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Technical Information

New Software for VG9000

MassCare Ltd is pleased to announce that a completely new software suite for control of the VG9000 is in the later stages of development and testing. The package has been named **MCAT9000** after the two companies involved in its development.

“MC” represents MassCare Ltd, a company set up by Peter Robinson in 2004. As most of you will know, Peter has been intimately involved with the VG9000 since its conception in 1981. “AT” is derived from **ATProg Ltd**, a company set up to develop software. Its founder, Alan Turnbull, has worked in electronics and software for many years, writing code for projects in the nuclear industry, air traffic control and, over the last few years, mass spectrometry.

It has long been recognized that there has been a need for modern software that will run on modern computers. MCAT9000 sets out to combine the familiar with the new. Those of you familiar with the current VG9000 software will find it quite simple to navigate through the new package, while it will remove the total dependency on obsolete hardware.

MassCare and ATProg spent long hours considering the “platform” that will be used for the software. We have chosen a modern tower system, a monitor with resolution 1280x1024 and a Laser Printer. We are happy to provide this as part of the package, but we are equally happy to define the full specification for you to buy locally. (By the way, you can use ANY printer for which you can find a driver, more choice than with DOS!)

The operating system gave us something to think about. We decided to launch our efforts with XP Pro rather than wait for Vista. After all, this project has been progressing for nearly a year now, time that would have been lost had we waited. Now Vista is available we will investigate the compatibility.

A copy of Excel is included with the package as we intend to make extensive use of this in handling data.

Instrument control has long been a worry with the VG9000. All systems use an ISA card for IEEE control. Others may use an Ion Counting Card built into the computer (again ISA) or an Ortec Bin system. The Bin system has been obsolete for many years now, and spares are becoming harder to find. In fact the "ACE" card from Ortec is also obsolete and has been replaced by a purpose built card (also ISA) only available from the original instrument manufacturer.

MCAT9000 pulls the control hardware back into the modern day. We have chosen PCI cards for both IEEE control and for replacement of the "ACE" card functions. Rather than going to small or specialist manufacturers, we have chosen off-the-shelf cards manufactured by National Instruments.

We have tested these thoroughly and there is no indication of speed problems for communications. And, as an added benefit of the flexibility of writing new software, we have designed a small module that can convert the pulses from the NIM form used by the Ortec Bin into TTL, thus removing the Photon Counter from the loop.

While on the subject of testing, we are extremely indebted to Hydro Aluminium High Purity GmbH for access to their two systems. They are (relatively) close geographically and have enabled us to test the software on both types of ion counting as well as Solartron and Keithley DVM's. And the canteen serves a good lunch!

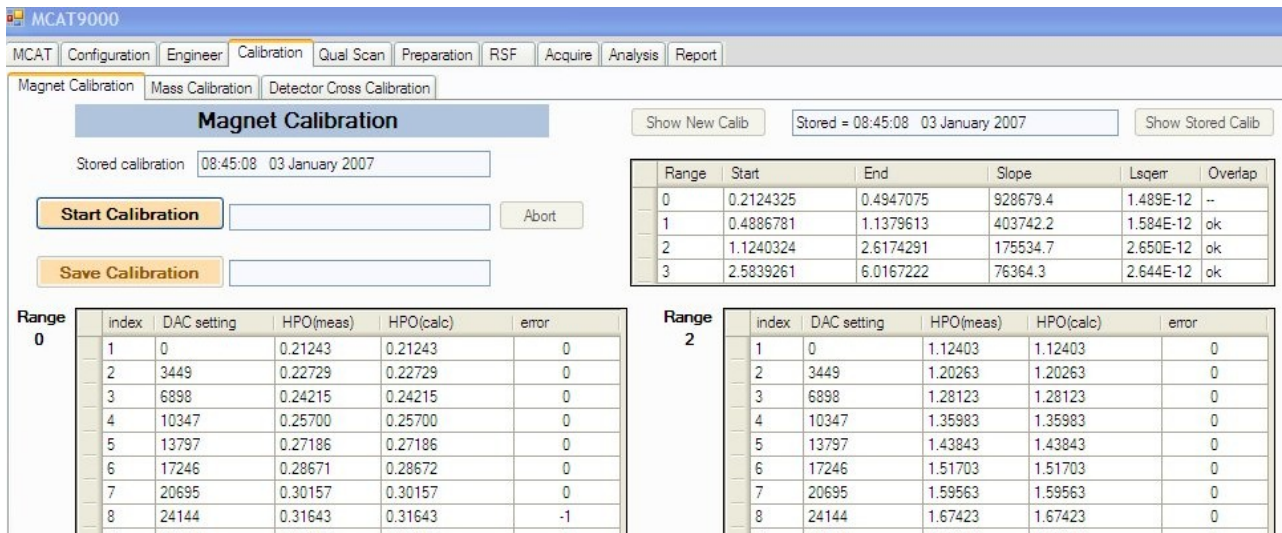
This document is intended to give you an oversight of the software as well as keeping you up to date on progress. We hope to have something new to report every two weeks or so, and have decided to post the updates on MassCare's web site, www.masscare.co.uk. In this way you can check it out when it suits you, rather than being inundated with emails that may not interest you.

So here goes.

As the software loads, you will be asked to **log on**. This will, in the future, allow a **two level, manager and technician**, access to the system. Any suggestions on how this could be structured or implemented would be appreciated. (In fact, if you have any suggestions that would make the software beneficial to you, the user, then please don't wait to be asked; email them to masscare2000@aol.com. We don't promise to implement them, but every suggestion will be considered at length).

Once into the software you will see a series of tabs at the top of the page. Each of these tabs has a sub menu (also tabs). By using this structure, it is possible to allow the user to do more than one thing at a time. For example when running a Magnet

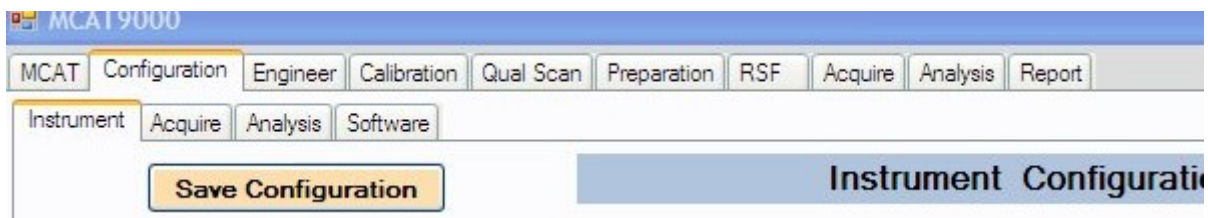
Calibration it is possible to analyse old data or set up an analytical procedure. The example below shows (top of) the Magnet Calibration page active, and the tabs for other functions can clearly be seen. Obviously some functions are mutually exclusive. For example you can't acquire data from a sample at the same time as you run a Magnet Calibration.



Let's take a look at each of the tabs and its sub menu in turn. We'll try to make clear what is currently working and tested, what is planned for inclusion before release, and what is planned for the update stage. Remember that your comments are welcome.

The MCAT tab is simply a welcome page loaded when the software is first run. In the future it may have the facility to log out and log back in again.

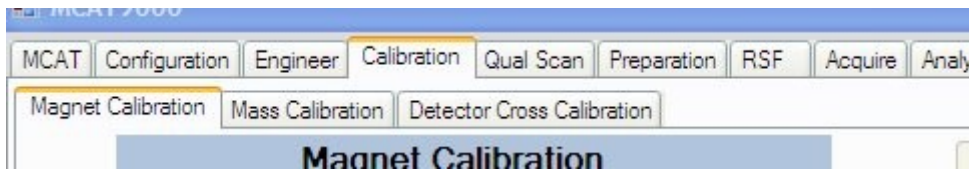
The Configuration Tab has 4 tabs in its sub menu. The Instrument tab will include essential information such as DVM type and Ion Counting type. It will also have the option to define the various generations of electronics units that are in the system, enabling easier discussion for ongoing support,



The acquire tab will hold default values for scan parameters for various functions, eg Short range scan, mass mark, sample data acquisition. The analysis tab and software tabs are currently unused, but it is expected that they will define path names for data storage.

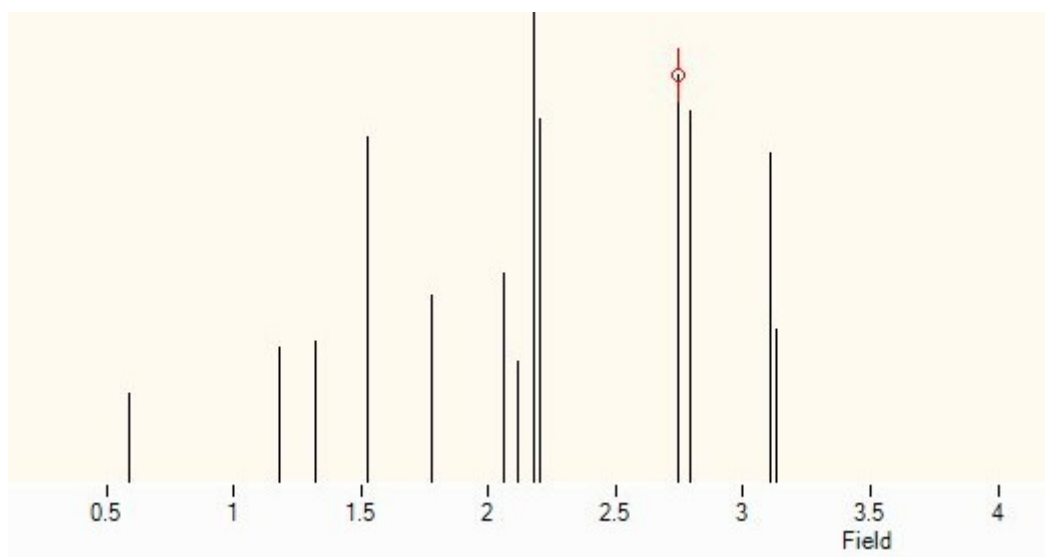
The Engineer Tab is designed to enable us to control the instrument at the lowest level. It will be developed further before release and the sub menu will reflect the functions found in the current diagnostics block, but with expansion so that some of the things we have all wanted for years are present.

The Calibration Tab has three operations in the sub menu, Magnet Calibration, Mass Calibration and Detector Cross Calibration (previously Ion Counting Efficiency).



Not much can change with the Magnet Calibration, after all it is only fitting a straight line to a Digital-to-Analogue Converter. We've tried to make it more user friendly, highlighting any large DAC errors and missing overlaps, but it's hard to do more.

The mass calibration offers more scope. For now we have adopted the familiar Faraday scan of the entire mass range, followed by peak identification. One hidden, but very important, improvement is the fact that if the Multiple Interface suffers from a "glitch", MCAT9000 can recover. With the original software you would see "Hardware Not Responding". We tested by introducing "glitches" by running a difficult sample in a flat cell and found that in more than 90% of cases the software recovered, clearing the "bus", cycling the magnet and returning to the field it was previously up to. This ability to recover is quite a complex process, but having found it we plan in the future to build it into other programs, particularly the multi element acquisition.



The mass calibration program also helps with peak identification. A spectrum of the peaks found is displayed and a cursor can be moved across the peaks using the mouse.

The software will highlight in the table the peak on which the cursor is sitting, allowing you to identify its mass in the way familiar to you. Even after all these years I find this feature useful.

Detector Cross Calibration is very similar to the Ion Counting Efficiency program from the original suite. However, because of the way the software is structured you can find the peak using a short range scan (see later), and then leave the magnet sitting on top of the peak while you switch to the calibration. Again, after years of measuring manually, I find that I use this feature to find the peak. After all, why complicate life when it can be simple.

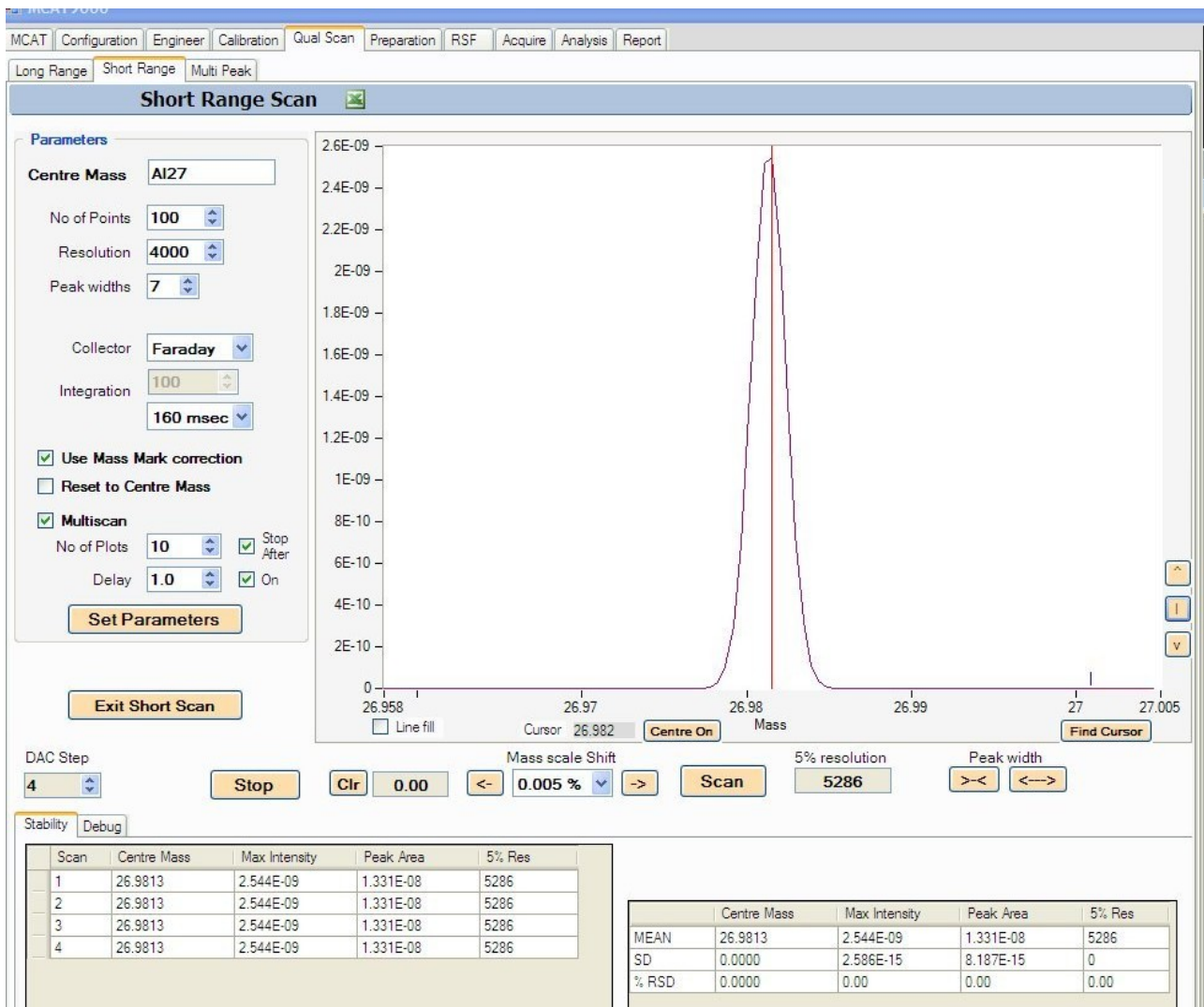
A small addition to the Detector Calibration is to store the mass at which the measurement was made. This can be a useful diagnostic.

The QualScan Tab will ultimately offer three functions; long range scan, short range scan and multi scan.

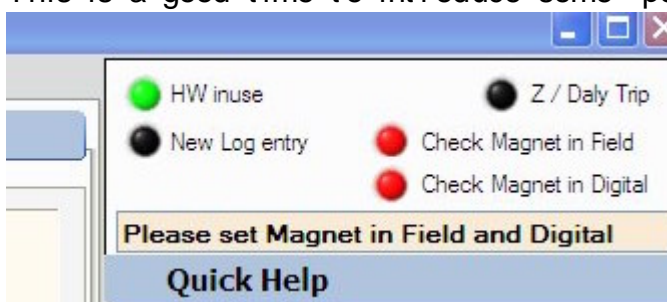
The long range scan will offer a simple chart recorder function, scanning from Field1 to Field2. This is considered low in the priority list and will probably be offered after release as a free update.

The Short Range scan is very similar to the current Stability program. The operator can choose single or multi scans and in the latter case the software will calculate the statistics on the data before outputting it to Excel. However, this program has additional features. The width of the scan can be varied graphically as well as by numerical input. If the peak is not centred then corrections can be made with an on-screen cursor. And the data acquired during mass mark can be used in calculating peak centres.

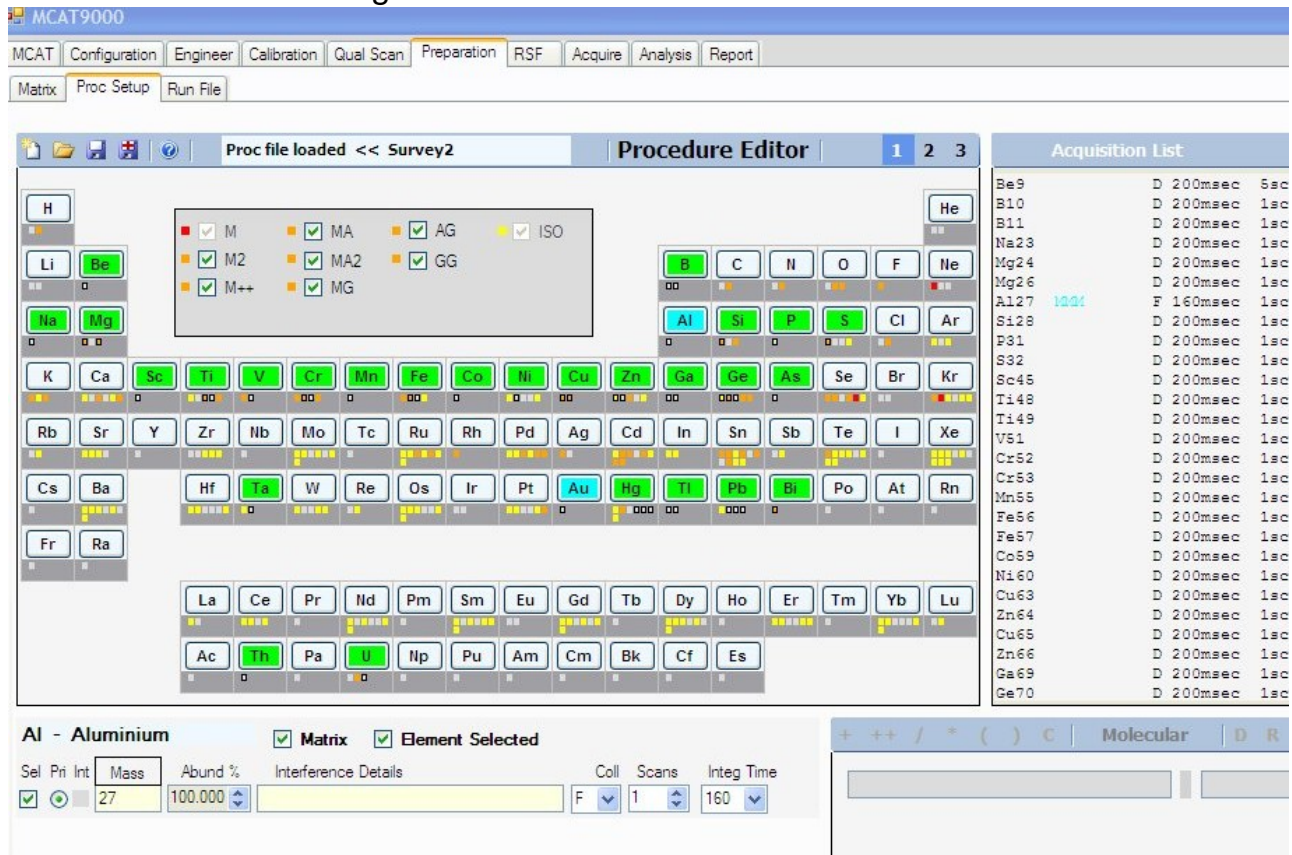
The picture below shows a few of these features.



This is a good time to introduce some “policing” features. Where necessary the software will check that the Magnet is in the correct settings, normally Digital and Field. If not then red “buttons” highlight this and the program will wait for you to correct it. You can also see a “Hardware In Use” button. This stops you trying to perform conflicting operations where there will be different demands on the Hardware. The “New Log Entry” will turn amber when an Error has been handled. A brief description of the error will be logged for you to view and also saved to file so that we can investigate.



The **Preparation Tab** accesses the software that defines the analysis to be undertaken. In many ways you will find it familiar from previous suites, but this has many additional features. There are many short cuts to enable smooth input of data; full use is made of the right mouse button.



Analytically, the most obvious difference is the ability to change not only the number of scans, but also the integration time from peak to peak. So, if you have impurities at PPM levels you may wish to scan these quickly, while spending more time on the lower, possibly more critical elements. This feature is available now for counter card systems and it is expected to be available for Ortec Bin systems when the conversion to counter card is fully proven.

A more complex interference guide is to be developed in the future. You will see in the sub menu a tab labeled "Matrix". This currently enables you to define default isotopes and integration times for a specific matrix. Obviously there may be some interferences present in one matrix that isn't there in another, thus necessitating a different approach. By holding this information in a "template" for creating the Procedure File, you only have to think through the problems once. This "Matrix Driven" concept will develop further in the future.

The tab labeled "Run File" will, in the near future, enable you to define a series of acquisitions on the same sample. This will be further enhanced to enable some quality control; for example if an element is found below a required detection limit then it

can be removed from the procedure for the next run (on the same sample). Of course, you can already manually change a procedure as you are analyzing the sample, ready for the next run. There is no need to wait until the acquisition is finished.

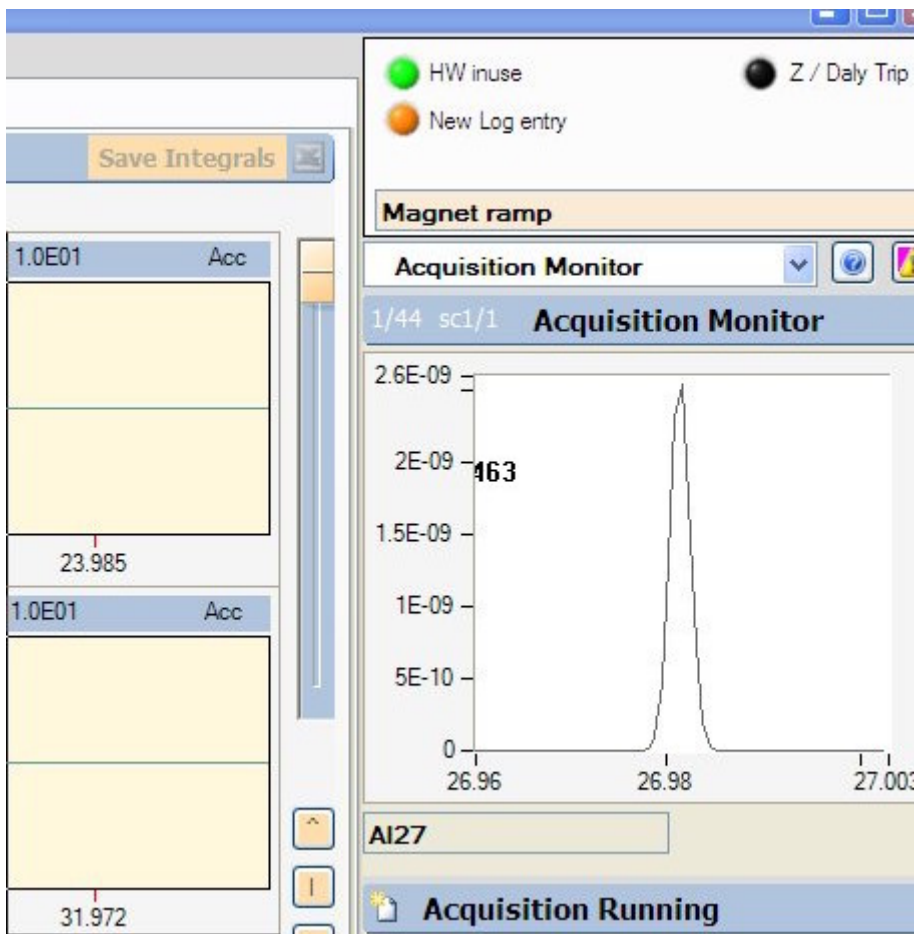
The RSF Tab at the moment simply allows you to define a table of RSF's. This will be developed before release to enable you to define more than one table and store them in a library. Naturally a reference element is needed for all tables as they may be used for multi-element matrix calculations.

The Acquire Tab has a submenu of five items, the first of which is Mass Marking. This again is familiar and provides a localized mass calibration to "fine tune" the fundamental curve. The biggest current difference to the old software is that you can change the number of points, and the DAC step via the Procedure Editor. The integration time can currently be changed for Daly peaks only for the counter card version, but hopefully by release this will have changed to include the Ortec Bin as well. This will save a lot of time in systems that are basically stable.

The screenshot shows the 'Mass Mark Acquisition' window in the MCAT software. The window title is 'massmark1.roc'. It features a grid of ten mass spectra plots, each with a peak labeled with its mass value and an offset. Below the plots, there is a 'Mass Mark Acquisition' panel with a 'Get MassMark' button and a 'Change Procedure' button. A table at the bottom right lists the acquisition parameters for each peak.

Use	Name	Mass	Offset
<input checked="" type="checkbox"/>	ar40/6	6.6604	-48
<input checked="" type="checkbox"/>	ar40/5	7.9925	-16
<input checked="" type="checkbox"/>	ar40/4	9.9906	-16
<input checked="" type="checkbox"/>	ar40/3	13.3208	-8
<input checked="" type="checkbox"/>	Ar40/2	19.9812	-8

The second tab under Acquire is the Multi Element Acquisition Control. Again this will



be familiar to you with some improvements. An Acquisition Monitor window is displayed to the right hand side of the screen. This monitor stays visible even if you go off to another part of the software (eg Procedure Definition).

Another difference is that the file being acquired is given its own multi element display so that you can work on the file as it's acquiring, but you can also work on old files at the same time (upto a further two files –

does anyone want more?).

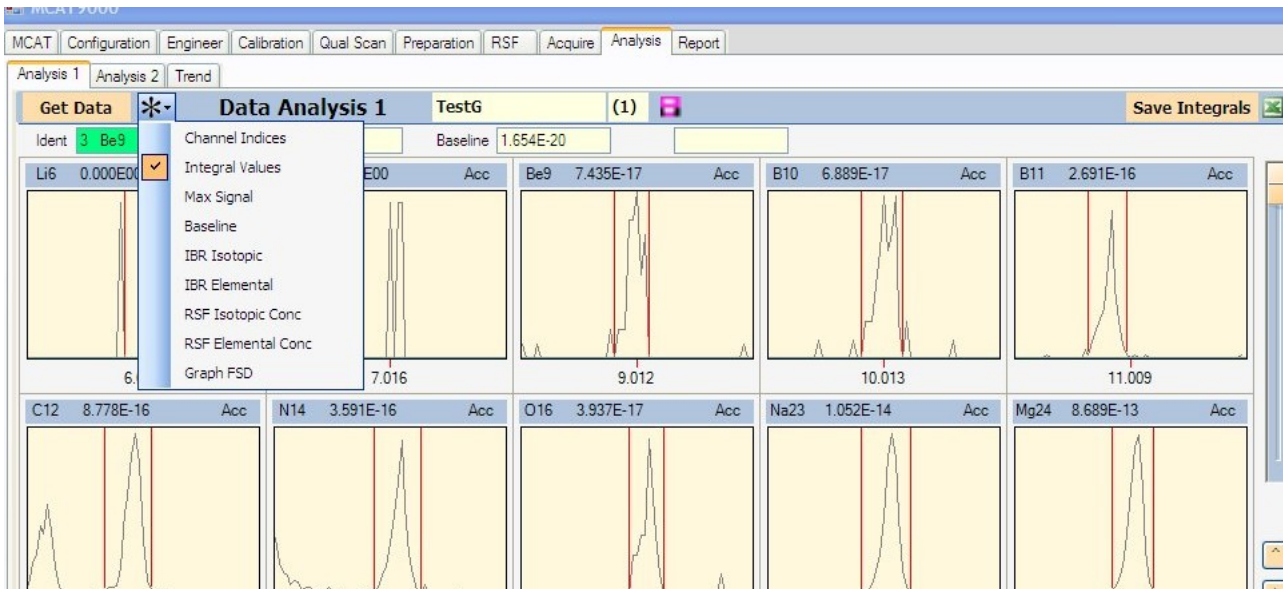
But the biggest difference is that you can set a flag to tell the system to measure the matrix peaks first (up to a maximum of 5). This will cause the program to measure all the element(s) defined as matrix in a quick 20ms scan before starting the normal cycle around the analytes. When the sequence reaches the matrix in the normal order of things then it will be measured using the parameters (integration time, scans) defined by the operator and the “quick scan” data will be replaced. This offers a couple of advantages. Firstly you can analyse the file and view PPM levels right from the start. Secondly, if something goes wrong, say your sample decides to short circuit or your exit slit becomes blocked, then you have matrix data that, while not measured as precisely as in the normal scan, can at least give you some results for the elements measured.

IR Acquire (Isotope Ratio) and DP (Depth Profiling – Real Time) will be offered after the launch of the main software – at an extra cost!

Finally under the Acquire tab, the Zoom Acquire allows the operator to take any of the smaller graphs and zoom in on the data to set limits, backgrounds etc with more

precision. At the time of writing this document this window was being developed and will appear in the first update.

The Analysis Tab offers some familiar and some new features.



The multi element display allows you to manipulate the data in the small windows for speed, or you will be able to zoom in on a graph. A variety of different values can be displayed on the graphs, the list is shown. All of this is familiar to you.

So what's new? You can open two files at once for analysis (as well as the currently acquiring file). Do you think that is enough? Let us know now if you'd like more.

If you look at the tabs you will see a "Trend" tab. This will allow you to pick a single isotope and display its value from a range of data files. Then you will be able to inspect for example its PPM value in each of the files while visualising the graphs. This is to be built in the future (hopefully before initial release) so any thoughts you might have now would be welcomed.

Also new, and definitely to be put into the release, is "post-acquisition mass marking". This will enable you to identify any peaks of which you are certain (eg the matrix) and use these to mass correct the other peaks for display only. This has proved useful in identifying unknowns.

When the zoom graph is finished, the next development will be the interference identification. You will be able (as now) to identify a peak that you believe could interfere and show its relative position on the graph. However, this software will allow you to show more than one peak at a time, and will remember in a library

anything you have previously entered. Hopefully this will be developed further to be matrix specific (you don't want to see Cd++ next to Fe if your matrix is Al).

The next major new feature is that when the calculations are complete, you simply click on a single button and the data is exported to Excel. Currently the program exports Integral, Isotopic PPM IBR, Elemental PPM IBR, Isotopic PPM RSF Corrected and Elemental PPM RSF Corrected. What else (if anything) do you think should be included? In future there will also be a separate feature to export all the raw data from each channel to Excel so that those of you who wish to push the detection limits will be able to investigate the data channel by channel.

It's probably worth stating at this point that the raw data has been analysed channel-by-channel to check that all the calculations are being done correctly, from baseline correction, to integration time, ion counting efficiency and, of course, the calculation of the ion beam ratios for single and multi element matrices. It's a lot easier with Excel than it was first time in 1982!

Finally, **the reports tab** is currently blank. This is for you to design. Do you feel that the program should offer some level of report generation, or is the output to Excel enough for you to make your own from Macros? We know we will get more than one answer!!

OK, that's a long document and a lot to take in. Updates will be issued frequently as the progress is made. All will be uploaded to the web site where you found this, so keep looking. But above all, remember that this is YOUR chance to suggest which features you've always dreamed of (or those that have given you nightmares in the past). So do write to us, talk to us, whatever is easier for you. It's important to us that this software is what you, the user, wants.