NON-LINEAR BEAM DYNAMICS IN HIGH RESOLUTION MULTI-PASS TIME OF FLIGHT MASS SEPARATOR*

V. A. Shchepunov†, ORAU, Oak Ridge, TN 37831-6374, U.S.A.
H. Wollnik, JIHIR, Oak Ridge, TN 37831, U.S.A.

Abstract

A multi-pass time-of-flight mass separator (MTOF-MS) is under development by the University Radioactive Ion Beam (UNIRIB) collaboration. The MTOF consists of two coaxial electrostatic mirrors, focusing lenses and auxiliary injection, extraction and separation elements. The injected ions having almost the same energy but different masses undergo hundreds or thousands of reflections between the mirrors. In the course of this periodic motion, the ions of different masses and hence velocities are spatially separated in longitudinal direction. The periodic motion in the MTOF has been investigated with a recently developed ray tracing program utilizing the canonical integration technique. Results of the performed numerical simulations are discussed. The simulations displayed the nonlinear character of the ions' behaviour both in transverse and longitudinal phase spaces. The ions' transverse stability and longitudinal isochronicity were the matters of primary attention. It is shown in particular that at transverse tunes of around Q=0.75 the system can be adjusted to be isochronous up to at least the 3rd order of the time-of-flight (ToF) optical aberrations.

INTRODUCTION

Mass measurement or mass separation based on multi-pass motion in a periodic structure make use of the fact that ions of different masses, extracted from an ion source or trap with the same energy, have different velocities and hence are separated longitudinally in the course of their motion. A fast separator placed behind such a periodic structure works as a time gate opened for ions of a certain mass and closed for ions of all other masses that arrive earlier or later. To achieve high values of mass resolving power, the extraction pulse length must be short compared to the overall flight time, while the periodic structure should minimize the dependence of the ions' flight times from their initial phase space coordinates. Ideally, such a system should be optimized so that the ions' flight time from a source to a detector or separator depend only on their masses. In other words, the entire system should be isochronous.

One such system, a 0.4m long mass spectrometer, had been built and demonstrated mass resolving power of m/Δm≥18,000 [1,2]. Our next step is a new 1.3m long multi-pass time of flight separator for a 1.5kV beam, which was designed for the UNIRIB collaboration. Similar to [1], in the new design, the mirror and lens electrodes are coaxially arranged (see Figure 1). The ion optics of the new system has been optimized and investigated numerically. Some of the new results of this work are reported in this paper.

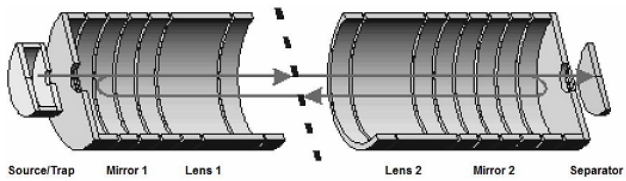

Figure 1: Sketch of the multi-pass time-of-flight mass separator that consisting of coaxially arranged electrostatic mirrors and lenses built as ring electrodes. Further downstream a fast ion separator selects ions of a certain mass.

NUMERICAL METHODS

Optimization Procedure

Voltages on the MTOF electrodes are adjusted to minimize ToF optical aberrations up to the 5th order. The following goal function characterizing the time spread due to ToF aberrations ($t|x^{n1}a^{n2}y^{n3}b^{n4}\delta^{n5}$) is minimized:

$$F_t=\sum\left[f_{n1,n2,n3,n4,n5}(t|x^{n1}d^{n2}y^{n3}b^{n4}\delta^{n5})x_m^{n1}d_m^{n2}y_m^{n3}b_m^{n4}\delta_m^{n5}\right]^2, \quad (1)$$

where (x, y) are transverse coordinates, (a, b) transverse angles, δ relative energy deviation [3], index m denotes that maximally possible values of the phase space coordinates are used, the weight factors $f_{n1,n2,n3,n4,n5}$ are defined according to [4] and the summation in (1) is performed for all possible values with indices $1\le n1+n2+n3+n4+n5\le 5$. In addition to (1), constraints on transverse phase advance per turn or the 1st order matrix elements can be imposed. The optimization is performed using an improved version of the previously developed 3rd order optimizing program [5].

Ray Tracing

A ray tracing program has been developed to investigate single particle dynamics in the MTOF and verify the validity of found optimal geometries and voltage settings. It can do the following:

- Calculate electrostatic fields created by a set of axially symmetric electrodes by the charge density method [6].
- Read from a file or generate randomly initial ion coordinates.

*Work supported by UNIRIB collaboration and Oak Ridge Associated Universities
†shchepunov@orau.gov

- Perform ion ray tracing through the MTOF using either a standard 4th order Runge-Kutta algorithm or Neri's 4th order symplectic integrator [7].
- Graphically represent the calculated field, the electrode geometry and results of ray tracing (phase space scatter plots).

SIMULATION AND DISCUSSION

Since ions trapped between the mirrors of Figure 1 can move inside the MTOF for hundreds or thousands of turns, its electrostatic potential should provide not only maximally possible isochronicity, but also transverse stability. Simulation results presented below are obtained for the 1.3m long MTOF under construction for the UNIRIB collaboration.

Transverse Motion

Two lens electrodes, located next to the mirrors (see Figure 1), are foreseen in the MTOF for transverse focusing. Varying lens potentials one can change the value of the transverse tune Q in the range from 0 to approximately 1.5. (Due to the axial symmetry, both the transverse tunes are equal, $Q_x=Q_y=Q$). Figures 2, 3 and 4 demonstrate the ions' motion in the plane (x-a) for Q close to 1, 1/2 and 3/4 respectively as seen by a monitor placed in the center of the MTOF.

As one can see from Figures 2 and 3, the motion near Q=1.0 is stable, while at Q≈0.5 stable ions are only those, which move sufficiently close to two fixed points. In general, Q can be of any value except those close to 0.5 or 1.5. Convenient values of Q are, for example, 2/3 or 3/4 since, at these resonance points, the optic has additional symmetries, which allow one to achieve smaller values of time spreads evaluated with function (1). An example of motion when Q≈3/4 is shown in Figure 4. Apart from the island structure typical for the 4th order resonance, one can also see numerous islands at the border of stability at large x and/or a values.

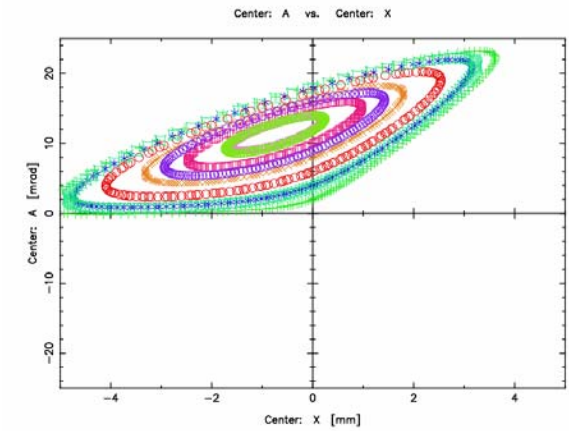

Figure 2: Stable motion of ions in the phase plane a[mrad]-x[mm] around the 1st order fixed point. The tune Q is close to 1.0, number of turns N=320.

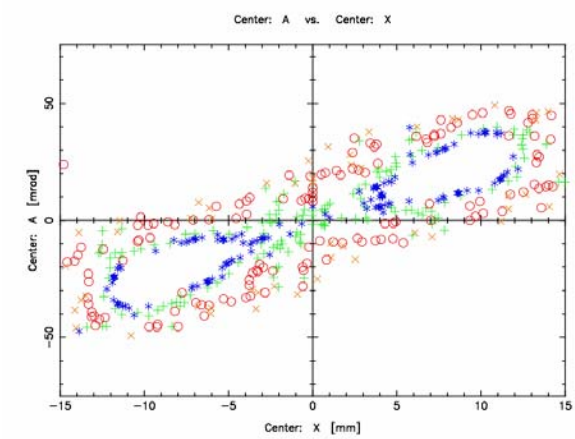

Figure 3: Motion of ions in the phase plane a[mrad]-x[mm] at Q close to 0.5. All shown ions are unstable and lost after less than 100 turns.

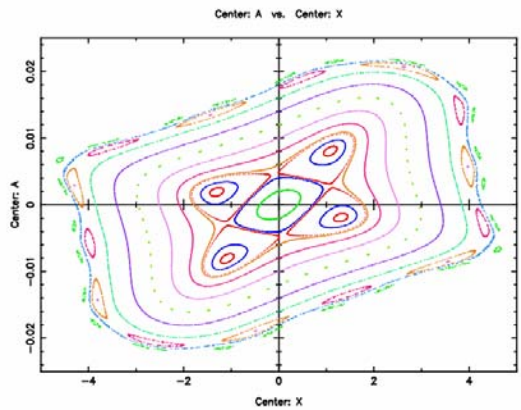

Figure 4: Motion of ions in the phase plane a[rad]-x[mm] for tune Q=0.73. Number of turns N=2000. The shown stable area is around 80π mm*mrad.

Note that even if the area of stable motion in Figure 4 is relatively large, around 80π mm*mrad, the area, in which the motion can be adjusted to be isochronous with high precision, is much smaller, typically an order of magnitude less depending on the requested level of time/mass resolution (see next sections). In practice this means that emittance of a beam injected into the MTOF must match such an 'isochronicity acceptance', otherwise ions travelling at large transverse coordinates, but still stable, will arrive at a detector or separator behind the MTOF with flight times quite different from that of a reference ion thus contributing into unwanted long tails of ToF spectra.

Isochronicity

The ToF deviation δτ of an arbitrary ion undergoing oscillations around optical axis relative to the ToF of a reference ion depends on the number of turns N as follows:

$$\delta\tau = kN + terms\ oscillating\ with\ N \qquad (2)$$

where k is a coefficient depending on initial phase space coordinates. This δτ is minimized together with function (1). Figure 5 gives an example of such behaviour.

The performed MTOF optimization showed, in particular, that for Q=3/4 electrode voltages can be adjusted so that all the ToF optical aberrations up to the 3rd order can be totally eliminated. Such an adjustment, however, is not optimal in comparison with a more general minimization (1), since the 4th and 5th order aberrations can become rather large.

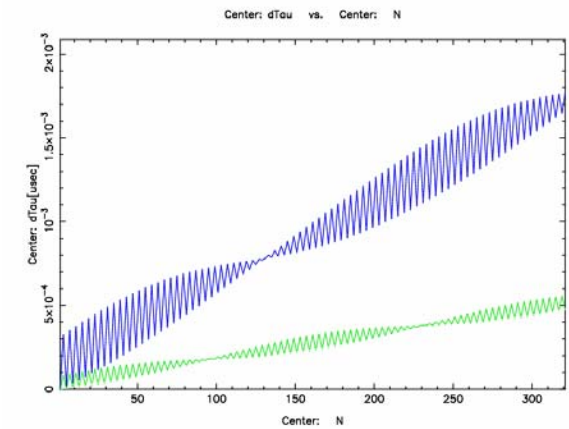

Figure 5: As function of the number of turns N, δτ [μsec] is plotted, the deviation of the ToF of the two ions that are closest to the optical axis in Figure 4 relative to that of a reference ion.

Time Spread per Turn versus Beam Emittance

Using the above described numerical techniques, one can estimate the r.m.s. time spread δT that ions gain per turn (starting from and arriving at the same point in the middle of the MTOF) due to the dependency (2). Figure 6

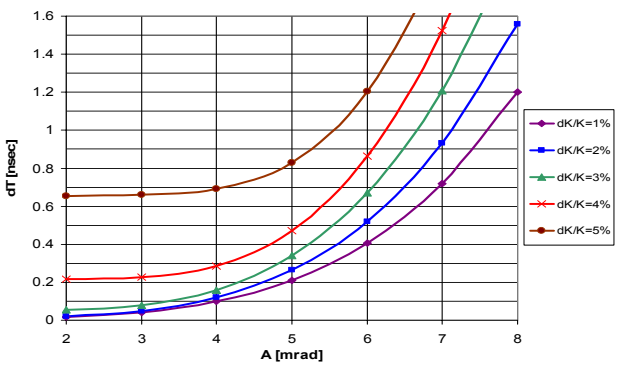

Figure 6: The MTOF time spread per turn versus beam r.m.s. angle ±A for different r.m.s. energy spreads δ=±dK/K and r.m.s. X=±1.5mm. (Beam energy K=1.5kV, mass A=100 a.m.u., period T_0=51.8μs.)

shows this δT as a function of the r.m.s. beam parameters for a beam energy of 1.5kV and a period of longitudinal oscillations of T_0=51.8μs. From this δT one finds an upper limit of the achievable mass resolving power $R_{m,max}=0.5T_0/\delta T$, while for a realistic resolving power one must take into account also other sources for time spreads like the initial time spread in an ion source or instabilities of power supplies. They also limit the resulting mass resolving power. The discussion of these matters are, however, beyond the goal of this paper.

CONCLUSION

The performed simulations demonstrated the importance of the optimization of the isochronous properties of a multi-pass system with respect to all phase space coordinates, not only to the energy deviation. Minimizing higher order (the 4th and 5th) ToF aberrations is essential to achieve high values of mass resolving powers. Additionally, transverse stability issues have been investigated.

REFERENCES

[1] H. Wollnik and A. Casares, "An Energy-Isochronous Multi-Pass Time-of-Flight Mass Spectrometer Consisting of Two Coaxial Electrostatic Mirrors", Int. J. Mass Spectrom. 227 (2003) 217.

[2] H. Wollnik et al., "Multi-Pass Time of Flight Spectrometers of High Resolving Power", Nucl. Instr. and Meth. A519 (2004) 373.

[3] H. Wollnik, "Optics of Charged Particles", Academic Press, New York, 1987.

[4] H. Wollnik and M. Berz, "Image Aberrations for Beams Filling Elliptical Phase-Space Areas or Volumes", Nucl. Instr. and Meth. A263 (1988) 280.

[5] H. Wollnik, M. Svedentsov, M. Yavor, private communication.

[6] A. Kalimov, M. Svedentsov, private communication.

[7] F. Neri, "Lie Algebras and Canonical Integration", Dept. of Physics, Univ. of Maryland, preprint (1987).