behavior has been detected for the H_2^+ and H_3^+ ions.

The spatial distribution of the electrostatic potential at the beginning of the simulation ($t = 0$) and at the quasi steady state regime ($t \approx 1\mu s$) are shown in Fig. 4. In the initial state the external electric field deeply penetrates inside the plasma chamber in both systems Fig. 4 a), c). For instance, the potential isoline of 100 V is shifted from x~14 mm at the beginning to x~23 mm for the steady state of IS01 and from x~15 mm to x~ 23 mm for the IS02 system. However, when the plasma screening occurs, the potential isolines are pushed towards the extraction aperture. Therefore, in quasi steady state regime the potential isoline of 100 V is located at the entrance plane of the extraction aperture for both systems ~23 mm - Fig. 4. b), d). The neutrality of the systems is maintained at the initial plasma region ($0 < x \leq 12.5$ mm). The potential is constant or slowly varies in most of the volume inside this interval.

If the electrons or NI cross the right boundary of the simulation domain they are eliminated from the system and counted as extracted current. The typical evolution of the extracted negative ions and co-extracted electron currents for IS01 system is shown in Fig. 5 a). One can see that the electron current grows very fast in the beginning, because the extraction potential is not screened yet. This growing continues up to $0.3\,\mu s$. At this time, the screening of the extraction potential starts being efficient, reducing thus the fraction of the co-extracted electrons. After this transitory phase, the NI and electron currents stabilize and the system evolves to a quasi steady state for time $>0.6\,\mu s$.

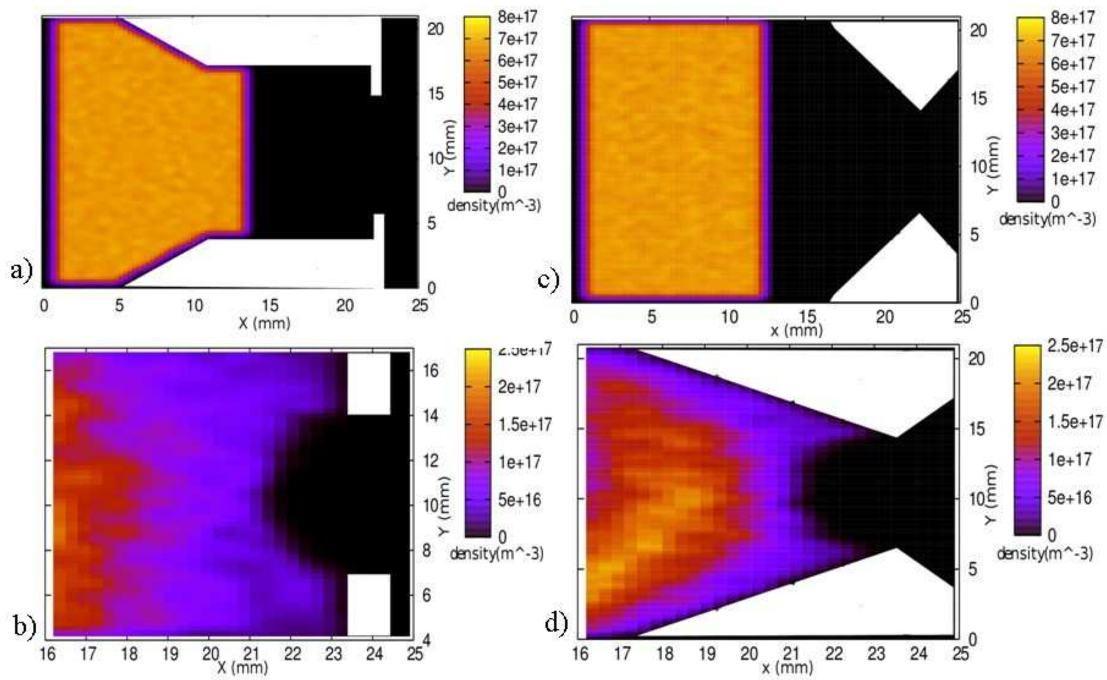

FIGURE 3. Positive ion spatial density distributions in the middle z=10 mm plane: a) IS01- initial H^+ b) IS01- steady state H^+, c) IS02- initial H^+ , d) IS02- steady state H^+.

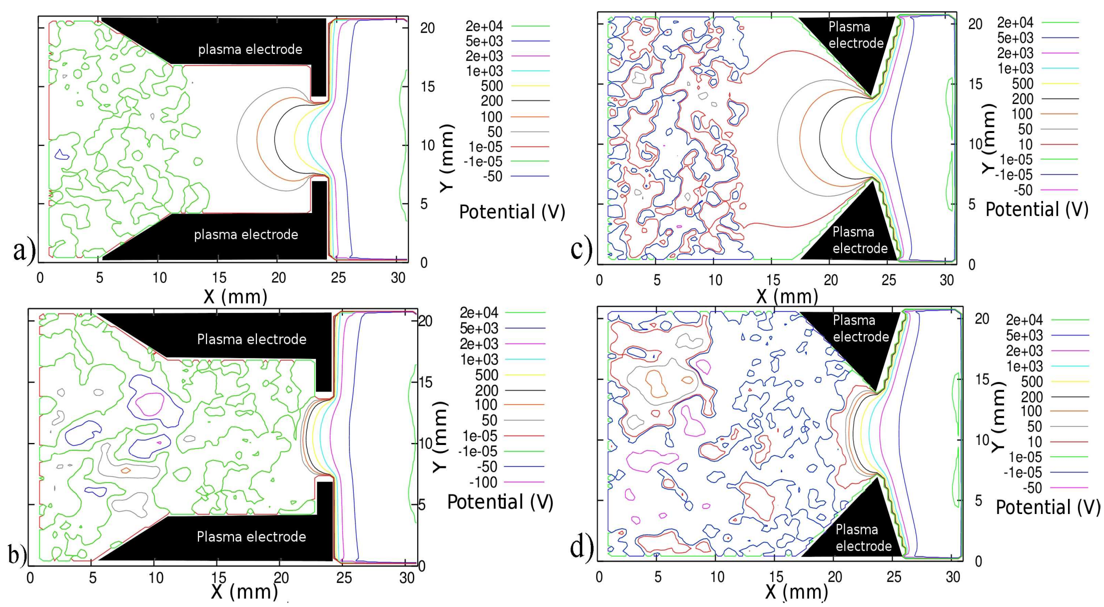

FIGURE 4. Spatial potential distribution at the beginning of the simulation: a) IS01, c) IS02 and at the quasi-steady state regime: b) IS01, d) IS02.

The asymptotic value of the extracted NI current obtained in the simulation $I_{NI} \approx 12 \pm 2$ mA. The simulated value of the co-extracted electron current ($I_e \approx 70 \pm 35$ mA) is in ~6 times larger than NI one (inset Fig. 5 a).

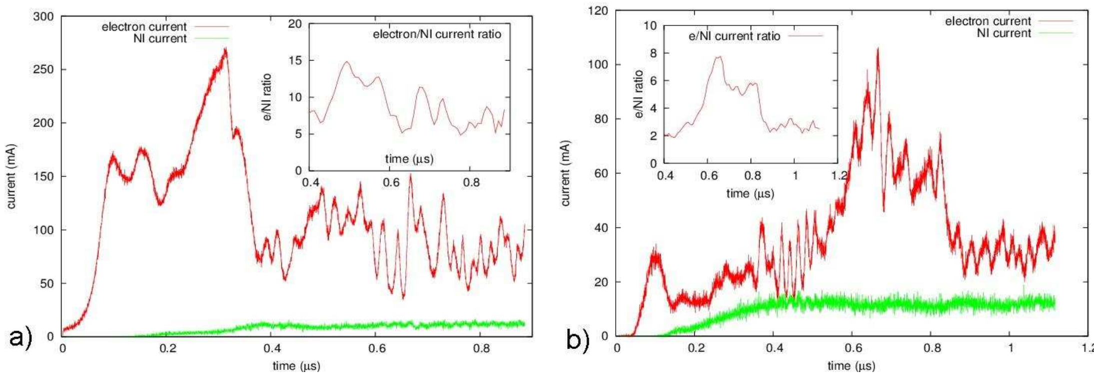

FIGURE 5. Time evolution of the extracted NI (green line) and co-extracted electron (red line) current for IS01 a) and IS02 b) extraction systems using 25kV extraction potential. Inset represents e/NI current ratio.

The time evolution of the extracted currents from IS02 extraction system is shown in Fig. 5 b. As one can see, the quasi steady state regime is reached later than for IS01. The transitory phase continues up to ~0.8 µs, after this point the fluctuations of co-extracted electron current stabilize and a steady state is achieved. Continuing current fluctuations in both systems could be explained by the particle reinjection procedure for keeping neutral plasma. The first negative ions are extracted at ~0.15µs and NI current stabilizes at ~0.4µs, similar to IS01 system.

The asymptotic value of the extracted NI current from IS02 extractor is very similar to IS01: $I_{NI} \approx 12 \pm 2\,\mathrm{mA}$ (Fig. 5 b.). However, the co-extracted electron current (Fig. 5 b.) is smaller in comparison with IS01: ($I_e \approx 40 \pm 20$ mA). Therefore, the value of the electron/NI current ratio is about 3 (inset Fig. 5 b.).

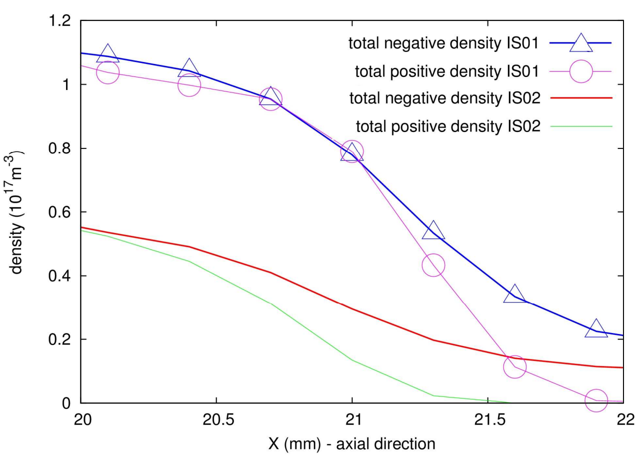

FIGURE 6. Total positive and negative 1D (mid *x-y* and mid *x-z* plane) density axial distributions in the meniscus region from the simulations of IS01 and IS02 extraction systems.

One of the reasons of decreasing the co-extracted electron current from the IS02 extractor is the local electric field map in vicinity to the extraction aperture (meniscus region). Fig. 6 represents the 1D axial distribution of total negative and positive charge density close to the plasma electrode (PE starts at x = 23 mm), averaged in time. The chamfered geometry of the plasma electrode changes the particle dynamics in the meniscus region. The slope of the charge separation is sharper in the case of IS01 extractor that creates stronger local electric field, thus accelerating electrons towards the puller electrode. Together with higher charge density it causes the increase of the co-extracted electron current.

Cusp and Filter magnetic fields

One of the main issues of the NI source is the suppression of co-extracted electrons that causes deleterious effect on source performance. On one hand, extracted electrons waste acceleration power, induce additional space charge and could destroy NI even after their extraction. The electron dump field is chosen high enough to trap the electron beam, but it does not perturb the NI trajectories.

Hallbach's offset octupole cups-like magnetic field is implemented around the cylindrical plasma chamber. A magnetic dipole filter field is installed in the plasma expansion region between plasma chamber and beam extraction hole. Two different magnetic filter field of 10 or 20 mT are available for IS01 or IS02 obtained by magnetization of the permanent magnet pairs (Fig. 7 a.).

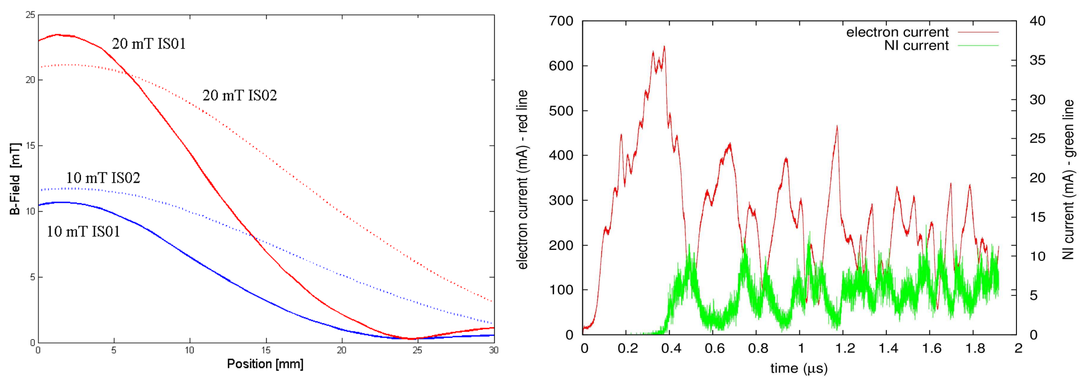

FIGURE 7. (left) Coaxial plot of the total magnetic field distribution for IS01 (solid lines) and IS02 (dashed lines) extraction systems. Top corresponds to the 20 mT configuration of the filter field; bottom – 10 mT configuration. (right) time evolution of the extracted NI (right y axis) and co-extracted electron (left y axis) current for IS01 extraction system using a 10 mT filter field configuration.

The extracted NI and electron current for the 20 mT magnetic field configuration was shown in Fig. 5 a) and discussed above. The time evolution of the extracted current for 10mT B filter field is depicted in Fig. 7 b. The asymptotic value of the co-extracted electron current increases in ~2.5 times ($I_e \approx 200 \pm 100$ mA) in comparison with the 20 mT configuration ($I_e \approx 70 \pm 30$ mA). The electrons become the dominant negative species in the vicinity to the plasma electrode reducing the fraction of the extracted negative ions. Therefore, extracted NI current is twice lower; from $I_{NI} \approx 12 \pm 2$ mA @20mT filter field to $I_{NI} \approx 6 \pm 1$ mA @10 mT.

Simulation of the NI surface production

One of the main Linac4 source requirements is to produce NI beam with current $I_{NI} = 80$ mA. The results presented above show that such current could not be obtained only from the volume produced NI at plasma density $n_0 = 10^{18}$ m^{-3} and dragged out by 25 kV extraction voltage. In order to increase negative ion production yield, Cs vapor with low work function (Cs ~2eV) is planned to be injected in the source. Cs covering the surface of the plasma electrode can effectively create NI releasing electrons to energetic neutral gas (3) or positive ions impinging the PE (4) [5,12]:

$$H + e_{surface} \rightarrow H^- \tag{3}$$

$$H^+ + e_{surface} \rightarrow H \Rightarrow H + e_{surface} \rightarrow H^- \tag{4}$$

The amount of the surface produced NI can be theoretically calculated from the conversion yield and the number of impelling neutrals/positive ions. The atoms flux to the wall is calculated from the density (n_H) and thermal velocity (v_{th}) as:

$$\Gamma_H = \frac{1}{4} \cdot v_{th} \cdot n_H \tag{5}$$

Because of the relatively small density of the positive ions close to the plasma electrode ($n_{H^+} \approx 10^{17}$ m^{-3}) with respect to the *H* gas density ($n_H \approx 10^{20}$ m^{-3}) the NI production rate via positive ion impact is much smaller than via neutrals. The negative ion conversion yield could reach up to 20 percent for all production channels [13, 14]. Therefore, the NI emission rate from the Cs covered plasma electrode surface was estimated ~7000A/m^2.

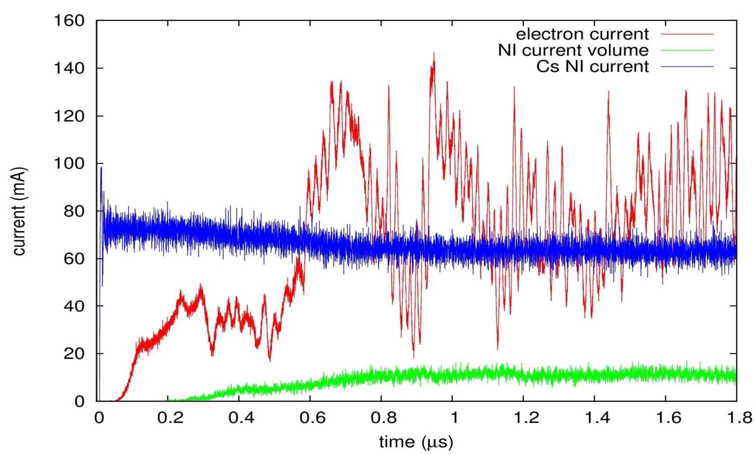

FIGURE 8. Time evolution of the extracted electron and NI currents for IS02 system. From bottom to top: Extracted NI current from the volume; extracted NI current from the plasma electrode surface and co-extracted electron current.

Results from the simulation of the NI surface production for IS02 are shown in Fig. 8. NI extracted currents originating from the volume and from the plasma electrode aperture surface are compared as well as co-extracted electron current. The surface produced NI from the inner aperture leads to ~6 time higher ($I_{H^- surface} \approx 70 \pm 5$ mA) current than one extracted from the volume ($I_{H^- volume} \approx 12 \pm 2$ mA), whereas the extracted current from the outer side of the aperture is 0.

The limitation of the NI extraction from the aperture surface causes the reverse negative field ("double layer") along the wall. This phenomenon is discussed in details in the previous paper [6]. However, more simulations with different NI production yield are required in order to specify the behaviour of the reverse field from both (inner and outer) sides of the plasma electrode.

CONCLUSION

The plasma property extraction capability of both extraction systems (IS01, IS02), recently developed at CERN, were studied using a modified version of self-consistent 3D PIC MCC code ONIX. Simulations show the self-consistent positive ions “meniscus” formation in the vicinity to the extraction aperture. It was found that co-extracted electron current significantly decreases in the case of the double chamfered extraction aperture geometry due to the most efficient deflection of the electron trajectories to the aperture walls related with different interception angle of the meniscus isopotential lines with the inner chamfered part of the aperture.

The effect of the filter magnetic field has been studied for IS01 extraction system. It was found that the 10 mT configuration of the filter field not only increases co-extracted electron current, but also reduces the extracted NI beam.

The NI surface production has been simulated for IS02 extractor. When the Cs vapor is used the total extracted NI current from both production channels (volume and surface) achieves the target source value of 80 mA.

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