ISBN: 978-3-95450-184-7 doi:10.18429/JACoW-IPAC2018-THPAK075

SIMULATION OF PARTICLE INTERACTIONS IN A HIGH INTENSITY RADIO-FREQUENCY QUADRUPOLE FOR MOLECULAR HYDROGEN IONS

Matthew J Easton*, Haipeng Li, Yuanrong Lu, Zhi Wang, Peking University, Beijing, China
Ji Qiang, Lawrence Berkeley National Laboratory, Berkeley, USA

Abstract

High-intensity deuteron accelerators run the risk of deuteron–deuteron interactions leading to activation. For this reason, in the commissioning phase, a molecular hydrogen ion (H_2^+) beam is often used as a model for the deuteron beam without the radiation risk. However, composite ions are susceptible to particle interactions that do not affect single ions, such as stripping of electrons and charge exchange. Such interactions affect the beam dynamics results, and may lead to production of secondary particles, which in high-intensity beams may cause damage to the accelerator and reduce the quality of the beam. In order to understand these effects, we have modified the IMPACT-T particle tracking code to include particle interactions during the tracking simulation through a high-intensity continuous-wave (CW) radio-frequency quadrupole (RFQ). This code is also designed to be easily extensible to other interactions, such as collisions or break-up of heavier ions. Preliminary results and possibilities for future development will be discussed.

INTRODUCTION

High intensity continuous wave (CW) radio-frequency quadrupole (RFQ) linear accelerators are important as the first acceleration stage for many different ions and many different applications, including neutron sources [1], nuclear fusion materials research [2], and cancer therapy using Boron Neutron Capture Therapy (BNCT) [3].

Most high intensity CW RFQs are designed to accelerate proton or deuteron beams [4]. Molecular hydrogen H_2^+ ions are often used in the commissioning stage for deuteron machines, to avoid activation from deuteron–deuteron collisions [5]. Molecular hydrogen ions have also been suggested as the first stage of proton acceleration, where the electron is stripped from the ion to leave two protons for further acceleration [6, 7].

However, molecular hydrogen ion beams do introduce a number of difficulties, as experienced by the Fusion Materials Irradition Test (FMIT) project at Los Alamos National Laboratory (LANL) in the 1980s [8]. Stripping, charge exchange and dissociation interactions affected the molecular hydrogen ions, producing a large halo of charged and neutral particles, which severely damaged several components of the accelerator.

To investigate these complex interactions of molecular hydrogen ions during acceleration in such a high-current CW RFQ, we have modified the particle tracking code IMPACT-T to include particle interactions during the tracking simulation.

IMPACT-T

The IMPACT code suite is a three-dimensional multi-particle tracking code, designed for high intensity accelerator applications. It uses the particle-in-cell (PIC) method of modelling space-charge effects, and runs in parallel for scalability. IMPACT-T is the time-dependent implementation. We recently added an RFQ module [9], including benchmarks with TOUTATIS and PARMTEQM. More information on the IMPACT-T code can be found on the project website [10].

The space-charge calculations already handle the Coulomb interaction between particles in the beam, but other interactions are also possible, especially with the presence of residual gas in the beam pipe. We have added an interactions module to IMPACT-T, with the ability to define different types of interactions in an input file and apply these throughout the tracking simulation. Interactions can change the state of the particles involved, such as stripping or capturing of electrons, or break-up of composite ions into smaller constituent parts.

To model these changes efficiently, we introduced separate interaction bunches for each type of particle modelled. Each interaction bunch has a reference particle for that particle type, and the space-charge calculation includes particles from all interaction bunches as well as the main beam bunch. When an interaction occurs, particles may be lost from one bunch type and added to another bunch type. For example, stripping the electron from a molecular hydrogen H_2^+ ion will remove one ion from the main beam bunch and add two protons to a proton interaction bunch. After the interaction, the particles in each bunch are tracked through the rest of the accelerator, and continue to contribute to the space-charge calculation.

MOLECULAR HYDROGEN SIMULATIONS

We implemented three different types of interactions to apply to a high-intensity molecular hydrogen ion beam in a CW RFQ accelerator. The first interaction is the stripping of the electron from a molecular hydrogen ion to produce two fast protons ($H_2^+ \rightarrow 2H^+ + e^-$). The second interact ion is charge exchange—the capture of an electron from the residual gas that neutralizes the ion ($H_2^+ + e^- \rightarrow H_2$). The third type of interaction is a composite, including both

* matt.easton@pku.edu.cn; matteaston.net/work

ISBN: 978-3-95450-184-7 doi:10.18429/JACoW-IPAC2018-THPAK075

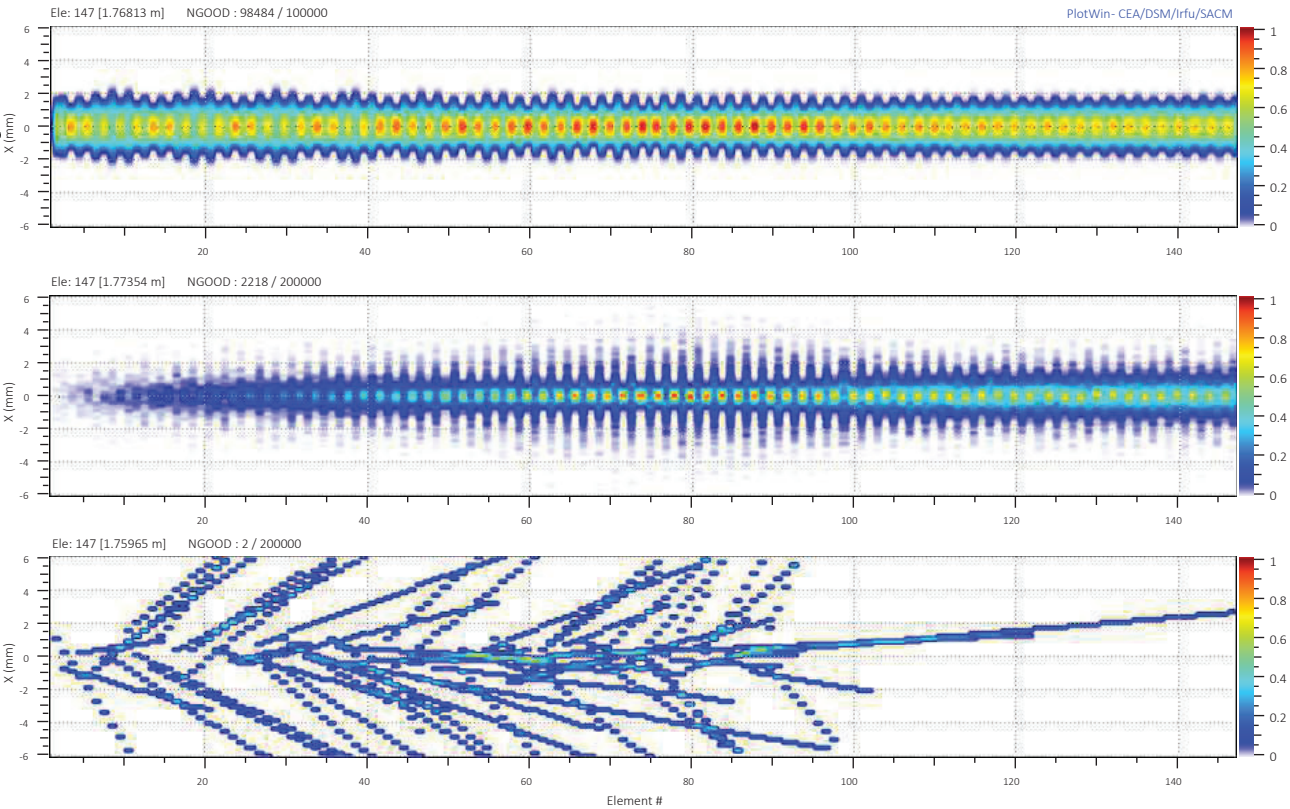

Figure 1: Plots of different particle species along the length of the simulated RFQ. Top: Molecular hydrogen ions; Middle: Protons; Bottom: Neutral hydrogen atoms.

charge exchange occurs and dissociation, producing two neutral hydrogen atoms ($H_2^+ + e^- \rightarrow 2H$). Note that the products of these interactions have different charge-to-mass ratios, and some of the products are neutral. All the product particles are tracked through the accelerator from the point where they are produced.

We modelled the transmission of a 50 mA molecular hydrogen ion beam through a 1.8 m RFQ, including these interactions. The IMPACT-T simulation included 100,000 macroparticles. The RFQ is an existing design [11], optimized to accelerate deuterons from 50 keV to 1 MeV. Figure 1 shows the three different types of particles in one simulation (plotted using PLOTWIN [12]). In this particular simulation, about 1.5% of the molecular hydrogen ions interact in one way or another. The plot for protons shows a steady increase in the proton beam current, with the protons being (imperfectly) contained and accelerated within the RFQ. The lower plot shows the production of neutral atoms by electron capture, which are not contained by the electric field and are lost towards the walls of the RFQ.

Figure 2 shows a histogram of the energy of all particles at the end of the RFQ. The main peak is the molecular hydrogen H_2^+ ions at the design value of 1 MeV, but there is also a small peak of protons at 0.5 MeV. The charge-to-mass ratio of the protons is double that of the molecular hydrogen ions, hence the final energy is halved. Most of the neutral atoms are produced at lower energies, and as they are not confined or

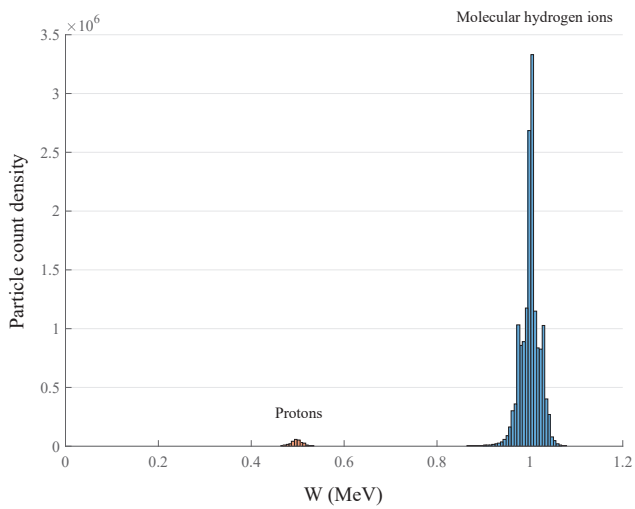

Figure 2: Energy spectrum at the end of the RFQ.

accelerated by the electromagnetic field, very few make it to the end of the RFQ, which is why they cannot be seen on the final energy spectrum.

Figure 3 shows the effect of adjusting the vacuum level within the accelerator. For the lowest pressures, no interactions take place and the losses are fixed. As the residual gas pressure increases, more and more interactions take place, reducing the transmission for the main beam and increasing the numbers of protons produced, as expected.

ISBN: 978-3-95450-184-7 doi:10.18429/JACoW-IPAC2018-THPAK075

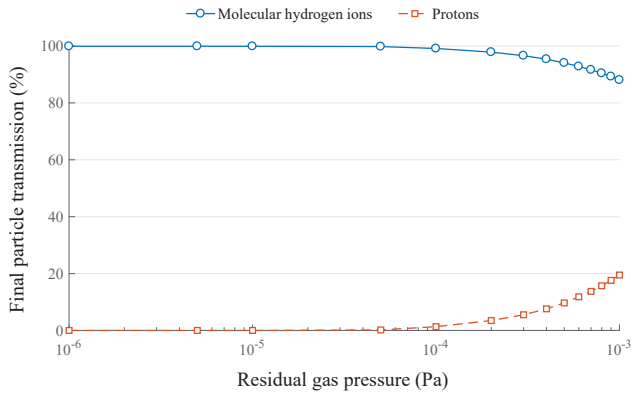

Figure 3: Final particle transmission for molecular hydrogen ions and protons with different values for the residual gas pressure inside the RFQ.

DISCUSSION

Using the reported cross-sections [13, 14], we found that at reasonable values for the quality of the vacuum in the beam pipe (of the order of 10^{-6} Pa), losses due to such interactions should be negligible. This doesn't match with our experience, in that molecular hydrogen beams often exhibit slightly higher loss rates than equivalent deuteron beams in the same RFQ. There are a number of possibilities as to why losses in our simulations are lower than expected. Firstly, the simulations so far use a simple probabilistic algorithm for determining particle interaction rates based on cross-sections. A full Monte Carlo implementation would be a more robust algorithm. Secondly, the extrapolation functions to calculate the interaction probability from the known cross-sections may not be accurate.

We hope to follow up these simulations with some experimental tests using a molecular hydrogen in an existing high intensity RFQ, in order to validate the new code and to investigate the interaction cross-sections empirically. We are also looking at other codes that could complement IMPACT-T for these investigations, such as OPAL [15], which already implements both a Monte Carlo algorithm and a PIC space-charge algorithm, but as yet does not have an RFQ module. Modelling the same interactions in multiple simulation codes should allow us to benchmark results from one against another, along with comparisons to experimental results.

The interaction code is not specific to molecular hydrogen beams, and future work could also include modelling break-up of heavy ions into constituent parts, interactions with electron clouds in a beam pipe, or other particle interactions during acceleration. Future work could also investigate different types of accelerating structures using the same interactions module.

ACKNOWLEDGEMENT

This work was supported in part by the Natural Science Foundation of China (NSFC) under the 973 program 2014CB845503.

REFERENCES

[1] H. P. Li, Q. Fu, P. P. Gan, Y. R. Lu, Z. Wang, and K. Zhu, "Beam dynamics design of the 3 MeV RFQ for BISOL project," in *Proceedings of IPAC 2017: the eighth International Particle Accelerator Conference*, Copenhagen, Denmark, May 2017, pp. 2328–2331. DOI: 10.18429/JACOW-IPAC2017-TUPVA103.

[2] J. Knaster and Y. Okumura, "Accelerators for fusion materials testing," *Reviews of Accelerator Science and Technology*, vol. 08, no. 11, pp. 115–142, Jan. 2015. DOI: 10.1142/S1793626815300078.

[3] X. W. Zhu et al., "2.5 MeV CW 4-vane RFQ accelerator design for BNCT applications," *Nuclear Instruments and Methods in Physics Research Section A*, vol. 883, pp. 57–74, Mar. 2018. DOI: 10.1016/j.nima.2017.11.042.

[4] A. Pisent, "High power RFQs," in *Proceedings of PAC 2009: the 23rd Particle Accelerator Conference*, Vancouver, BC, Canada, May 2009, pp. 75–79. http://jacow.org/PAC2009/papers/MO3GRI04.pdf

[5] R. Gobin et al., "A 140 mA cw deuteron electron cyclotron resonance source for the IFMIF-EVEDA project," *Review of Scientific Instruments*, vol. 79, no. 2, 02B303, 2008. DOI: 10.1063/1.2801976.

[6] J. R. Alonso and the DAEδALUS Collaboration, "High current H_2^+ cyclotrons for neutrino physics: The IsoDAR and DAEδALUS projects," *AIP Conference Proceedings*, vol. 1525, pp. 480–486, Mar. 2013. DOI: 10.1063/1.4802375.

[7] D. Winklehner, R. W. Hamm, J. R. Alonso, and J. Conrad, "An RFQ direct injection scheme for the IsoDAR high intensity H_2^+ cyclotron," in *Proceedings of IPAC 2015: the sixth International Particle Accelerator Conference*, Richmond, VA, USA, Jul. 2015, pp. 3384–3386. http://jacow.org/IPAC2015/papers/WEPTY048.pdf

[8] W. D. Cornelius, "CW operation of the FMIT RFQ accelerator," *IEEE Transactions on Nuclear Science*, vol. 32, no. 5, pp. 3139–3143, Oct. 1985. DOI: 10.1109/TNS.1985.4334300.

[9] J. Qiang, Z. Wang, and H. P. Li, "A new RFQ model and symplectic multi-particle tracking in the IMPACT code suite," in *Proceedings of HB 2016: the 57th ICFA advanced beam dynamics workshop on high-intensity and high-brightness Hadron Beams*, Malmö, Sweden, Jul. 2016, pp. 562–566. http://jacow.org/HB2016/papers/THPM7Y01.pdf

[10] Impact-t code homepage at nersc. http://portal.nersc.gov/project/m669/IMPACT-T

[11] F. J. Jia et al., "Beam dynamics design of a 50 mA D+ RFQ," *Chinese Physics Letters*, vol. 33, no. 7, p. 72 901, Jul. 2016. DOI: 10.1088/0256-307X/33/7/072901.

[12] Plotwin code homepage at cea irfu. http://irfu.cea.fr/en/phocea/page/index.php?id=263

[13] E. M. Kellogg, "Ion–gas collisions during beam acceleration," *IEEE Transactions on Nuclear Science*, vol. 12, no. 3, pp. 242–246, Jun. 1965. DOI: 10.1109/TNS.1965.4323628.

[14] M. Abs et al., "Multimegawatt DAEδALUS cyclotrons for neutrino physics," Online preprint at arXiv:1207.4895 [physics.acc-ph], Jul. 2012.

[15] Opal code homepage at psi. https://gitlab.psi.ch/OPAL