
Program Documentation
S3-Flux

Technical Note
ISR TN-1030-3
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INTERNATIONAL SAFETY RESEARCH

Safety Support Software (S3) Flux

TABLE OF CONTENTS

| | |
|--------------------------------------------------------|----|
| 1. Overview of Application..... | 1 |
| 1.1 Installation..... | 1 |
| 1.2 Location of Installed Files | 3 |
| 2. Interface | 4 |
| 2.1 General Description | 4 |
| 2.2 Menus..... | 6 |
| 2.2.1 File Menu | 6 |
| 2.2.2 Detector | 6 |
| 2.2.3 Library..... | 7 |
| 2.2.4 View..... | 7 |
| 2.2.5 Process..... | 8 |
| 2.2.6 Graph Customization Dialog..... | 12 |
| 2.3 Program Operation | 13 |
| 3. Program Theory | 15 |
| 3.1 Energy Calibration | 15 |
| 3.2 Detector Resolution Function..... | 15 |
| 3.3 Peak Identification | 16 |
| 3.4 Maximum Entropy Spectrum Deconvolution | 17 |
| 3.4.1 Theory | 17 |
| 3.4.2 Detector Response Function | 18 |
| 3.4.3 Implementation | 19 |
| 3.5 Isotope Identification..... | 21 |
| 3.5.1 Decay Chains | 23 |
| 3.5.2 Isotope Libraries | 24 |
| 4. Visual Basic Code | 28 |
| 4.1 Introduction..... | 28 |
| 4.2 Forms..... | 28 |
| 4.2.1 S3Flux | 28 |
| 4.2.2 Calibration Plot..... | 29 |
| 4.2.3 Manual | 30 |
| 4.2.4 MaxEnt | 30 |
| 4.2.5 Resolution | 30 |
| 4.2.6 Spectrum..... | 31 |
| 4.3 Creating the Install CD-ROM..... | 31 |
| 4.3.1 New Install or Adding Files to the Install | 31 |
| 4.3.2 Updating Existing Files | 31 |
| 5. References..... | 33 |
| Appendix A: Contents of Spectra Files..... | 34 |
| Appendix B: Calibration peaks | 35 |

SAFETY SUPPORT SOFTWARE (S3)-FLUX

1. OVERVIEW OF APPLICATION

S3-Flux is a Windows program that allows spectra to be visualized, calibrated, filtered and processed to obtain the fluence incident on the detector. The program implements the Maximum Entropy algorithm developed by ISR for unfolding scintillation detector spectra. It can also perform isotope identification.

1.1 Installation

The CD-ROM contains the setup program and the cabinet (CAB) file necessary to install the application. Before installing S3Flux, you must uninstall any previous version of the program. You should check that the following files have been removed. If necessary, remove them manually.

TABLE 1: Old files that should be removed

| File | Location |
|------------------------------------------------------------------------------------------|------------------------------------------------------------------|
| READRESP.DLL READDATA.DLL UNFOLD.DLL UNFOLDME.DLL FMATHDLL.DLL FIODLL.DLL | Windows System directory (\WinNT\System32 or \Windows\System) |

After running Setup.exe, all DLL's and system files will be installed automatically. Test files are also included on the CD-ROM.

TABLE 2: Content of the installation disk

| File | Description |
|-------------------------------------------------------------------------------------------|------------------------------------------------------------|
| [Bootstrap Files] | |
| SETUP.EXE | Installs the program |
| SETUP1.EXE | Setup program specific to the application |
| SETUP.LST | List of files that will be installed |
| ST6UNST.EXE | Application removal utility |
| VB6STKIT.DLL | Library containing various functions used by the setup kit |
| COMCAT.DLL OLEPRO32.DLL STDOLE2.TLB ASYCFILT.DLL OLEAUT32.DLL MSVBVM60.DLL | Visual Basic 6.0 Run-time DLLs |

| File | Description |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p>[S3Flux Files]</p> <p>S3FLUX.EXE KERFAC.TXT ITER.OUT READRESP.DLL READATA.DLL UNFOLD.DLL UNFOLDME.DLL FMATHDLL.DLL FIODLL.DLL</p> | <p>S3Flux application Air kerma factors (Gy) Maximum entropy module iteration log Reads the response matrix for the selected detector Reads a raw spectrum Performs the LT Deconvolution Performs the ME Deconvolution Absoft Fortran Run-time DLLs</p> |
| <p>[VB Controls Files]</p> <p>COMDLG32.OCX TABCTL32.OCX PEGO32a.OCX PESGO32a.OCX PEGRP32A.DLL ACTIVEEX.DLL MSSTDFMT.DLL MSDERUN.DLL</p> | <p>Common dialogs OCX Tabbed control OCX Bar Graphs OCX Scientific Graphs OCX Graph support DLL Active-X Controls (OCX) DLL Microsoft Data Formatting Object Library Microsoft Data Environment Instance 1.0</p> |
| <p>[Detector Files]</p> <p>BGO1.M BGO5.M BGO8.M BGO9.M CSI1.M CSI2.M NAI0.M NAI1.M NAI2.M NAI3.M NAI4.M NAI5.M NAI8.M</p> | <p>Detector response matrices</p> |
| <p>[Library Files]</p> <p>CANDUOPS.LIB DEPOSITION.LIB SEALED.LIB</p> | <p>Isotope library for normal Candu operation Isotope library for reactor accident ground contamination Isotope library for sealed sources</p> |

| File | Description |
|----------------|------------------------------|
| [Test Files] | |
| BCK_OFF1.DP3 | DosSpec 3 File |
| 203HG21%.DP2 | DosSpec 2 Files |
| 226RA22%.DP2 | |
| 232TH9%.DP2 | |
| 60CO_20%.DP2 | |
| 60CO_95%.DP2 | |
| BACK10.DP2 | |
| CAL10.DP2 | |
| CSBANA14.DP2 | |
| MIX8%.DP2 | |
| ALCF252C.BTI | MicroSpec (BTI) Files |
| ALCFBACK.BTI | |
| HA2X510.CNF | Inspector (CNF) File |
| BG1G405B.MCA | Canberra S100 (MCA) Files |
| PU1G501F.MCA | |
| V14MEV01.MCA | |
| CHERNOBYL1.MCA | |
| CHERNOBYL2.MCA | |
| PUBCFG.SPC | Robitaille PDP-11 (SPC) File |
| SPEC1.EXP | Exploranium (GR-130) Files |
| SPEC2.EXP | |

1.2 Location of Installed Files

The S3Flux files are installed in the S3Flux application directory. The detector files are installed in a subdirectory (S3Flux\Detect). The isotope library files are copied in subdirectory (S3Flux\Library). The test files are copied in another subdirectory (S3Flux\TestFiles). The VB run-time DLLs and the VB controls files are copied to the Windows System directory (either \WinNT\System32 or \Windows\System directory). The bootstrap files are deleted after installation.

2. INTERFACE

2.1 General Description

The program uses a combination of standard menus and tabs to select the various options.

The program gives the user the option of viewing the raw spectrum vs. channel number or vs. energy (refer to Figure 1). The calibration specified in the input file can be updated using a calibration screen accessible under the process menu.

By default, a 2" x 2" NaI detector, with a maximum energy of 3 MeV and 150 bins is selected (file NAI8.M). Other types of detectors, of varying size and maximum energy can also be selected. Each detector file contains the default resolution parameters of the detector. These parameters can be updated using the resolution screen, accessible under the process menu.

The binned raw energy spectrum can be displayed, using the energy binning of the selected detector. The spectrum can be unfolded using one of two methods. The first method uses a lower triangular (LT) matrix solver, which solves the system of equations from the highest energy equation to the lowest energy equation. The second method consists in using a Maximum Entropy (ME) solver, which seeks the best solution through an iterative process.

The parameters controlling the Maximum Entropy method are accessible under the process menu. The iteration log of the Maximum Entropy method can also be viewed under that same menu.

The isotope identification tab shows the currently selected spectrum, or if a background file has been selected, can show a histogram of the isotopes that generated the spectrum.

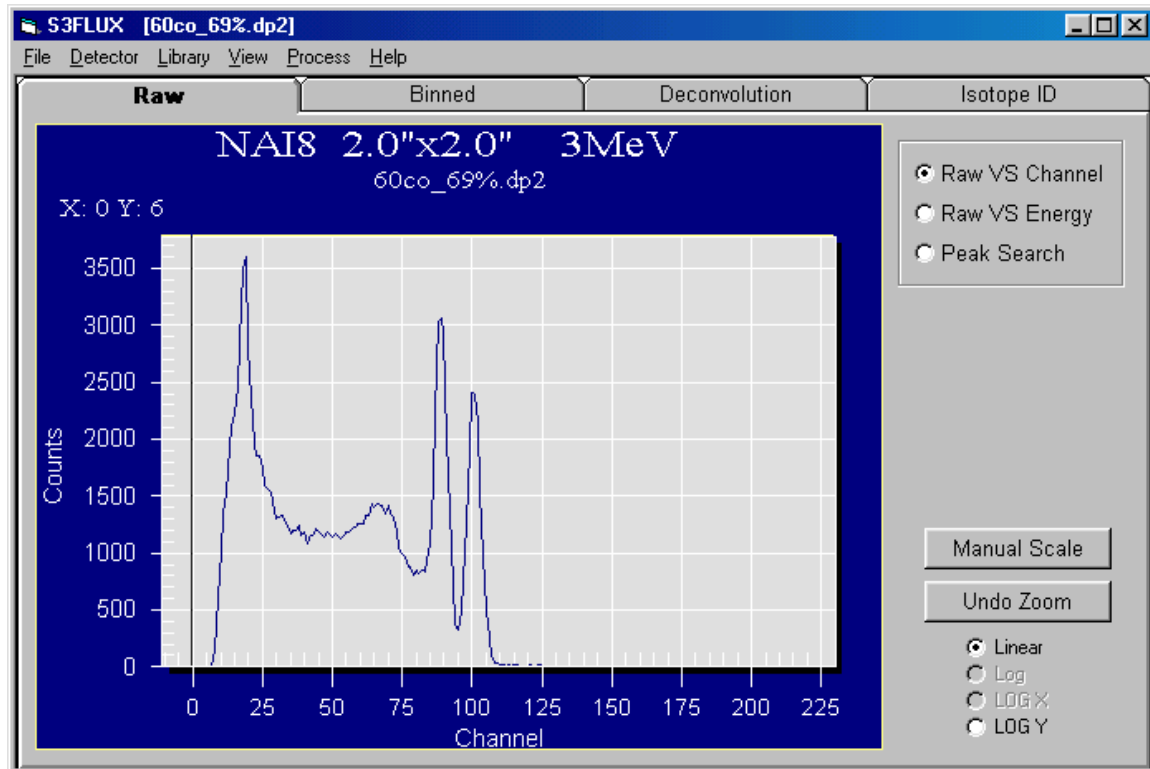


Figure 1: Main program screen

2.2 Menus

2.2.1 File Menu

TABLE 3: File menu items

| Operation | Description |
|-------------------|----------------------------------------------------------------------------------------------------------------|
| Open | Reads a spectrum file and converts the information to graphical form. |
| Close | Resets program variables and viewable interface area. Prompts user to save. |
| Save As | Saves current graph data to a file. Can be either text or graphical. |
| Copy to Clipboard | Copies the graph image or data text to the clipboard for use in other applications. Shows export dialogue box. |
| Print : Graph | Changes the viewable graph to a printable format and shows export dialogue box. |
| Print : Data | Changes the viewable graph to printable text data. |
| Print Setup | Allows user to change or set current printer and printing options. |
| Exit | Closes S3Flux. |

The **File | Open** menu reads in a spectrum. The program can read the following file formats:

| | |
|-----------|---------------------------------------------------------------|
| (DP2-DP3) | Dospec |
| (BTI) | Microspec |
| (CNF) | Inspector files |
| (MCA) | Canberra S100 files |
| (SPC) | Robitaille files (older custom PDP-11 data collection system) |
| (EXP) | GR-130 exploranium files |

2.2.2 Detector

The “Detector” menu lists a selection of detectors that can be selected by the user. The user’s input will be reflected in the title of the graph and will change the energy scale for the binned spectrum.

The program reads the detector files from a sub-directory of the main S3Flux directory:

Detector directory: ..S3Flux/detect

2.2.3 Library

The “Library” menu lists various isotope libraries that can be selected by the user. The default is the *sealed source* library. The *deposition* library is appropriate for ground contamination following a nuclear reactor accident, while the *CanduOps* library contains radioisotopes frequently found in Candu nuclear generating stations during normal operation. The library selection is used in the isotope ID module, which is selected with the ‘Isotope Identification’ tab.

The program reads the selection of libraries from a sub-directory of the main S3Flux directory:

```
Library directory:    ..S3Flux/Library
```

2.2.4 View

The “View” menu controls the graphical representation of the spectrum file selected under the current detector. Using the view menu to change graphs will automatically update all the information, which is to be presented with that graph. Refer to Table 4 for descriptions of the view options.

TABLE 4: View menu items

| Menu Selection | Description |
|------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Raw vs. Channel | Displays the raw data (counts) plotted against the channel number. Linear and Log Y views available. |
| Raw vs. Energy | Displays the raw data (counts) plotted against the calculated energy (MeV) at the channel. Linear, Log X, Log Y, and Log views available. The energy scale is initially given by the calibration read from the file spectra (when available). After the user has re-calibrated the spectrum, the new calibration is used. |
| Peak Search | Displays the raw data (counts) plotted against the channel number and of the raw filtered data (counts) plotted against the same channel. Linear view only is available. |
| Binned | Displays the binned raw data (counts) against the energy. The energy binning is a function of the current detector selected. Linear, Log Y, Log X and Log views available. |
| LT Deconvolution | Graphic representation of the flux per cm ² plotted against the energy. The flux is obtained with a Lower Triangular (LT) solution of the response matrix. The energy binning is a function of the current detector selected. Linear, Log, Log X, and Log Y views available. |

| Menu Selection | Description |
|------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ME Deconvolution | Graphic representation of the flux per cm^2 plotted against the energy. The flux is obtained by Maximum Entropy (ME) solution of the response matrix system of equations. The energy binning is a function of the current detector selected. Linear, Log, Log X, and Log Y views available. |
| Reconstructed Raw vs. Energy | A comparison graph of the binned raw data (counts) against the energy, and the reconstructed counts against the same energy. The energy displayed is a function of the selected detector. Linear and Log Y views available. |
| Isotope Identification | Brings up the tab where binned data is displayed and isotope identification can be carried out. Linear, Log, Log X, and Log Y views available. |

2.2.5 Process

The “Process” menu regulates how the spectrum file is delivered by controlling the variables used to graph the selection. Refer to Table 5 for a listing of the process options.

TABLE 5: Process menu items

| Process Option | Description |
|-----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Calibrate | This option will display a new window called “Calibration Plot”. This allows the user to enter pairs of channel and energy data points that define an energy calibration curve. |
| Resolution | This option will display a new window called “Resolution Plot”. The user can enter pairs of energy and FWHM values that define a detector resolution curve. |
| MaxEnt Parameters | This option will display a new window that gives the user the option of changing the calculation parameters used by the Maximum Entropy method. |
| View ME iteration log | This displays the latest Maximum Entropy iteration log file in a separate window. |

2.2.5.1 Calibration Window

The *Raw Counts vs. Channel number* graph can be calibrated by entering the location of peaks (channel number), along with their energy. Up to five peaks may be used to calibrate the current spectrum file.

One pair of points gives a linear calibration, which passes through the origin. Two pairs of data points give a linear calibration with offset at the origin. When more than 2 peaks are entered, the program generates a second order least square calibration curve.

The original calibration values, a_0 , a_1 , and a_2 , are shown, along with the new calibration values, b_0 , b_1 , and b_2 . The calibration window also displays the original calibration curve, along with a new calibration curve.

A peak can be selected in the main graph window by using the vertical cursor. The corresponding channel number can be entered in the channel text box by pressing the "Acquire From Graph" button. It is possible to restore the original calibration contained in the spectrum file by using the "Default" button.

The secondary peak calculators calculate the energy of the Compton edge, the first and second escape peaks from the energy of the full energy peak. If such spectrum features are present in the measured spectrum, they may be used in the calibration.

The **Calibration** window is shown in Figure 2.

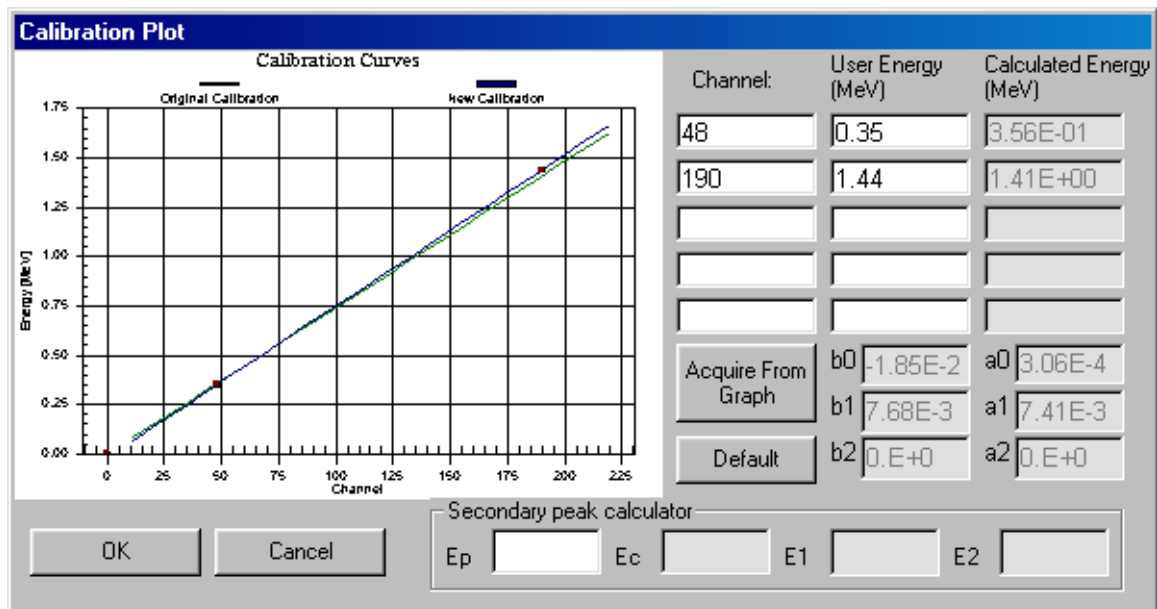


Figure 2: The Calibration window

2.2.5.2 Resolution Window

The resolution of the detector can be calibrated using the FWHM at up to five energies. The original calibration values, ar_0 , br_0 , and cr_0 , are shown, along with the new calibration values, ar , br , and cr . The energy of the peaks can be acquired from the main graph window by using the "Acquire From Graph" option.

The default button restores the resolution parameters that were contained in the detector file.

The equations describing the resolution function are discussed in section 3.2. The **Resolution** window is shown in Figure 3.

adjustment of the other parameters, of the spectrum calibration or the detector response may be necessary.

Spectra acquired with the Microspec II often contain several low energy channels without counts. The Maximum Entropy method will not converge on these spectra. To fix this problem, a user specified number of low energy bins can be set to 1% of the total counts by entering a non-zero value in the appropriate text box. In practice, 5-10 energy bins need to be adjusted in this manner.

2.2.5.4 Iteration Log

An **iteration log** is shown in Figure 5. The description of the columns is given in Table 6.

| Iteration | Test | Entropy | Chi_Target | Chi_Squared | Alpha |
|-------------------|-----------|------------|------------|-------------|-----------|
| 0 | 0.000e+00 | -5.297e+02 | 1.500e+02 | 1.416e+05 | 0.000e+00 |
| 1 | 5.808e-01 | -5.317e+02 | 1.500e+02 | 1.415e+05 | 0.000e+00 |
| * dist constraint | | | | | |
| 2 | 5.554e-01 | -5.252e+02 | 1.411e+05 | 1.415e+05 | 4.319e+00 |
| * dist constraint | | | | | |
| 3 | 5.583e-01 | -5.178e+02 | 1.410e+05 | 1.415e+05 | 8.635e+00 |
| * dist constraint | | | | | |
| 4 | 5.595e-01 | -5.098e+02 | 1.410e+05 | 1.416e+05 | 8.640e+00 |
| * dist constraint | | | | | |
| 5 | 5.454e-01 | -5.015e+02 | 1.411e+05 | 1.417e+05 | 4.322e+00 |
| * dist constraint | | | | | |
| 6 | 5.437e-01 | -4.924e+02 | 1.410e+05 | 1.418e+05 | 8.649e+00 |
| * dist constraint | | | | | |
| 7 | 5.265e-01 | -4.829e+02 | 1.410e+05 | 1.419e+05 | 8.656e+00 |
| * dist constraint | | | | | |
| 8 | 5.252e-01 | -4.731e+02 | 1.410e+05 | 1.421e+05 | 8.663e+00 |
| * dist constraint | | | | | |
| 9 | 5.062e-01 | -4.631e+02 | 1.407e+05 | 1.422e+05 | 1.301e+01 |

Figure 5: View ME iteration log window

Table 6: Description of the columns in the ME iteration log file

| Column | Description |
|-------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Iteration | Iteration number |
| Test | Degree of non-parallelism between ∇S (gradient of entropy) and ∇C (gradient of chi squared), which is zero for a true maximum entropy image. Should be less than 0.1 for unique ME solution. |
| Entropy | $S(f) = -\sum_{j=1}^N (f_j / \Sigma f) \log(f_j / \Sigma f)$ where the f_j are the flux values at each energy. |
| Chi_Target | Approximately equal to M , the number of bins. |
| Chi_Squared | $C(f) = \chi^2 = \sum_{k=1}^M (F_k - D_k)^2 / \sigma_k^2$ where the D_k are experimental points and F_k is the simulated data. |
| Alpha | Lagrange multiplier in the minimization problem $Q = \alpha S - C$. |

2.2.6 Graph Customization Dialog

The Graph customization dialog allows the user to customize the graph. The dialog is made up of tabs. This dialog is invoked by either 1) the space bar, 2) double clicking on the graph, 3) right-mouse clicking to show the pop-up dialog, or 4) pressing the "Q" key to invoke the pop-up menu.

General

The General menu allows changes to the title, sub title, numeric precision, grid lines, viewing style (colour or monochrome) and font size.

Plotting Method

The graph offers the following plotting methods: Line, Bar, Area, Points, Points plus Best Fit Curve, Points plus Best Fit Line, Points plus Line, Points plus Spline, Spline. The Scientific Graph supports two plotting methods per left/right axis pair. Each axis pair can contain a primary plotting method and a secondary plotting method. Comparison subsets are plotted in the secondary plotting method.

Subsets

This group consists of a listbox of subsets and scrollbar/slider controlling the Scrolling Subsets quantity. These allow the user to view subset information in a variety of ways.

| Selected Subsets | Scrolling Subsets | Results |
|------------------|-------------------|-----------------------------------------------------------------------------------------------------------------------------------|
| no | no | Display all subsets |
| yes | no | Display only those selected subsets |
| no | yes | Scroll through subset information via the scrollbar by the amount defined by Scrolling Subsets |
| yes | yes | Maintain those selected subsets as permanent subsets and revolve through the remaining subsets in increments of Scrolling Subsets |

Axis

This group allows the user to view axes as linear or log. It also allows the user to adjust how the axis range is determined. Possible selections are Automatic, Manual Min, Manual Max, and Both Manual Min and Manual Max.

Style

This group allows the user to adjust a subset's colour, line style, and point style. Double clicking the colour selection box will invoke a custom colour selector. Note that the point style cannot be modified unless the plotting method selected includes "point".

2.3 Program Operation

Program operation is summarized through the following steps, the bold text highlights in which order the menu items should be activated:

1. Open a file
File | Open → Choose a file
 The file is displayed in the raw spectrum view by default. Move the vertical cursor on the screen by clicking on the graph and using the left and right arrow keys. The cursor point is displayed in the upper-left-hand corner of the graph.
2. Choose the required display option.
 Once a file is loaded, choose a tab and display option to see the various data forms. The view may also be selected from the **View** menu.
3. Re-calibrate the initial energy calibration from the spectrum file
Process | Calibration
 This window allows pairs of channel and energy data points to be entered until the required calibration is achieved.

4. Choose an appropriate detector
Detector
The default detector is a 2" x 2" NaI detector with a maximum energy of 3 MeV. Each detector contains a response matrix, resolution parameters, and an energy bin grid.
5. Select the binned display according to the energy grid specified in the detector file
View | Binned or by using the Binned tab
When the detector's energy grid properly matches the spectrum's energy range, the binned spectrum is a good representation of the original spectrum. The reconstructed spectrum is a useful diagnostic that can be used to verify the results of the deconvolution or the isotope identification calculations.
6. Reset the resolution parameters if required.
Process | Resolution
This will display the raw spectrum vs energy in the main window and the resolution window. The resolution equations are described in section 3.2.
7. Display the flux incident of the detector.
View | LT Deconvolution or **View | ME Deconvolution**
Or select the Deconvolution tab followed by the appropriate choice. The LT Deconvolution uses a lower triangular solver that is fairly robust, but gives less accurate spectra. The maximum entropy solver (ME) uses iterative methods that may diverge. However, it has the potential of producing very high quality flux spectra. To verify the quality of the reconstructed flux spectra, go back to the Binned tab (**View | Reconstructed raw vs energy**) to display the original binned data along with the counts corresponding to the flux solution obtained at the deconvolution step.
8. Isotope Identification
View | Isotope ID or select the Isotope ID tab.
A background file must initially be loaded. See Step 1. After the background file has been loaded, click the "Set as Background" button to initialize the file. Load another file that you wish to perform the isotope identification on. Again, see Step 1. The binned spectrum will be displayed in the main window. Select the Isotopes button to display the relative intensity of isotopes in its library. By adjusting the minimum and maximum half-lives allowed, the list of isotopes considered can be narrowed down.
9. Changing the Isotope identification library
Library
The content of each library is given in section 3.5.2. As default, the program loads the "Sealed Source" library.

3. PROGRAM THEORY

3.1 Energy Calibration

The energy is calculated using a second order equation, numbering the channel numbers from zero to $n-1$, where n is the number of channels.

$$E(\text{MeV}) = a_0 + a_1 \cdot c + a_2 \cdot c^2$$

The parameters a_0 , a_1 , a_2 are the energy calibration parameters.

3.2 Detector Resolution Function

The Resolution screen of the S3Flux allows a graphical view of both the original and new resolution required by the user. The plotted resolution in both cases is calculated as follows.

The shape of a Gaussian peak is given by

$$f(E) = C \cdot e^{-(E-E_a)^2 / \sigma^2}$$

The parameter σ is given by

$$\sigma = \frac{a_r + b_r \sqrt{E} + c_r E}{2 \ln 2}$$

This parameter has units of Energy and is related to the FWHM

$$FWHM = a_r + b_r \sqrt{E} + c_r E$$

This also has units of Energy. Given one pair of data points, the value of b_r can be set. Given two pairs of data points, both a_r and b_r are defined. With three pairs of data points or more, a quadratic curve fit is calculated.

The relative resolution, in % is given by

$$R = \frac{100 \cdot FWHM}{E}$$

This is the quantity that is displayed in the “Resolution” boxes. It should be noted that when the energy of the channel is negative (due to a bad calibration) the resolution is set equal to a_r . In this instance, it is important that a_r be greater than zero, otherwise, the filter function used in the peak identification routine (section 3.3) is undefined.

3.3 Peak Identification

The peak identification graph shows the raw spectrum vs. channel number along with the filtered spectrum. The latter is obtained using a Routti-Prussin filter that produces the filtered second derivative of the flux resolution function.

Given a Gaussian peak, its shape is given by

$$f(E) = C \cdot e^{-(E-E_a)^2 / A^2}$$

The second derivative of this peak shape is

$$\frac{\partial^2 f(E)}{\partial^2 E} = C \cdot e^{-(E-E_a)^2 / 2\sigma^2} \left[\frac{(E-E_a)^2}{\sigma^4} - \frac{1}{\sigma^2} \right]$$

The filtered counts at channel i are given by

$$f'_i = \sum_{j=0}^n A_j(E_i) \cdot f(E_j) \cdot E_j^2$$

where the raw counts are given by $f(E_j)$ and the filter coefficients by

$$A_j(E_i) = e^{-(E_j-E_i)^2 / 2\sigma_i^2} \left[\frac{(E_j-E_i)^2}{\sigma_i^4} - \frac{1}{\sigma_i^2} \right]$$

3.4 Maximum Entropy Spectrum Deconvolution

3.4.1 Theory

The response of the detector to an incident flux can be modeled as a linear system of equations. The observational data consists of a measured pulse-height spectrum. The desired data reconstruction is the flux incident on the detector. The matrix coupling the data reconstruction with the resulting observational data represents the effect of interactions inside the detector. A coupling matrix for several detectors is included with the program.

There are many mathematical problems of this type for which there is no unique solution. The problem is either underdetermined, i.e. there are fewer equations than unknowns, or the measurements contain considerable uncertainty, which makes a range of solutions possible.

The Method of Maximum Entropy offers a way to combine the least square method with additional constraints that make the solution unique. The additional constraints consist in maximizing the entropy of the data reconstruction. The theory is connected to Shannon's theory of information contents and communications [2].

The theoretical foundation of the Maximum Entropy method in data analysis is that this method is the only consistent way of selecting a single data set from the many data sets that fit the data. It answers the following question: *Given the observational constraints, where should the next photon come from?*

From a probabilistic point of view, it appears interesting to choose the solution that can be created with the largest number of combinatorial configurations. To describe the search for the Maximum Entropy solution in a simplistic fashion, it could be achieved by the following device: throwing photons at random in all allowed flux energy bins, keep only the data reconstructions (flux spectra) that are compatible with the experimental constraints. When a very large number of such acceptable data reconstruction sets have been accumulated, rank them according to the number of times they occur. The data reconstruction that occurs most frequently and satisfies the experimental constraints is to be preferred. Although this could be done using the Monte Carlo method (at considerable expense), it was demonstrated that the data reconstruction that would occur most frequently has the largest entropy [4]. The problem becomes computationally manageable because it consists of maximizing a single function (entropy) while fitting the data.

The practical merit of maximizing the entropy is that the resulting data reconstruction has the minimum configuration information, so that there must be evidence in the data for any observed structure. In addition, the physically important requirement of a positive solution is automatically invoked, since the entropy does not exist if any of the solution elements are negative. Numerically, it is far easier to ensure a positive value via a single, smooth function such as the entropy, than via N separate inequality constraints for each solution element.

The observational constraints on the permitted reconstruction come from observational

data D_k , related to the incident flux f_i through the detector response matrix R , and subject to noise of amplitude σ . Thus for additive noise

$$D_k = \sum_j R_{kj} f_j + n_k \sigma_k$$

n_k is a random variable of zero mean and unit variance. The observational constraints are set up by comparing the actual measurement data D_k with the simulated data,

$$F_k = \sum_j R_{kj} f_j$$

which would be obtained in the absence of noise, if the observed spectrum were generated by a flux f_j

The chi-squared function is used to measure the misfit between the simulated and the measurement data.

$$C(f) = \sum_k \frac{(F_k - D_k)^2}{\sigma_k^2}$$

The original lower triangular (LT) solver implemented simply minimized this chi-square function. However, for the chi-squared statistics, the largest acceptable value at 99 per cent confidence is approximately

$$C_{aim}(f) = (M + 3.29 \cdot \sqrt{M})$$

where M is the number of measurement bins. So a range of solutions is possible and the least square solution is not necessarily the most plausible solution. The Maximum Entropy method consists of maximizing the entropy of the flux.

$$S(f) = - \sum_j \frac{f_j}{\sum_j f_j} \ln \frac{f_j}{m_j \sum_i f_i}$$

(where m_j is the initial model of the flux) while at the same time constraining

$$C(f) \leq C_{aim}(f)$$

In essence, the method allows some misfit of the data (within the statistically acceptable range) in order to obtain a “simpler” flux shape.

3.4.2 Detector Response Function

The response matrix for each detector is obtained using MCNP 4b [1], running the problem as a coupled photon-electron simulation. The response matrix of a 2”x2” NaI detector, calculated at every 20 keV up to 3 MeV, is presented in Figure 6. The broadened response matrix is shown in Figure 7.

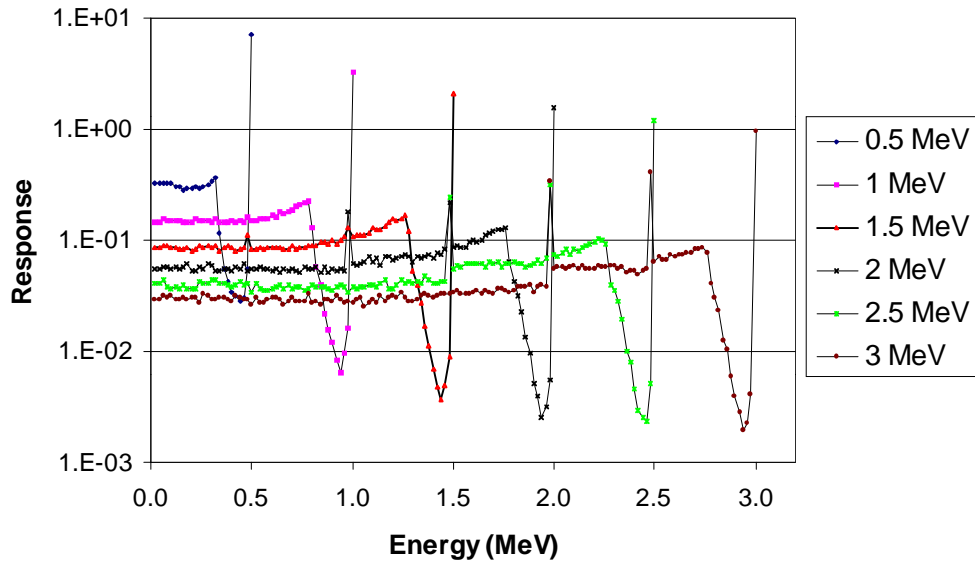


Figure 6: Raw detector response function at selected energies

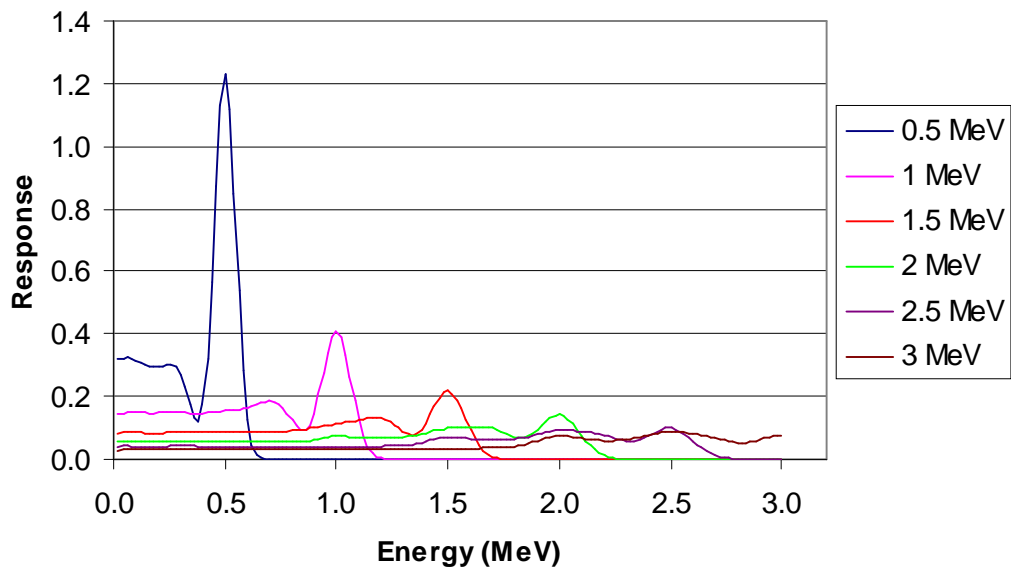


Figure 7: Broadened detector response function at selected energies

3.4.3 Implementation

Los Arcos [5] recently described the use of the Maximum Entropy method to unfold NaI detector spectra. His article was the impetus for the creation of the current program. The Maximum Entropy algorithm to be tested is described in the article by Skilling and Bryan [3]. An implementation created by Lizamore [6] was used as the basis for the

unfolding software.

3.5 Isotope Identification

The isotope identification module compares an experimental spectrum with spectrum shapes contained in the isotope's library. It uses the maximum entropy method to find the most likely list of isotopes matching the experimental spectrum.

This process can be described by the following system of equations

$$\begin{pmatrix} S_1 \\ S_2 \\ \vdots \\ S_p \end{pmatrix} = \begin{pmatrix} D_{11} & D_{12} & D_{13} & \cdots & D_{1i} \\ D_{21} & D_{22} & D_{23} & \cdots & D_{2i} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ D_{p1} & D_{p2} & D_{p3} & \cdots & D_{pi} \end{pmatrix} \begin{pmatrix} N_1 \\ N_2 \\ N_3 \\ \vdots \\ N_i \end{pmatrix}$$

$$\text{or } S_i = \sum_k D_{ik} \cdot N_k$$

Where S is the simulated experimental spectrum that must match the real spectrum
 D is a non-square matrix coupling the list of nuclides with the simulated experimental spectrum
 N is the unknown relative intensity of each nuclide in the library.

Given that the system of equations coupling the flux and the simulated measurements is

$$F_i = \sum_j R_{ij} f_j$$

Where R is the square detector response matrix coupling the flux with the simulated experimental spectrum.
 f is the flux spectrum incident on the detector.

The flux spectrum is proportional to the gamma spectrum emitted by nuclide. A matrix of gamma spectra for each nuclide can be created:

$$f_j = \sum_k G_{jk} N_k$$

Thus, the non-square matrix D of simulated measurements is obtained as

$$D_{ik} = \sum_j R_{ij} \cdot G_{jk}$$

Figure 8 shows the *gamma intensities* for a ^{137}Cs source. From these intensities, a *binned source* spectrum is obtained, using the same energy grid as the detector response matrix. The *binned source* spectrum is a column of the matrix G . The *binned counts* spectrum shown in Figure 8 is a column of matrix D . Figure 8 also shows an experimental ^{137}Cs spectrum acquired with a 2"x2" NaI detector. The calibration of the *experimental counts* spectrum is slightly wrong, the resolution doesn't match that of the detector and the spectrum is truncated at low energies. These artifacts are challenging for any isotope identification method.

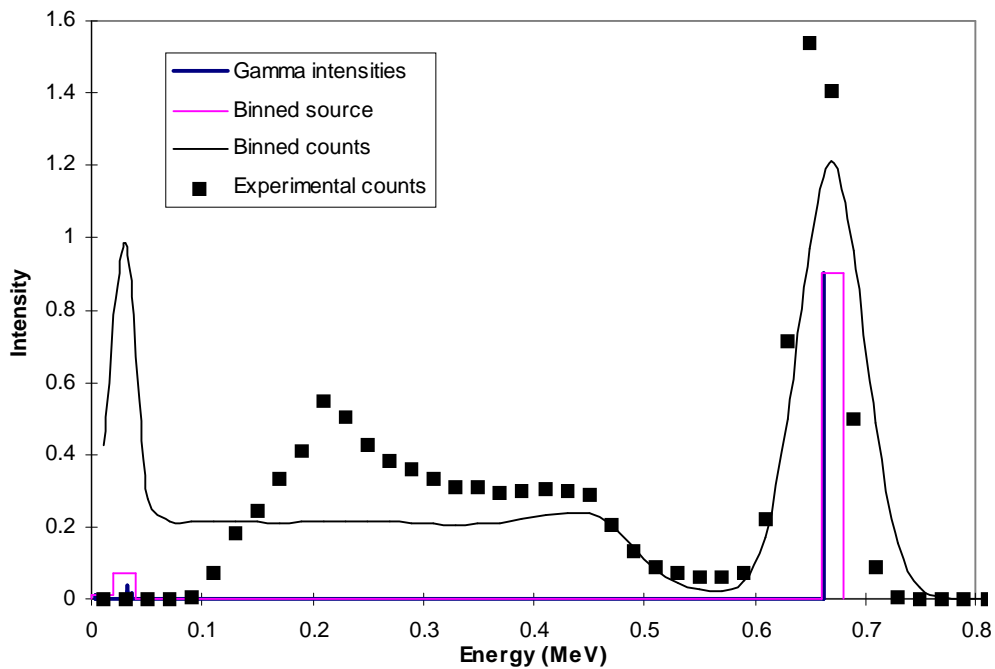


Figure 8: Isotope identification matrix for ^{137}Cs .

3.5.1 Decay Chains

In the isotope identification module, the decay chains are modeled assuming “secular equilibrium” (meaning that the parent activity does not decrease appreciably relative to the daughter activity). This means that the activity of all the decay products is the same as that of the parent, therefore we simply sum the spectra of all the decay products. An exception arises when the branching ratio of the daughter product is less than one. The code takes this into account, and will multiply all the daughter products that follow by the same branching ratio (fraction). If the other branch needs to be modeled, the fraction should be multiplied by the inverse of the first branch. Figure 9 illustrates this.

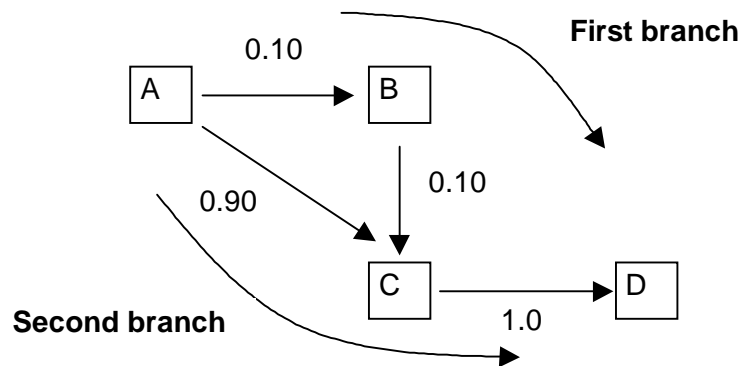


Figure 9: Isotope identification branches

This decay chain would be modeled as in Table 7.

Table 7: Isotope Decay Fractions

| Isotope | Decay fraction | |
|---------|-----------------|---------------|
| A | 1.0 | |
| B | 0.1 | First Branch |
| C | 1.0 | |
| D | 1.0 | |
| C | $0.9/0.1 = 9.0$ | Second Branch |
| D | 1.0 | |

The first branch includes isotopes B, C and D. The gamma lines for isotopes C and D are multiplied by 0.1, since this is the decay fraction for the first branch. The second branch includes isotopes C and D. The decay fraction for this branch is 0.9, but it must also be divided by 0.1. This is necessary since the fractions are always carried forward for the remainder of the decay chain. Also note that the decay fractions for the two branches leading to isotope D add up to 1.0 (as they should).

3.5.2 Isotope Libraries

The following nuclides (including the full progeny, when appropriate) are included in the isotope libraries.

Table 8: Isotope libraries

| Libraries | | |
|----------------------|------------------|------------------|
| Sealed | CanduOps | Deposition |
| Background | Background | Background |
| Ba-133 | Na-24 | Kr-88 (Rb-88) |
| Cd-109 (Ag-109m) | Cr-51 | Sr-89 |
| Cs-137 (Ba-137m) | Mn-54 | Sr-91 |
| Co-57 | Mn-56 | Zr-95 |
| Co-60 | Co-58 | Cs-138 |
| Hg-203 | Co-60 | Ce-144 |
| I-129 | Sr-89 | Rb-89 |
| Mn-54 | Sr-91 | Ru-103 |
| Na-22 | Zr-95 | Ru-106 (Rh-106) |
| Ra-226 (and progeny) | Nb-95 | I-129 |
| Th-232 (and progeny) | Sb-124 | Te-131m |
| | Cs-134 | I-131 |
| | Cs-137 (Ba-137m) | Te-132 |
| | Cs-138 | I-132 |
| | Ce-144 | Te-133 |
| | Eu-152 | I-133 |
| | Gd-153 | Te-134 |
| | Gd-159 | I-134 |
| | Kr-88 (Rb-88) | I-135 |
| | Rb-89 | Cs-134 |
| | W-187 | Cs-137 (Ba-137m) |
| | Te-131m | Co-60 |
| | I-131 | |
| | Te-132 | |
| | I-132 | |
| | Te-133 | |
| | I-133 | |
| | Te-134 | |
| | I-134 | |
| | I-135 | |

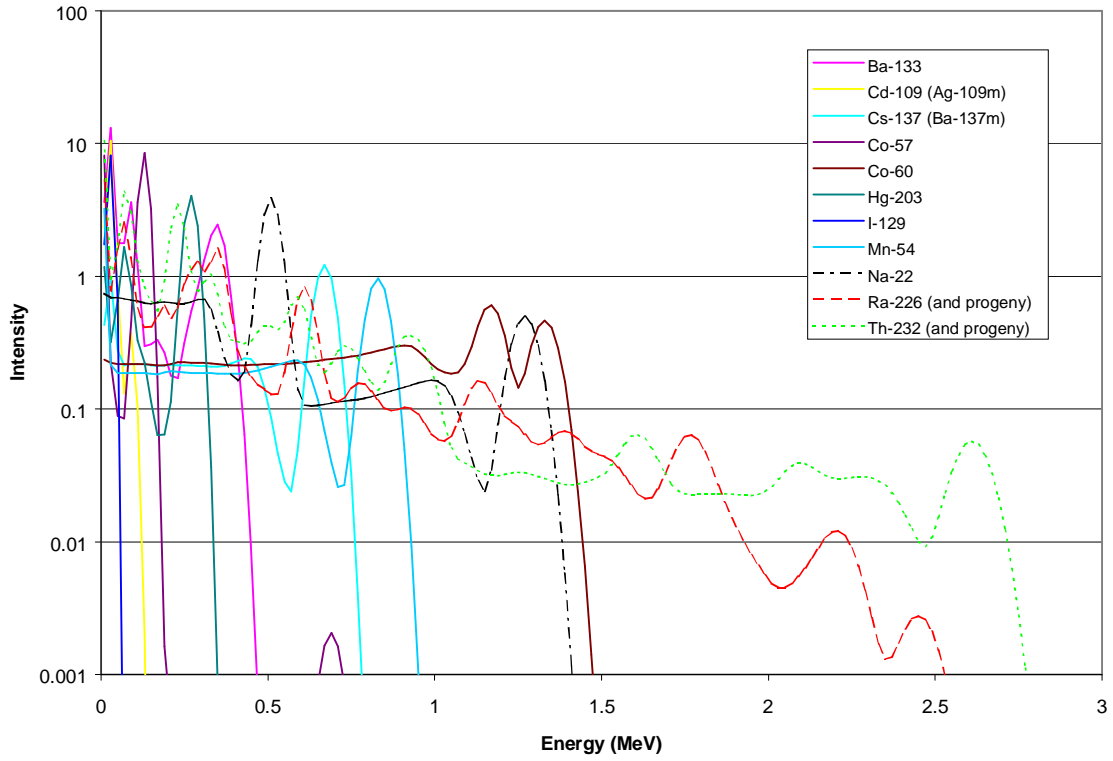


Figure 10: Basis spectra for sealed source library (Sealed.lib)

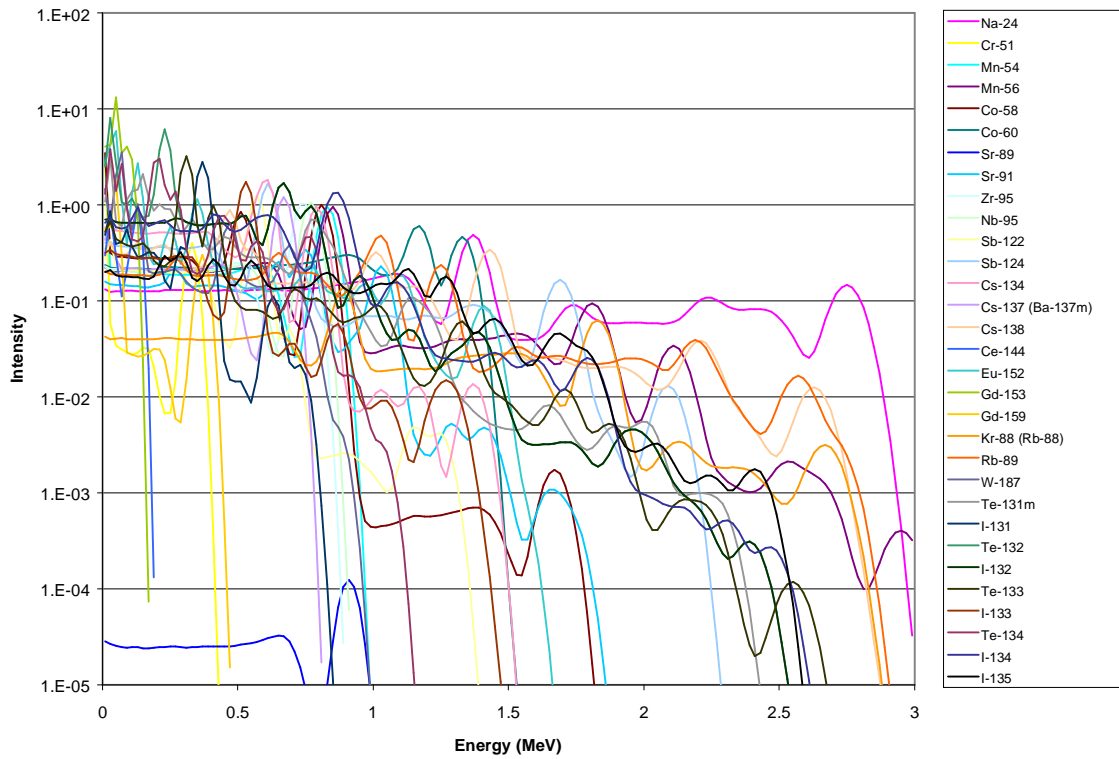


Figure 11: Basis spectra for CanduOps library (CanduOps.lib)

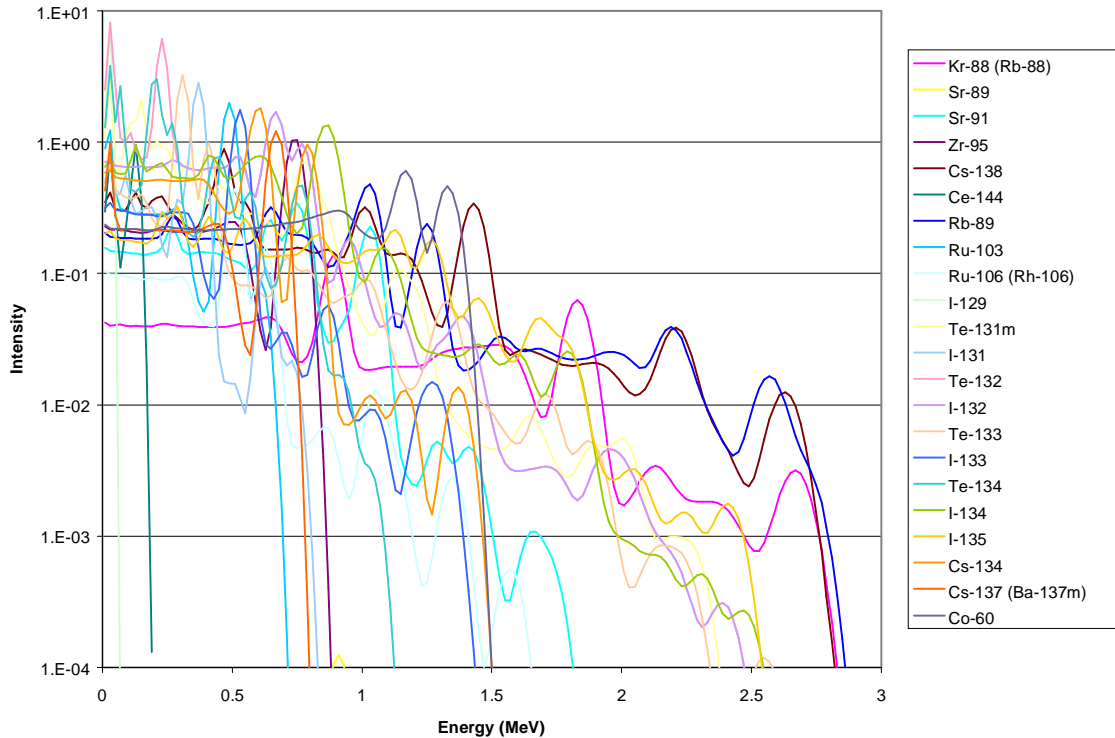


Figure 12: Basis spectra for deposition library (Deposition.lib)

The CanduOps and Deposition libraries contain a large number of isotopes. Consequently, there is considerable overlap between the spectra of the isotopes. To minimize such an overlap and to ensure that the basis spectrum set is orthogonal, it is important that the user select a range of half-lives that matches the conditions for which the spectra was acquired. The isotopes that fall outside the selected range of half-lives are not considered in the calculation, which reduces the number of spectra included in the basis spectra.

As an example, the basis spectra for the deposition library when the maximum half-life is one day are shown in Figure 13. There is considerably less overlap here than when the full library is selected, as shown in Figure 12.

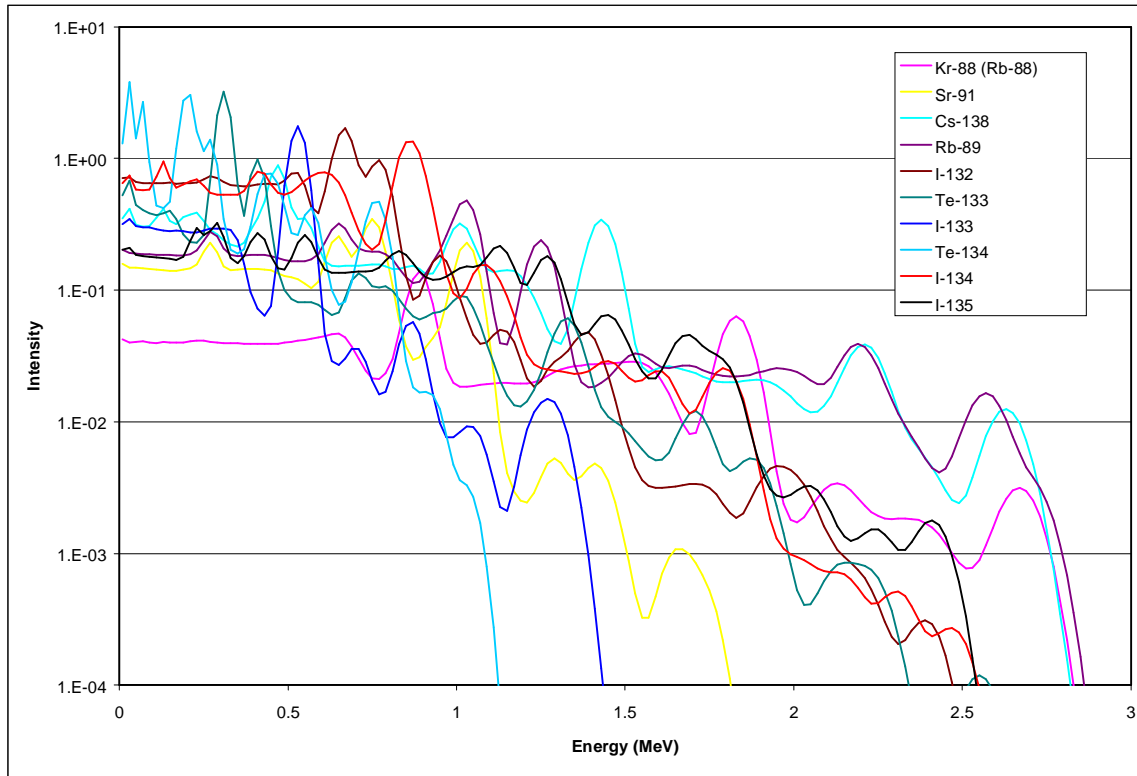


Figure 13: Basis spectra for deposition library for less than one day

The library is organized by isotope and lists the emission gamma lines. When the isotope decays into a daughter product with a half-life shorter than the parent isotope, the progeny name and gamma lines follow without a blank line. The entire data group for an isotope is separated by a blank line.

| | | |
|---------------------------------------|--------------|-----------------------------------------|
| Ba-133 | 3.31E+08 | 22 character name, half-life (seconds) |
| 0.004290 | 0.167990 | Energy (MeV), intensity |
| 0.030625 | 0.342460 | |
| ... | | |
| 0.356010 | 0.605000 | |
| 0.383850 | 0.086697 | |
| Blank line (end of isotope & progeny) | | |
| Cd-109 (Ag-109m) | 4.01E+07 | Next isotope |
| 0.002980 | 0.058184 | |
| 0.021990 | 0.186150 | |
| 0.022163 | 0.352560 | |
| 0.024900 | 0.113670 | |
| Ag-109m | 3.96E+01 1.0 | Progeny name, half-life, decay fraction |
| 0.002980 | 0.052940 | |
| 0.021990 | 0.098760 | |
| 0.022163 | 0.187050 | |
| 0.024900 | 0.060305 | |
| 0.088032 | 0.037200 | |
| Blank line (end of isotope & progeny) | | |

4. VISUAL BASIC CODE

4.1 Introduction

The S3Flux program was written primarily in Visual Basic. Fortran and C were used in implementation of the dynamic link libraries (DLL's). Since the graphical user interface (GUI) was developed solely in Visual Basic 6.0, the code structure must be understood in order to make any changes or updates.

Since the structure relies heavily of the use of "Forms" and their interaction, the code will be explained according to the location in each of the interface forms.

4.2 Forms

4.2.1 S3Flux

This is the main interface dialogue. The S3Flux screen controls all controls, variables, DLL declarations and internal calculations. Since the main control for this program is the Graph object (Gigasoft ProEssentials), all graph initializations must take place before any information is placed with the graphing object.

The main pitfall of working with Visual Basic code is the tendency for objects and file menus to have the same events which, simply, causes duplicate procedure calls. All new procedures must be thoroughly checked to avoid this case.

The layout for the S3Flux form code is as follows:

Form_Load

Initialize: This is used to initialize the graph, the user forms, and all required variables.

LoadDetector: Loads all the available detectors into the S3Flux "Detector" menu item

SortDetector: Sorts the detector names before loading them into the menu.

LoadLibrary: Loads all the libraries into the S3Flux "Library" menu

Read_Kerma: Reads Kerfac.txt, included in the S3Flux directory from ICRU report #47 Table A.1 pg 23

The above forms the initialization procedures of the S3Flux code. All other code calls are activated by user events. I.e.: when a control is clicked on.

A list of the controls and their menu options follows:

SSTab1
 Graph1
 ManualScale
 UndoZoom
 LinearOption
 LogOption
 LOGXOption
 LOGYOption
 CommonDialog1

| | | |
|-------------------|---|--------------|
| Raw | | mnuView |
| RawChannelOption | → | mnuRaw |
| RawEnergyOption | → | mnuRawE |
| PeakSearchOption | → | mnuPeak |
| Binned | | |
| BinnedOption | → | mnuBinned |
| RERawEnergyOption | → | mnuRecRawE |
| Deconvolution | | |
| LTOption | → | mnuLT |
| MEOption | → | mnuME |
| FluxOption | | |
| FluxEOption | | |
| KermaText | | |
| IntegralText | | |
| Isotope ID | → | mnuIsolident |
| GraphID | | |
| IDBinned | | |
| IDBackground | | |
| IDIsotopes | | |
| MinLife | | |
| MaxLife | | |

MnuDetector
 MnuLibrary
 MnuProcess

- MnuCalib
- MnuRes
- MnuMaxEntParm
- MnulterationLog

 MnuHelp

- MnuAbout
- MnuHelpS3

4.2.2 Calibration Plot

Calibration Plot is a form that requires Channel and Energy points to be entered to the purpose of adjusting the calibration of the chosen detector file. The new calibration is shown plotted against the original calibration and may be adjusted as necessary.

A list of controls follows:

| | | |
|-----------------|-----|---------------------------------------------------------------------|
| CalibGraph | | |
| ChannelText() | 0:4 | |
| EnergyText() | 0:4 | |
| CalEnergyText() | 0:4 | |
| B() | 0:2 | A and B are output variables for the original and new calibrations. |
| A() | 0:2 | |
| AcquireClick | | |
| DefaultClick | | |
| OKClick | | |
| ClosePlot | | |
| Ep_text | | These four variables are for calculating the secondary peak values. |
| Ec_text | | |
| E1_text | | |
| E2_text | | |

4.2.3 Manual

This form is directly associated with the S3Flux main form. Using minimum and maximum values for both X and Y co-ordinates, the viewable area for the main graph can be set using the Manual form. This is a more exact method of setting the zoom area rather than using the mouse to zoom into an area.

The controls on this form are simple. TxtXMin, txtXMax, txtYMin, txtYMax, Ok, and Cancel. The values for the minimum and maximum co-ordinates are checked for validity before the graph properties are set.

4.2.4 MaxEnt

This is the maximum entropy parameter form. Values for the initial guess, the baseline, number of iterations, and number of bins can all be adjusted. These values are used in the maximum entropy calculations to help ensure that the values converge within a reasonable number of iterations.

4.2.5 Resolution

This form is used to adjust the resolution of the given detector file. Pairs of energy and FWHM are entered to adjust the original resolution. The original and new resolutions are plotted for comparison purposes and may be adjusted as necessary. The graph view may also be switched from a linear plot to that of a square root plot.

A list of controls follows:

| | | |
|--------------|-----|----------------------------------------------|
| Resgraph | | |
| EnergyText() | 0:4 | |
| UserFWHM() | 0:4 | |
| CalFWHM() | 0:4 | |
| r() | 0:2 | r and r0 hold the variables for the original |
| r0() | 0:2 | and new resolution curves. |
| Aquire | | |
| DefaultClick | | |
| SqrSwitch | | |
| OK | | |
| Cancel | | |

4.2.6 Spectrum

This is a small utility form that is used in conjunction with the S3Flux main form to facilitate the selection of spectrum when a file is opened that contains a multiple number of spectrums.

4.3 Creating the Install CD-ROM

4.3.1 New Install or Adding Files to the Install

Visual Basic 6.0 allows an add-in to automate the process of compiling an end product and its associated install.

1. Choose the "Add-In Manager..." from the "Add-Ins" menu.
2. Load "Package and Deployment Menu", then select from the "Add-Ins" menu
3. Select "Package" from the Deployment Wizard.
 - a) Follow through all prompts, making sure the following files are in their appropriate places.
 - i) The following DLL's must be present:
 - Unfold.dll
 - UnfoldME.dll
 - ReadResp.dll
 - ReadData.dll
 - Fiodll.dll
 - Fmathdll.dll
 - Pegrp32A.dll
 - ii) All files must be placed in the application directory in the "Install Location".
 - Kerfac.txt
 - Isotopes.dat

4.3.2 Updating Existing Files

If changes have been made to existing files that are included in the current Install version. A faster method may be used to update the install program.

1. Recompile the S3FLUX.EXE
2. Copy and paste the S3FLUX.EXE to ..Package/Support in the working directory. Overwrite the existing S3FLUX.EXE
3. If there has been any DLL changes, or other file changes, copy and paste the files into the ..Package/Support directory.
4. Run: ..Package/Support/S3FLUX.bat. This will recreate the install package.
5. Copy [S3FLUX.cab, setup.exe, setup.1st] from ..Package to destination. (ie, the CD-ROM) Also copy any documentation needed.

5. REFERENCES

- [1] J. Briesmeister, *MCNP – A General Monte Carlo N-Particle Transport Code*, version 4B, March 1997.
- [2] C.J. Shannon, *A Mathematical Theory of Communication*, Bell System Technical Journal, **27**, pp. 379-423 and 623-656, 1948.
- [3] J. Skilling, R.K. Bryan, *Maximum Entropy Image Reconstruction: General Algorithm*, Mon. Not. Royal Astronomical Society, **211**, pp. 111-124, 1984.
- [4] S.F. Gull, J. Skilling, *Maximum Entropy Method in Image Processing*, IEE proceedings, **131**, part F, No. 6, pp. 646-659, October 1984.
- [5] J.M. Los Arcos, *Gamma Ray Spectra Deconvolution by Maximum Entropy*, Nuclear Instruments and Methods in Physics Research A, **369**, pp. 634-636, 1996.
- [6] S. C. Lizamore, *The MaxEnt Method Applied to Spectral Analysis and Image Reconstruction*, Institute of Statistics and Operations Research, Victoria University of Wellington, 1995.
- [7] Dr. Ed Waller, personal communication.

APPENDIX A: CONTENTS OF SPECTRA FILES

Files Spec1.exp and Spec2.exp contain multiple spectra acquired at the Gentilly-2 Nuclear Generating Station using an Exploranium GR-130 NaI spectrometer. Table A.1 describes the contents of each file.

Table A.1 Contents of GR-130 files

| Spec1 | Description |
|-------|---------------------------------------------------|
| 1 | S2-101 Spent fuel pool |
| 2 | S2-103 Spent fuel transfer pool |
| 3 | S2-008 Cooling of end-shields |
| 4 | S2-161/162 Sampling station for coolant-moderator |
| 5 | S2-245 Ventilation of reactor building |
| 6 | S2-101e Waste storage |
| 7 | Background in administration building |
| Spec2 | Description |
| 1 | Control rod mechanisms |
| 2 | Cladding failure detector |
| 3 | Coolant purification |
| 4 | Reactivity liquid controllers |
| 5 | Moderator poison |
| 6 | Auxiliaries on fuelling machine |
| 7 | Moderator leaks recovery |
| 8 | Reflection North vault ceiling |

Files Chernobyl1.mca and Chernobyl2.mca contain two spectra obtained inside the 10 km Chernobyl NPP-4 Emergency Zone, near the MORAL12 location, in the fall of 1999. The dose rate due to ground contamination at that location was approximately 3 $\mu\text{Sv/h}$. The contamination due to ^{137}Cs was between $1.68 \times 10^6 - 2.85 \times 10^6 \text{ Bq/m}^2$ [7].

Chernobyl1.mca is the measurement of a soil sample obtained using a 3"x3" NaI detector inside a lead castle for 133 seconds. Chernobyl2.mca is an in-situ gamma spectrum obtained using the same detector, held one meter above the ground for a live time of 224 seconds.

APPENDIX B: CALIBRATION PEAKS

The main emission energy of the following calibration sources is given in Table B.1.

Table B.1 Calibration peaks for sealed sources

| Source | Energy (MeV) |
|----------------------|-----------------------------------------------------------------------------|
| Am-241 | 0.060 (α 5.486) |
| Ba-133 | 0.031, 0.081, 0.303, 0.356 |
| Cd-109 (Ag-109m) | 0.022, 0.025, 0.088 |
| Cs-137 (Ba-137m) | 0.662 |
| Co-57 | 0.122, 0.136 |
| Co-60 | 1.173, 1.333 |
| Hg-203 | 0.0729, 0.0826, 0.2792 |
| I-129 | 0.030, 0.034, 0.040 |
| Ir-192 | 0.317 (β 0.536, 0.672, e 0.303) |
| Mn-54 | 0.0054, 0.834 |
| Na-22 | 0.511, 1.2745 |
| Tc-99m | 0.141 |
| Ra-226 (and progeny) | 0.047, 0.077, 0.186, 0.242, 0.295, 0.352, 0.609, 1.765 (α 4.784) |
| Th-232 (and progeny) | 0.239, 0.338, 0.583, 0.727, 0.860, 0.911, 0.969, 2.615 |