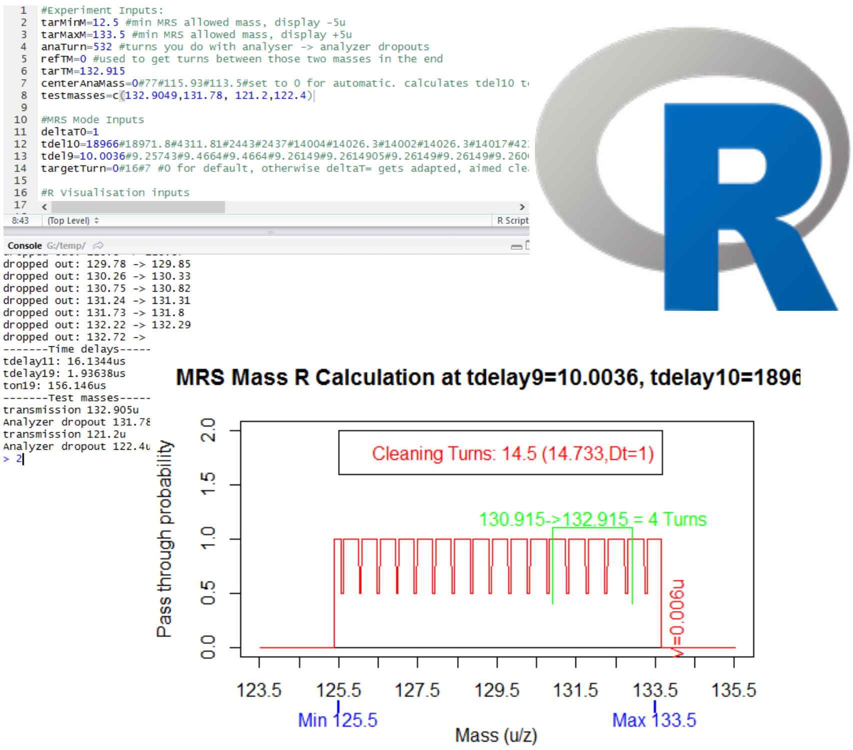
Mass Range Selector Settings

Manual for the R Script MRS.R

By Julian Bergmann

2017-11-01



```
#Experiment Inputs:
tarMinM=12.5 #min MRS allowed mass, display -5u
tarMaxM=133.5 #min MRS allowed mass, display +5u
anaTurn=532 #turns you do with analyser -> analyzer dropouts
refTM=0 #used to get turns between those two masses in the end
tarTM=132.915
centerAnaMass=0#77#115.93#113.5#set to 0 for automatic. calculates tdel10 t
testmasses=c(132.9049,131.78, 121.2,122.4)

#MRS Mode Inputs
deltaT0=1
tdel10=18966#18971.8#4311.81#2443#2437#14004#14026.3#14002#14026.3#14017#42
tdel9=10.0036#9.25743#9.4664#9.4664#9.26149#9.2614905#9.26149#9.26149#9.260
targetTurn=0#16#7 #0 for default, otherwise deltaT= gets adapted, aimed cle

#R Visualisation inputs
```

```
dropped out: 129.78 -> 129.85
dropped out: 130.26 -> 130.33
dropped out: 130.75 -> 130.82
dropped out: 131.24 -> 131.31
dropped out: 131.73 -> 131.8
dropped out: 132.22 -> 132.29
dropped out: 132.72 ->
-------Time delays-----
tdelay11: 16.1344us
tdelay19: 1.93638us
ton19: 156.146us
-------Test masses-----
transmission 132.905u
Analyzer dropout 131.78
transmission 121.2u
Analyzer dropout 122.4u
> 2
```

Contents

1 Introduction

This manual is divided into two parts. The first part will give a short overview about the use and using the R script for the MRS (Mass Range Selector) Settings. The second part will explain the basic concept behind the script.

This script can do three major things:

1. Calculate the timings for the MRS, so only a certain mass range passes the analyzer
2. Check for when the analyzer opens which masses will be dropped out due to reflector pulsing
3. visualize the transmitted masses

Coming from those points, there are additional features the script provides:

- determine the number of turns a mass has taken
- target a specific amount of cleaning cycles or delay time
- center a mass in the analyzer, scaling up for multiple turns

Throughout this manual the term *Cleaning Cycle* will refer to a full turn (regarding to an ion) inside of the analyzer. The MRS is supposed to cut two times during a cleaning cycle, since the ions pass it first in one and half a turn later in the other direction.

2 Using the script

2.1 Executing the script

I recommend *RStudio* to run the script using the *Source* button or Ctrl+⇧+A. This will give you a tabular view with the script at the top left, the output at the bottom left, the graphical output at the bottom right and a table of all calculated variables at the top right.

Native R will also work, but will miss syntax highlighting, tabular window arrangement and the variable-table. Also, in native R you need to use the command `Source(”path/to/script.mrs”)` to execute the file. You can also open the script in R and execute it by marking everything (Ctrl+A) and pressing Ctrl+R. However, then the output will be spammed by the command lines of the script.

2.2 Parameters

All parameters you will need to change are positioned at the top of the script.

Head		
Version	Date of last change to this file	please mark modified scripts here
triggerFile	file path to .tri file to load	overrides analyser and MRS inputs. ncc, plot settings and test masses are still in effect

Analyzer		
Variable	Description	Comment
anaTurn	Turns of mean target ion in analyzer	Ignored when tdel10 and tdel9 used Mean target ion comes from mean in flight time of tarMinM and tarMaxM or centerAnaMass
tdel10	Time in µs the analyzer stays reflecting after tdel9	Overrides anaTurn. Ignored when centerAnaMass is used
tdel9	Time in µs between ion injection and the ion of interest reaching the center of the analyzer	tdel9+tdel10 after the injection the analyzer is opened. Ignored when centerAnaMass is used.
centerAnaMass	Mass centered in the analyzer at extraction	Overrides tdel9 and Tdel10

MRS		
Variable	Description	Comment
MRS	switch for MRS calculation.	use T (TRUE) or F (FALSE). F will only simulate analyzer cutoff. Mean target mass comes from mean of tarMinM and tarMaxM or centerAnaMass
tarMinM / tarMaxM	Mass range in u you want the MRS to transmit	
deltaT0	time in µs that the MRS is ON per cut	ignored when targetTurn is used
ncc	non cleanin cycles	The number of cycles the MRS waits before starting
targetTurn	number of cleaning cycles to force. deltaT0 will be adapted	overrides deltaT0
mDelta	display parameter. Plot margin in u around mass range	overrides plotMin and plotMax
plotMin	min u for plot display	
plotMax	max u for plot display	

MRS Loading		
Variable	Description	Comment
tdel11	time in µs the MRS is OFF per cut	overrides MRS calculation
tdel19	time in µs the MRS waits after injection to trigger	Gatedelay
ton19	time in µs the MRS active.	Gate ON time

Markings		
Variable	Description	Comment
refTM	Reference mass in u for dropout calculation.	
tarTM	Target mass in u for dropout calculation.	All dropouts between refTM and tarTM will be counted (difference in turn number) and presented
testmasses	List of masses in u that are checked for dropping out	

Constants		
Variable	Description	Comment
step	precision the mass range is checked for cutting	default 0.01 u
CS1t	Time in µs ^{133}Cs needs for one turn in the analyzer	common default values are commented out
CSm	Mass of ^{133}Cs in u	other mass values can be used, if CS1t and CSdel are adapted.
CSdel	Time in µs ^{133}Cs needs after injection to reach the center of the analyzer	common default values are commented out
Ekin	Kinetic energy in eV the ions get at injection.	default: 1300. Used for cutting precision calculation.
fringeFieldSize	MRS fringe field size (one side, along flight axes) in m	default 9 mm (experimental result[1])

---

[1] internal document: MRS Investigation, Julian Bergmann, Samuel Ayet San Andres

2.3 Script Output

The direct output of the script (using `source()`) will look similar to this:

Listing 1: Text output of the MRS script

```
---------------script start---------------
 Clean in Turn 21
 Clean in Turn 21.5
 Clean in Turn 22
 Clean in Turn 22.5
 Clean in Turn 23
 Clean in Turn 23.5
 Clean in Turn 24
 Clean in Turn 24.5
 Clean in Turn 25
 Clean in Turn 25.5
 Clean in Turn 26
 Clean in Turn 26.5
 Clean in Turn 27
 Clean in Turn 27.5
 Clean in Turn 28
 Clean in Turn 28.5
 Clean in Turn 29
 Clean in Turn 29.5
 Clean in Turn 30
 Clean in Turn 30.5
 Clean in Turn 31
 Clean in Turn 31.5
 Clean in Turn 32
 Clean in Turn 32.5
 Clean in Turn 33
 Clean in Turn 33.5
 Clean in Turn 34
 Clean in Turn 34.5
 Clean in Turn 35
--------Analyzer Dropouts--------
 Analyzer dropped out:    100.073 -> 100.119
 Analyzer dropped out:    100.402 -> 100.449
 Analyzer dropped out:    100.734 -> 100.78
MRS contained:   100 -> 100.969
--------Time delays--------
 tdelay11:          5.50119us
 tdelay19:          631.862us
 ton19    :          465.036us
--------Crop Range--------
 Calculated min: 99.3565u
 Calculated max: 101.649u
--------Test masses--------
MRS Dropout        99u
 Transmission      100.5u
MRS Fringe Field          101u
 Analyzer Dropout          100.1u
```

Clean in Turn is mostly a progress message to the user. The last line will also show you, how many cleaning cycles were done. Cleaning cycles is refering to the target ion (mean in fliegt time of tarMinM and tarMaxM) arriving again at the center of the MRS.

Analyzer Dropouts is showing you all mass areas between *refTM* and *tarTM* that are dropped out by the reflector. These areas can be changed by changing tdel9 and tdel10, centerAnaMass or tarMinM and tarMaxM.

Time delays Are the timings you will need to enter into your TTL schematic. *ton19* and *tdelay19* is the MRS Gate (on-time and delay). *tdelay11* is the off time of the MRS per cut. *ton11* is not listed as it is an input parameter (deltaT0). *tdelay9* is the time until the reference mass reaches the center of the MRS and *tdelay10* the time it takes for its turns until the analyzer is opened. *tdelay9* and *tdelay10* are not printed when you set them manually.

Crop Range is the expected mass range after MRS cutting. This might deviate slightly from the target mass range since the MRS is cutting only twice per cleaning cycle.

Test masses is the result of your list at *testmasses*. If the mass comes through, *transmission* is printed, otherwise *dropout*. If the mass is kicked out by the MRS, *MRS dropout* is printed. If the reflector is kicking it out, *Analyzer dropout* is printed.

2.4 Plot

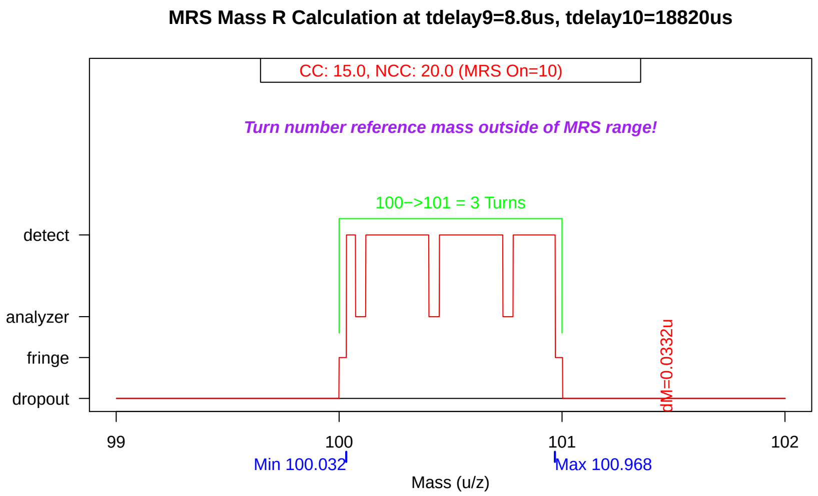


Figure 1: Graphical output of the MRS script.

The plot result gives you an overview about the resulting mass range. The red line shows you the mass transmission. At full height (*detect*) ions are transmitted. Half height (*analyzer*) indicates a loss at the analyzer end cap due to pulsing during opening the analyzer. At quarter height (*fringe*) ions can see the MRS fringe field at its last cutting cycle.

In blue at the bottom you can see the target mass range that you set up. This can differ from the implied mass range in red, since the MRS only cuts on every 0.5 turn. The title contains wether MRS was used and tdelay9 and tdelay10 when fixed or otherwise the target turn number are written. The box inside the plot will show you the cleaning cycles (actual and numerical, since cutting is only possible on half turns) and the ON time of the MRS (Dt in µs).

Inside the plot in green is the specified refTM and tarTM as well as the turn number difference between the two masses. The algorithm effectively counts the ridges between the two masses. This value is only valid when both masses are within the red transmission mass range.

At the right side 90° turned is an estimate for the cutting precision. This value is calculated using the kinetic energy and fringe field size to estimate the time which the maximum mass is seeing the fringe field. This is then converted using the total time of flight into a relative error and then into an absolute error in mass units. See 3.3.5 for more information.

3 Theory

This section describes the concept behind calculating MRS and reflector dropouts in this script.

3.1 Simplification and upscaling

The script makes a couple simplifications.

- the connection between time and mass is $m(t,n) = a\frac{(t-t_0)^2}{(1+b\cdot n)^2}$ with a, b, t_0 calibration parameters and t time of flight, m mass and n turn number.
- t_0 is neglected in the formulas to avoid needing a calibration
- instead of a full calibration, ^{133}Cs is measured in CSdel (time untill middle of MRS) and CS1T (Time per Turn) and all other masses are upscaled based on this.
- the simplified connection is $\frac{t_m}{t_{133_{\mathrm{Cs}}}} = \sqrt{\frac{m}{m_{133_{\mathrm{Cs}}}}}$
- this is used for the delay as well as for the turn time
- the script avoids using absolute ion positions requiring the kinetic energy. It calculates in flight times and relative turns.
- all analyzer timings assume that one reflector is used for injection and the other one for extraction to the detector.

3.2 Reflector dropout

Simulations have shown that ^{133}Cs is staying for 14 %[2] of its time per turn in the ciritcal area of the analyzer. When the analyzer is opened, the reflector that is switched off will temporarly create a electric field, that can kick ions out of their flight trajectory. To check if a mass is inside this region, the script is doing the following:

1. scale up the delay and turn time for this mass with ^{133}Cs:
   $frac_m = \cdot\sqrt{\frac{m}{m_{133_{\mathrm{Cs}}}}}$
   $t_{\mathrm{m,del}} = t_{133_{\mathrm{Cs,del}}} \cdot frac_m$
   $t_{\mathrm{m,1T}} = t_{133_{\mathrm{Cs,1T}}} \cdot frac_m$
2. Determine the time since this mass was doing turns:
   $t_{\mathrm{m,turns}} = tdelay9 + tdelay10 - t_{\mathrm{m,del}}$
3. Determine relative number of turns this mass has done:
   $n_m = \frac{t_{\mathrm{m,turns}}}{t_{\mathrm{m,1T}}}$
4. Check if the current turn is within the critical 14 % section:
   $n_m \bmod 1 \in [\frac{1}{4} - \frac{0.14}{2}, \frac{1}{4} + \frac{0.14}{2}]$

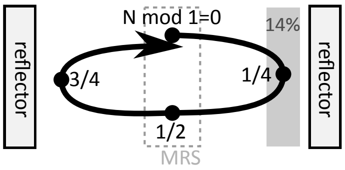


Figure 2: visualization of n_m mod 1 for ions in the analyzer.

3.3 MRS Concept

In this MRS mode the MRS is set to a fixed frequency with a fixed duty time starting at the extraction of the ions into the analyzer. The actual cut at the right mass position is happening only at the last cleaning cycle (turns while the MRS is cutting).

Each cycle the MRS is only dropping out masses that passes it during its ON time. This means that in principle you can start cutting later, but need a longer ON time to avoid letting masses outside the desired mass range through.

---

[2] Timo Dickel, personal conversation

The upside is that you can reach extremly high precision cuts using 1 µs (5% duty time) and need a very low amount of cleaning cycles for a broader mass range (20 u at 150 u in 7 cleaning cycles). The downside is that you need a very high amount of cleaning cycles for very small target areas (120 cleaning cycles for 1 u at 130 u with 1 µs).

An alternative is to use longer ON time and thus cut more on each cycle, reducing the amount of cleaning cycles needed. However, this also means you also loose cutting precision.

A combination of both methods is to start the MRS later with longer ON time, promising a high cutting precision due to the late cutting time and a low amount of cleaning cycles needed due to the high ON time. However, one needs to make sure that ON time and cleaning cycles are sufficient high to kick all unwanted ions out, not just a frame around the wanted mass range.

3.3.1 Amount of cleaning cycles

Using the simplifications and assumptions noted earlier, you can calculate the cleaning cycle at which you only let through your mass range. This is the point in time where the highest mass is just leaving the MRS field while the lowest mass is almost entering again from the same side.

For a reference of the parameters, see chapter 2.2. First we convert the target mass range into a time range, using upscaling from ^{133}Cs for *tdel9* (time till middle of MRS) and *tdel10* (time per turn). Note that t_{min} belongs to *tarMinM*, leading to $t_{min} < t_{max}$.

After the cleaning is done, we want the mass range fill the analyzer unambiguously. For this we focus on the lightest (fastest) ion *tarMinM* and the heaviest (slowest) ion *tarMaxM*. The time per turn for both ions is scaled from *tdel10* $t_{min,T}$ and $t_{max,T}$. To fill the analyzer unambiguously in the last cleaning cycle the fastest ion should be able to fly exactly one turn without being kicked out. This time-range would be exactly $t_{min,T}$. However, since we use the MRS two times during a turn, we only have half the analyzer, leading to a target time range of $\frac{1}{2}t_{min,T}$. Additionally we need to substract the cutting time of the MRS in the last cutting cycle: $\Delta t_{\text{target}} = \frac{1}{2}t_{min,T} - deltaT0$.

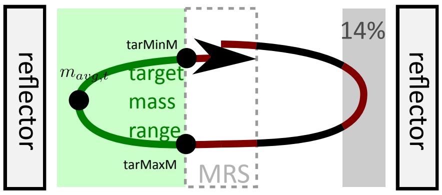


Figure 3: target time range

tarMinM and *tarMaxM* will increase their difference in time (when they would hit the detector) each time when they pass through the center of the analyzer by $\Delta t_{\text{Turn}} = t_{max,T} - t_{min,T}$. When they reach the analyzer they already have a spread of $\Delta t_{\text{initial}} = t_{max,del} - t_{min,del}$. By dividing the difference between the initial time spread and the target time spread by the time spread increase per turn, we can calculate the amount of cleaning cycles:

$$N_{\text{cleaning}} = \frac{\Delta t_{\text{target}} - \Delta t_{\text{initial}}}{\Delta t_{\text{Turn}}} = \frac{\frac{1}{2}t_{min,T} - deltaT0 - (t_{max,del} - t_{min,del})}{(t_{max,T} - t_{min,T})}$$

What is left is to align the MRS with the target window.

3.3.2 MRS Frequency and Phase

To make sure that the off time is done at the correct timing, we need to synchronize the MRS' frequency with a virtual ion that would be flying at the center of our desired time range (not the average mass).

This virtual ion $m_{t,avg}$ would need the average time per half turn of *tarMinM* and *tarMaxM*:

$$t_{avg,T} = \frac{1}{2} \cdot (t_{min,T} + t_{max,T})$$

Since the ON-time of the MRS was an input parameter (deltaT0), what is left to calculate is the OFF-time (tdel11) to sync its frequency to $m_{avg,t}$:

$$\text{tdel11} = \frac{1}{2} \cdot t_{avg,T} - \text{deltaT0} = \frac{1}{4} \cdot (t_{min,T} + t_{max,T}) - \text{deltaT0}$$

Now we need to make sure that the MRS starts at the correct time. This point in time is reached, when $m_{avg,t}$ first reaches the center of the extraction reflector. At this time $m_{avg,t}$ is the furthest away of the MRS and the resulting time range gets cut symmetrically around it.

$$t_{avg,del} = \frac{1}{2}(t_{min,del} + t_{max,del})$$

$$t_{avg,ref} = t_{avg,del} + \frac{1}{4} t_{avg,T} = t_{avg,del} + \frac{1}{8} \cdot (t_{min,T} + t_{max,T})$$

However, since the MRS will start with its delay after triggered, we need to subtract its delay time (tdel11) in addition from its triggering point. To realize this, we set the MRS gate delay:

$$\text{tdel19} = t_{avg,ref} - tdel11 = t_{avg,del} - \frac{1}{8} \cdot (t_{min,T} + t_{max,T}) + \text{deltaT0}$$

The cleaning cycles can be set by the on time of the MRS-gate:

$$\text{tdel19} = N_{\text{cleaning}} \cdot t_{avg,T}$$

3.3.3 Analyzer Timings

If the script is supposed to calculate tdelay9 and tdelay10 it will align m_{avg} at the center of the reflector that is opposing the one used for extraction. This ensures that the center of the transmitted mass range is not disturbed by the pulsing extraction field.

$$\text{tdelay9} = t_{avg,del}$$
$$\text{tdelay10} = t_{avg,T} \cdot \left(\text{anaTurn} - \frac{1}{4}\right)$$

3.3.4 Sampling

This chapter describes how the script is actually checking for MRS transition.

The script samples the mass range and checks on each cleaning cycle which mass to drop out. Each cleaning cycle the ion's distance to the time range center is checked and compared to the maximum time range the MRS would let through. If this maximum is exceeded, the mass is cut out. Since target time range is positioned in a way that the time range center is at a reflector, anything that is outside the target mass range will be in the MRS. Ions that are even beyond the MRS will be treated as if they have done half a turn less and remain in the time range.

Each cleaning cycle (n) the time difference (Δt_i) between the time range center (t_{avg}) and each sample (m_i) in the displayed mass range is calculated:

$$t_{avg} = t_{avg,T} \cdot n + t_{avg,del}$$

$$t_i = \sqrt{\frac{m_i}{m_{^{133}\text{Cs}}}} \cdot (t_{^{133}\text{Cs},T} \cdot n + t_{^{133}\text{Cs},del})$$

$$\Delta t_i = |t_{avg} - t_i|$$

To get rid of the problem of ions having done different amount of turn numbers within a cleaning cycle, we use the modulo operator. By calculating the modulo of Δt_i to half of the cycle time of our time range center ion, we get an indicator how far away m_i is from our time range, or if it entered it again within this cleaning cycle. Now we just need to compare this value with half the time the MRS is not cutting for the final time range:

$$b_i = \Delta t_i \mod \frac{1}{2} \cdot t_{avg,T} \geq \frac{1}{2} \cdot tdel11$$

b_i is a boolean indicator (true/false) whether the condition is true and indicates if an ion is transmitted (true) or kicked out (false).

In addition there is a condition to skip the check at cleaning cycle 0.5, since that would also kick out ions that haven't reached the MRS yet. Since ions would need to do a full turn until extraction anyway and the main (precise) cutting is done in the last cleaning cycle, this simplification has no negative influence on the plot result.

For this check, it is assumed that the gate delay and MRS frequency is set correctly. A wrong values would not make a difference in the plotted result, but would shift or completely block the resulting time range in the actual MRS.

3.3.5 Precision–estimate

For estimating cutting precision it is assumed that ions seeing the MRS' fringe field are in an undefined state of transmission. Since the MRS cuts the mass range further in every cleaning cycle, the precision error of former cleaning cycles is neglectable.

From Measurements [3] the fringe field size (at one side of the MRS) was deduced to be $x_{\text{fringe}} = 9\,\text{mm}$. With the ion's kinetic energy and mass one can now calculate the time they need to traverse the fringe field:

$$\begin{aligned} \text{Ekin} = \frac{1}{2} \cdot \text{tarMaxM} \cdot v_m^2 \quad &\Rightarrow v_m = \sqrt{\frac{2 \cdot \text{Ekin}}{\text{tarMaxM}}} \\ t_{\text{fringe}} &= \frac{x_{\text{fringe}}}{v_m} \end{aligned}$$

Now the precision in mass units is deduced by converting this value into a value relative to the total time of flight. This can then be converted to mass units using the relationship of $m \propto t^2$:

$$\begin{aligned} t_{\text{tot}} &= \text{tdel9} + \text{tdel10} \\ R_{\text{fringe}} &= \frac{t_{\text{tot}}}{2 \cdot t_{\text{fringe}}} = \frac{tarMaxM}{\delta m_{\text{max,fringe}}} \\ \text{dM} = \delta m_{\text{max,fringe}} &= \frac{tarMaxM}{R_{\text{fringe}}} \end{aligned}$$

3.3.6 Fringe fields

The electrical field on each side of the MRS will exponentially decrease after the electrodes end. Ions that reside in this field during switching the MRS on or off will experience small to large shifts in flight time or get completely kicked out. If this happens in an early cleaning cycle, influenced ions will be cut out in the nect cleaning cycle. As a result, only ions influenced during the last cleaning cycle will actually show influenced behavior. For this reason this region is calculated only for the last cleaning cycle and then displayed in the plot.

The fringe field size was measured in an experiment where the gate delay was stepwise increased to measure the effect of half an MRS cleaning cycle (one cut) on a fixed Mass (^{133}Cs). The fringe field effect

---

[3] *MRS Investigation*, internal paper, 2017-07, Julian Bergmann, Samuel Ayet San Andres

was shown as the slope between transmission and loss of those ions. With the kinetic energy known the field size was calculated to be around 9 mm. With the scaling methods mentioned before, this length is converted into flight time for ions at the maximum of the mass range.

3.4 Outlook

Things that can be improved:

- scaling formulas with $t_0 \neq 0$
- better estimation of field size and cutting precision
- switching between fast cutting (low cleaning cycles) and precice cutting mode
- check for scalability on different devices