SpecMaker

Prepared by Dr. Gordon Gilmore of Nuclear Training Services Ltd.

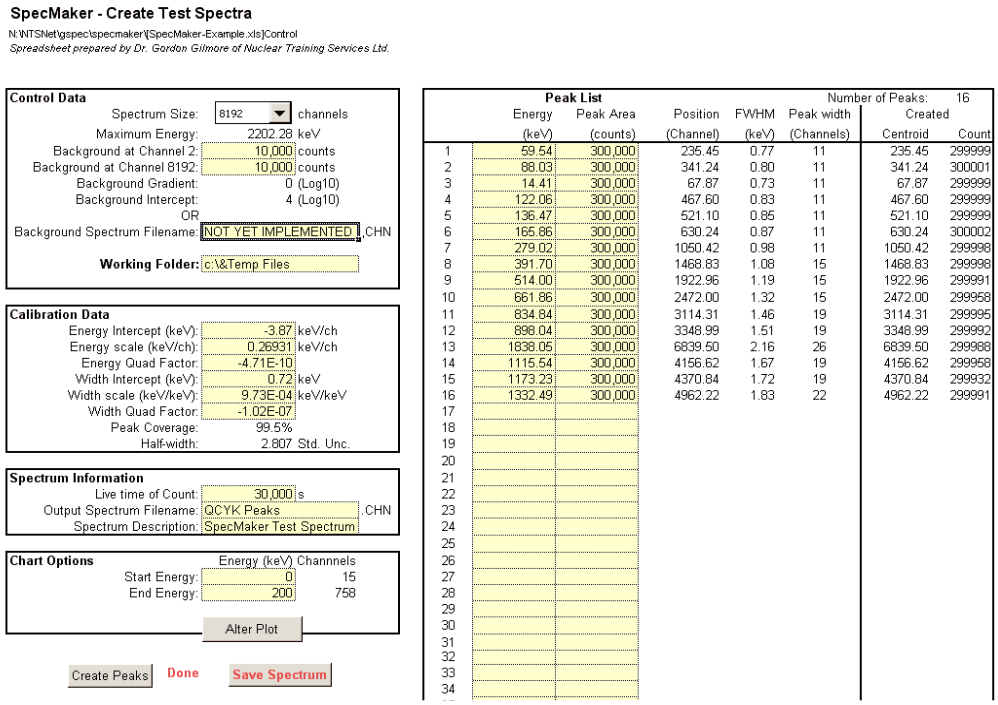
1 Introduction

SpecMaker was written to allow gamma spectrometrists to create spectra with which they can test their spectrum analysis program. The spectra generated comprise a continuum, which may be mathematically generated or be an imported background spectrum, on which are superimposed up to 50 peaks at user-defined positions and peak areas (i.e. number of counts within them).

All spectra are generated in the ORTEC .CHN format. The spectrum will be accompanied by a .csv (comma-separated-value) file listing the expected positions and peak areas. This is created so that it can be used by other programs, spreadsheets etc. to allow a comparison to be made between expected values and those measured by the spectrum analysis program. *SpecMaker* itself allows this comparison to be made. Because it is not always convenient to do that at the moment a spectrum is created, *SpecMaker* is accompanied by *SpecMaker-Assessment* – the assessment part of the workbook packaged alone.

These notes will continue by explaining the function of each worksheet in turn.

2 Control



SpecMaker - Create Test Spectra

N:\NTSNet\gspec\specmaker\[SpecMaker-Example.xls]Control

Spreadsheet prepared by Dr. Gordon Gilmore of Nuclear Training Services Ltd.

Control Data

Spectrum Size:	8192	channels
Maximum Energy:	2202.28	keV
Background at Channel 2:	10,000	counts
Background at Channel 8192:	10,000	counts
Background Gradient:	0 (Log10)	
Background Intercept:	4 (Log10)	
OR		
Background Spectrum Filename:	NOT YET IMPLEMENTED	.CHN
Working Folder:	c:\&Temp Files	

Calibration Data

Energy Intercept (keV):	-3.87	keV/ch
Energy scale (keV/ch):	0.26931	keV/ch
Energy Quad Factor:	-4.71E-10	
Width Intercept (keV):	0.72	keV
Width scale (keV/keV):	9.73E-04	keV/keV
Width Quad Factor:	-1.02E-07	
Peak Coverage:	99.5%	
Half-width:	2.807	Std. Unc.

Spectrum Information

Live time of Count:	30,000	s
Output Spectrum Filename:	QCYK Peaks	.CHN
Spectrum Description:	SpecMaker Test Spectrum	

Chart Options

	Energy (keV)	Channnels
Start Energy:	0	15
End Energy:	200	758

Alter Plot

Create Peaks Done Save Spectrum

Peak List — Number of Peaks: 16

	Energy (keV)	Peak Area (counts)	Position (Channel)	FWHM (keV)	Peak width (Channels)	Created Centroid	Created Count
1	59.54	300,000	235.45	0.77	11	235.45	299999
2	88.03	300,000	341.24	0.80	11	341.24	300001
3	14.41	300,000	67.87	0.73	11	67.87	299999
4	122.06	300,000	467.60	0.83	11	467.60	299999
5	136.47	300,000	521.10	0.85	11	521.10	299999
6	165.86	300,000	630.24	0.87	11	630.24	300002
7	279.02	300,000	1050.42	0.98	11	1050.42	299998
8	391.70	300,000	1468.83	1.08	15	1468.83	299998
9	514.00	300,000	1922.96	1.19	15	1922.96	299991
10	661.86	300,000	2472.00	1.32	15	2472.00	299958
11	834.84	300,000	3114.31	1.46	19	3114.31	299995
12	898.04	300,000	3348.99	1.51	19	3348.99	299992
13	1838.05	300,000	6839.50	2.16	26	6839.50	299988
14	1115.54	300,000	4156.62	1.67	19	4156.62	299958
15	1173.23	300,000	4370.84	1.72	19	4370.84	299932
16	1332.49	300,000	4962.22	1.83	22	4962.22	299991
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34							

On this worksheet, the parameters needed to generate the spectra are provided by the user. On all worksheets, cells where information should be put are coloured pale yellow. All other cells will be protected from alteration. Whenever units are specified, it is important that the parameter be provided in those units.

Control Data

Spectrum size from 256 to 8192 channels is selected on a drop-down list.

Background Continuum

a) If it is desired to create a mathematical background, specify the background level you require at channel 2 and again at the end of the spectrum. *SpecMaker* will then create a smooth exponentially decreasing background across the spectrum. This is intended to mirror, to some extent, the fact that in most spectra the continuum level decreases from low to high energy. If the two levels are equal, a linear background will be created. If a very low continuum levels are chosen, say less than 10, it is likely that many channels will have zero counts.

b) It will also be possible, as an alternative, to specify an existing real background spectrum to be used instead of the mathematical continuum. The background spectrum must be in .CHN format and be in the working folder specified below. If the spectrum file is not present in the folder, *SpecMaker* will fault.

Specifying a background spectrum will override any continuum instructions already specified.

Working Folder

This is the folder into which the created spectrum and its csv file will be put. If a background spectrum is to be used, it must be in this folder. If the folder specified does not exist, *SpecMaker* will fault.

Calibration Data

It is necessary to specify the following information:

a) **Energy calibration**: Intercept (in keV), energy scale (keV/ch) and, if a quadratic function is required the quadratic term (keV/ch^2)

b) **Peak Width Calibration** Intercept (in keV), energy scale (keV/keV) and, if a quadratic function is required the quadratic term (keV/keV^2)

If a pre-existing background spectrum is used, these factors will be taken from that.

Count Period

Specify the count period in seconds. Both real time and live time will be set to this value. No dead-time will be allowed for. This value has no significance for spectrum creation, but simply fills the necessity for a spectrum to have a count period.

Spectrum Filename

This is the name under which you wish the spectrum to be saved. Do not include the .CHN filename extension.

Spectrum Description

This is an optional field for you to put information about the spectrum in. It will be saved within the spectrum file as the Sample Description. The CHN file Detector Description will be automatically created is the form: `SpecMaker – Bgd: 1000/100 – 10 Peaks`, reflecting parameters provided by the user.

Peak List

In this area, the user should supply a list of required peaks – peak energy (keV) and peak area (counts). If no peaks are defined, *SpecMaker* will simply create a background continuum.

As the list is created, the worksheet will calculate the required spectrum position (in channels), the FWHM at the required energy and the peak width in channels.

It is not necessary to list peaks in numerical order, but the list must start on line 1 and have no blank lines within it.

Create Spectrum

When all the above items have been defined, clicking the `Create Spectrum` button will generate the required background continuum and superimpose the specified peaks. At this stage, the spectrum created will be smooth with no uncertainties. That smooth spectrum is then subjected to a scattering process that mimics the statistical scatter of radioactivity counting. The scattered data is stored as the spectrum.

At the conclusion of the spectrum generation process, the program will fill in the table to the right of the peak list, giving the actual peak centroid and peak area for comparison with that requested.

Do not click `Create Peaks` until all necessary parameters have been defined.

If a background spectrum is requested, the procedure is slightly different. The spectrum will be loaded into the continuum space onto which the peaks will be superimposed. Each peak will be superimposed on a continuum level calculated as the mean of the background counts within the peak region.

Chart Options

If you wish to see what the peaks look like, specify a plot region – ie. start and end energies in keV - in the `Chart Options` box. Click `Alter Plot` to reset the display parameters and display the portion of the spectrum in the *Chart1* worksheet.

Save Spectrum

When you are satisfied with the outcome, save the spectrum simply by clicking the `Save Spectrum` button. The spectrum will be saved in .CHN format to the `Working Folder` specified above.

At the same time, a csv file will be generated containing the following list of information:

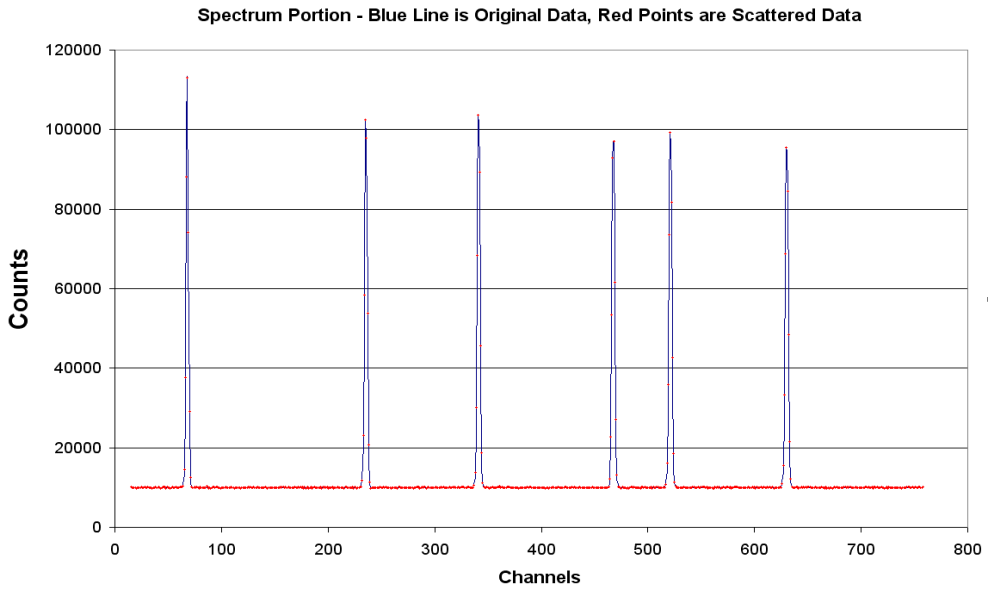
Peak energy
requested number of counts in the peak,
the requested peak centroid,
the requested FWM,
the actual number of counts,
the actual number of counts.

With a mathematically defined continuum, the complete scattered data will be saved as the spectrum. When a background is loaded, the original spectrum points will be transferred to the new spectrum, except within peak regions when the scattered points will be taken.

3 Chart1

This worksheet has no function other than to display portions of the spectrum selected by the `Chart Options` referred to above.

The chart is not protected, so it is possible to alter the scales manually, but be aware that *SpecMaker* will not reset all the display parameters after such intervention.



The blue line is the original continuum, the red dots the scattered data. When a background spectrum is loaded, it instructive to compare the scattered points with the spectrum points.

4 Spectrum

It is in this worksheet that the spectrum is created. The whole of it is protected and, while the data it contains can be viewed, none of it can be altered. Column A is the channel number, column B is the generated spectrum without scatter and column C the scattered data ready for saving as a spectrum. Column D will contain the peak counts added to the continuum.

You will see that if you press the F9 key to force a recalculate, column C will alter. This is simply another random scattering of the data. Each recalculation will create a different spectrum – different in detail, but each one statistically consistent with the original data. Saving more than one such spectra is equivalent to making successive count measurements on the same sample.

The worksheet also contains information representing the header and trailer information of the spectrum. This is here merely for convenience and to assist the Visual Basic coding that saves the spectrum.

5 Check

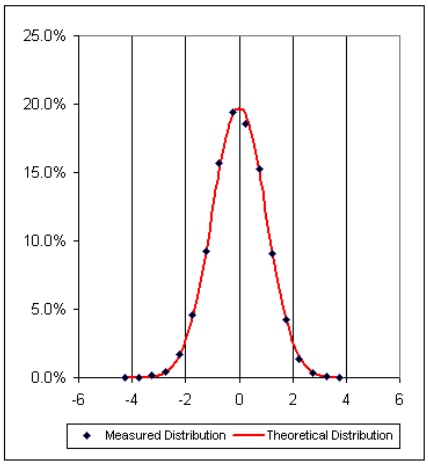
SpecMaker - Check Consistency of Results

N:\NTSNet\gspec\specmaker\[SpecMaker-Example.xls]Check

Spreadsheet prepared by Dr. Gordon Gilmore of Nuclear Training Services Ltd.

Only take notice of this sheet if there is no gradient on the continuum and there are no peaks superimposed.

Bin Edge in SU units	Centre of Bin	Bin Edge Counts	Frequency No. Cts	Frequency %	Theor. %	Difference
Bin Hwidth:						
-4	-4.25	873	0	0.0%	0.0%	0.0%
-3.5	-3.75	889	3	0.0%	0.0%	0.0%
-3	-3.25	905	11	0.1%	0.1%	0.0%
-2.5	-2.75	920	37	0.5%	0.5%	0.0%
-2	-2.25	936	137	1.7%	1.6%	0.1%
-1.5	-1.75	952	377	4.6%	4.3%	0.3%
-1	-1.25	968	757	9.2%	9.1%	0.1%
-0.5	-0.75	984	1282	15.7%	15.1%	0.6%
0	-0.25	1000	1590	19.4%	19.3%	0.1%
0.5	0.25	1015	1518	18.5%	19.3%	-0.8%
1	0.75	1031	1248	15.2%	15.1%	0.2%
1.5	1.25	1047	742	9.1%	9.1%	-0.1%
2	1.75	1063	347	4.2%	4.3%	-0.1%
2.5	2.25	1079	108	1.3%	1.6%	-0.3%
3	2.75	1094	25	0.3%	0.5%	-0.1%
3.5	3.25	1110	8	0.1%	0.1%	0.0%
4	3.75	1126	0	0.0%	0.0%	0.0%
Above			0	0.0%		
		Total Counts:	8190			0.27%



Total counts before randomization: 8,190,000

Total counts afterwards: 8,184,531

Difference: -5,469 -0.07%

Standard Uncertainty: 32 counts in each channel

Press F9 to re-scatter the data

This worksheet is here to allow user to gain some confidence in the scattering process. Under normal conditions, where peaks are superimposed on the continuum, or the continuum is varying, this sheet has no value whatsoever. However, if a constant continuum is defined and no peaks specified, this worksheet calculates the frequency distribution of counts across the whole of the spectrum. The graph on the right-hand side will display that distribution superimposed upon the theoretical (Normal) distribution. Pressing F9 will force recalculation and demonstrate the reproducibility of the scattering process.

The expectation, which is almost always borne out in practice, is that there will be a close match between actual and expected distributions.

6 Assessment

This worksheet compares the peak parameters used to create the spectrum with the parameters measured by the spectrum analysis program.

Program Details – are simply there for convenience to identify the assessment.

Peak Analysis – in this box the only user supplied value is the number of spurious peaks reported by the spectrum analysis program, from which the peak detection index is calculated.

Requested Values – these are echoed from the Control sheet.

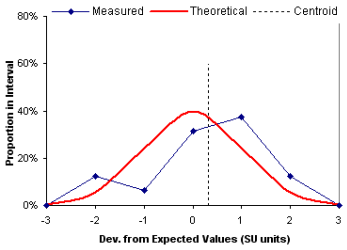
Given Values – again echoed from the Control sheet

SpecMaker - Spectrum Analysis Assessment

N:\NTSNet\gspec\specmaker\[SpecMaker-Example.xls]Assessment

Spreadsheet prepared by Dr. Gordon Gilmore of Nuclear Training Services Ltd.

QCYK Peaks.chn
GammaVision



Program Details	
Program:	GammaVision
Version:	5.22
Date of Analysis:	23-Feb-08
Comments:	QCYK peaks
Energy Calibration:	0.269309 keV/ch

Peak Analysis	
Number of peaks created:	16
Number of measured peaks:	16
Number of missed peaks:	0
Number of spurious peaks:	0
Peak Detection Index (Target =1):	1.00

Centroid and FWHM Differences	Channels	keV
RMS Centroid Difference:	1.863	0.502
RMS FWHM differences:		0.023

Area Estimation	
Centroid of Distribution:	0.313
	OK

	Requested Values				Given Values		Measured Values					Assessment		
	Peak Energy (keV)	Peak Area (counts)	Peak Centroid (channels)	FWHM (keV)	Peak Area (counts)	Peak Centroid (channels)	Peak Energy (keV)	Peak Area (counts)	Std. Uncery (%)	Peak Centroid (channels)	FWHM (keV)	Peak Area Significance z-score	Centroid Difference (channels)	FWHM Difference (keV)
1	59.54	300,000	235.447	0.774	299,999	235.447	59.54	300528	0.28%	235.44	0.812	0.63	-0.007	0.038
2	88.03	300,000	341.236	0.801	300,001	341.236	88.03	301852	0.26%	341.24	0.826	2.36 May be signif.	0.004	0.025
3	14.41	300,000	67.870	0.730	299,999	67.870	14.41	300338	0.27%	67.88	0.754	0.42	0.010	0.024
4	122.06	300,000	467.597	0.834	299,999	467.597	122.06	300875	0.28%	467.60	0.873	1.04	0.003	0.039
5	136.47	300,000	521.104	0.847	299,999	521.104	136.47	301106	0.27%	521.11	0.861	1.36	0.006	0.014
6	165.86	300,000	630.236	0.875	300,002	630.236	165.86	298571	0.26%	630.23	0.888	-1.84 Prob. Not Signif.	-0.006	0.013
7	279.02	300,000	1050.424	0.980	299,998	1050.424	279.02	299927	0.27%	1050.42	1.023	-0.09	-0.004	0.043
8	391.70	300,000	1468.830	1.082	299,998	1468.830	391.70	300677	0.21%	1468.83	1.085	1.08	0.000	0.003
9	514.00	300,000	1922.957	1.189	299,991	1922.957	514.00	300143	0.24%	1922.95	1.190	0.21	-0.007	0.001
10	661.86	300,000	2471.996	1.315	299,958	2471.996	661.66	299128	0.24%	2471.25	1.333	-1.16	-0.746	0.018
11	834.84	300,000	3114.313	1.457	299,995	3114.313	834.84	298477	0.24%	3114.31	1.468	-2.12 May be signif.	-0.003	0.011
12	898.04	300,000	3348.990	1.508	299,992	3348.990	898.04	300232	0.23%	3348.99	1.511	0.35	0.000	0.003
13	1838.05	300,000	6839.504	2.159	299,988	6839.504	1836.05	299887	0.20%	6832.09	2.159	-0.17	-7.414	0.000
14	1115.54	300,000	4156.624	1.674	299,958	4156.623	1115.54	300473	0.23%	4156.62	1.704	0.75	-0.003	0.030
15	1173.23	300,000	4370.842	1.717	299,932	4370.841	1173.23	301415	0.23%	4370.85	1.727	2.14 May be signif.	0.009	0.010
16	1332.49	300,000	4962.217	1.831	299,991	4962.217	1332.49	300606	0.21%	4962.22	1.849	0.97	0.003	0.018
17														
18														
19														

Measured values – these must be supplied by the user from the spectrum analysis program report. Note that the standard uncertainty should be provided at a coverage factor of 1.

The assessment results are reported as follows:

Peak Detection Index – this represents the performance of the peak search process. If all peaks are detected with no spurious peaks, this would be 1.00. Peaks missed and spurious peaks reduce this index. It can become negative if the number of spurious peaks is high.

Peak area z-score – numerically this is the difference between actual and measured peak areas divided by the standard uncertainty of the measured result. From that score, a degree of significance of the difference is reported. No message in that column means the difference is not significant.

The distribution of z-scores is plotted in the graph at the top right hand corner of the worksheet superimposed on the theoretical (Normal) distribution. Ideally, the measured data will be consistent with the expected distribution, However, for small numbers of peaks that may not be apparent.

Centroid Difference – is the difference between actual peak position and measured peak position. Obviously, one hopes that this is small.

FWHM Difference – is the difference between actual peak width and measured peak width, both expressed as FWHM. Again, one hopes that this is small.

Centroid and FWHM Differences – this box summarizes data in the Assessment columns. The overall centroid differences are expressed as an RMS (root-mean squares) value expressed in channels and keV. The RMS of FWHM differences is only given in keV.

Area Estimation – this box displays the calculated centroid of the measured z-score distribution. Large deviations from zero indicate bias in the peak area measurement process. A message to that effect will appear whenever the value exceeds 1.96 times the standard uncertainty of the centroid value.

7 Stats

This worksheet merely provides the information for the graphical display on the Assessment sheet.

8 The SpecMaker-Assessments spreadsheet

This independent spreadsheet has exactly the functionality of the Assessment worksheet of *SpecMaker*. However, the Required and Given data, which is automatically echoed in the parent program, must be entered manually in the independent *SpecMaker-Assessments*. That can most easily be done by loading the relevant csv file into *Excel* and then copying and pasting the data into *SpecMaker-Assessments*. When doing that, it is advisable to use the `Paste Special…/Text` procedure; otherwise formatting of the cells will be lost. It will also be necessary to insert manually insert the spectrum energy calibration factor.

The *Stats* worksheet is not normally accessible in *SpecMaker-Assessments*.

9 Disclaimer

The *SpecMaker* worksheets are provided in good faith for for the convenience of gamma spectrometrists and readers of 'Practical Gamma-Ray Spectrometry'. The author cannot be held responsible for any inconvenience or loss of any kind arising from the use of these spreadsheets or the conclusions drawn from them.

Please note that this spreadsheet does not take account of all circumstances. Unreal values for some parameters may give ridiculous results with no error messages. In other cases, the error messages will be rudimentary. *Caveat utilitor.*

Dr. Gordon Gilmore
02/03/08