CIDA/STARDUST Example of Data Calibration

Jochen Kissel and Johan Silen

Abstract

We present a step by step tutorial of how to calibrate CIDA/STARDUST data using laboratory spectrum. We convert the numerical units of the instrument readout into meaningful physical values. A guide for the interpretation of this time-of-flight signal as a mass spectrum is outlined.

1   The Calibration Principle

The CIDA instrument is described in the document *"Cometary and Interstellar Dust Analyzer for comet Wild 2"* by Kissel, J., et.al., *J.Geophys.Res., 108*(E10), 8114, doi: 10.1029/2003 JE002091, 2003. Be sure to have understood this document before proceeding.

The term *calibration* is used here for the conversion of the digital output of the instrument into physical values. Calibration can be done to

1. the housekeeping data
2. the target-channel
3. the spectrum data

Among them, 3 needs a more sophisticated procedure, which is outlined here and demonstrated with a laboratory and in-flight examples.

The data as provided by the instrument consists of housekeeping information and science data in one or several redundant hardware channels. The housekeeping data serves as technical support information and is not normally needed for data analysis. The data to be analysed therefore consists of four 8192 samples long vectors, representing two high and two low sensitivity channels. Two of the vectors may contain zeros to indicate missing data. For details of the experiment see the paper we refer to in the beginning of the section; the data format is described in FMT files in the DATA directory. A nonzero channel is used for two purposes. The first half (samples 1 to 4096) carries the output of the charge sensitive amplifier connected to the target, the second half is redundant to the previous nonzero data channel, i.e. serves as an additional measurement of the same signal, but with slightly different gain properties. At the end of each data vector, a calibration sequence of four distinct current pulses is injected. The sequence usually produces an unwanted transient at its start. The calibration pulses are the response to the four injected currents with the values shown in Table 1. Note, that the starting positions of calibration signals vary and must be determined independently for each spectrum.

A sample laboratory spectrum is shown in Figure 1. The y-axis indicates instrument digital numbers; the x-axis shows instrument 25 ns bin number. The left upper corner shows the primary signal (the charge released from or introduced to the target) recorded in low-sensitivity delayed channel (blue line). The middle bottom part of the figure shows the spectra recorded in redundant channels: high-sensitivity direct

Table 1: Values of injected calibration signal into a TOF-spectrum for Channel 1 as an example

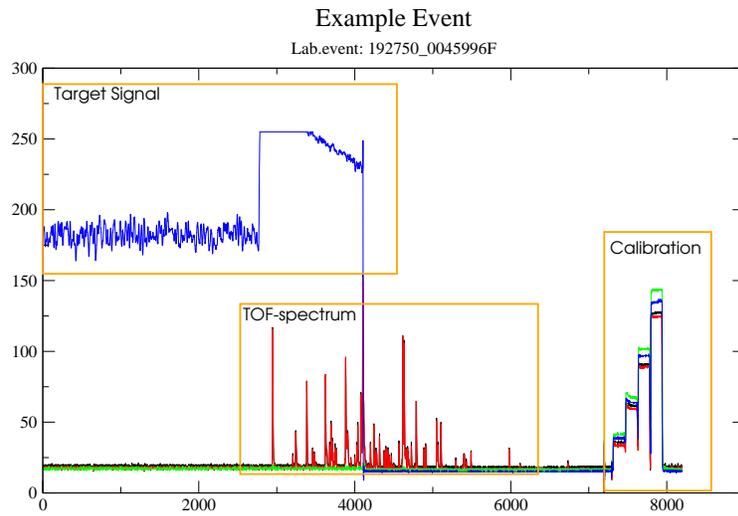| Name	Injected Signal $[\mu A]$	Start Position
Cal-1	53.2	7351
Cal-2	167	7501
Cal-3	532	7651
Cal-4	1670	7810
Background	0	8101

Figure 1: Example spectrum used to demonstrate the calibration process.

(black) and delayed (red) channels and low-sensitivity direct (green) channel. The right lower corner shows the calibration signals for the four channels.

The relation between the current I (in μA) and the numerical reading N is described by a theoretical equation:

$$N = C_1 + C_2 I + C_3 \log(1 + I/C_4) \tag{1}$$

A useful inverse solution to reconstitute the current I from the digital number N is given by

$$I = c_1(N - N_0)e^{c_2(N-N_0)} \tag{2}$$

We prefer to use eq. (2) for any practical work. Using the values from Table 1 it is possible to solve it in a least square sense to get the values for c_1 and c_2. Here N and N_0 are respectively the numerical reading and the spectrum numerical background level of the recorded, compressed raw signal.

The relation between time-of-flight and ion mass is:

$$t = a\sqrt{m} + b \tag{3}$$

This relation holds for all ions, which are formed simultaneously, are stable during their flight time and are accelerated to the same kinetic energy. The instruments reflector compensates for initial energies the ions might have. Ions with different distribution functions for their initial energy may be represented by different peak shapes and thus provoke a slightly different set of a-, b-values determining the peak mass. Note that there is a small $\sim 1\%$ variation of a depending on whether the impact is central or peripheral due to a small difference in the ion trajectories from the target to the detector. Also, there may occasionally be some spurious peaks present because of ion chemistry processes or collisions with the walls.

Knowing positions of two or more mass peaks in a given spectrum, it is possible to find the constants a and b defining the relation between mass and sample time.

2   Application to Laboratory Spectrum

The example presented is chosen to demonstrate how to produce a time of flight spectrum from the recorded raw signal. The steps involved are the following:

1. Compute the mean background of the spectrum: This is conveniently done by taking the very last samples in the spectrum, positions starting at, e.g., 8101. The result is slightly different for the different channels. Make sure that the region used for the background estimation does not contain any real signal.

2. Compute the mean of say 50 samples from each of the channels present starting from the positions given in Table 1. The difference indicates directly the difference in gain. Make sure that there is no contamination by real signal.

3. Knowing the injected currents (Table 1) and the levels (step 2), the constants c_i and N_0 can be calculated from formula 2.

4. Having the constants c_i and N, one can build a lookup table for $I = I(c_i, N_0, N)$. Knowing this completes the amplitude calibration. The spectrum amplitude I is given in μA sampled at 40 MHz (samples are 25 ns apart).

5. Looking at the TOF-spectrum and knowing (or guessing) that the first major peak seen is Hydrogen and that the large double peak at end of the spectrum is Silver, it is possible to compute an estimate for a and b (Equation 3) connecting the mass and the time of flight

It is important to note that the relative yields of ions are strongly dependent on the detailed chemical properties of the incident dust grain and of the local target composition and structure. Therefore it is incorrect to infer relative elemental abundances from the above procedure directly. Filters in the detector amplifier eliminate the difference in amplitude due to the smaller flight time of the light ions where the peak width would be below 200 ns.

3 Numerical Values for the Example Spectrum

This section provides values for the example spectrum (Figure 1).

3.1 Background and Calibration Injection Levels

The background and the calibration levels estimated from 50 samples starting at the positions indicated in Table 1 are shown in Table 2.

Table 2: Background and calibration injection levels computed for the example spectrum

	Background	Cal-1	Cal-2	Cal-3	Cal-4
Ch1	18.58	35.84	62.32	90.46	126.86
Ch2	17.16	33.78	59.92	88.76	124.18
Ch3	16.64	41.12	68.24	101.58	143.00
Ch4	15.24	38.78	64.34	96.84	134.36

3.2 Computation of Constants

The computation of the numerical constants has to be made numerically iteratively using some standard technique. The result is shown in Table 3 which contains the results obtained based on Equations 1 and 2. The solution based on Eq. 2 is more stable and sufficiently accurate. C_1 in Eq. 1 is identical to N_0 in Eq. 2. For calibration,

Table 3: Coefficients connecting the numerical raw value and the physical current as calculated from the example spectrum using the values in Table 1.

	c_1	c_2
Ch1	2.01	0.0183
Ch2	2.10	0.0181
Ch3	1.35	0.0179
Ch4	1.38	0.0192

one can either use a lookup table built from Eq.(1) or calculate the current directly from inverse Eq.(2). The first approach may be numerically unstable but when it works

gives somewhat more accurate results. The second approach is stable and simple to use but for amplitudes larger than the highest injected calibration impulse can be somewhat inaccurate. However, the errors are smaller than the uncertainties in the physics of ion production rates.

3.3 Transforming Time-of-Flight Spectrum into a Mass-Spectrum

Identifying the Hydrogen peak at $t = 2944$, ^{107}Ag at $t = 4614$ and ^{109}Ag at t=4632 gives the three equations:

$$2944 = a + b$$
$$4614 = a\sqrt{107} + b \tag{4}$$
$$4632 = a\sqrt{109} + b$$

The solution is $a = 178.8$ and $b = 2765$. In an analog way, one can identify a larger number of masses and solve the corresponding linear equations in a least square manner. The mass expressed in sample coordinates would then be:

$$m = \frac{(t - b)^2}{a^2} = \frac{(t - 2765)^2}{3.1969 \cdot 10^4} \tag{5}$$

Equations (2) and (5) together with data from table (3) and the values for a and b completes the calibration procedure. The resulting impact mass spectrum is shown in Figure 2. The interpretation of it requires a solid knowledge of mass spectrometry and is beyond the scope of this paper.
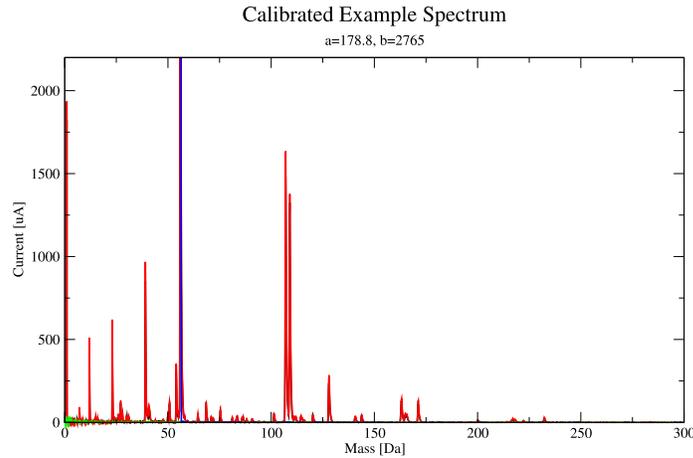

Figure 2: Calibrated spectrum. The mass is fixed using equation (5) and the amplitude using equation (2) and the data values in Table 3.

4 Calibration of Negative Mode Flight Spectrum

We selected the event NEG31 as an in-flight data example. Its spectrum is shown in Figure 3. The negative mode is indicated by the information in the housekeeping header data.
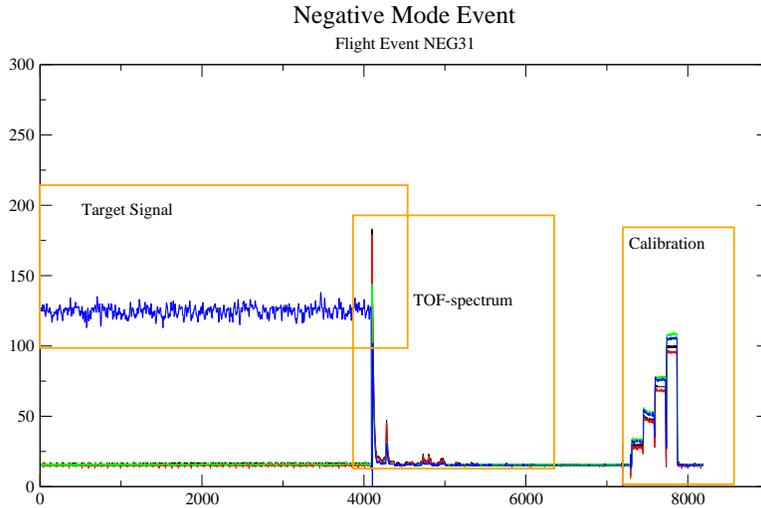

Figure 3: Flight spectrum, event NEG31 used as an example illustrating the calibration procedure. The amplitude calibration data shown at the end of the spectrum represent the data given in Table 4.

4.0.1 Background and Calibration Injection Levels

The background and the calibration levels are estimated from 120 samples starting at the positions indicated in Table 4.

Table 4: Values of injected calibration signal into a TOF-spectrum, sample position and average value of signal for channel 1 as an example.

Name	Injected Signal $[\mu A]$	Starting Position
Cal-1	53.2	7310
Cal-2	167	7460
Cal-3	532	7600
Cal-4	1670	7740
Background	0	8000

4.0.2 Computation of Constants

We use equation (2) to perform the amplitude calibration. The logarithm of this equation gives

$$\log(I) = \log(c_1) + \log(N - N_0) + c_2 \cdot (N - N_0) \tag{6}$$

6

This equation has to be solved for c_1 and c_2 which can be made in a least square sense using standard techniques, see *eg. Menke(1984), Geophysical Data Analysis, p 57-59.* Here we use a constrained least square fit requiring that the multiplier for the term $\log(N - N_0)$ equals 1. Table 5 contains the values representing the average calibration injection levels computed from the injected signal levels.

The resulting values for c_1 and c_2 are shown in Table 6. No lookup table is required

Table 5: Background and calibration injection levels computed for the NEG31 spectrum

	Background	Cal-1	Cal-2	Cal-3	Cal-4
Ch1	15.88	29.24	48.31	71.06	99.29
Ch2	15.01	27.75	46.94	68.18	95.58
Ch3	15.35	33.30	53.24	77.42	108.18
Ch4	15.09	32.02	51.67	75.95	105.26

since Eq. (2) provides an analytic function, which describes the relation between physical current expressed in μA and the numeric value of the data. The constrained least square fit provides values for the constants which are given in Table 6.

Table 6: Constants c_1 and c_2 computed for the NEG31 spectrum using a constrained least square solution to equation (6), expressing currents in μA in equation (2)

	c_1	c_2
Ch1	0.978	0.0237
Ch2	1.01	0.0245
Ch3	0.612	0.0245
Ch4	0.681	0.0246

4.1 Transforming Time-of-Flight Spectrum into a Mass-Spectrum

Determining the mass scale requires identifying some peaks in the spectrum. This can most conveniently be made by identifying at least two peaks. Using these as an initial guess providing an estimate for a and b in Eq. 3, gives a simple approximate scale which can be refined by identifying additional peaks. This is an iterative process which does require general knowledge about the interpretation of mass spectra.

In general, negative mode spectra do not show a pronounced step in the target signal. Instead it usually contains a large electron peak indicating the impact time (mass zero). Often also a M=1 is present as is M=13 (CH^-). For this example an inspection of the spectrum shows that there are peaks at positions shown in Table 7.

The mathematics is similar to section 3.3, equations (4) and (5). The results are indicated as calculated mass in Table 7. The calibrated mass spectrum (amplitude and mass both calibrated) is shown in Figure 4.

Table 7: Peaks identified from the data for channel 1. The mass is computed together with the values for a and b using equations (4) and (5). The values for the constants are calculated to be $a = 174.05$ and $b = 4104$. The resulting masses are shown.

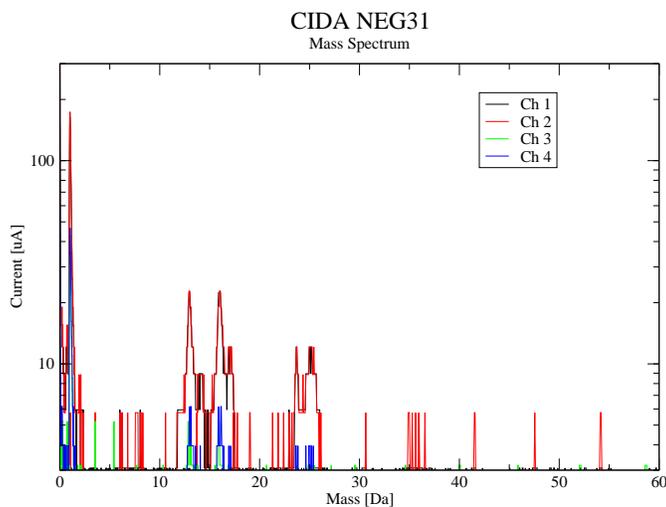| Peak Position	Identification as mass	Calculated Mass
4100	0	$5.9 \cdot 10^{-4}$
4283	1	1.05
4707	12	12.00
4731	13	12.97
4800	16	15.98
4827	17	17.25
4951	24	23.67
4976	25	25.09

Figure 4: Enlarged portion of the calibrated mass spectrum. Note the well behaving channels 1 and 2 superimposed to well within 1 bit accuracy. The low sensitivity channel is not accurate at this low 2-bit amplitude level.