Simulation of ion trajectories in an electrostatic Bessel-box type energy filter

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Introduction

The Bessel-box is a kinetic energy filter, first introduced in 1976 by Allen et al. Herein a beam of charged particles with a certain kinetic energy distribution enters a cylindrical electrode through a pinhole entrance. The beam is deflected from its straight path through the cylinder by a small center electrode. Consequently, only particles with a kinetic energy matching the forces of the electrical field inside the box follow a trajectory around the center plate and can leave the Bessel-box through a second pinhole in the exit electrode. This energy filter is used, e.g., by Hiden Analytical, upstream of the quadrupole analyzer. We present numerical results on the transmission and filter characteristics of this particular Bessel-box.

Methods

The geometry of the Bessel-box under investigation was taken from the user's manual of the HPR60 quadrupole mass spectrometer from Hiden Analytical Ltd.. Electrical fields and corresponding ion trajectories were simulated with Simion 8.1. Custom Lua scripts and python code allowed for automated simulation processing, data visualization and analysis. Each simulation started with an initial ion population of 10 000 singly charged particles with a mass of 3 Da and an evenly distributed initial kinetic energy ranging from 0 to 10 eV.

Goal

- Simulation of ion trajectories inside a Bessel-box type energy filter with SIMION®
- Investigate the relation between the different potentials and ion trajectories, transmission range and transmission width
- Determination of energy distributions of the transmitted ions in dependence of the applied potentials

Geometry

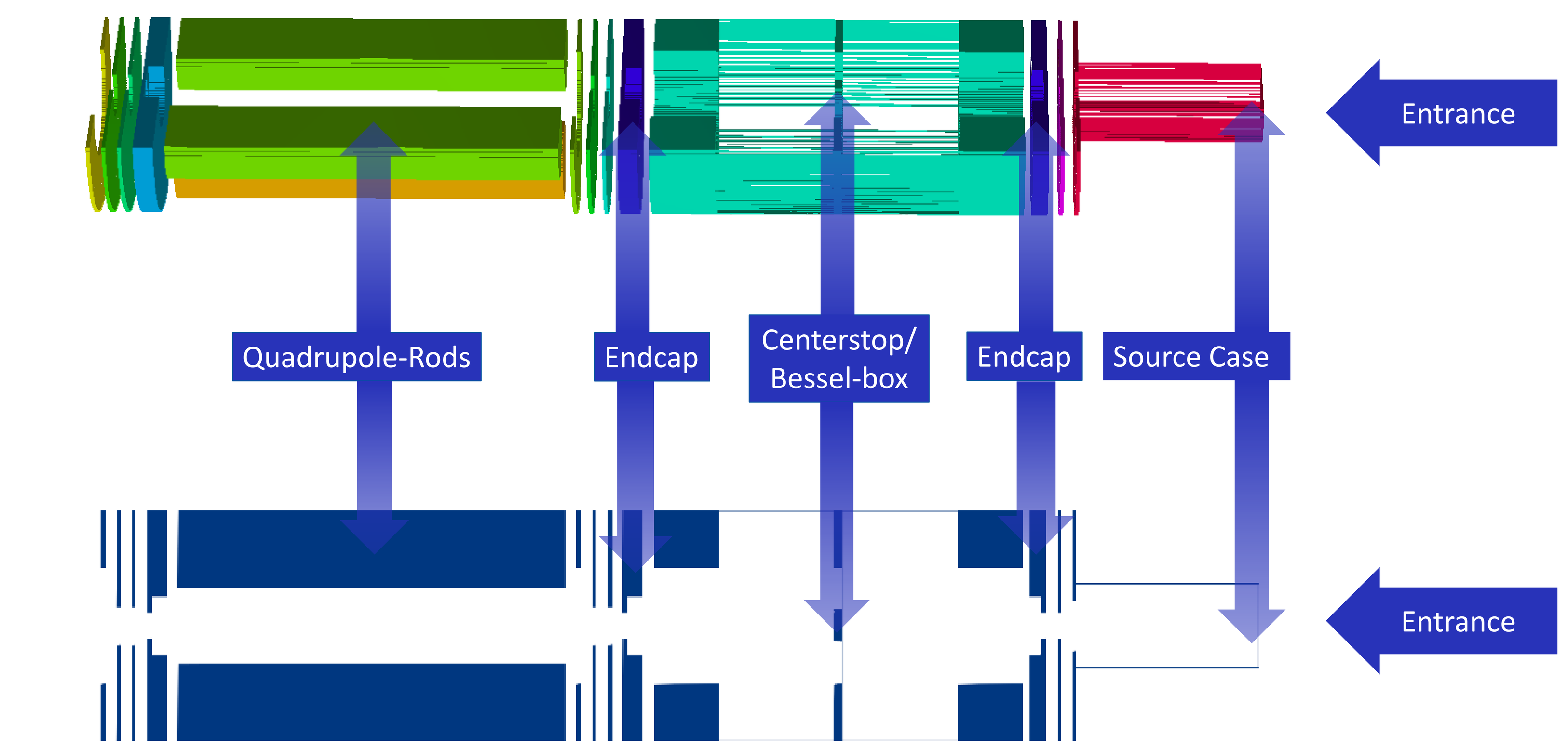


Fig. 1: 3D and 2D schematic drawing of the ion source, simulated bessel-box and subsequent quadrupole analyzer (HPR60, Hiden Analytical Ltd.).

Transmission

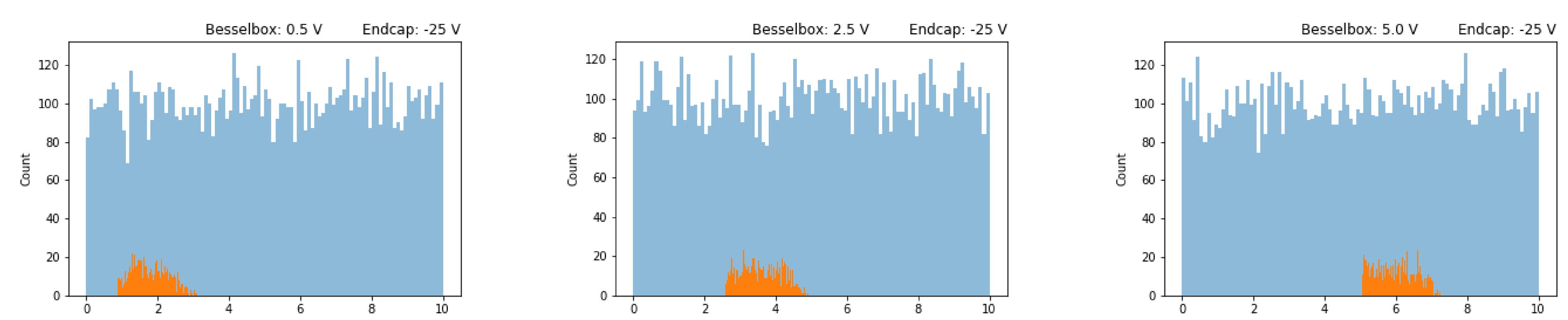


Fig. 7: Kinetic energy (KE) distribution of transmitted ions (orange) in contrast to the KE distribution of all simulated ions (blue) with varying bessel-box voltage at -25 V endcap potential.

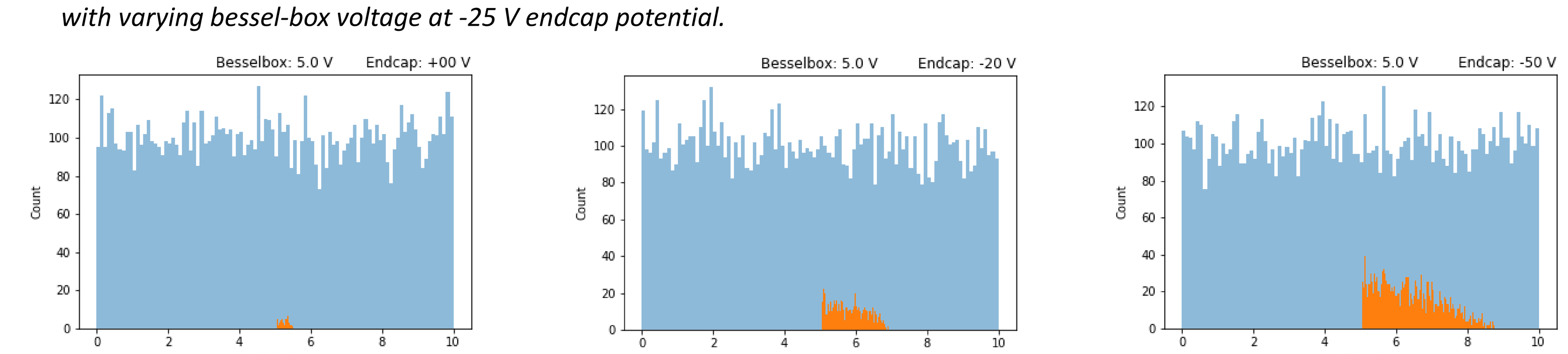
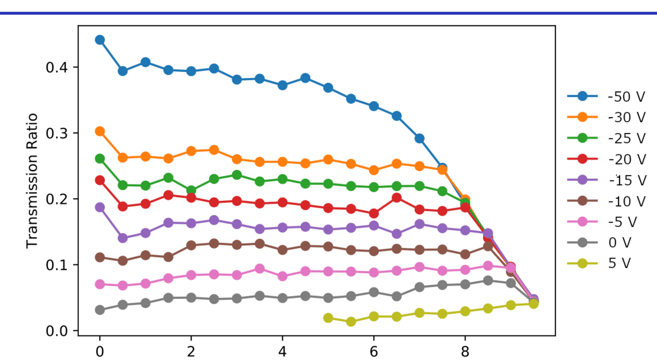


Fig. 8: Kinetic energy distribution of transmitted ions (orange) in contrast to the KE distribution of all simulated ions (blue) with varying endcap voltage at 5 V bessel-box potential.

Fig. 9: Transmission ratio as a function of the bessel-box voltage for different endcap settings.



- the ratio of transmitted ions is virtually ***independent*** of the ***bessel-box voltage***
- the ratio of transmitted ions strongly ***depends*** on the ***endcap voltage***
- bend slope for bessel-box voltages > 8 V due to simulation conditions

Maximal transmitted kinetic energy as measure for the transmission range

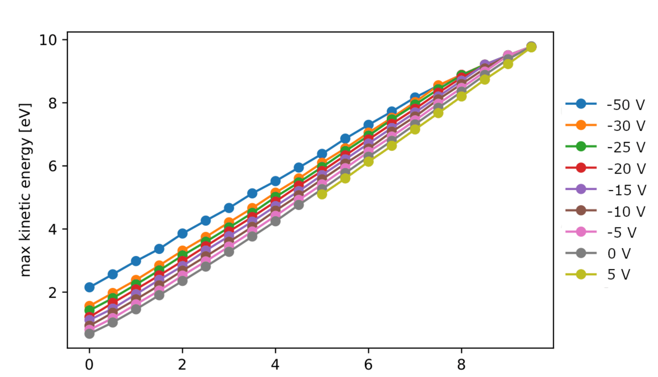


Fig. 10: Maximal transmitted kinetic energy as a function of the Bessel-box potential for several endcap voltages.

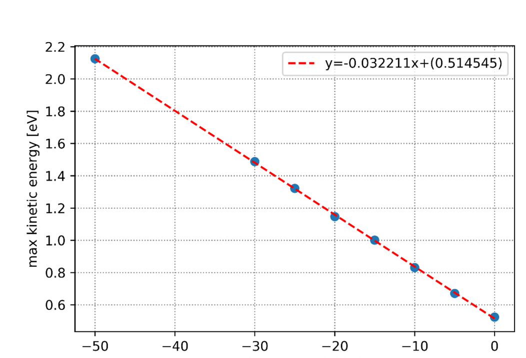


Fig. 11: Maximal transmitted kinetic energy as a function of the endcap potential at zero bessel-box voltage (y-intercepts of the fitting functions from Fig. 10).

Potential Dependency

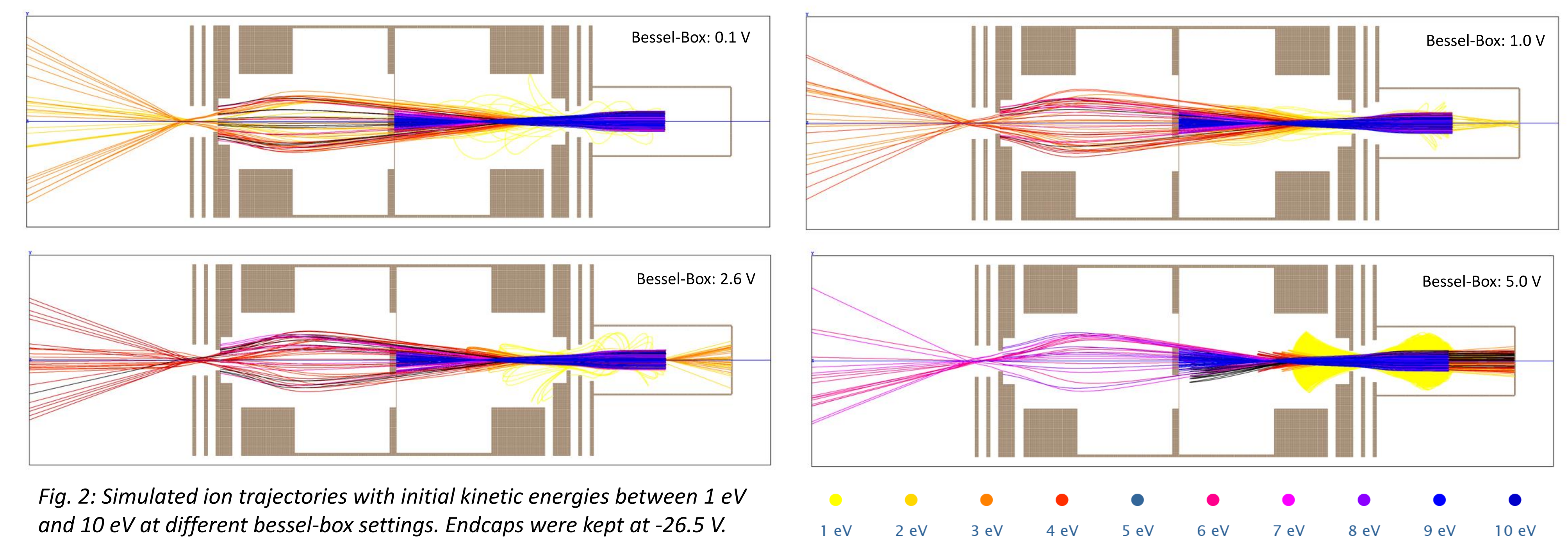


Fig. 2: Simulated ion trajectories with initial kinetic energies between 1 eV and 10 eV at different bessel-box settings. Endcaps were kept at -26.5 V.

Transmission range correlates strongly with bessel-box Potential

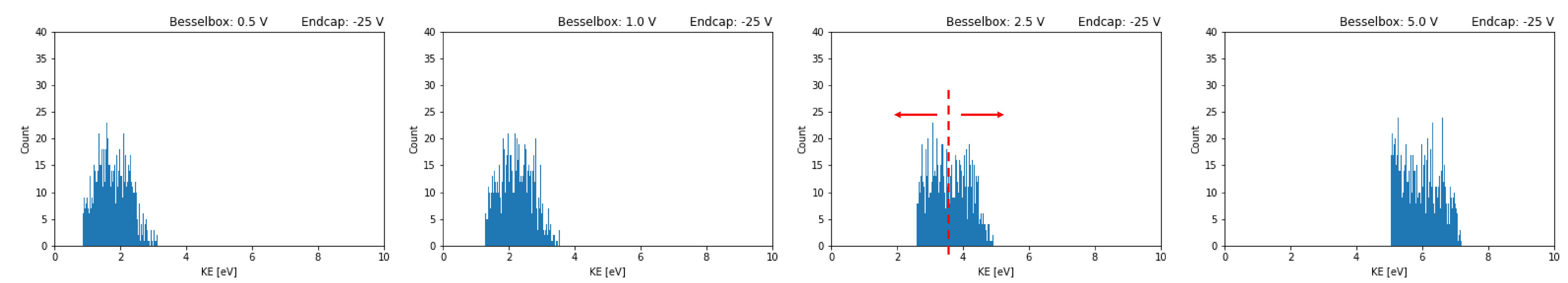
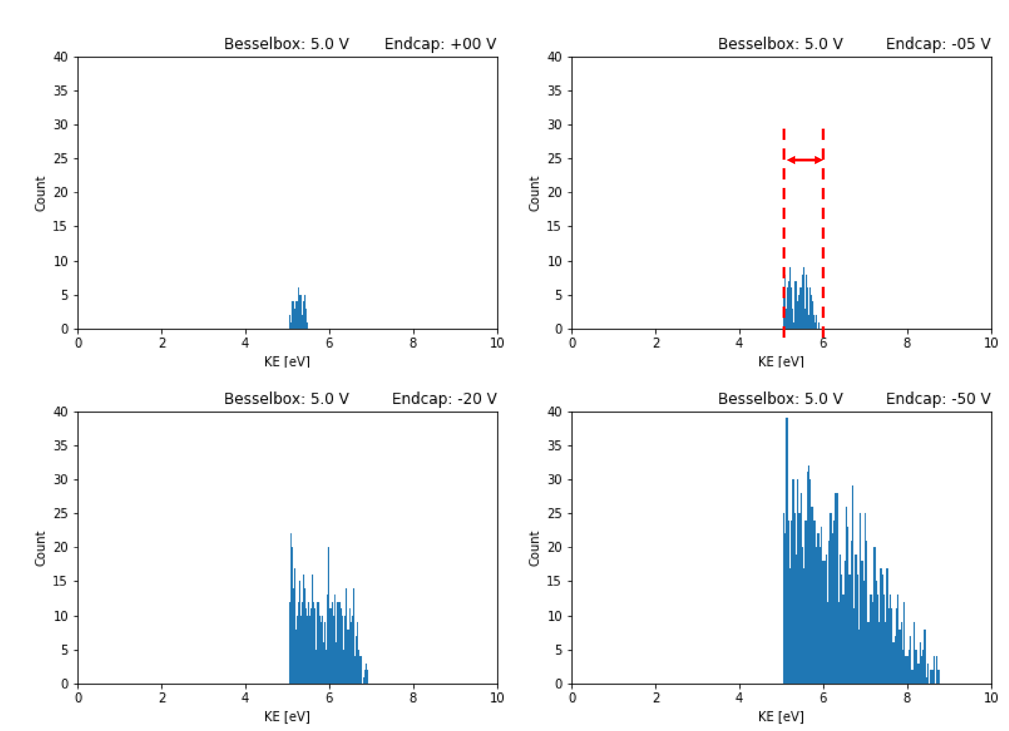


Fig. 3: Initial kinetic energy (KE) distribution of transmitted ions with varying bessel-box settings and -25 V endcap potential.

Transmission width and intensity correlates strongly with Endcap Potential



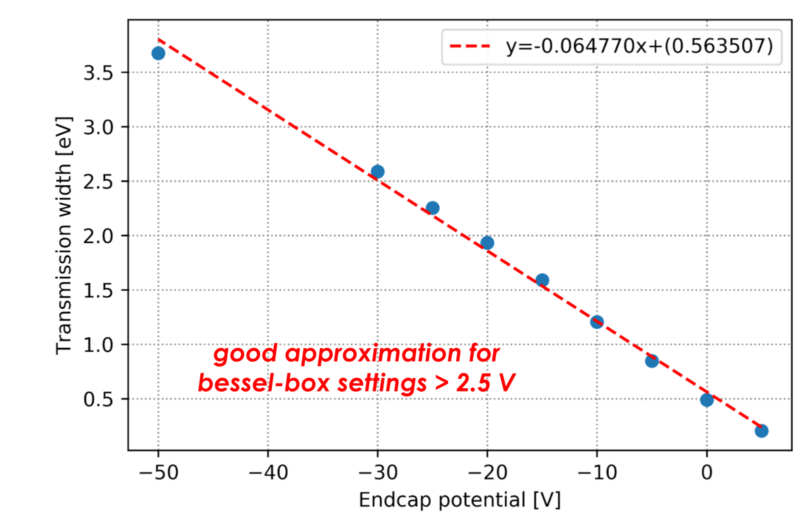


Fig. 4: (above) Kinetic energy (KE) distribution of transmitted ions with constant bessel-box potential. (right) The transmission width as a function of the endcap potential at a fixed bessel-box voltage of 5 V (good approximation for bessel-box seetings >2.5 V).

- Figure 3 depicts the gaussian like distributions for bessel-box settings below 2.5 V.
- The transmission distribution for bessel-box settings at 2.5 V and higher show a clear KE cut off on both sides.

Fig. 6: Transmission width as a function of the endcap voltages for bessel-box settings below 2.5 V.

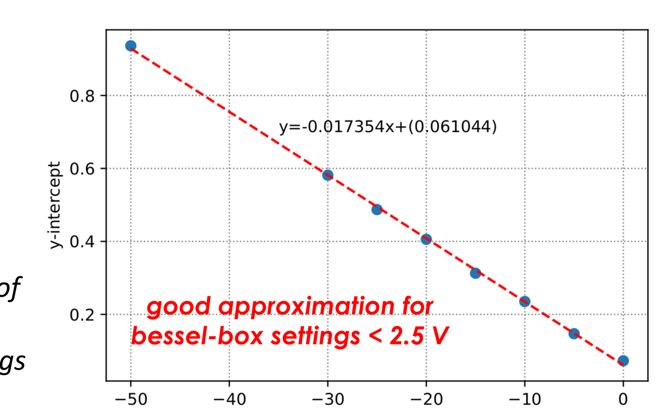
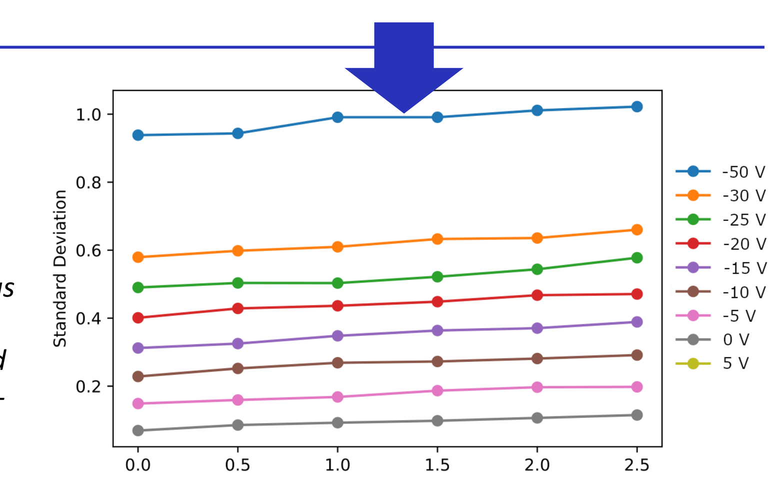


Fig. 5: The standard deviation of the transmission distribution as a measure for the transmission range plotted as a function of the bessel-box voltage for different endcap settings.



Conclusions

- The ***bessel-box voltage*** U_B adjusts the transmitted kinetic energy ***range*** with virtually constant transmission width.
- The transmission ***width*** σ is essentially a linear function of the ***endcap voltage*** U_E for bessel-box voltages $U_B > 2.5V$:

$$\sigma(U_B, U_E) = \begin{cases} 0.0278 \cdot U_B + (-0.0174 \cdot U_E + 00611), & U_B < 2.5\,V \\ 00648 \cdot U_E + 0564, & U_B \geq 2.5\,V \end{cases}$$

- The transmission ***efficiency*** mainly depends on the ***endcap voltage*** and ranges between 5 and 30%.
- Fitted functional correlation between the high energy cut-off of the transmitted energy range and U_B/U_E:

$$E_{kin}[eV](U_B, U_E) = 0.937 \cdot U_B + (-0.0322 \cdot U_E + 0.5146)$$

Outlook

- Additional simulation of the subsequent quadrupole geometry.
- Simulation of the overall ion transmission efficiency (bessel-box and analyzer).
- Experimental validation of the simulated results.

Literature

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Acknowledgement

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