

THE IMS1270 CIPS USER'S MANUAL (3)
Appendices

Customizable Ion Probe Software

Version 4.0

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12. Appendices

12.1 Appendix 1: The EM Physical principles

12.1.1 Overview

The IMS 1270 is equipped with electron multipliers (EM) working in a direct pulse counting mode.

- An AF150H EM, manufactured by ETP is mounted on the main axial detection block. It is made of 21 active film dynodes.
- The multicollector trolleys are equipped with R4146 EM, manufactured by Hamamatsu. R4146 is made of 16 CuBeO dynodes.
- The multicollector trolleys can also be equipped with ETP AF151H, smaller than AF150H, with only 19 dynodes.

A secondary ion striking the first dynode (conversion dynode) of the EM induces a secondary electron emission. Then, these electrons are accelerated through the successive dynode stages in order to amplify the secondary electron current. A *gain* (mean number of electron per secondary ions) of about 10^8 is obtained. For most of the secondary ions reaching the detector, a charge pulse is produced at the last dynode output. The charge amplitude is converted in voltage, and the pulse amplitude, in Volt is proportionnal to the EM gain. Note that some incident ions do not produce any signal at the EM output (See below the sections § [EM output and discriminator threshold](#)).

It may occur that two or more ions impinge the EM first dynode within a time interval small enough to be detected as a single ion. This effect is known as EM dead time and is developed in the section § [Dead time and Yield corrections. Dependance on the gating](#).

The amplitude of every pulse is randomly distributed according to a distribution law currently displayed by the *PHA Distribution Curve* (PHA states for Pulse Height Amplitude). The knowledge of this distribution is therefore very helpful to optimize the setting of the EM High Voltage (HV), and Threshold (See the section § [EM output and discriminator threshold](#)). Checking this curve shape also used for controlling the EM aging (See the section § [EM aging](#)).

12.1.2 EM output and discriminator threshold

Definitions

Due to the statistical variation of the secondary electron emission, every secondary ion reaching the first dynode of the electron multiplier does not produce the same number of electrons. Note that the percentage of those producing at least one electron is called **DQE** (Detection Quantum Efficiency).

More generally, the *ion/electron conversion efficiency* corresponds to the response of the first dynode. It includes the *DQE*, and the *P(k)* distribution law which gives the

probability for one ion to produce k electrons. The *ion/electron conversion efficiency* depends on the incident ion features: mass, velocity and nature (single or molecular) species.

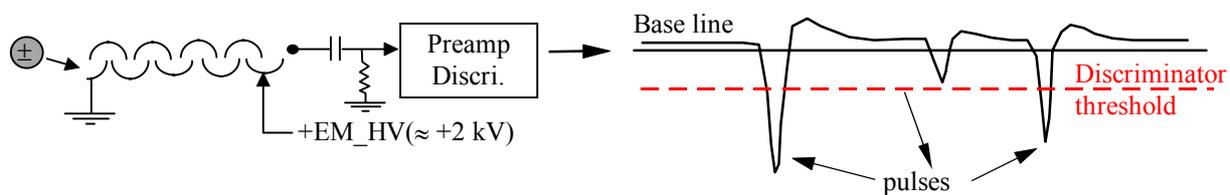
The **EM gain** is the ratio between the electron output current and the ion input current. It involves both the first dynode *ion/electron conversion efficiency* and the other dynodes amplification effect. This last amplification depends on the *EM HV* and also on the EM age.

The **PHA distribution** is the probability $P(V)$ for an EM output pulse to have a voltage amplitude V . As the EM gain, it depends also on both the first dynode *ion/electron conversion efficiency* and the other dynode amplification effect.

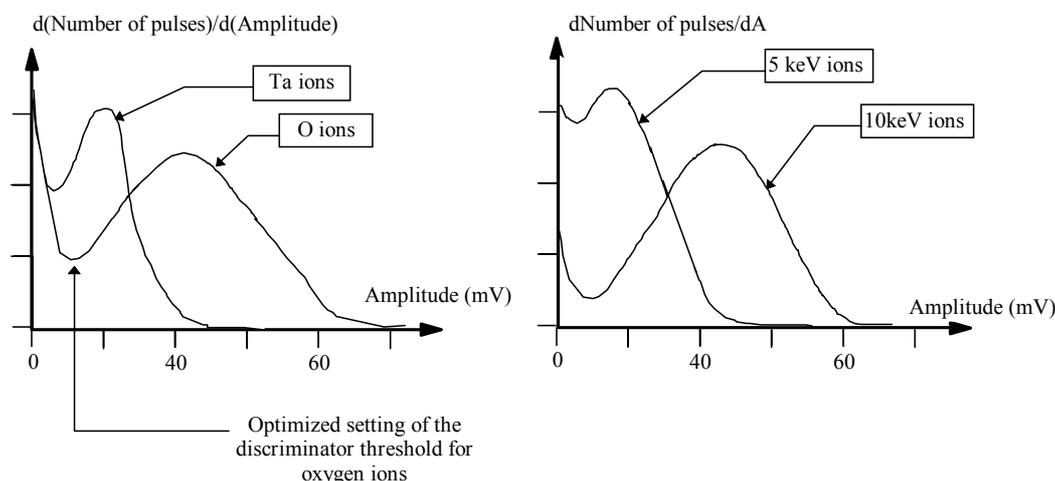
The **EM Yield** is the ratio between the number of output pulses counted after the EM discriminator (see below) and the number of incident ions.

The EM detection channel

The first electrons produced by the first dynode when impinged by an ion are amplified by the successive stages the electron multiplier with a gain in the range of 10^8 (EM gain). As it is displayed on a PHA distribution curve, the pulses detected at the EM output do not have the same amplitude (see the figure below). A preamplifier converts the charge pulses into voltage pulses and amplifies them. Then, a discriminator selects the pulses larger than a given *threshold*.



Typical PHA distribution curve



The large number of pulses with a small amplitude (first part of the pulse amplitude distribution) are due to the system noise. These pulses are therefore eliminated by using a discriminator with an adjustable threshold. The setting of the threshold is the result of an optimization which minimizes the *EM background* (typically < 5 counts/mn) and to EM detection efficiency (number of counted pulses per secondary ion). This optimized threshold corresponds to the first minimum of the *PHA distribution curve*. For displaying a *PHA curve*, See the main *CIPS user's manual*, § *Tools/The EM PHA*

Note that, for instance, when the secondary ion extraction voltage is varied the discriminator threshold should be re-adjusted in order to work under optimized conditions.

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12.1.3 Dead time and Yield corrections. Dependence on the gating

Dead time τ

At a given accuracy, the highest secondary ion intensity which can be measured is limited by the time resolution of the pulse counting system. The so-called *dead time* of the pulse counting system is the time spent after each event before being able to detect the next one.

Let N_c the number of counted pulses per second at the pulse counting system, and τ the dead time of this system. Assuming that the system was unabled during $N_c * \tau$, it is possible to deduce the *EM* output count rate N'

$$N' = \frac{N_c}{1 - N_c * \tau}$$

This is the basic dead time correction formula. For a dead time of 25 ns and a true pulse rate of 10^6 pulse/s, a dead time correction of 2.4 % must be applied to the counted rate. As it can be easily corrected by a mathematical formula, the EM dead time is not an instrument limitation, providing τ is precisely known. That is why a delay line circuit is implemented on the discriminator board. Switches on this PCB allow to set the dead time (See the *User's guide for Multicollector*)

EM detection Yield Y_{EM}

The *EM* detection Yield Y_{EM} is defined as

$$Y_{EM} = (EM \text{ output pulse rate} / EM \text{ input ion rate})$$

It can be measured on the instrument by comparing the measured EM count rate and the FCs count rate in the range of 10^6 c/s.

$$N = Y_{EM} * N'$$

$$N = Y_{EM} * \frac{N_c}{1 - N_c * \tau}$$

The deadtime correction depends also on the gating

Some analyses may be achieved with an optical or an electronic gating. It consists of rastering the primary spot and masking (either by optical means or by electronic means) the secondary ions generated outside of a central zone of the rastered frame. It is worth to emphasize that whenever either *optical* or *electronical* gating is set. The instantaneous count rate, within the gate, can be much larger than the measured count rate averaged over a frame. The dead time correction must therefore take into account the ratio η_{GATE}

$$N = \frac{I}{Y_{EM}} * \frac{N_c}{1 - \frac{N_c}{\eta_{GATE}} * \tau}$$

The ratio η_{GATE} is the area ratio gate/frame, so that N_C/η_{GATE} is actually the instantaneous count rate since N_C is the count rate averaged over the whole frame while all the counts occur only over the gate.

For determining η_{GATE} , both electrical and optical gate must be considered.

- In the electrical gate case, the calculation of η_{GATE} is quite straight. For example, if the electrical gate is determined as a square of $p \times p$ pixels within the 1024×1024 frame.

$$\eta_{GATE} = \frac{p * p}{1024 * 1024}$$

- In the optical gate case, both the *raster size* and the *Analysed area* must be correctly calibrated. The *raster size* is defined as the scanned field size, in μm at the sample plane in the case of a punctual primary spot. The *Normal Area* is defined as the sample field diameter limited by the *Normal field aperture size*. So, the *Analysed area* is simply defined as

$$\text{Analysed Area} = \frac{\text{Field Aperture size}}{\text{Normal field aperture size}} * \text{Normal Area}$$

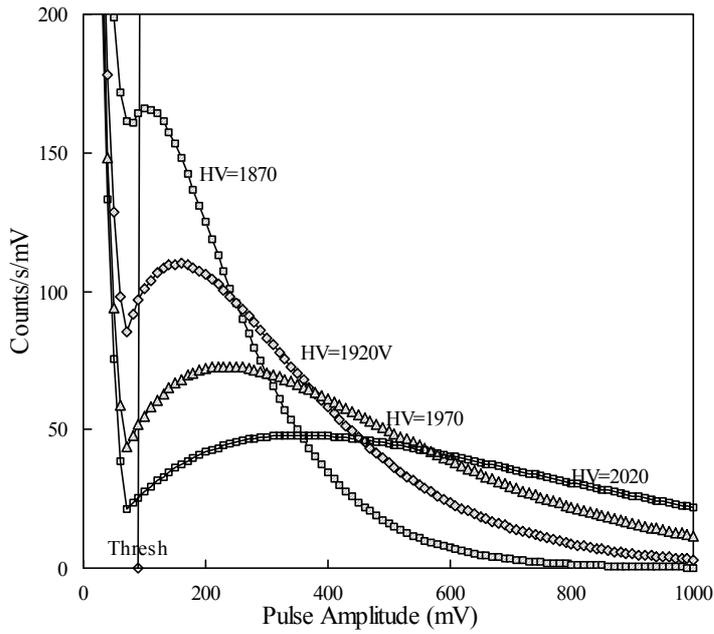
$$\eta_{GATE} = \frac{\text{Analysed Area}}{\text{Raster Size}}$$

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12.1.4 EM aging

When an EM is getting older the EM gain (*output electrons per ion*) decreases, leading to a Y_{EM} decrease if the EM HV is kept constant. For recovering the original gain and yield, The EM HV must be increased (See the figure below)

Note that the life time of an electron multiplier depends on the gain and the total number of ions counted (total integrated charge). Frequent high intensity measurements shorten the EM life time.



THE EM PHA Distribution Curve

The PHA distribution curve is obtained by scanning the discriminator voltage from 0 to 1000 mV. The obtained curve is then derivated.

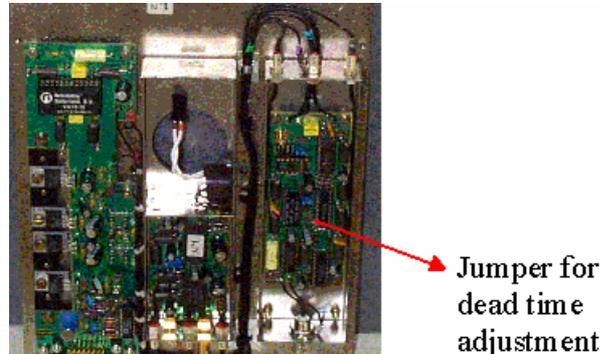
Different plotted curves correspond to different EM high Voltages.

The aging effect is equivalent to an EM HV decrease so that the aging must be compensated by increasing the HV Voltage.

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12.1.5 The EM electronic dead time adjustment

The preamplifier / discriminator assembly is shown in the hereunder image. It can be noticed that the preamplifier and the discriminator are independently shielded in order to reduce the electronic noise of the overall system.



The dead time value is adjustable by positioning a jumper. The available dead time values are : 20, 24, 28, 36, and 40 ns.. The jumper label on the board is TB2. The jumper position corresponding to 20 ns is at the top. The dead time value is the sum of the delay time (determine by the delay line) and the extra time for the signal propagation.

$$\text{Dead Time} = 2 * \text{delay_line} + 4\text{ns (propagation time)}$$

Dead time (ns)	Delay line (ns)	Jumper position
20	8	1 (top)
24	10	2
28	12	3
36	16	4
40	18	5 (bottom)

For most of the applications the jumper position #2 is recommended.

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12.2 Appendix 2: The EM drift correction principles

12.2.1 Introduction

12.2.1.1 Overview

The EM Y_{em} Yield is the *counted electrons/incident ions* ratio. As a matter of fact, Y_{em} corresponds to the rated working discriminator threshold which is called *Thr1* in this document. It is wellknown that Y_{em} drifts down along the time when yhe incident ion rate is large. This is a big issue in the case of an isotopic ratio measurement achieved in the multicollecion mode, since the different EMs, which received different ion intensity, will not drift at the same rate.

The first approach in order to by-pass this drift effect is to run frequently a standard sample, but a counterpart of this method is to require a motion of the sample holder.

Moreover, a high precision of the drift estimate requires for the standard measurement duration to be practically as long as the sample measurement.

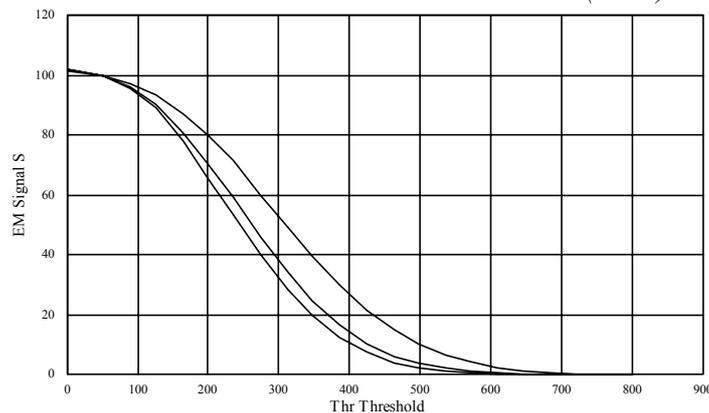
The method which is considered in this section is an intrinsic measurement of a given EM drift, targetted for correcting the data. Typically, along a one hour analysis, drift measurement could be run automatically every 6 minutes, and the data acquired during the last six minutes would be corrected, by taking into account the drift measurement.

The correction method is derived from a model taking into account the assumption that the EM drift is basically an homothetic shrinking of the curve $S=f(Thr)$ which is easily recorded by scanning the threshold Thr and measuring the EM signal S . The drift phenomena transforms $S=f(Thr)$ into $S=f(k*Thr)$, $k>1$. What is usually called *PHA* is the derivative of $S=f(Thr)$.

The method main idea is to measure the shrinking k , not at the working threshold $Thr1$, since the S variation is very low in its neighbourhood, but at $Thr3$, a threshold such as $S(Thr3)$ is close to $S(Thr1)/2$. the method is therefore insensitive to any incident ion beam drift, resulting from a primary beam drift or any other cause.

12.2.1.2 Example of EM drift measurement

The 3 $S(Thr)$ curves plotted hereunder have been recorded on an IMS1270 multicollector R4146 EM. These curves are normalized so that $S(Thr1)=100$.



Init (left hand side) is the curve recorded at the time t_0 , while *Drift1* (middle) was recorded at t_0+1 hour and *Drift2* (right hand side) at t_0+3 hours. The ion rate was several hundred of thousands counts per seconds. This plot shows that obviously, the shrinking k can be measured easily in the middle region while it would be more tricky at the neighbourhood of $Thr1=50$.

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12.2.2 Processing

12.2.2.1 Introduction

The different processing stages are presented hereunder. This processing requires a limited number of measurement points,

On présente ci-dessous les différentes phases du traitement. Ces différentes phases ne requièrent qu'un nombre limité de points de mesures (S , Thr), mais à chaque étape, pour justifier et discuter le traitement proposé, on est amené à considérer l'ensemble des courbes $S(Thr)$ qui ont été présentées en guise d'exemple.

Pour coder le traitement, il suffit de lire les sections (description du traitement)

12.2.2.2 Before analysis, $S(Thr)$ overall featuring σ and α calculation

12.2.2.2.1 Processing Description

$Thr1$ is the *working* threshold, set during an analysis.

$Thr3$ is a threshold such as $S(Thr3)$ is close to $S(Thr1)/2$.

$Thr4$ is a threshold slightly larger than $Thr3$. (Typ, $Thr4=1.11*Thr3$)

- $S1=S(Thr3)$, $S1=S(Thr3)$, $S4=S(Thr4)$, $S3$ and $S4$ are normalized at $S1=100$.
- σ et α parameters are calculated so that the relationship

$$S(Thr) = S3 * e^{\left(\left(\frac{Thr3}{\sigma} \right)^\alpha - \left(\frac{Thr}{\sigma} \right)^\alpha \right)} \quad (1)$$

is checked for the 3 points $(Thr1, S1)$, $(Thr3, S3)$ and $(Thr4, S4)$.

The σ and α computation routine accepting these 3 points as input is described further in the section § [sigma et alpha computation routine](#)

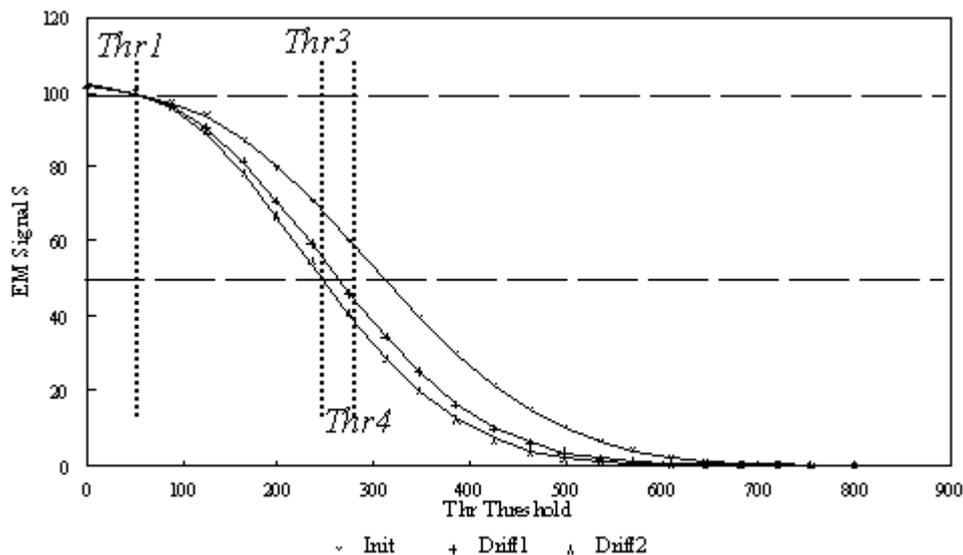
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12.2.2.2.2 Example.

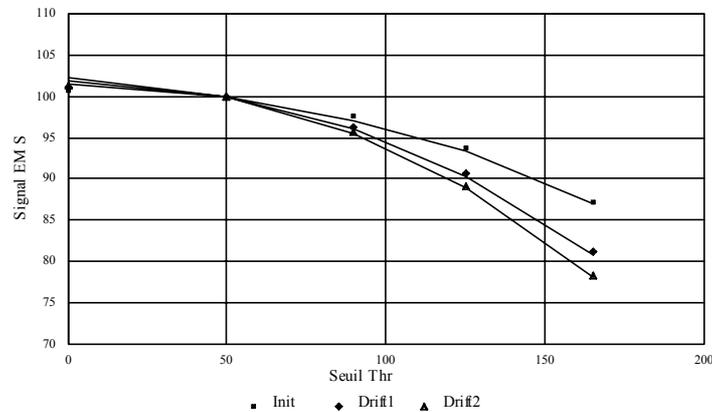
In the proposed routine, only 3 points are measured. However, for demonstrating the method relevancy, all the $S(Thr)$ curve is considered in this section. The hereunder plot shows that

- $\alpha=2.5$ and $\sigma=357.3$ make it possible to rebuild the overall *init* curve.
- Keeping the same $\alpha=2.5$, a new value of σ makes it possible to rebuild the overall *drift1* and *drift2* curves ($\sigma=302.59$ et $\sigma=284.21$)

In the hereunder plot, lined curves, corresponding to measurement, are the same as in the previous plot while symbol points are calculated according the analytic formula (1).



A first look on the plot may suggest that the experimental measurements are correctly modeled by the analytical relationship (1), but a finest look close to the working threshold ($Thr1=50\text{ mV}$) does not demonstrate a good fitting in this region.



Analytical relationship (1) gives, for *Drift2*, $S(0)=101.31$, instead of 102.2 , that is an underestimate of 50% of the actual drift. A finest analytical model must therefore be used in the working region.

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12.2.2.3 Before analysis, $S(Thr)$ fine modelization, β and λ computation

12.2.2.3.1 Processing description

Additionally to the point $(S1, Thr1)$, one takes into account 2 other points $(S0, Thr0)$ and $(S2, Thr2)$ located on both sides of $Thr1$. Typically

$$\begin{aligned} Thr0 &= Thr1 - (Thr3 - Thr1)/10 \\ Thr2 &= Thr1 + (Thr3 - Thr1)/10 \end{aligned}$$

- Both $S0=S(Thr0)$ and $S2=S(Thr2)$ intensities must be measured. (practically, the five intensities, corresponding to $Thr0, Thr1, Thr2, Thr3$ and $Thr4$ will be measured in the same routine)
- β and λ parameters are computed so that the relationship

$$S(Thr) = S1 * e^{\lambda * \left(\left(\frac{Thr1}{\sigma} \right)^\beta - \left(\frac{Thr}{\sigma} \right)^\beta \right)} \quad (2)$$

is checked for the 3 points $(Thr0, S0)$, $(Thr1, S1)$ et $(Thr2, S2)$.

The β and λ computation routine accepting these 3 points as input is described further in the section § [Lambda and Beta computation routine](#)

12.2.2.3.2 Example

In the hereunder table, columns 2, 3 and 4 are measurements while columns 5, 6 and 7 are calculated according to the analytical expression (2) with the numerical values of σ , β and λ which are displayed in the table.

Thr	meas init	meas drift1	meas drift2	Calcul (1) init	Calcul (2) drift1	Calcul (2) drift2
0	101.48	101.81	102.20	101.48	102.03	102.29
50	100.00	100.00	100.00	100.00	100.00	100.00
90	97.04	96.01	95.60	97.04	95.97	95.47
			σ	357.3	302.59	284.21
			β	1.895	1.895	1.895
			λ	0.61	0.61	0.61

For understanding correctly this table, it must be clear that β and λ have been computed once only before the analysis, and that only σ is re-computed along the analysis. The last analytical model (2) fits fairly better the measurement at the neighbourhood of *Thr1*.

Whenever a measurement of σ is achieved, the yield can be deduced, by assuming that the $S(Thr)$ curve is shrunked of a factor σ/σ_i , σ being the value calculated along the analysis, and σ_i the value calculated before the analysis. This computation processing is described in the next section.

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12.2.2.4 During analysis, determining the current σ and therefore the yield drift

12.2.2.4.1 Processing Description

Along an analysis, whenever the yield is to be estimated again, the two points $S(Thr1)$ and $S(Thr3)$ are only required to be measured.

- The threshold is successively set to *Thr1* and *Thr3*, $S1=S(Thr1)$ and $S3=S(Thr3)$ are measured and normalized to $S1=100$.
- Parameter σ is calculated so that the relationship (1)

$$S(Thr) = S3 * e^{\left(\left(\frac{Thr3}{\sigma} \right)^\alpha - \left(\frac{Thr}{\sigma} \right)^\alpha \right)}$$

is checked for both points (*Thr1*, $S1$) and (*Thr3*, $S3$). α is kept to its previously determined value. This routine for computing σ is described below in the section § [sigma computation routine, alpha being kept constant](#)

- The Yield is derivated from the formula

$$Y_{EM}(\sigma) = e^{\lambda * \left(\left(\frac{Thr1}{\sigma_i} \right)^\beta - \left(\frac{Thr1}{\sigma} \right)^\beta \right)} \quad (3)$$

σ_i and λ being kept to their previously determined value.

Regarding the considered example:

For Drift1: $Y_{EM}=99.46\%$

For Drift2: $Y_{EM}=99.21\%$

12.2.3 Computation routines

12.2.3.1 Sigma et alpha computation routines

Let $(Th1, 100)$, $(Th2, y2)$, $(Th3, y3)$ be a set of 3 points so that $Th1 < Th2 < Th3$ and $100 > y2 > y3$ (attention, in this section, the indexes, 1, 2, 3, may have not the same meaning as in the previous sections.)

The routine targets to determine the hereunder function parameters α and σ

$$y(x) = y2 * e^{\left(\left(\frac{Th2}{\sigma} \right)^\alpha - \left(\frac{x}{\sigma} \right)^\alpha \right)}$$

$y(x)$ must be checked for the 3 points. Note that this function is always checked for $(Th2, y2)$, for any α and σ .

The issue is therefore to determine α and σ for checking the relationship for $(x=Th1, y=100)$ and $(x=Th3, y3)$. (α, σ) are initialized to $(2.5, Th2)$ and then an iterative calculation is carried out. Let (α', σ') be the new values calculated at the step $i+1$, from the step i (α, σ) values:

$$\begin{aligned}\sigma' &= \sigma * (1 - 0.5 * (y(Th1)-100)/(Th1-Th2)) \\ \alpha' &= \alpha * (1 + 1 * (y(Th3)-y3)/(Th1-Th2))\end{aligned}$$

The iterative calculation stops when

$$|(\sigma-\sigma')/\sigma| < 0.001 \quad \text{and} \quad |(\alpha-\alpha')/\alpha| < 0.001$$

And then

$$\sigma = \sigma'; \quad \alpha = \alpha'$$

maximum number of loops : 50

12.2.3.2 sigma computation routine, alpha being kept constant

Let $(Th1, 100)$ and $(Th2, y2)$ be a pair of 2 points so that $Th1 < Th2$ and $100 > y2$ (attention, in this section, the indexes, 1 and 2, may have not the same meaning as in the previous sections.)

The routine targets to determine the hereunder function parameter σ , α being kept constant

$$y(x) = y2 * e^{\left(\left(\frac{Th2}{\sigma} \right)^\alpha - \left(\frac{x}{\sigma} \right)^\alpha \right)}$$

$y(x)$ must be checked for the 2 points. Note that this function is always checked for $(Th2, y2)$, for any σ .

The issue is therefore to determine σ for checking the relationship for $(x=Th1, y=100)$. σ is initialized to $Th2$ and then an iterative calculation is carried out. Let σ' be the new value calculated at the step $i+1$, from the step i value of σ :

$$\sigma' = \sigma * (1 - 0.5 * (y(Th1)-100)/(Th1-Th2))$$

The iterative calculation stops when

$$|(\sigma-\sigma')/\sigma| < 0.001$$

And then

$$\sigma = \sigma'$$

Maximum number of loops : 50

12.2.3.3 Lambda et Beta computation routines

Let $(Th0, y0)$, $(Th1, 100)$, $(Th2, y2)$ be a set of 3 points so that $Th0 < Th1 < Th2$ and $y1 > 100 > y2$

The routine targets to determine the hereunder function parameters λ and β

$$y(x) = 100 * e^{\left(\lambda * \left(\frac{Th1}{\sigma} \right)^\beta - \left(\frac{x}{\sigma} \right)^\beta \right)}$$

$y(x)$ must be checked for the 3 points. Note that this function is always checked for $(Th1, 100)$, for any λ and β .

The issue is therefore to determine λ and β , σ being given, for checking the relationship for $(Th0, y0)$ and $(Th2, y2)$. (λ, β) are initialized to $(2.0, 0.6)$ and then an iterative calculation is carried out. Let (λ', β') be the new values calculated at the step $i+1$, from the step i (λ, β) values:

$$\beta' = \beta - 10 * (y(Th0)-y0)/(Th0-Th1)$$

$$\lambda' = \lambda + 4 * (y(Th2)-y2)/(Th2-Th1)$$

The iterative calculation stops when

$$|(\beta-\beta')/\beta| < 0.001 ; \quad |(\lambda-\lambda')/\lambda| < 0.001$$

And then

$$\beta = \beta'; \quad \lambda = \lambda'$$

maximum number of loops: 100

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12.3 Appendix 3: The QSA effect

The QSA (Quasi Simultaneous Arrivals) effect may be taken into account for the EM counting, additionally to the deadtime correction.

Secondary ions are often considered to be only a small fraction of the bunch of sputtered particles resulting from the impact of a single primary ion. However, for some applications, which combines both high ionization yields (by using Cs^+ primary ions for instance) and high collection efficiencies, the average number K of secondary ions (of a given species) ejected per primary ions may reach values as high as 20% for some elements. In such conditions, the probability to get more than one secondary ion per primary impact is not negligible so that one must contemplate situations where a single primary impact produces two secondary ions, which in return infers that those ions will arrive at nearly the same time on the conversion dynode of the electron multiplier (EM). Quasi-simultaneous arrivals (QSA) are registered as single pulses so that the registered number of counts is slightly lower than the actual number of incoming ions. Assuming a Poisson statistics, the correction factor is given by $(1 + K/2)$ in a first order approximation. In the case of an EM measurement of the complete set of Oxygen Isotopes (^{16}O , ^{17}O , ^{18}O), with wellknown abundancies of (2000, 1, 4), ^{16}O must be corrected for the QSA effect whereas corrections will be completely negligible for ^{17}O and ^{18}O , the low abundant isotopes. Similar observations can be made for others elements like carbon, silicon or sulfur. It should be emphasized that the QSA effect is not linear with the mass difference between isotopes and does not depend upon the counting rate.

Reference: *G. Slodzian, M. Chaintreau, R. Dennebouy and G. Rousse : Precise in situ measurements of isotopic abundances with pulse counting of sputtered ions. EPJ Applied Physics, 14, n°3, 199, June 2001*

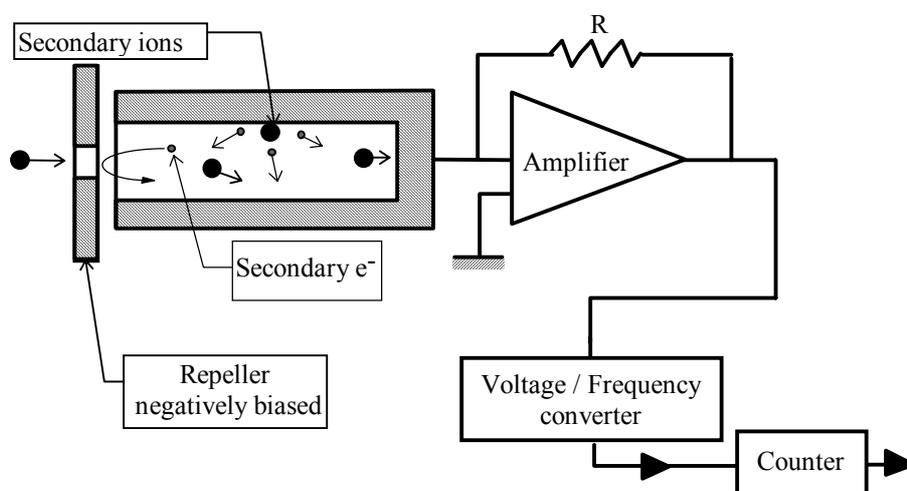
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12.4 Appendix 4: The Faraday cup Measurement principle

12.4.1 The Faraday cup description

The Faraday cup is a hollow cylinder with large ratio length/diameter isolated from the instrument ground. In order to measure accurate secondary ion intensities it is mandatory to prevent the secondary electrons induced by the ion bombardment of the Faraday cup walls from escaping of the Faraday cup. This is achieved by placing a repeller (a plate negatively biased) in front of the Faraday cup.

A schematic drawing of the IMS Faraday cup system is shown in the here under figure :



The charges brought by the secondary beam focused into the Faraday cup produces a current which is converted into a voltage by a high impedance amplifier. This voltage is sent at the input of a voltage/frequency converter.

12.4.2 The FC resolution and thermal drift

The maximum input voltage of the V/F converter is 10 V and the resistor R is of $10^{10}\Omega$ for the FC1 amplifier, $10^{11}\Omega$ for the standard multicollector amplifiers. The maximum count rate which can be measured with the multicollector Faraday cups therefore

$$I_{max} = 10 / (10^{11} \times 1.6 \cdot 10^{-19}) = 6 \times 10^8 \text{ c/s}$$

The typical thermal drift is $400 \text{ c/s}/^\circ\text{C}$ for the multicollector, and $4000 \text{ c/s}/^\circ\text{C}$ for FC1

In order to work in the linear range of the V/F converter an offset is applied on the preamplifier (typically equivalent to few Millions of c/s). The intensities measured by means of the Faraday cup must be corrected of the offset (See the Software user's guide,)

The polarity of the preamplifier is automatically adjusted by the automation system according to the polarity of the secondary ion beam.

12.4.3 The FCs Channel settling time .

The FCs channel response time order of magnitude is of one second with a $10^{11}\Omega$ resistor and 0.1 second with a $10^{10}\Omega$ resistor. Any Faraday cup measurement involved within an analysis must therefore take into account both the Faraday channel T_{fcs} time constant and the required precision *prec*.

$$\textit{Settling Time} = T_{fcs} * \left(4.6 + \ln\left(\frac{1}{\textit{prec}}\right) \right)$$

prec is expressed in %.

That leads, for the multicollector $10^{11}\Omega$ resistor, to

$$\begin{aligned} \textit{Settling Time} &= 4.6 \text{ seconds if } \textit{prec}=1\% \\ \textit{Settling Time} &= 9.2 \text{ seconds if } \textit{prec}=0.01\% \end{aligned}$$

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12.5 Appendix 5: Fundamental of Statistics

12.5.1 Binomial law, poisson law, Normal law

The binomial law

A is an event which may occur along a test. If A does not occur, the opposite event B occurs. p is the probability that A occurs. So the probability of B is $q=1-p$

Let run n tests. Let be $P_n(k)$ the probability that A occurs exactly k times (and thus B , $n-k$ times)

$$P_n(k) = C_n^k p^k q^{n-k} = \frac{n!}{k!(n-k)!} p^k q^{n-k}$$

Let's assume now that n is a large number. It is possible therefore to calculate the mean \bar{k} and its spread σ .

$$\begin{aligned}\bar{k} &= np \\ \sigma &= \sqrt{npq} \\ \frac{\sigma}{\bar{k}} &= \frac{\sqrt{1-p}}{\sqrt{\bar{k}}}\end{aligned}$$

if p is very small

$$\boxed{\frac{\sigma}{\bar{k}} = \frac{1}{\sqrt{\bar{k}}}} \quad (1)$$

The Poisson law and the Gauss law or Normal law

This very simple relationship can also be deduced from the *Poisson law* which gives $P_n(k)$ when n is large

$$P_n(k) = \frac{e^{-np} (np)^k}{k!}$$

When n is very large, $P_n(k)$ can be estimated by the *Gauss law*, also called *Normal law*.

$$P_n(k) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(k-\bar{k})^2}{2\sigma^2}}$$

As a matter of fact, (1) can also be deduced from the Gauss law.

12.5.2 Properties of the normal law

Calculating the uncertainty of a measurement

So far it is established that the result R of a given counting test must follow the *normal law*

$$P_n(R) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(R-\bar{R})^2}{2\sigma^2}}$$

Let's define σ as the measurement uncertainty.

Let $X_1, X_2, \dots, X_i, \dots, X_N$ the actual results of N tests. The better estimation of σ which can be made with these N results is

$$\sigma = \sqrt{\frac{\sum_i (X_i - \bar{X})^2}{N-1}}$$

It is called the *sample standard deviation* or *experimental standard deviation* and currently written STDE.

Confidence interval

If a serie of n tests for determining gives an arithmetic mean of \bar{x} , so far the *normal law* is observed, there is a probability of 95% that the interval

$$\bar{x} \pm \frac{2\sigma}{\sqrt{n}}$$

contains the actual mean x_0 .

More generally, if a serie of n tests for determining gives an arithmetic mean of \bar{x} , there is a probability $\Theta(k)$ that the interval

$$\bar{x} \pm \frac{(\sqrt{2} k) * \sigma}{\sqrt{n}}$$

contains the actual mean x_0 .

$$\Theta(k) = \frac{2}{\sqrt{\pi}} \int_0^k e^{-k^2} dk$$

$\Theta(k)$ is called the *error function*.

$\Theta(k)$	$\sqrt{2} k$
0.9	1.163
0.99	1.821
0.999	2.327
0.9999	2.751

Estimating the accuracy of a measurement consisting of n sub-measurements

Let's define the accuracy as the standard deviation which would be observed if the measurement was repeated a large number of times.

If the sample standard deviation of the n sub-measurements is σ , the uncertainty of the measurement is

$$\frac{\sigma}{\sqrt{n}}$$

So far the statistical law ruling the n sub-measurements is actually a normal law.

Standard deviation of a Sum

Let's assume that $Z=X+Y$, X and Y being 2 random variables following a normal law characterized respectively by their mean arithmetic value \bar{X} and \bar{Y} and their standard deviation σ_X , σ_Y .

Z distribution will also follow a normal law characterized by

$$\bar{Z} = \bar{X} + \bar{Y}$$

$$\sigma_Z = (\sigma_X^2 + \sigma_Y^2)^{1/2}$$

Standard deviation of a product

Let's assume that $Z=X*Y$, X and Y being 2 random variables following a normal law characterized respectively by their mean arithmetic value \bar{X} and \bar{Y} and their standard deviation σ_X , σ_Y .

Z distribution will also follow a normal law characterized by

$$\bar{Z} = \bar{X} * \bar{Y}$$

$$\frac{\sigma_Z^2}{\bar{Z}^2} = \left(\frac{\sigma_X^2}{\bar{X}^2} + \frac{\sigma_Y^2}{\bar{Y}^2} \right)^{1/2}$$

Standard deviation of a ratio

Let's assume that $Z=X/Y$, X and Y being 2 random variables following a normal law characterized respectively by their mean arithmetic value \bar{X} and \bar{Y} and their standard deviation σ_X , σ_Y .

Z distribution will also follow a normal law characterized by

$$\bar{Z} = \frac{\bar{X}}{\bar{Y}}$$

$$\frac{\sigma_Z^2}{\bar{Z}^2} = \left(\frac{\sigma_X^2}{\bar{X}^2} + \frac{\sigma_Y^2}{\bar{Y}^2} \right)^{1/2}$$

12.5.3 Consequence for the ion counting

When the mean number of counted ions is N during a given time τ , it can be said it is the result of repeating $N*M$ tests for which the probability of counting one ion is $1/M$. As M can be as large as desired, the formula (1) is relevant for calculating the standard deviation test result ($N^{1/2}$) which can be considered as the uncertainty of the test.

Consequently, when a ratio is defined as $R = \frac{S_1}{S_2}$, Where S_1 and S_2 , expressed in counts per seconds (cps), are derived from two numbers of counts N_1 and N_2 ,

$$S_1 = N_1/T_1 \qquad S_2 = N_2/T_2$$

Where T_1 and T_2 are the respective counting times, accordingly to above formula giving the standard deviation of a ratio, there is an unavoidable uncertainty which can be expressed as

$$R = \frac{S_1}{S_2} * \left(1 \pm \left(\frac{1}{\sqrt{N_1}} + \frac{1}{\sqrt{N_2}} \right) \right) = \frac{S_1}{S_2} * \left(1 \pm \left(\frac{1}{\sqrt{T_1 S_1}} + \frac{1}{\sqrt{T_2 S_2}} \right) \right)$$

In the field of isotopic ratios, it can be relevant to define some more sophisticated ratios (for example, in the case of zircon analysis for achieving a common lead correction)

$$R = \frac{a_0 + \sum_{m=1}^{m=M} (a_m * S_m)}{b_0 + \sum_{m=1}^{m=M} (b_m * S_m)} = \frac{num}{deno}$$

Where it is assumed that each signal S_m , expressed in cps, derives from a given number of counts:

$$S_m = N_m/T_m$$

It is possible to calculate the uncertainty of R by calculating firstly separately the absolute σ of both the numerator and the denominator (these σ are added in quadrature), and then, by adding in quadrature the relative standard deviations:

$$\frac{\sigma}{R} = \sqrt{\frac{\sigma_{num}^2}{num^2} + \frac{\sigma_{deno}^2}{deno^2}}$$

$$\frac{\sigma}{R} = \frac{1}{\sqrt{n}} * \sqrt{\frac{\sum_{m=1}^{m=M} \frac{a_m^2}{T_m} S_m}{num^2} + \frac{\sum_{m=1}^{m=M} \frac{b_m^2}{T_m} S_m}{deno^2}}$$

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12.6 Appendix 6: LabVIEW® graph options and graph cursors

13. Questions

Q1 Amplifiers calib: Comment y accéder ?

Q2 Overlapping Crater, ça marche ?

Q3 boites pour EMDrift, Beam centering et Overlapping crater.

Q4 Comment remplace-t-on l'option Auto/Manual, pour le waiting time présente autrefois dans Analysis Definition ? Je vois 2 tableaux de masse différents. Il semble que la fonction soit présente sur l'un d'entre eux (Compute waiting time...), mais dans ce cas, pas de définition d'isotopes. Quelle est la différence entre *analysis_species_table_bp.gif* et *analysis_species_table_monop.gif* ?

AUTO/MANUAL If "Auto" is selected, the waiting time corresponding to the magnet settle time is computed according to the formula

$$wt = \frac{\Delta B}{100000} * \sqrt{\frac{MR}{300} + 0.1}$$

Where B is the magnetic field in digits and MR the Mass Resolution

Q6 Dans boîte *Analysis Definition*, "Edit Last conditions" est alternatif à quoi ? et New ?

Q7 Où retrouve-t-on les fonctions autrefois accessibles à partir de Analysis Definition ?

DEFINE CONDITION (EDIT/LOAD/SAVE/SAVE AS)

EDIT loads the last analysis condition related to the current acquisition mode.

LOAD loads the analysis file selected by the operator among all the files corresponding to the current acquisition mode.

SAVE saves the analysis definition under the current filename.

SAVE AS saves the analysis definition under a new filename.

CALIBRATE (FROM TABLE/ FROM CONDITION)

Launches the *Mass Calibration* process

- **FROM TABLE** In the Mass Calibration process, for each species M_i , the magnetic field B_i will be initialized by the value as it is deduced from the current mass table [M, B]
- **FROM CONDITION** In the Mass Calibration process, for each species M_i , the magnetic field B_i will be initialized by the value recorded in the analysis definition species table. These recorded values are resulting from a previous calibration.

Q8 Dans le panneau "Analysis Definition" qu'est-ce qui est alternatif avec EDIT LAST CONDITIONS ? Comment ouvre-t-on *Isotope box* ? Elle s'ouvre en même temps que la *Species table*, quand on fait *New* dans Analysis definition ?

Q9 Est-ce que le panneau *semi-auto Mass Calibration* (avec Cycling, Display calib etc...) est identique au panneau *Manual Mass Calibration* (exception faite du bargraph) ?

Q11 Multicol: Modify Position, ça fait quoi ? Park, ça fait quoi ?

Q10 Le tableau de masse de Mass cali: Nécessite des explications détaillées, de vive voix

Q12 Panneau EM HV Adjust: En haut du panneau, il y a des champs de saisie x et y dont je ne comprends pas bien la signification. (dans set thresholds aussi)

Q13 Panneau Measure set_up: Le tableau "calibration table" concernant les amplis FC, que l'on retrouve en bas du panneau, est-il purement passif ou peut-on l'éditer ?

Q14 Panneau de contrôle Multicollection: A discuter de vive voix.

Q15 Table périodique: A discuter de vive voix.

Q16 Dans Panneau PHA, les champs de saisie "min value", "max value" ont disparu. Par quoi ont-ils été remplacés ?

Q17 Il y a un panneau "Préférences", avec "IMS 1270 with Turbo-pumps", une sélection de directory etc... ? Il faudra que j'ai la liste de toutes les options possibles.

Q18 Dans le panneau "Detection setup", Multicol waiting time, c'est quoi ?

Q19 Dans panneau "Detection Set-up", dans le menu déroulant, Detection Setup est alternatif avec quoi ?

Q19 Dans panneau "Detection Set-up", bouton "Define Set-up", c'est quoi ?

Q20 Download + Global: MOT veut bien dire qu'on charge les moteurs, et DET, les paramètres de la multico ?

Q21 petit panneau permanent L'2/L2.L1... Quit Comment ça marche ?

Q22 Stop Source: Différence entre cancel et Quit ?

Q23 Compteur de source: Set Status ? Si on fait quit, le panneau disparaît, et si on veut le faire revenir ?

Q24 Dans Scan panel, Snap c'est quoi ?

Q25 Dans Scan panel, print to file, où est-ce qu'entre le filename ?

Q26 Dans la boîte de définition d'analyse Multicoll (table de masses), comment se calcule le champ avant le "Trolley Centering"? Avant, on avait l'option "from table/ from condition", présente dans le premier panneau Analysis definition qui traitait différemment le Pb selon la sélection.

Q27 Single/Multi dans le panneau graphique Mass Cali

Q28 Est-ce qu'on peut sauver la table de masse avec les masses de référence ?

> Q1 Amplifiers calib: Comment y accéder ?

tuning > FC_CALIB> OFFSET ou GAIN/OFFSET

>

> Q2 Overlapping Crater, ça marche ?

Jamais utilise, donc je ne sais pas,

La nouvelle fonction pre-sputering permet de changer la taille du raster,

c'est peut-etre equivalent a la fonction Overlapping Crater.

>

> Q3 boites pour EMDrift, Beam centering et Overlapping crater

> (pas vraiment une question, je n'ai pas regardé toutes les

> boites)

>

> Q4 Comment remplace-t-on l'option Auto/Manual, pour le

> waiting time présente autrefois dans Analysis Definition ?

> Je vois 2 tableaux de masse différents. Il semble que la

> fonction soit présente sur l'un d'entre eux (Compute waiting

> time...), mais dans ce cas, pas de définition d'isotopes.

> Quelle est la différence entre analysis_species_table_bp.gif

> et analysis_species_table_monop.gif ?

le bouton Auto/Manual est remplace par compute waiting time dans le panneau du tableau de masses. Ca marche en monocollection.

Il y a plusieurs presentations du tableau de masses suivant le type d'analyse, mono,multi, isotope , line scan etc... j'ai du sans doute impimer les tableau isotope multi et mono.

>

> Q6 Dans boite Analysis Definition, "Edit Last conditions"

rapelle les conditions de la derniere analyse du meme type.

> est alternatif à quoi ?

load analysis

et New ?

le bouton (racourci) est a supprimer , New de la liste <File> ouvre un tableau vierge pour le type d'analyse choisi.

- >
- > Q7 Où retrouve-t-on les fonctions autrefois accessibles à partir de Analysis Definition ?
- >
- > DEFINE CONDITION (EDIT/LOAD/SAVE/SAVE AS) dans la liste <File>
- >
- > CALIBRATE (FROM TABLE/ FROM CONDITION) bouton CALIBRATE dans le panneau tableau de masses l'option From table,condition est dans le programme de mass calib
- >
- > Q8 Dans le panneau "Analysis Definition" qu'est-ce qui est alternatif avec EDIT LAST CONDITIONS ? Comment ouvre-t-on Isotope box ? Elle s'ouvre en même temps que la Species table, quand on fait New dans Analysis definition ?

Avec Species table quand on choisi analysis type = isotope

- >
- >
- > Q9 Est-ce que le panneau semi-auto Mass Calibration (avec Cycling, Display calib etc...) est identique au panneau Manual Mass Calibration (exception faite du bargraph) ?

le mode Manual > centrage du champ a la main a l'aide du bargraph ou du MCP.

Semi_auto : mode standart centrage par l'operateur a l'aide du scan automatique des pics.

mode auto : = mode standart avec centrage par le soft : cache et oublie pour l'instant.

- >
- > Q10 Le tableau de masse de Mass cali: Nécessite des
 - explications détaillées, de vive voix

Repone a Q26 :Le champ se calcule a partir de la masse entree dans le champ monocollection de la table multicoll. et en choisissant <FROM TABLE> dans mass cali.

On peut aussi rentrer a la main le champ dans la premiere ligne de la table de definition multi et choisir <FROM CONDITION> dans mass cali.

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