

Does our software tell us the truth?

(Should we burn the black box?)

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Disclaimer:

The results quoted in this presentation were generated using particular versions of the programs used. It is possible that later versions of the same program perform differently – for better or worse. That applies to their manuals as well.

I make no absolute value judgements on these programs; I merely quote experience. It is possible that other people using different parameters might achieve better results.

GammaVision was version 5.30

FitzPeaks was version 3.63

The Genie manual was for Genie-PC

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My brief...

- I was asked to share my experience of working with different programs.
- CompAct - my own program LOTS
- GammaVision (ORTEC) LOTS
- FitzPeaks (Jim Fitzgerald) SOME
- Genie (Canberra) LITTLE

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When I was asked to give this talk, it was suggested that I share my experience of different gamma spectrometry software systems. I can only do that to a limited extent. Like most people, my experience, and the systems I have used, was dictated by the commercial situation I found myself in.

In my early gamma spectrometry days, from 1966 to 1993, I ran a small Activation Analysis Service. It was up to me to provide the spectrum analysis software – by which I mean to create it. At the time, the commercial programs were only just appearing, and certainly were not aimed at Activation Analysis. That program, or rather the successor to it, is called CompAct, standing for Comparative Activity measurement.

The experience of writing spectrum acquisition and analysis software means that I can judge other programs with some understanding of the underlying difficulties that those other programs have had to overcome. It also means that I feel justified in being somewhat critical of programs that do not function as well as they might.

Much later, in 2000, I was asked to help set up the gamma spectrometry lab for NIRAS (now part of AMEC) in the UK. That lab was committed to using GammaVision, and so I gained considerable experience of the inner workings of that program.

FitzPeaks I have a little experience of, but I am generally impressed by it. The author, Jim Fitzgerald, used to work for Canberra in the UK providing software support. The nice thing about FitzPeaks is that Jim is resident in the UK and is approachable – unlike the software writers for the large companies.

Genie I have little real practical experience of, but I have, from time to time, sought to compare its performance against other programs.

Does our software tell the truth?

- The short answer is...
- ...probably most of the time,
- but not all of the time

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So to the point...

Does our software tell the truth?

The answer is probably most of the time, but not all of the time.

What is this 'black box'?

- It's the mental box many people live by:
- Samples go into the box at one end...
- ...results come out of the other...
- ... and are accepted with complete and utter, uncomprehending and untested, trust.
- That will not do!
- Bear in mind that the manufacturers live by selling systems – not by generating results.

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I should explain what I meant, in the sub-heading to my talk, by 'the Black Box'. It is the system, be it spectrometer, program, whatever, that unaware people use for their measurements. The sample, or spectrum, goes in at one end and results come out of the other and are accepted with complete and utter, uncomprehending and untested, trust. The box is black because no light – or should we say, enlightenment – penetrates it.

It is a great concern to me that the 'Black Box' mentality is rife in many gamma spectrometry labs. In my opinion it will not do!

You must always bear in mind that the manufacturers live by selling systems and software – not by generating results. They don't lose jobs or clients if their systems give the wrong results – but YOU might.

You may think that is a very cynical view of the manufacturers, but I have spent many years observing and trying to communicate with them.

Article of Faith...

- All software will let you down under the right circumstances...
- ...the trick is to know what those circumstances are!
- Read the manual – but they sometimes lie!
- Play with your software – change the settings, see what happens
- Above all - resolve inconsistencies

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As some people here may remember, on my gamma spectrometry course, I present one of my articles of faith as

‘All software will let you down under the right circumstances’. The trick is to understand what those circumstances are.

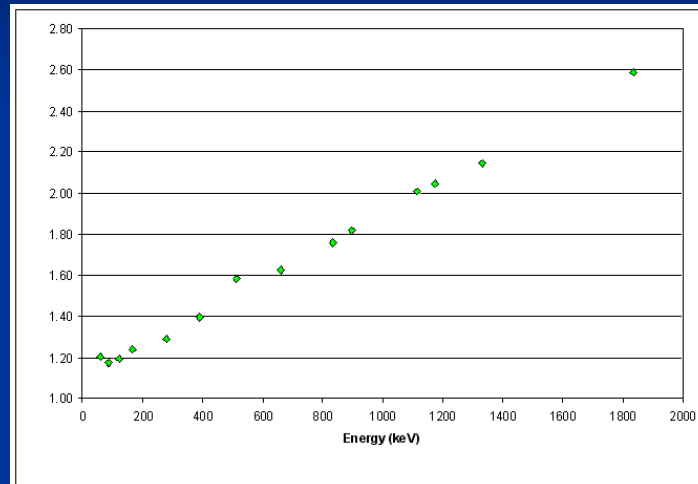
That knowledge can only be acquired by reading the manuals (which, as we shall see, may themselves tell lies!) and playing with the software; changing parameters to see what happens to the analysis. It might be necessary to do some manual calculations, both of activity and uncertainty, to check whether the program give justifiable results.

The most profound learning experiences are to keep ones eyes open for inconsistencies: situations where the results look odd, or the peaks don't look right, or something just doesn't seem right. When that happens, don't just say ‘Oh, how odd!’ - find out why it's odd!

Resolving inconsistencies can be particularly satisfying.

By way of example, I want to bring to your attention a few inconsistencies and, while discussing them, point out various pitfalls in trying to understand your software

A Calibration

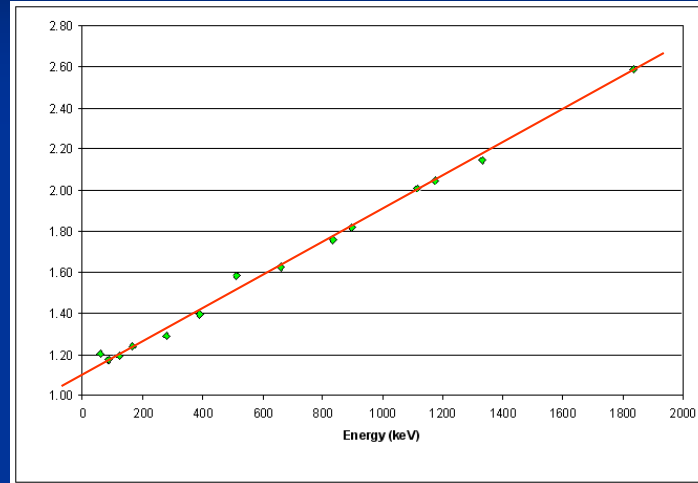


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This is a calibration – it doesn't matter what calibration (although any experienced gamma spectrometrists should recognize it). Look at it from a simplistic point of view – what calibration line would *you* fit to the data?

A Calibration

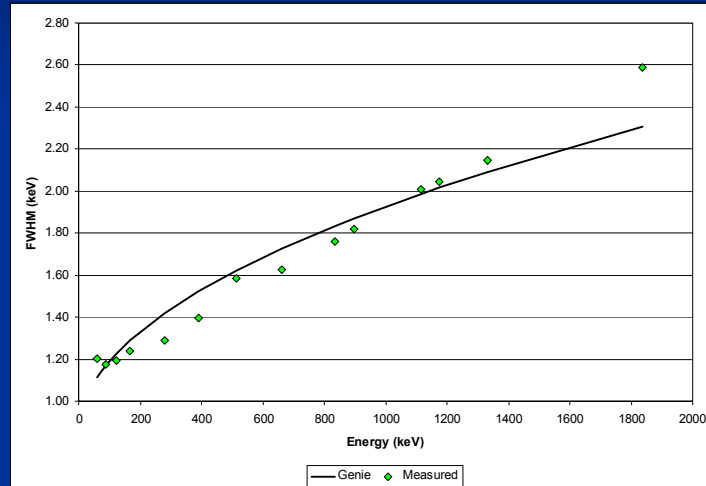


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Well, I'm a simple soul! A straight line looks fine to me.

Canberra Genie FWHM Calibration



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In fact, of course, this is a peak width calibration – in fact it is part of the data within the calibration spectrum provided as an example with the Genie-2000 software.

Do you think it fits? I certainly don't. As far as I'm concerned the data and the fitted function are inconsistent.

Why do Canberra use that function?

Canberra Peak Width Calibration

2. Peak full-width at half-maximum (FWHM in units of channels) as a function of energy

Page B.12

$$\text{FWHM} = \frac{F_0 + F_1\sqrt{E}}{C_1}$$

where E is the energy in keV, C₁ is the “gain” term from the energy calibration equation, and F₁ and F₀ are the coefficients of the FWHM equation.

This is the appropriate page from the Genie manual...

The calibration is a function involving the square-root of the gamma-ray energy: an Intercept + a gradient times square-root of the energy.

Canberra Peak Width Calibration

2. Peak full-width at half-maximum (FWHM in units of channels) as a function of energy

Page B.12

$$\text{FWHM} = \frac{F_0 + F_1\sqrt{E}}{C_1}$$

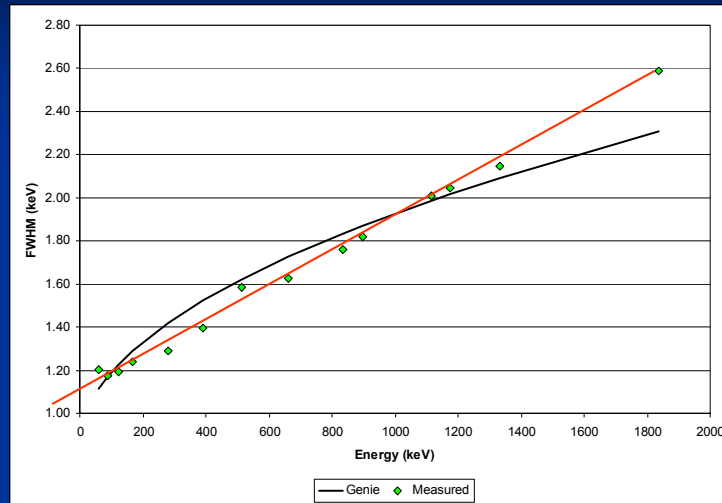
Debertin and Helmer: $\text{FWHM} = \sqrt{[F_0 + F_1 \cdot E]}$

where E is the energy in keV, C₁ is the “gain” term from the energy calibration equation, and F₁ and F₀ are the coefficients of the FWHM equation.

In their book, Debertin and Helmer suggest the square-root function shown in red: the square-root of an Intercept + gradient times the energy. There is theoretical justification for this equation. There is no theoretical justification for the Genie equation.

I suspect that the Canberra programmer thought he/she was using a rearrangement of this Debertin and Helmer equation. That is not the case and there is no theoretical justification at all for it. As far as I am concerned it is wrong and, bearing in mind that our programs make judgements based up peak width, this must have unwanted consequences for our analyses.

Canberra Genie FWHM Calibration



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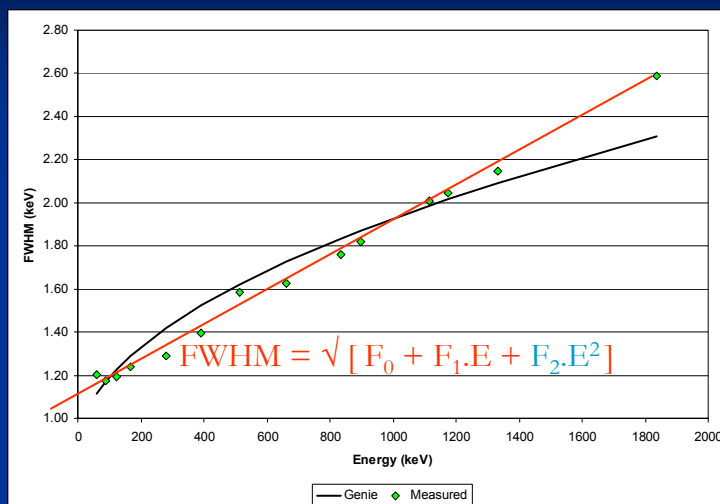
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Again I invite you to judge whether the Genie function fits the data properly.

UPDATE:

In discussion with Gerhard Fritz, of Canberra, at this Seminar, he admitted that perhaps there had been a mistake in the FWHM calibration but insisted that the Genie algorithms are relatively insensitive to the actual form of the FWHM calibration.

Canberra Genie FWHM Calibration



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Having looked at this matter in some depth while preparing the second edition of 'The Book', taking theoretical considerations into account, I have come to the conclusion that a square root quadratic function best fits FWHM data. There is reasonable theoretical justification for that view.

GammaVision uses an un-square-rooted quadratic and for some time I have been critical of that choice as being an easy, unimaginative choice by a badly advised programmer. There is no theoretical justification for it but, to my surprise (and some embarrassment) in practice it appears to fit actual data almost as well as the square-rooted quadratic function I propose.

Canberra again...

$$F_i = H e^{-\frac{(x_i - c_p)^2}{2\sigma^2}} \quad (1)$$

where

F_i is the value of the peak model function at channel x_i ,

H is the height of the peak,

c_p is the peak centroid, and

σ is the width of the Gaussian (approximately $2.355 \cdot \text{FWHM}$, where FWHM is the width of the peak at half height after the subtraction of the continuum).

So, we had there an example of a fundamental inconsistency within the software itself.

But sometimes even the manuals may frustrate our attempts to understand the software.

This is another page from the Genie manual – the statement made is simply incorrect.

Canberra again...

$$F_i = H e^{-\frac{(x_i - c_p)^2}{2\sigma^2}} \quad (1)$$

where

F_i is the value of the peak model function at channel x_i ,

H is the height of the peak,

c_p is the peak centroid, and

σ is the width of the Gaussian (approximately 2.355*FWHM, where FWHM is the width of the peak at half height after the subtraction of the continuum).

No! FWHM = 2.355 × σ

this is what it should be. In this case, I suspect that within the software the correct relationship is used. The problem is the manual compiler. But it is not helpful is it?

UPDATE:

Gerhard Fritz pointed out to me that the current versions of the Genie manual do have this function defined correctly. Excellent!

And ORTEC...

GammaVision Manual – version 5.30:

The random uncertainties are:

- Counting
- Additional
- Random summing
- Absorption correction

The systematic uncertainties are:

- Nuclide uncertainty from library
- Efficiency fitting uncertainty from calibration
- Calibration source uncertainty
- Geometry correction
- Additional

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Another example...

This is from the GammaVision 5.30 manual.

While trying to create an uncertainty budget for the AMEC lab, I found that the uncertainties given by GammaVision did not agree with manual calculations based upon the list here...

And ORTEC...

GammaVision Manual – version 5.30:

The random uncertainties are:

- Counting
- Additional
- Random summing
- Absorption correction

The systematic uncertainties are:

- Nuclide uncertainty from library
- Efficiency fitting uncertainty from calibration
- ~~Calibration source uncertainty~~
- Geometry correction
- Additional

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– unless, that is, I left out the calibration source uncertainty.

I contacted Ametek and, on my behalf, they contacted ORTEC in the USA who went back to the source code for GammaVision and agreed with me – GammaVision does not take that into account.

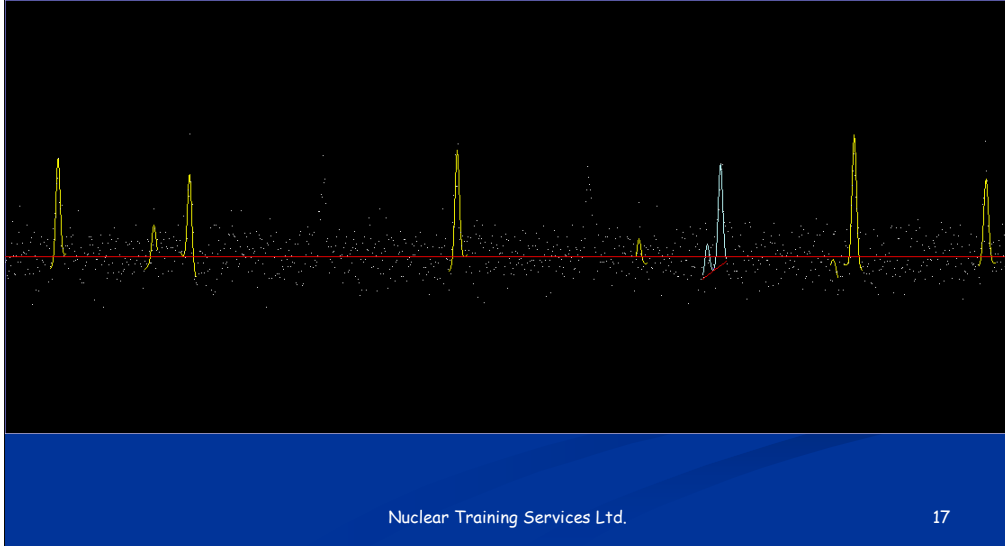
They then said ‘We will alter the next version of the manual’! Hmmph. As it happens they haven’t. And, of course, what they should have said is that they would alter the program!

There is another problem with this uncertainties list, which is not immediately obvious. GammaVision assumes all random uncertainties have a Gaussian distribution, and all systematic uncertainties as having a rectangular distribution.

This is not ORTEC’s fault, they were following common usage at the time, where uncertainties were split into random and systematic. Experience has shown that there is no clear-cut distinction between two categories. Modern usage is to split into Type A, determined by repeated practical measurements (counting uncertainties are a special Type A case) and Type B, determined by any other means – including guesses!

Clearly, when setting up an uncertainty budget, all that should be borne in mind.

GammaVision: Peak background



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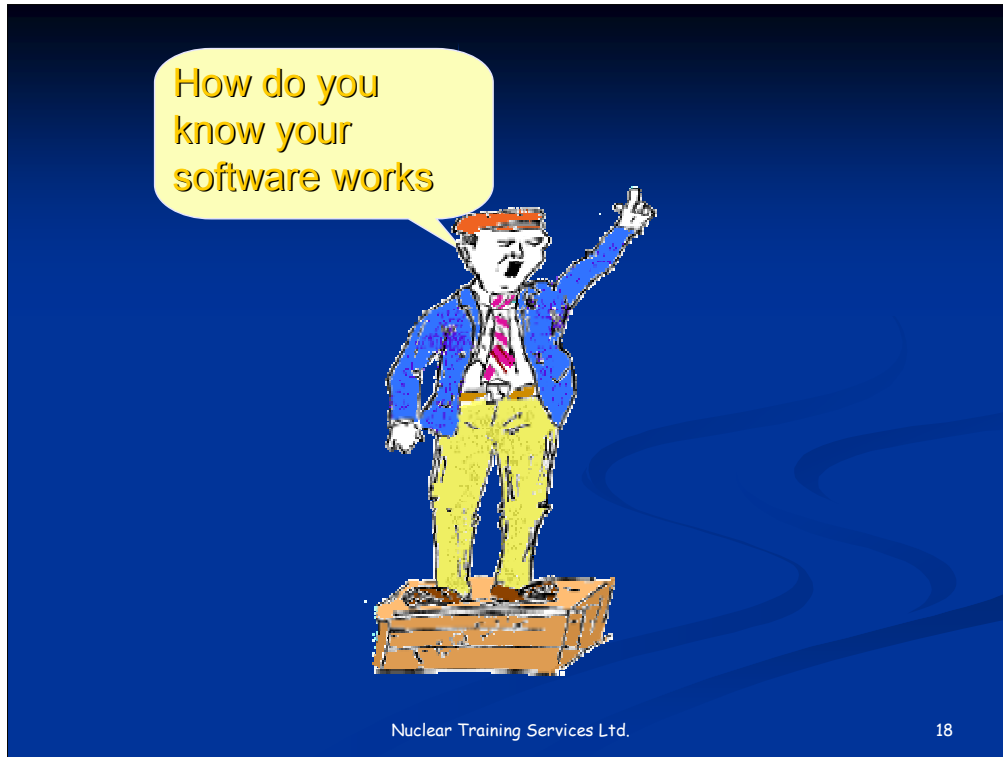
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Let's have a look at a spectrum inconsistency...

This is a spectrum with the peaks detected by GammaVision superimposed. This is a spectrum created by SpecMaker, for which I happen to know exactly what the mean background is – that is represented by the red line.

The thing to note is that the lowest point of most of the peaks is below that mean line. Anybody who has worked with GammaVision and bothered to examine their spectra will recognize that this is very common for GammaVision.

But, if the base of the Gaussian is below the mean background level it must mean that the area of the peak is overestimated. Quite so! The problem is proving that...



How do you know that your program gives you accurate peak areas?

It is not good enough to say 'Well, ORTEC or Canberra or Jim Fitzgerald or anybody else says so'. You really have to convince yourself by doing some sort of testing.

This is more difficult than it sounds. You need spectra with peaks at known positions, with known peak areas and known widths. There are a number of sets of test spectra available, but none of them are without criticism by somebody.

The problem is that if the spectra are created mathematically, some people will cry 'not real detector peaks'. If the spectra are created by counting, one can never know how many counts in a peak region are due to background and how many actual counts. You can easily estimate those numbers of counts, but never measure them.

Test spectra available

- IAEA G1 1976 – tests peak area measurement
- Sanderson 1992
- IAEA 1995 – tests peak area measurement
- NPL 1997 – tests activity measurement
- IAEA 2002 – tests activity measurement
- Intercomparison Exercises - e.g. NPL – test activity measurement
- SpecMaker – prepare your own test spectra

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These are sets of test spectra available. Most of them are available for download on the gammaspectrometry.co.uk website.

The G1 spectra were created mathematically from real detector spectra counted for such a long time that statistical scatter was negligible. They test the basic peak detection and area measurement of the software.

The Sanderson 1992 spectra were mathematically generated spectra and again test peak area measurement.

IAEA 1995 spectra were created by Menno Blauuw of Delft. They test area measurement and Menno claims that the quoted areas are absolute and traceable.

NPL 1997 spectra were created by counting and are designed to test the whole analysis process. Unfortunately, there are problems with these spectra. In a report dealing with an assessment of various programs using the spectra, the originators criticise the lack of true coincidence summing corrections, but their calibration spectra supplied did not include the spectra needed to make those corrections. Some of the spectra are also subject to random summing, although that has gone unrecognized in the assessment report by NPL, the software manufacturers and the NPL's expert analyst. The means to make those corrections are present, but not obvious.

IAEA 2002 spectra were again created by Menno Blauuw and this time test activity estimation. This set of spectra does include all the spectra necessary to perform TCS corrections on both Genie and GammaVision.

Of course, all laboratories should be participating in intercomparison exercises. If you get the right answer, you can be confident that everything is working fine. If not, then one may have to go back through the individual analysis stages to seek the problem.

SpecMaker

- You provide calibration data – energy and width
- You specify peaks positions (up to 50)
- You specify number of counts in each peak
- SpecMaker creates the spectrum
- You use you own program to analyse it...
- ...and compare the results with expected values
- SpecMaker Assessment spreadsheet

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SpecMaker is a spreadsheet based program that will create spectra up to 16k in size with peaks of known shape, position and area with realistic statistical uncertainty imposed upon the channels.

The idea is that you should create a suitable spectrum for your purposes, by specifying where you want the peaks to be and how big they should be. The peak widths are determined by the calibration data supplied by the user.

SpecMaker provides a page to compare the actual versus the measured peak information. The program also exports the actual data into a .CSV file, which can then later be loaded into the SpecMaker Assessment spreadsheet to do the comparison.

SpecMaker – Test Spectra

- Three spectra – 100, 1000, 10000 cts/ch bgd
 - 50 peaks ALL with **Critical Limit** number of counts
 - 50% probability of detection – i.e. expect to find 25
- Three spectra – 100, 1000, 10000 cts/ch bgd
 - 50 peaks ALL with Limit of Detection number of counts
 - 95% probability of detection – i.e. expect to find 47-48
- Three spectra – all have 50 peaks of 1000 counts
 - Backgrounds: 100, 1000, 10000 – some below critical limit
- One spectrum – 50 peaks 10000 counts on 1000 cts/ch bgd – expect to find all

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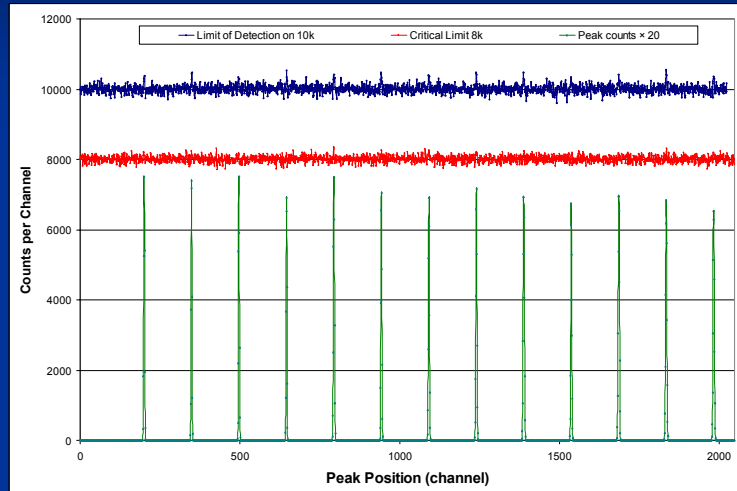
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I have created a number of simple spectra designed to test the peak search function of spectrum analysis programs.

All these spectra contain 50 peaks on a flat continuum. The first peak is centred at 50 keV and the others are then inserted at 40 keV intervals. In all cases, when calculating limits, the background region widths are assumed to be 5 channels

- 1) Three spectra containing peaks containing a number of counts equivalent to the Currie Critical Limit at the particular peak energy and peak width on different continuum levels.. We would expect these peaks to be significant in 50% of cases, so our spectrum analysis programs should be able to detect 25 peaks.
- 2) Three spectra containing peaks containing a number of counts equivalent to the Currie Limit of Detection at the particular peak energy and peak width on different continuum levels. We would expect these peaks to be significant in 95% of cases, so our spectrum analysis programs should be able to detect at least 47 peaks.
- 3) Three spectra with 1000 count peaks on continuums of 100, 1000 and 10,000 counts/channel. The peaks in the third of these spectra are below the Detection Limit.
- 4) One spectrum with 10,000 count peaks on a 1000 counts/channel continuum. All these peaks should be easily measured.

Peaks at Critical Limit and Limit of Detection



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At the top is part of a spectrum containing 50 peaks on a 10k background that contain exactly the number of counts equivalent to the 95% confidence Limit of Detection.

At the bottom are the peaks added.

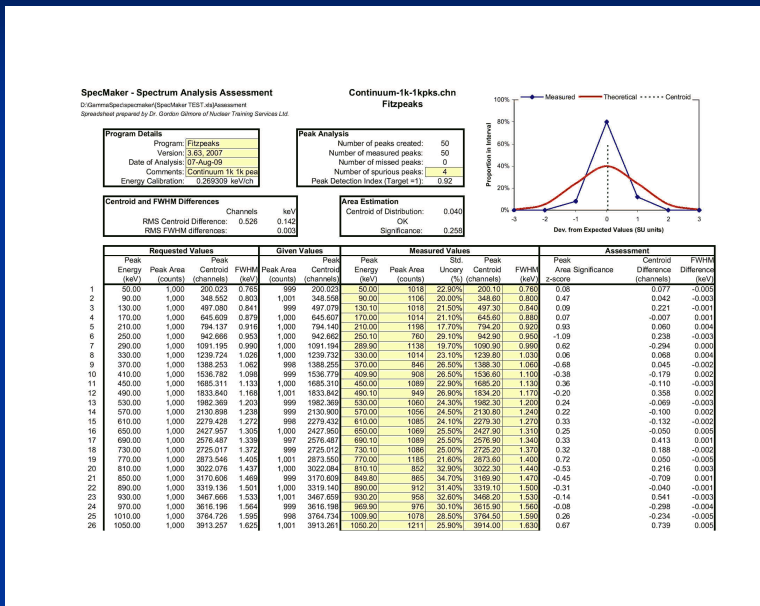
Statistically, we would expect any program to be able to detect 95% of those 50 peaks – 47 or 48.

Would you agree with me that all the peaks at the Limit of Detection are visible by eye?

The red spectrum contains peaks that are at the Currie Critical Limit on an 8k background. We would expect to be able to detect 50% of those peaks, because in half of cases the peak area would be below the critical limit and half above.

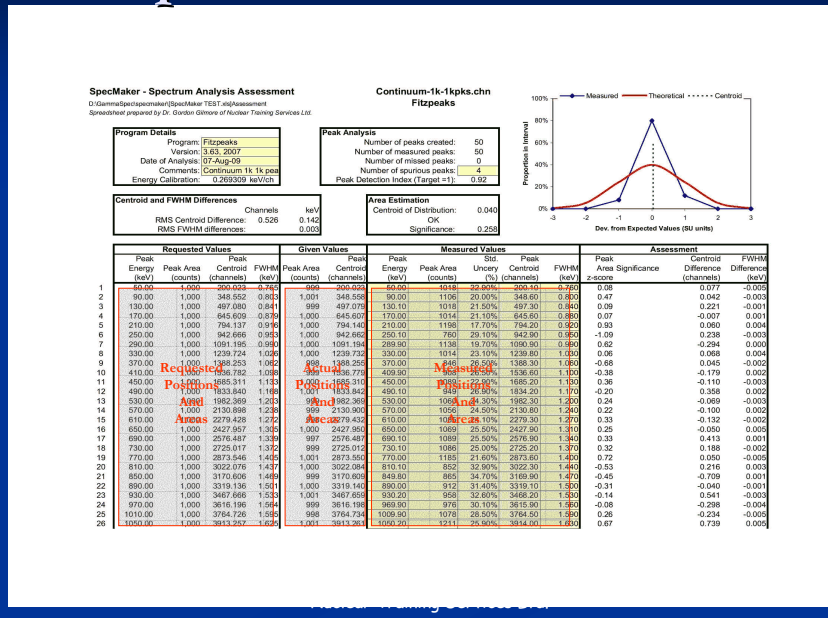
At least some of those peaks are visible by eye.

SpecMaker Assessment



This is an overall view of the SpecMaker Assessment spreadsheet.

SpecMaker Assessment



The left hand four columns specify where the user asked SpecMaker to put the peaks and how big they should be.

The next two columns list the actual peak positions and the actual number of counts in the peaks,

The next four columns are the results gleaned from the user's spectrum analysis program. The right hand four columns give the significance of the difference between actual and measured areas, the difference in peak position and width.

SpecMaker Assessment

SpecMaker - Spectrum Analysis Assessment

D:\GammaSpec\specmaker\SpecMaker TEST.xls\Assessment
 Spreadsheet prepared by Dr. Gordon Gilmore of Nuclear Training Services Ltd.

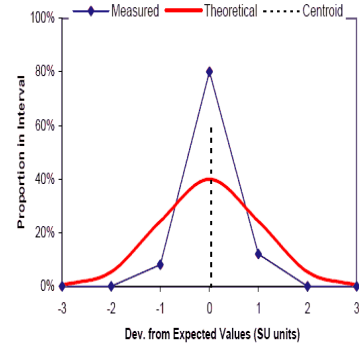
Continuum-1k-1kpks.chn
 Fitzpeaks

Program Details	
Program:	Fitzpeaks
Version:	3.63, 2007
Date of Analysis:	07-Aug-09
Comments:	Continuum 1k 1k pea
Energy Calibration:	0.269309 keV/ch

Peak Analysis	
Number of peaks created:	50
Number of measured peaks:	50
Number of missed peaks:	0
Number of spurious peaks:	4
Peak Detection Index (Target =1):	0.92

Centroid and FWHM Differences		
	Channels	keV
RMS Centroid Difference:	0.526	0.142
RMS FWHM differences:		0.003

Area Estimation	
Centroid of Distribution:	0.040
	OK
Significance:	0.258



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At the top of the screen are a number of assessment summaries:

Peak Analysis box – how many detected, how many spurious, how many missed

Position and Width box – the mean differences – measured and actual

Area Estimation – the centroid of the distribution of peak area difference (measured – actual) and whether it is significantly different from that expected

A plot of the distribution of area differences – (Measured – Actual) – in units of standard uncertainty.

L_D on 1k c/ch



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This shows part of the upper spectrum I showed you before – each peak has the number of counts corresponding to the limit of detection on a 1000 ct/channel background.

I would suggest that you can easily pick them out by eye.

Do you agree?

Think about this...

- If you are 95% certain of detecting the peak, do you not think you should be able to see it yourself (in most cases)?
- Based up long experience, I am convinced that that is so.
- If you don't believe me, look at the example spectra and make up your own mind.

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A question...

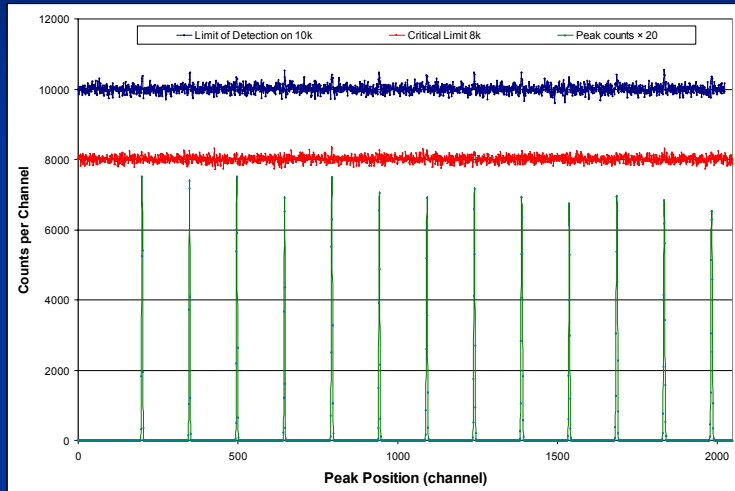
If I'm right, if you can't see a peak, the actual number of counts must be less than the 95% Limit of Detection.

So why do our programs quote that limit when they can't find a peak?

UPDATE

I was informed at the Seminar that both GammaVision and Genie now include upper limit option to be quoted when peaks are not found. Hallelujah!

Peaks at Critical Limit and Limit of Detection



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This is simply another opportunity to see if you can pick out the Ld peaks by eye.

CompAct and FitzPeaks

Spectrum	FitzPeaks				CompAct			
	Detected	Spurious	Centroid	Signif?	Detected	Spurious	Centroid	Signif?
Target: 50%	25	0	0.000		25	0	0.000	
Lc 100	13	3	0.231		11	9	1.364	YES
Lc 1,000	20	2	0.350		17	10	0.941	YES
Lc 10,000	17	4	0.235		14	6	1.357	YES
Target: 95%	48	0	0.000		48	0	0.000	
Ld 100	50	2	0.220		49	5	0.367	Maybe
Ld 1,000	49	5	-0.020		47	4	1.511	YES
Ld 10,000	49	1	0.143		47	4	0.213	
Target: 100%	50	0	0.000		50	0	0.000	
Peak 10,000 on 1,000	50	0	0.180		50	3	-0.060	
Peak 1,000 on 10,000	21	1	0.143		18	6	0.772	Maybe
Peak 1,000 on 1,000	50	4	0.040		50	7	-0.100	
Peak 1,000 on 100	50	3	0.020		50	4	-0.180	

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This slide compares the performance of FitzPeaks with my own program CompAct. I have never used FitzPeaks myself in practice, but I have to say that analyzing these test spectra suggests to me that it is well worth looking at.

The general conclusions are:

Critical Limit spectra: both programs find less than expected peaks, but CompAct appears to be significantly overestimating these small peaks areas. CompAct finds rather more spurious peaks than FitzPeaks.

Limit of Detection spectra: both programs find the expected 95% of peaks, at the same time generating few spurious peaks. Unfortunately, for me, CompAct is again overestimating peak areas.

1k Continuum spectra: both programs find all the peaks with few spurious peaks and little or no area bias.

(I am not discussing the 10k continuum spectrum because the peaks are below the Critical Limit by a variable amount, which makes assessment difficult.)

GammaVision and FitzPeaks

Spectrum	FitzPeaks				GammaVision			
	Detected	Spurious	Centroid	Signif ?	Detected	Spurious	Centroid	Signif ?
Target: 50%	25	0	0.000		25	0	0.000	
Lc 100	13	3	0.231		1	11	Not analysed	
Lc 1,000	20	2	0.350		5	14	0.800	Prob. Not
Lc 10,000	17	4	0.235		6	11	1.667	Prob.
Target: 95%	48	0	0.000		48	0	0.000	
Ld 100	50	2	0.220		16	7	0.563	Maybe
Ld 1,000	49	5	-0.020		12	13	0.333	
Ld 10,000	49	1	0.143		25	13	0.560	Maybe
Target: 100%	50	0	0.000		50	0	0.000	
Peak 10,000 on 1,000	50	0	0.180		50	0	0.440	Maybe
Peak 1,000 on 10,000	21	1	0.143		7	14	0.429	
Peak 1,000 on 1,000	50	4	0.040		35	10	0.571	Prob.
Peak 1,000 on 100	50	3	0.020		49	8	0.510	Prob.

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Comparing GammaVision to FitzPeaks is, at first sight, rather worrying.

The general conclusions are:

Critical Limit spectra: GammaVision performs disastrously with these spectra, finding few peaks and measuring them with a possible positive bias.

Limit of Detection spectra: again GammaVision does not find the expected number of peaks. In fact, visual inspection of the GammaVision results reveals many visually perceptible peaks that haven't been detected.

1k Continuum spectra: GammaVision has very variable performance on these easy spectra and again the result suggest a positive bias on the areas.

GammaVision is generally prone to finding spurious peaks. My experience with the program is that it is not possible to remove these without compromising further the ability to detect peaks.

However, maybe we are being to hard on GammaVision. These analyses were done as a blind peak search. ORTEC themselves suggest that it is better to use a peak library and tell the program where to look for peaks.

GammaVision using Library

Spectrum	GammaVision				GammaVision - Library			
	Detected	Spurious	Centroid	Signif ?	Detected	Spurious	Centroid	Signif ?
	Target: 50%							
Lc 100	25	0	0.000		25	0	0.000	
Lc 1,000	1	11	Not analysed		30	18 (28)	0.839	YES
Lc 10,000	5	14	0.800	Prob. Not	31	22(31)	1.065	YES
	6	11	1.667	Prob.	41	15(22)	0.854	YES
	Target: 95%							
Ld 100	48	0	0.000		48	0	0.000	
Ld 1,000	16	7	0.563	Maybe	49	7	0.837	YES
Ld 10,000	12	13	0.333		49	12	0.551	Prob
	25	13	0.560	Maybe	50	18	0.880	YES
	Target: 100%							
Peak 10,000 on 1,000	50	0	0.000		50	0	0.000	
Peak 1,000 on 10,000	50	0	0.440	Maybe	50	12	0.440	Maybe
Peak 1,000 on 1,000	7	14	0.429		44	17(20)	0.841	YES
Peak 1,000 on 100	35	10	0.571	Prob.	50	11	0.560	Maybe
	49	8	0.510	Prob.	50	8	0.054	Prob

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So let us compare GammaVision's performance with and without a library.

Critical Limit spectra: now GammaVision tends to find more peaks than expected. Unfortunately, there is still a large number of spurious peaks found and the positive area bias is definitely significant. Careful examination of the results reveals that some of the peaks GammaVision has found are, in fact, below the Critical Limit area and should be rejected.

Limit of Detection spectra: GammaVision now finds all the peaks, but with the usual positive area bias.

1k Continuum spectra: As above.

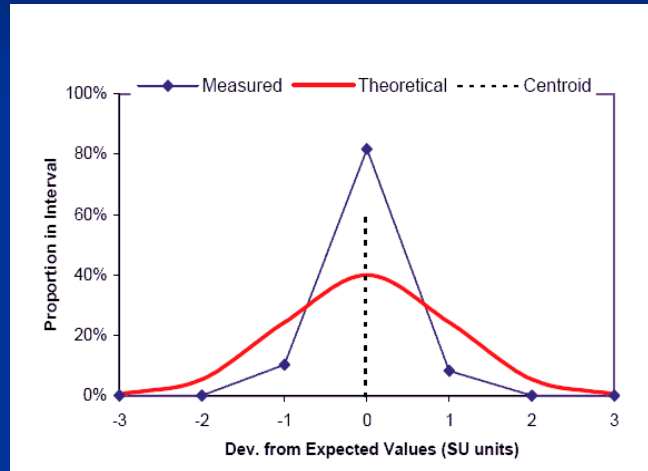
GammaVision...

- Blind search is poor
- Library directed better - but gives results for non-significant peaks
- Peak areas are consistently overestimated
- ...because of that, many spurious peaks
- Unless peak/continuum ratio is high, then poor estimation of peak position
- Unless peak/continuum ratio is high, then awful estimation of FWHM

To summarize:

One of the hidden problems of GammaVision is that it can easily miss very visible peaks if they are not in the library. It means that manual examination of the spectrum and the analysis results are necessary if the spectrum is in any way out-of-the-ordinary.

FitzPeaks: L_D on 1000 c/ch



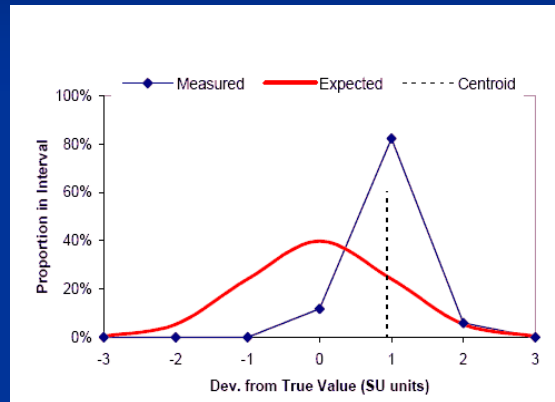
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This is the distribution of area differences (measured-actual) for a FitzPeaks analysis of the Limit of Detection peaks on a 1k counts/channel background.

Fitzpeaks often seems to measure peak areas more accurately than would be expected statistically. I'm not sure how that can be so, but there it is.

CompAct: L_C on 1000 c/ch

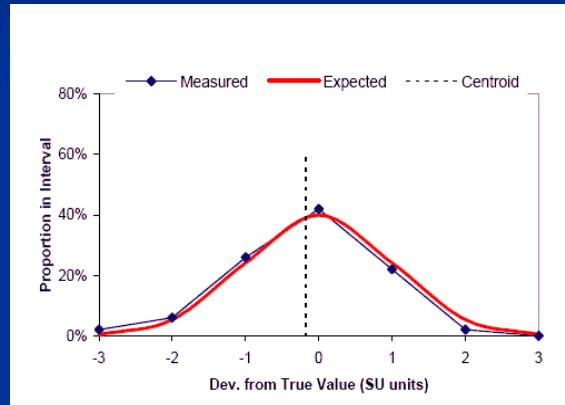


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This distribution of area differences generated by my own program CompAct shows graphically the positive bias.

CompAct 1k peaks on 100 c/ch

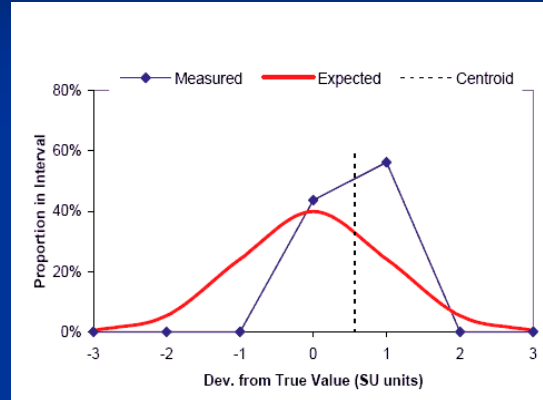


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But when peaks are better defined, CompAct shows an area distribution exactly matching the statistical expectation.

GammaVision: L_D on 100 c/ch

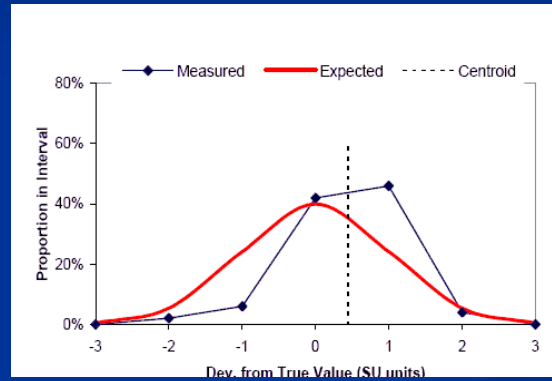


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This is a typical distribution from GammaVision – peaks areas significantly biased high, regardless of the peak/continuum ratio.

GammaVision: 10k peaks on 1k c/ch



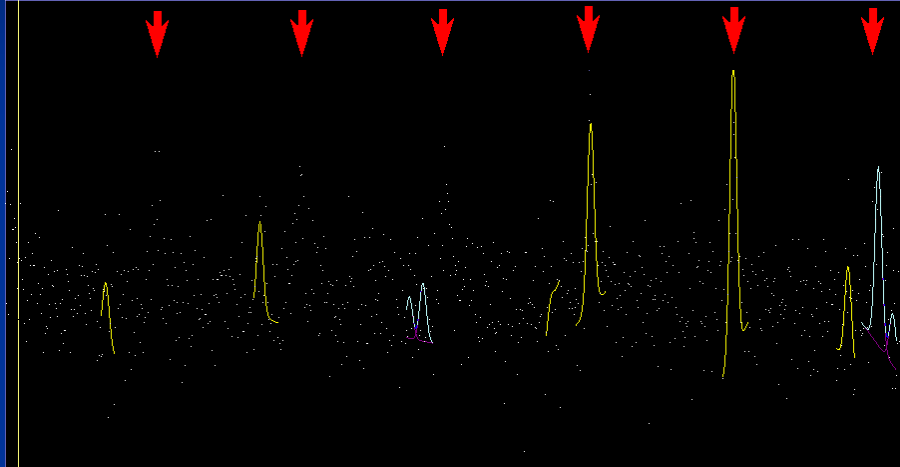
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These are very well-defined peaks on a low background. As with all these assessments of GammaVision, small peaks or well-defined peaks, the pattern here common to all. GammaVision consistently overestimates peak areas.

This is an inconsistency – and I haven't yet explained it.

GammaVision: L_D on 1k c/ch



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Let's return to the Limit of Detection peaks on the 1k background

These are the peaks GammaVision fitted. Note the missing, visually perceptible peaks and the fitted peak shapes dipping below the mean of the background scatter. This was the inconsistency we started off discussing.

The reason for it is revealed in the GammaVision manual. GammaVision does not work out the peak limits using the peak width calibration, which would seem to be the sensible thing to do. It finds the limits by searching for a group of 5 points together forming a minimum point on each side of the centroid. Simple logic tells us that the resulting peak area MUST be at a maximum – hence the positive area bias.

The message is...

- Look at your spectra!
- When you find inconsistencies – follow them up – resolve them
- Test your software – make sure you understand it's weaknesses – and it's strengths
- If necessary, arrange some sort of post-analysis correction of results

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My messages are:

Look at your spectra! THE MARK 1 EYEBALL CONNECTED TO A SENSIBLE BRAIN IS A REMARKABLE DEVICE – in many ways better than any of the software

Test your software – make sure you understand it's weaknesses – and it's strengths
YOU HAVE TO TAKE THE TIME

When you find inconsistencies – follow them up – resolve them
THAT'S THE WAY YOU LEARN

If necessary, arrange some sort of post-analysis correction of results
In practice, you have your software, if you replace it you may have just as many (probably different) problems.
It may be possible to correct some of the problems after the software has done it's work.

FOR EXAMPLE...

Post analysis correction...

- **Fred** - AMEC radiometric lab at Birchwood
- Summarizes the GammaVision .rpt data
- Removes some spurious peaks
- Does a correct peaked background correction
- Corrects random summing correction uncert.
- Does a proper weighted mean of individual peak results
- When appropriate, calculates activity upper limit, rather than MDA
- Checks that correct calibration were used etc.

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The link program 'Fred' was written for the gamma spectrometry laboratory at NIRAS, now part of AMEC, Birchwood in the UK.

Fred takes the GammaVision .rpt output and performs a number of operations on. Some of them are for convenience, others are necessary.

Of particular note are the following (all are handled by Fred):

GammaVision does not do a correct peaked background correction because it does not take into account the uncertainty on the amount subtracted. This has the effect of leaving false positive peaks.

Although the random summing correction is accurate, the empirical uncertainty is unrealistically high,

If more than one peak is used to measure a nuclide, GammaVision does not use the intermediate results to calculate the final result. It adds all the individual peak areas together to calculate it. This give equal weight to all peaks whether measured with small or large uncertainty. The correct procedure would be to calculate a weighted mean based on the uncertainties of the individual peak measurements.

GammaVision uses the Limit of Detection to calculate MDA instead of upper limit – although I am informed that that may now be an option.

Further information...

- www.gammaspectrometry.co.uk
 - www.gammaspec.co.uk
 - www.gammaspec.org.uk

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This website was created in tandem with the book 'Practical Gamma-ray Spectrometry Second Edition'.

It carries the following:

The appendices from the book

Fully analysed example spectra: QCYK, long background, NORMS

Some of the spreadsheets used to generate figures for the book

SpecMaker and example spectra

Publicly available test spectra

Links to other relevant websites

References and links to Data

A bulletin board for exchange of information