How to reduce SWS AOT01 Data in the ISAP GUI

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Before you begin:

This guide is intended to give a basic description of how to use ISAP in the GUI mode to reduce the Auto Analysis Results (AARs) for SWS AOT01 data: it explains the basic principles and shows in a representative way how and in which order to work through each of the possible steps of data processing. It assumes that you are working with ISAP version 2.0. For a full description and alternate uses of a particular routine, consult the ISAP help. This help is accessible on the web: http://www.ipac.caltech.edu/iso/isap/isap.html or http://www.mpe.mpg.de/www_ir/ISO/observer/isap/isap.html. From within the GUI simply use the "Help!" button and select "WWW pages." The help pages contain - among other things - a beginners GUI guide, a description of all the GUI Buttons, and links to the detailed help text of each individual ISAP routine ("Command Line Routines"). Here you'll also find the necessary information about routines that are not mentioned in this recipe. A lot of fundamental information about the SWS instrument and its behaviour is contained in the SWS handbook. The latest version is always available on the web: http://www.iso.vilspa.esa.es/ (follow the link to "ISO Documentation"). Before trying to reduce SWS data we **strongly recommend** to carefully read at least the beginners' GUI guide, which will make you familiar with the basic principles of the ISAP GUI, and the handbook!

If your AAR has been produced with a pipeline version earlier than 7, you should seriously consider/ask for a reprocessing of your data. The pipeline version can be found in the header of the FITS file. Note that the data in the official ISO Post Mission Archive are all processed with version 8 (or higher). Also note, OSIA and IA3 do not update the pipeline version in the header (but you can use the header editor in ISAP to overwrite it manually).

These instructions suggest saving the intermediate products of the data processing after particularly time-consuming steps; the user should weigh the value of additional saves against the constraints of disk space.

Before starting ISAP, you should close all applications which use color (e.g., Netscape, or additional IDL sessions), as they will interfere with the ISAP color table. After ISAP has been started, you may restart these applications without affecting the ISAP session.

Finally: Whenever you have comments, suggestion or complaints about this manuscript (e.g., if you are missing some information), please let me know! Please check the web site for modifications of this document - from time to time.

1) **getting started / data input**

Start ISAP in the GUI mode (possibly "isap" or "isap_gui" - see the readme text of your installation). The first thing to do of course is to read in the data: Click on "Read data..." and then select "FITS" (provided you have your AAR available in its original fits format). Choose the desired file from the file selection tool which pops up (i.e. double click on the file name).

2) **Quick look**

To see the full data set, select all scans (should be only one for SWS01), detectors (or bands), lines, and scan directions, then click on plot. For a closer (but still quick) look at your data, plot the spectrum line by line (if your data have been processed with a pipeline version prior to 7, click on "Special Fns..." first and select "Convert Line →AOT Band," see below). Make use of the different color coding options offered by ISAP (click on "Select Plot Style"). Note, that **plotting** of large data sets in plot modes **other than the default** "dot cloud" **mode** can take a **long time**. If you want to interrupt a plotting process, and you are running UNIX, type "Ctrl-C" in the command line of your IDL window, and then type "return". You should now be able to reset the plot style and to plot again.

Here follow some criteria you can use for a first cut evaluation of the data quality and to spot potential problems:

- *Are the flux values non-negative (on average)?*
  If the answer is NO, then the dark current subtraction in the automatic pipeline processing has not been optimal (the dark current has been over-subtracted). In this case you could very likely improve the result by going back to OSIA (the Observer's SWS Interactive Analysis system, which operates on SPD level) and performing an interactive dark current subtraction (with OSIA's routine dark_inter). Note that *on average* means that many individual points might still be negative in the case of a faint, noisy source.

- *Are there inconsistent trends in the continuum shape?*
  If some of the detectors within a line (AOT Band) have continuum slopes that are tilted with respect to the other detectors, or if the whole AOT band has a different tilt then the neighbouring AOT bands, this could again be due to problems in the automatic dark current correction. Going back to OSIA is recommended.

- *Are there significant systematic differences between the two scan directions?*
  If so, it is recommended to use OSIA's tool updown1_inter, which is able to remove

Table 1: The relationship between AOT band, order, aperture and SWS01 line tag.

AOT Band	order	aperture	converted line tag	OLP 7+ line tag
1A	4	1	911	1
1B	3	1	912	2
1D	3	2	914	3
1E	2	2	915	4
2A	2	2	921	5
2B	1	2	922	6
2C	1	3	923	7
3A	2	1	931	9
3C	2	2	932	10
3D	1	2	934	11
3E	1	3	935	12
4	1	3	940	13

such differences on a level before the relative spectral response function and absolute flux calibration are applied to the data (but see also step 8 below).

3) **Remove bad data - I)**

Sometimes the pipeline AAR (prior to version 7) contains data with a scan counter 0, line number 0, and/or a scan direction 0. Those data usually can be dropped. Also, if there are any data of band 5 or 6 (the FP bands) in your SWS01 data, they can be disregarded, too. In this case select all scans, lines, scan directions and bands, except those with a zero value and bands 5 and 6, plot everything (select the default plotmode, i.e. unconnected, no color preference, which is fastest), and catch everything with the right mouse button. Choose "make aar" in the tool box, enter a new name and store the result.

4) **Line tag conversion**

This is an operation which is required for SWS AOT1 data only, and only for those that have been processed prior to version 7 of the pipeline. The SWS AOT bands are defined as certain combinations of detector material (the "bands"), aperture and order (see the SWS Observer's Manual or the IDUM). For pipeline version 7 and higher the line tag reflects these AOT bands already (see Table 1).

The routine "Convert Line →AOT Band(SWS AOT 1)", accessible under "Special Fns...Convert" enables you to easily select the various AOT bands separately. The line tag is mapped to reflect the AOT band as described in Table 1.

In principle the line tag of pipeline 6 AARs (SWS01) already does code aot bands (continuous counting from 1 to 13), which is, however, not always reliable.

Don't forget to STORE the converted AAR.

5) **Split**

The SWS AOT1 data consist of 12 different sub-spectra according to the 12 different grating AOT Bands (see step 4 above). The spectra of neighbouring AOT bands have overlapping wavelength regions. To avoid mixing of data which belong to different orders and/or apertures and/or detector material during the data reduction it is recommended to process the individual AOT bands separately. Click on "Special Fns..." and choose "Split Apart AAR". Then check the "lines" box and apply. This will automatically split the AAR according to the line tag, and will store the result, i.e. the 12 new sub-spectra, in "Stored Data Sets..."

6) **Start loop**

Now you can select the first of the 12 sub-spectra: click on "stored data sets...", then on the name of the band 1A (line 1 or 911, name=filenamename_l1) spectrum, and then on "make prime" (under "apply function to"). The following steps describe what should be done for each of the 12 spectra separately (i.e. in a loop).

7) **Remove bad data - II**

The next step should be the removal of all kinds of bad data. First of all ISAP offers a method to visualize and, if required, to delete data points that have been marked as "bad" by the pipeline. These are "nodata","glitch", and (partially or totally) "out of limit". Under "Special Fns..." you'll find a function to overplot these bad data, and several functions to remove them. If you want to have these data removed automatically on read-in (i.e. without plotting them first), you can set this option in "Bad Data Removal..." before you clik on "Read Data...."

For bad data that have not been identified by the pipeline you can choose between "Tippex", "Mask" and "Zap" (invoked via the tool box which pops up if you select some data with the right mouse button). With TIPPEX a single point is replaced by a linear interpolation between the two corresponding neighbouring points. This is done as unique as possible, i.e. the two points choosen as basis for the linear interpolation are of the same detector, scan and scan direction, if any of this information is available. MASK simply masks out the selected data, i.e. they will not be taken into account for the computation of correction functions in the subsequent processing steps (e.g. in AVERAGE they won't contribute to the average). But the masked data stay in the data set, and shift, for instance, shifts masked points as well (without using them for the computation of the correction). With ZAP you really get rid of the data, they are thrown away. To remove single outliers you could use TIPPEX, but for an SWS AOT1 it is usually a good idea to simply ZAP all bad data, because the redundancy in the data and the spectral sampling is high enough.

Besides single outlying points another kind of "bad data" can be sudden jumps in flux (a glitch) followed by a subsequent exponential-like decrease over several seconds/data points, due to memory effects. You should zap the entire memory tail.

In the decision of what is a glitch and what is a line you should make use of the redundancy in your data: If the feature is seen only in one of the twelve detectors it is a glitch. If it is seen in several or all twelve detectors at the same time but at slightly different wavelengths it is a glitch which caused some electronic cross-talk (that's why it is seen in more than one detector). A line is only a feature which is seen in at least most of the detectors at the same wavelength and which is present in both scan directions (up and down, or -1 and 1). In the overlap region between different AOT bands there is even more redundancy to classify a feature as glitch or real. The different possible color codings (per detector, per scan, per scan direction), adjustable via the "Set Plot Style" button, and the ability to plot different detectors, scans or scan directions separately, are usually a great help in this business. E.g. you could choose the plot style "unconnected, plot symbol = +" - this sometimes helps to identify lines. Then you can select "connected, color code detectors", which helps identifying "bad" detectors (see below). Finally you should try "connected, color code scan direction". This will help to detect differences between the two scan directions (see below). Don't zap away lines! In the low resolution ATO1 data it is easy to confuse lines with glitches!

Sometimes a whole detector seems to produce much worse quality than the others (e.g. detectors 21, 26, 29 or 34 are known to behave strangely sometimes). This can be checked if you set the color preference to "Detector Number." With the MIDDLE MOUSE BUTTON you can always get information about a single data point. Just click on the desired point (or near to it). In the info field at the bottom of the GUI you'll get e.g. the detector number, scan number, scan direction etc. In this way you can identify the detector number. To get rid of a whole detector use "Zap assoc", which will zap all points associated with the selected data points (,so, simply select a few points of both scan directions for the detector under consideration with the right mouse button and apply "zap assoc").

The removal of bad data can take quite a while (in fact it can be the most time consuming part of the whole processing), but it is definitely one of the most important steps and will improve the quality of the final product significantly. It is certainly a good idea to STORE the result and perhaps even write it to disk (select the data under "Stored Data Sets...", click on "Write to Disk in..." and choose the format).

If you have to zap (mask/tippex/etc.) a lot you can make use of the "Preselect" button: Click on it and choose "Zap". From now on ISAP will automatically zap whenever you catch data points with the right mouse button. Don't forget to switch preselect off when you are done with zapping. (If you do forget, the "undo" button in the upper right corner of the GUI might come in handy...).

An alternative to zapping "by hand" is automatic "Clipping".

8) **Differences between up and down scans**

Each AOT1 scan actually consists of two scans of different SCAN DIRECTION:
+1: up scan (increasing grating positions, decreasing wavelength)
-1: down scan (decreasing grating positions, increasing wavelength)
The sequence is always up $\rightarrow$down. Due to hysteresis/memory effects of the detectors there can be differences in the shape of the continuum between the up and down scan

of a given scan number (see the SWS handbook). In ISAP there is no optimal tool to correct for this effect. If these effects are strong, you should go back to OSIA and try to correct them on SPD level. In ISAP you can at least mask out or zap the portion (sometimes a full scan direction) which you believe to be the worse/more effected one. Note that masking-out might be preferable because the affected data points might still be usefull for the distinction between lines and glitches, and for the identification of lines and other features. Usually the down scan is considered the more trustworthy scan, because it follows after the up scan in the observation sequence, i.e. the detectors have had more time to settle. However, this is true only if the memory effect was caused *before* the scan sequence started (by a large signal between the science scans, e.g. a photometric check). If the memory effect is caused *during* the scan itself, e.g. by scanning across a strong line, both scan directions may be similarly affected. (In the example of a strong line in band 4 the red part of the lineprofile would be more reliable in the up scan, whereas the blue part would be better traced in the down scan.) Note that averaging of scan directions within "average" (see step 11 below) is not possible directly, because up and down scans have different wavelength grids (contrary to, e.g., AOT02 scans). Only if all 12 detectors show more or less the same differences, these differences may be averaged out when averaging across detector and scan direction later on. Alternatively, you could rebin all up scans, using the down scans as reference, and then average. Again, the redundancy between all 12 detectors and overlapping regions should help to make the best decision.

9) **Flatfielding**

Although the best effort has been made in the offline processing pipeline to ensure that the variation in response between detectors has been accounted for, there will inevitably be some residual discontinuity between detectors. To normalise all detector data to a common level use "Shift". You can either adjust all 12 detectors to the mean level or adjust 11 detectors to the level of a 12th, "good" detector. Please see the web help for more details. If the signal is weak the differences between the spectra of the 12 detectors can be attributed to uncertainties in the dark current subtraction. Hence, the "offset" mode should be choosen. Only for strong signals (above several 100 Jy) the dark current can be neglected and differences are due to gain effects, i.e. multiplicative effects. In this case "scaling" would be the right option. No general rules can be given here to decide which of the modes is the best. The same is true for"weighted" or "unweighted". However, in many cases "offset", "preserve mean", and "unweighted" is a good default.

An example for a problematic case is the combination of a strong line on a weak continuum: the continuum may be better corrected in "offset" mode, whereas the line itself might need a "gain" correction. If the continuum flux is around zero, both modes may fail, however. In this case you could try the following: freeze the plot range, mask out either the line or the continuum (depending on what you are interested in most), and shift in offset or gain mode. Then unmask again. (Note: shift will not use the masked data for the computation of the correction, but it will apply the correction to the masked data as well).

If you did not average across scan directions before, each scan direction will be shifted separately.

For band 1 and 2 data, flatfielding usually does not improve the data quality significantly, but for band 3 and 4 data this can be a very important step.

Be aware, however, that shifting in offset mode, i.e. adding or subtracting a constant, at this stage of processing is in principal wrong, because the relative spectral response function has been applied to the data (multiplicative). Nevertheles a shifting at this stage can improve your data quality. The result of the shifting should in any case be examined critically.

10) **Remove bad data - III**

After shifting you might want to do some additional zapping. Don't zap away lines!

11) **Averaging**

Now you can go on and average the spectra of all 12 detectors (and both scan directions if not done already in step 8) to get a single, mean spectrum. Select all data and choose "Average". For a detailed description of the average tool please read the web pages (see "GUI Buttons"). You should average across detectors and scan directions (i.e. don't select the corresponding buttons). The bin size should correspond to the spectral resolution (= FWHM of the Instrumental Profile). The resolution of an AOT1 observation depends on its' speed. The measured resolution at certain key wavelengths for a speed 4 observation (slowest speed, highest resolution, point source) is given in Table 2.

The resolutions of speed 3, 2, and 1 are approximately 0.5, 0.35, and 0.3 times the resolution of speed 4. For extended sources the resolution of all 4 speeds is $\approx$ 0.6 - 0.7 times smaller then for point sources.

To preserve the oversampling the 12 detectors provide, the bin size should be smaller than the actual resolution element. FWHM/5 is usually a value which gives good results (for a band 1A, speed 4 spectrum, e.g., 0.002/5=0.0004). These FWHM/5 (or resol x 5) values are offered as default values in the average tool (whenever ISAP is able to automatically deduce the resolution element from your data, i.e. whenever the data are unique and the status word is present).

The plotstyle options in combination with the possibility to zoom in (with the left mouse button), e.g. into a small range around a line, and to freeze the plot range in both windows to identical values, should help you to judge the result. To adjust the plot ranges in both windows use "Replot Max" in the left window, then use "Copied Range" in the right window. In addition, ISAP overplots the result directly in the left hand side plot window (if the oplot button is checked), so that you can directly compare e.g. line profiles before and after averaging.

In oplot mode you will also see the points that have been clipped by the clipping routine (in red). Note, that the small bin sizes associated with sws spectra can be too small for a significant clipping. In this case try to lower the sigma value (e.g. 2 or 1). Alternatively, there are two stand alone clipping routines available. A very basic one is available under the "arithm" button (in the tool box). It performs a kapp x sigma clipping on the basis of all selected data (i.e. the bin size is the entire selected wavelength range). Kappa can

Table 2: Approximate resolution of speed 4 SWS01 observations at certain key wavelengths. The values are for point sources. For extended sources the resolution is approximately a factor of 0.6 - 0.7 smaller.

AOT Band	Wavelength	Resolution (λ/FWHM)	FWHM
1A	2.407	1388	0.0017
1B	2.626	1216	0.0022
1D	3.092	1458	0.0021
1E	3.741	1143	0.0033
2A	4.052	1236	0.0033
2A	4.487	1366	0.0033
2A	4.530	1347	0.0034
2A	4.654	1422	0.0033
2B	5.610	818	0.0069
2B	6.986	1144	0.0061
2C	7.319	1149	0.0064
2C	7.460	1031	0.0072
2C	7.653	1227	0.0062
2C	7.902	1123	0.0070
2C	9.666	1550	0.0062
2C	10.51	1697	0.0062
3A	12.81	1149	0.0111
3A	13.10	1186	0.0110
3A	13.52	1176	0.0115
3A	14.32	1357	0.0106
3A	15.55	1411	0.0110
3C	18.71	1663	0.0113
3D	24.32	1004	0.0242
3D	25.89	1049	0.0247
3E	28.5	1000	0.0285
4	34.81	1619	0.0215
4	36.02	1459	0.0247

be specified by the user (e.g. 2.5). Outliers more than kappa x sigma off will be masked. You can then use the plot option "show masked data" to view the result. If you like it: "zap masked", if not: "unmask". A more advanced clipping tool is available under "Clipping". This routine allows you to adjust a bin size.

You can choose between different methods of averaging (see the description on the web). Try all of them to find the best method for your data set.

Don't forget to STORE!

12) **Defringe / RSRF**

For strong sources you may see periodic modulations in the continuum of band 2 and 3 data (and sometimes in band 1, too). These are the fringes, which are described in more detail in the SWS IDUM. ISAP offers a tool to defringe these data. Use the tool "SWS_Defringe", which can be found under "Special Fns...". Please read the very detailed on-line help text for this tool.

To check if you have residual fringes in your data you can read in the Relative Spectral Response Functions (RSRF, calibration files Cal25_xx, found in your ISAP installation under .../data/cal_sws), overplot those to the spectrum, and compare the frequency of the modulation. Note, that the unit of the cal files is microvolt/second/jy. So you will have to scale the RSRF to the level of your spectrum (which is in Jy). For more details please see the SWS handbook.

The overplotting of the RSRF function can also help to address the question of "fake" features in the spectrum. See the handbook.

13) **Smooth**

This function reduces the noise in the flux values of an AAR (either in unique parts, such as detectors, or all together) by convolution with a selected function: Boxcar, Gaussian, Lorentzian, Median, Hanning, or Sinc. If you are interested in line profiles you should, however, be very careful when choosing the function width (in other words: don't smooth too much!). Stay well below the FWHM of your lines (or try using the boxcar or median filter).

14) **Loop over all AOT bands**

Store the processed spectrum and go back to step 6 to reduce the other AOT bands in the same manner. Be aware of the plot style!

15) **Further steps**

After you have cycled through all AOT bands in the way described above, the basic reduction of SWS01 data is complete. If you wish to combine all the single spectra to one complete spectrum again, you can do so: make one of the spectra the prime data set and then select the other bands one after the other ("Stored Data Sets") and use "Stored Data Sets" →"Merge with Prime Data Set". This operation simply combines all selected data into one, larger AAR. A quicker way is provided by "Merge group of AARS" under

"Special Fns...". Before you merge, you should consider to mask out in the overlap region of two AOT bands the data of one of the bands, if these are of lower quality than the corresponding data in the other band. Alternatively you could average across the overlap region (by using the line tag, i.e average across lines). Note, however, that a higher flux value in a higher AOT band could be real, if the source is extended. E.g. the aperture of band 4 is much larger then the aperture of band 3E. In this case, of course, do not average.

A further option of data processing is REBINning (see the web documentation). ARITHM may be helpful for all kinds of arithmetic operations (e.g. to subtract or add two spectra or to add a constant, etc.).

Finally you may wish to analyse the processed spectrum, e.g. measure some line fluxes. The "Line Fit" tool, accessible via the tool box for selected data, provides all you need to fit a baseline and the line itself, it returns the fit parameters, line fluxes etc., and suggests several possible line identifications, based on the specified redshift (radial velocity) and a built in line list (including unidentified infrared bands – UIBs – and some unidentified lines).

You can also compare your flux densities with photometric measurements, like the IRAS measurements at 12 and 25 μm. This can be done using the "syn_phot" routine of ISAP. From within the GUI it is invoked via the "Photometry" button in the toolbox. Basically the ISO spectrum is convolved with the filter profile of the photometry. ISAP has built in the IRAS filter files as well as others, like KAO and ISOCAM. You can also specify your own filter curves. In this respect the unit conversion tool (accessible under "Special Fns...") may also be of interest for you.

"Zodiacal" can be used to subtract the dominant foreground at SWS wavelengths. "Dered" (available in the command line mode only) allows to deredden the spectrum according to a given extinction law.

When you exit the GUI you will be in ISAP's command line mode. By typing *aar=gui_output()* you'll get the aar which was prime on exit of the GUI. You can then work on your aar just like in a normal IDL command line environment. You can go back to a GUI session any time by typing *start_gui* or *start_gui, aar_in=aar*. The latter command passes an aar from your command line session directly into the GUI (see the information on the ISAP web page under "IDL-ISAP interface").

If you need more help, you should contact (or consider to schedule a visit to) IPAC, MPE, VILSPA or one of the other national ISO data centers. Informations about IPAC, MPE or the VILSPA IDC can be found on the web:
http://www.ipac.caltech.edu/iso/
http://www.mpe.mpg.de/www_ir/ISO/
http://www.iso.vilspa.esa.es/
You can also email us any kind of problems with ISAP and any suggestions you have:
isap_dev@ipac.caltech.edu. (Within the GUI just click on "Send Mail".)
The author of this recipe can be contacted via: sturm@mpe.mpg.de

If you are going to publish results which are based on a data reduction and/or analysis with ISAP we would very much appreciate the following acknowledgement:
"The ISAP Spectral Analysis Package (ISAP) is a joint development by the LWS and SWS Instrument Teams and Data Centres. Contributing institutes are CESR, IAS, IPAC, MPE, RAL and SRON."

And now: Good luck with the reduction and analysis of your ISO data!