

ISOTOPIC V4 represents a **SUBSTANTIAL** move forward from previous versions of this program. Improvements to algorithms have been made, but in addition, great attention has been paid to improvements to useability.

ISOTOPIC V4 Benefits

- Provides quantitative assay of gamma-emitting waste samples with an emphasis on ease of use and practicality.
- Analyzes all types of gamma-emitting waste, fissile and non-fissile.
- Measure containers of many shapes and sizes, surfaces and even soils; via independently verified analysis methods; new algorithms for CLOSE geometry measurements.
- Use your own HPGe detector(s) and electronics or as part of an integrated ISO-CART™ system. Calibrate ANY detector on site, TRACEABLY, in minutes.
- Ideal for use with the revolutionary ORTEC trans-SPEC-100 portable HPGe spectrometer.
- Multiple measurements on a single object easily combined.
- Easy system expansion.
- New algorithm includes detector characterization parameters for improved accuracy.

ISOTOPIC V4 provides a practical solution to a wide range of gamma-ray measurement problems encountered in site characterization prior to remediation and decontamination and decommissioning (D&D) operations. ISOTOPIC is based on work done originally at several US DOE sites in the analysis of thousands of fissile waste containers¹ and in methods developed at the US Energy Measurements Laboratory^{2,3} (EML-NYC) to measure wide-area contamination of soils and surfaces.

In version 4, algorithms have been refined, user interaction has been simplified and reporting has been greatly improved in response to user suggestions.

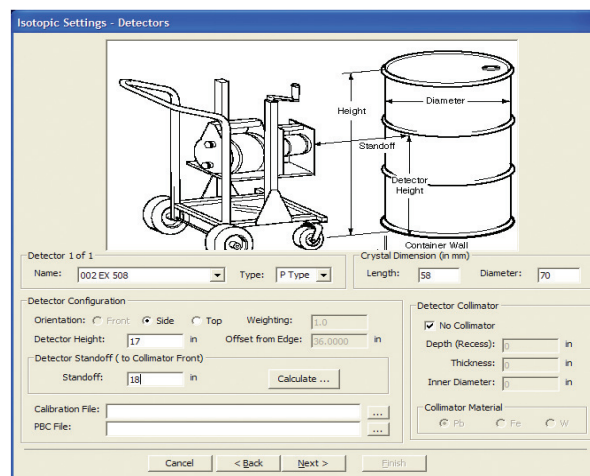
Extensive improvements make the latest version of ISOTOPIC easier to use than ever before. The job gets done with a minimum of complication. No special procedures are required to get an HPGe detector ready for use with ISOTOPIC. It can be used with almost any HPGe detector⁴ and can be calibrated and ready to go in minutes. A practical, semi-empirical approach to efficiency calibration is used.

Applicability

The following geometries are easily accommodated:

- Boxes
- Drums
- Pipes
- Surfaces (Collimated Detector)
- Wide Area Assay of Soils and Surfaces (Uncollimated Detector: M-1 Methodology)

ISOTOPIC provides a number of standard geometry "templates" from which a specific measurement configuration may be developed. These include cylinders (from top and side; including lined cylinders (pipes)), boxes, point source (far field), and infinite plane. The infinite plane (soils) mode is for uncollimated measurement of contamination, fall out or wide area spills, either washed into or on top of an infinite plane surface, most typically soil on the ground.



Methodology

In container mode, for the counting of packages, pipes and surfaces, the detector is characterized by a single point-source measurement, even when a collimator is to be used. This primary calibration, which can be traced to a certified standard, for any detector, is extrapolated or modeled to match the physical situation of the sample; container geometry, material, and matrix composition. The model is based on "point-kernel" methods in which the entire measurement problem is broken down into multiple source/matrix voxels and their contribution to the composite spectrum are calculated and summed. The approach, which is similar to Monte-Carlo Methods, utilizes detector parameters (crystal diameter, crystal length, dead layer, and end cap thickness) which the user supplies as part of the measurement configuration. No special separate measurements are needed to characterize the detector other than one point-source calibration.

ISOTOPIC V4 includes improved algorithms for "close geometry" where the detector to container distance is less than 15 cm.

¹Hagenauer, R.C., "Nondestructive Assay Quantification of Poorly Characterized Radioactive Isotopes," Proceedings of the 4th Nondestructive Assay and Nondestructive Waste Characterization Conference, Salt Lake City, 1995.

²H.L. Beck, et al., "In Situ Ge(Li) and NaI(Tl) Gamma Ray Spectrometry," U.S. Dept. of Energy, Environmental Measurements Laboratory, HASL-258, September (1972).

³I.K. Helfer and K.M. Miller, "Calibration Factors for Ge Detectors Used for Field Spectrometry," Health Physics, Vol. 55, No. 1, pp 15–29 (1988).

⁴For use in M-1 mode for soil characterization, an HPGe with crystal length/diameter in the range of 0.5 to 1.3 is recommended. 80% of HPGe detectors meet this criteria. The ORTEC PROFILE M Series detectors are ideal for this and the ISOTOPIC container measurements.

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For the uncollimated wide-area counting of soils, the "1-meter" methodology developed by the US DOE EML² and later extended³ is used. It is applicable in many situations:

- Decontamination assessment of previously used sites
- Assessment of nuclides deposited during emergencies
- Routine environmental monitoring near nuclear facilities

The EML methodology reduces a complex measurement problem to the product of three, simply-determined factors. The gamma-ray peak areas are related to the nuclide-specific activity by the product of the three factors. These factors have been determined for a range of detector types and soil conditions and are tabulated within the program. The efficiency calibration is determined using the stated efficiency according to the usual ANSI/IEEE 325-1996 convention at 1.33 MeV, and from the crystal length and diameter.

For improved accuracy at low energy, the user can use the same calibration used for container mode as an alternate to the EML method.

No special (and costly) Monte-Carlo characterizations of the detector are necessary. The attenuation correction is determined by selection of the soil type and type of nuclide distribution: recent (surface) deposits, older (washed-in) deposits or natural (uniform) deposits. The energy and peak shape calibration are performed using any multiline source and may be entirely automated. However you plan to use ISOTOPIC, there will be no unexpected detector calibration costs.

Support for Multiple Measurements of a Single Container

In the measurement of any large container of waste, several measurements are usually made from different directions to ensure the best results are obtained. This will be done sequentially if only one hardware system is available or simultaneously if there is access to multiple sets of hardware. ISOTOPIC can automatically combine the results taken either way by a user-defined weighted average. When multiple detectors are used at the same time, live spectra may be displayed on screen simultaneously from each detector, increasing user confidence.

Reporting

ISOTOPIC V4 provides GREAT flexibility in reporting within the standard product. All changeable parameters may be included in the standard output report. Analysis results are stored in an MS Access-compatible database, from which they are easily printed or exported for further processing into summary reports.

Hardware Support

ISOTOPIC V4, like all ORTEC *CONNECTIONS-32* Applications software products, is compatible with all ORTEC MCA hardware. In particular, it is ideal for use in conjunction with the trans-SPEC-DX-100, a complete rugged and portable HPGe spectrometer system which does NOT require the use of liquid nitrogen.



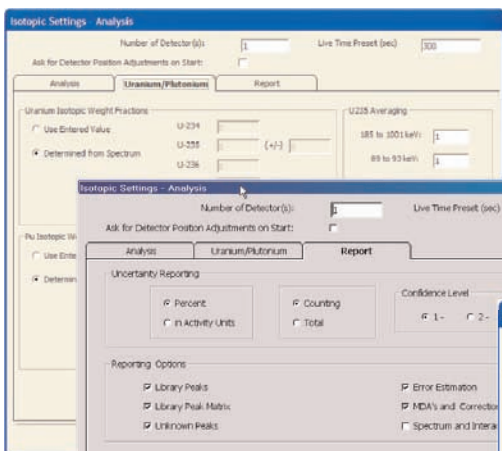
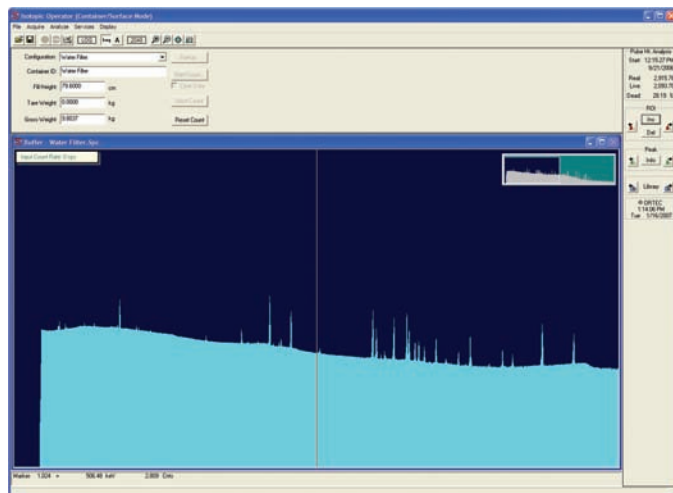
ISOTOPIC In Use

ISOTOPIC V4 has two modes: supervisor and operator. The operator need make choices only from the minimum subset of system options defined by the supervisor. The supervisor mode defines what operations the operator is allowed to carry out. A wizard guides the supervisor through the process of setting up the operator procedures. The wizard presents the parameters on logically grouped screens, with an emphasis on clarity of approach.

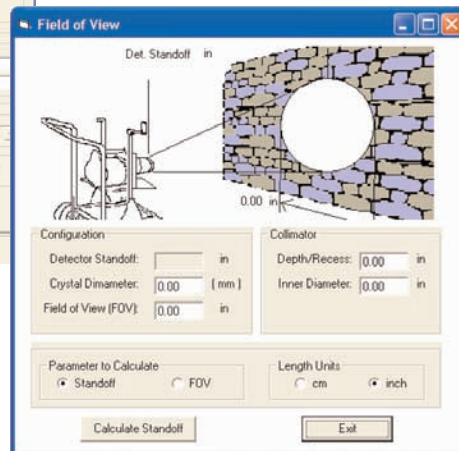
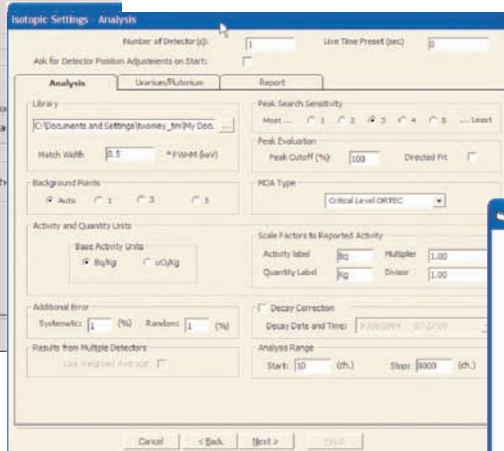
The supervisor/operator partitioning means that even semi-skilled operators in the field will collect good data with less wasted time for repeats (lower cost per measured item). Of course a skilled user may choose to run both modes.

Supervisor calibrates the system, creates libraries, defines sample geometries, matrices, collimators to be used, and other functions for later use by the operator. Supervisor can also define which features operator may access.

A handy "field of view" calculator provides a simple way to set up the detector-to-sample distance for the current collimator.



The operator main screen, which is customized by the permissions granted by the supervisor, is much simpler than the supervisor screen. In routine use, for container analysis, the operator need only start the acquisition, select the configuration (nearest standard container configuration), and enter the "book keeping data" such as container ID, type, weight, and the critical measurement data, such as detector-to-container distance.



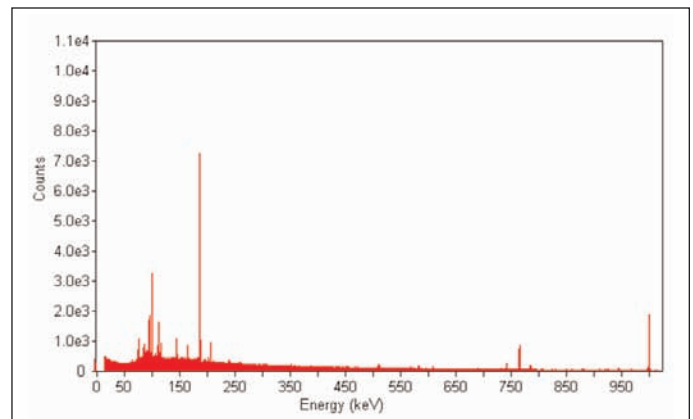
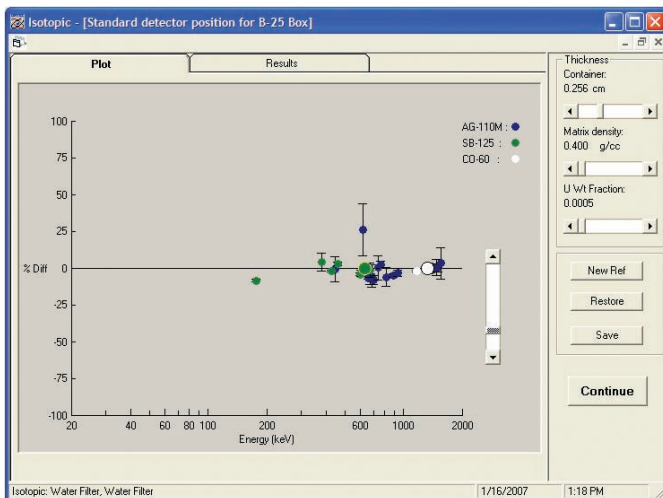
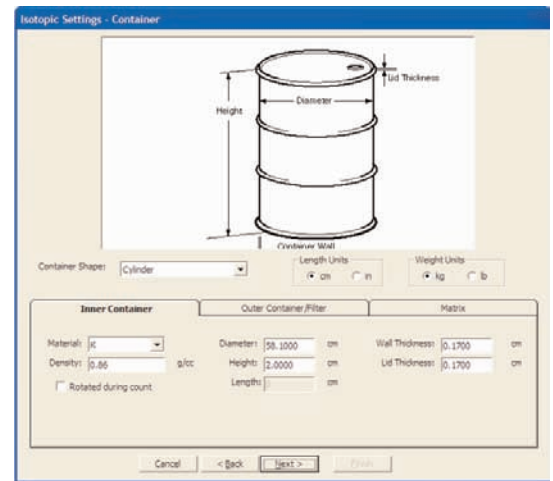
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The standard container configurations and collimator configurations are defined and specified by the supervisor. A container configuration includes the default dimensions, materials, and matrix detail. Any number of these configurations may be specified and recalled by the operator when needed.

When the analysis is complete, the operator can adjust the container/matrix physical parameters (such as matrix density or container wall thickness) to optimize the results by use of the nuclide plot.

The plot shows the percentage difference between the corrected measured activity and the activity calculated for the reference peak for each nuclide. The supervisor selects the reference peak. The operator may optimize the analysis, adjusting the container, matrix, and weight fraction uranium, to refine the results. The visual evidence of a good result is immediately seen when the points from a multi-peaked nuclide are distributed normally about the "zero-line." In the case of uranium analysis, if the U-235 enrichment is known, it may be entered and then the U-238 and U-234 values are computed more accurately for samples containing weak uranium activity. Homogeneous and inhomogeneous samples are analyzed with increased accuracy by this method. A good indication that a package contains an inhomogeneous distribution of materials is that the user can obtain a combination of parameters which makes the activity plot flat for some nuclides but not others. This plot can form part of the output report, along with a plot of the spectrum itself.



Accuracy of Results

It is not easy to give a precise estimate for the accuracy to be expected. Several factors are influential: statistics and counting time, matrix density and inhomogeneity, calibration uncertainty, and the number of measurements carried out on a single container or object. A range of 10 to 50% accuracy should be considered representative, the smaller being for well-defined geometries in homogeneous and light matrices.

Reports

When the fine-tuning is finished, the operator selects a report for each nuclide showing the activity and weight. These results may then be printed and archived. The report files are written in either a database summary or as complete reports showing all input and correction information. Custom reports may be generated by the use of the report generator option. The tabulated components of error estimates can be used to help reduce overall uncertainties, for example, by extending count time or repositioning the detector. The user is also warned if any of the corrections appear to be excessively large. Minimum Detectable Activities (MDA) are calculated for each nuclide. Activities, grams of U or Pu, or MDAs from multiple measurements may be reported as weighted averages. The weighting is user definable.

Sample Name: Uranium from ISPRA

Spectrum File Name: C:\User\Uranium from ISPRA Buf00460.An1

Acquisition information			
Start time	3/6/2001 12:54:38 PM		
Live time:	2500	Real time:	2570
Detector:	DSPE-044No detector	Dead time (%):	2.72

Calibration		
File name	C:\User\Uranium from ISPRA.Clb	
Energy calibration	Created	3/6/2001 11:29:29 AM
	Zero offset	0
	Gain	0.1249744
	Quadratic	0
Efficiency calibration	Created	3/6/2001 10:17:31 AM
	Type	Quadratic
	Uncertainty Above Knee	20.91%
	Uncertainty Below Knee	9.19%
	Coefficients (Above the Knee)	-24.71316, 5.465302, -0.4830579
	Coefficients (Below the Knee)	0, 0, 0
	Detector calibration point-source reference distance	30.0 cm

Library	
Main analysis library	C:\User\Uranium only.lib
Library match width	0.5

Analysis parameters			
Start channel:	20	Stop channel:	16000
Peak cutoff (%):	50.0	Peak search sensitivity:	3
MDA type:	ORTEC Traditional	Background type:	Auto
Base Activity Units:	Bq/Kg	Activity scaling factor:	1.000E+0/1.000E+0
Activity Label:	Bq <input type="checkbox"/>	Quantity Label:	
Random error (%):	0.0	Systematic error (%):	0.0
Directed fit:	No	Uncertainty in percent:	Yes
Counting uncertainty only:	Yes	Confidence level (sigma):	1
U235 89-93 keV averaging:	1	U235 186/1001 keV averaging:	1

Spectral corrections			
Decay correct to date:	No	Decay correction date/time:	N/A
PBC correction:	No	PBC File:	N/A

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Library peaks								
Nuclide	Channel	Energy	Bkg Counts	Net Counts	CPS	1 Sigma	FWHM (keV)	Flags
U-235	202.34	25.26	4132	116	0.046	90.47	2.564	s
U-238	393.52	49.15	4237	493	0.197	31.98	1.639	s
U-234	430.00	53.71	2779	-27	-0.011	334.13	0.000	s

s - Peak fails shape tests.
D - Peak area deconvoluted.
M - Peak is close to a library peak.

Library peak matrix						
Nuclide	Ave. activity	Energy	Activity	Codes	MDA	Comments
U-234	6.445E+6	53.71	0.000E+0	&	1.999E+6	G
		120.93	6.445E+6	(4.913E+6	GK

General Configuration info			
Configuration name:	Recall	Has Collimator:	NO
Orientation:	Side	Height:	10.0 cm
Detector standoff:	20.0 cm	Collimator depth/recess:	N/A
Database	C:\User\OrtecDB.mdb		

Container			
Type:	Cylinder	Material:	Fe
Thickness (entered):	0.10 cm	Thickness (effective):	0.10 cm
Height:	20.0 cm	Fill Height:	20.0 cm
Diameter:	20.0 cm		
Tare weight:	5.0 kg	Container density:	7.60 g/cc
Sample weight:	1.847 kg		

Matrix			
Material:	Combustible	Density (initial estimated):	0.300 g/cc
U total fraction (initial estimated):	0.0	Pu total fraction (initial estimated):	0.0
Thickness	19.80 cm		
Weight fraction of U (eff.)	0.0		
Volume	6.16E+3 cc		
Gross weight	6.847E+0 kg		
Net weight	1.847E+0 kg		
Density (measured)	0.300 g/cc		
Density (adjusted)	0.300 g/cc		

Peak Correction Factors

Energy	Nuclide	Activity* (Bq/Kg)	Air	Container Correction	Coll.	Activity** (Bq/Kg)
58.32	U-235	1.033E+04	1.010	1.68E+3	1.00E+0	1.75E+07
63.39	U-238	4.044E+03	1.009	9.08E+2	1.00E+0	3.70E+06
81.24	U-235	8.272E+03	1.009	2.16E+2	1.00E+0	1.80E+06
84.17	U-235	6.897E+03	1.009	1.84E+2	1.00E+0	1.28E+06
89.97	U-235	5.472E+03	1.008	1.39E+2	1.00E+0	7.69E+05
92.39	U-238	2.490E+04	1.008	1.25E+2	1.00E+0	3.14E+06
92.81	U-238	2.033E+04	1.008	1.23E+2	1.00E+0	2.52E+06
93.36	U-235	2.376E+03	1.008	1.20E+2	1.00E+0	2.88E+05

Uranium Analysis	
Grams of uranium	3.800E+3
Weight% U-235 (186 to 1001-keV region)	0.3 (+-) 0.1032
U235 Enrichment calculated (%)	0.297 (+-) 0.103

Isotopic results			
Nuclide	Weight(g)	Activity (Bq)	% Uncertainty (1Sigma)
U-235	1.130E+01	9.034E+05	25.295
U-238	3.832E+03	4.722E+07	24.791
U-234	5.999E-02	1.381E+07	45.905

Total activity	
Total Activity	6.19E+07 Bq
Total Alpha Activity	6.19E+07 Bq

ISOTOPIC Specifications

General

The acquisition control and quantitative analysis functions are integrated into a concise package for use in PC-based *in situ* gamma spectroscopy systems for the determination of radioactive content of containers, objects, surfaces, and soils.

Operating System

32-bit application for Windows 2000/XP network capabilities; support for preemptive multitasking; and ORTEC *CONNECTIONS-32* compliant.

Spectroscopy Hardware Support

ISOTOPIC is recommended for use with the ORTEC digiDART® Portable MCA system. However, all ORTEC MCBs (past and present) and all other devices supported by ORTEC *CONNECTIONS-32* (see *CONNECTIONS-32* literature) are compatible. Support is built-in for advanced operations (where provided in hardware): amplifier gain/shaping control, Auto-PZ, "optimize" and InSight™ mode, digiDART field mode, graphical setting of MCB spectrum stabilizer and statistical uncertainty peaks. Specifically, the trans-SPEC-DX-100 is recommended for *in situ* measurements (literature on request).

File Formats Supported

ORTEC .SPC and .CHN, and ASCII ".SPE" are supported as standard in file save, recall, and compare functions. Other file formats may be imported by the use of A49-B32 Data Master.

Quantitative Spectrum Analysis Methods

Peak Search

Peak Search by library direction for specified nuclides, plus Mariscotti peak search for non-specified nuclides, both main library and supplemental ("suspect") library are used.

Interactive Bulk Sample Parameter Adjustments

Interactive Matrix and container adjustments and automatic attenuation correction for new matrix. Easy to use graphical display of relative analysis results to show the best matrix.

Deconvolution Method

Both peak finder and library are used to direct the deconvolution process. Automatic recalibration of Energy/channel based on identified peaks where possible.

Choice of Detection Limit Formalisms

ORTEC Traditional
ORTEC Critical Level
No MDA (report zeros if less than MDA)
KTA Rule
Detection Limit 2 sigma — Japan
Detection Limit 3 sigma — Japan
Currie Limit
RISO MDA
ORTEC LLD
Peak Area
Air Monitor — Gimrad method
Reg. Guide 4.16 Method
Counting Lab — USA
DIN 25 482.5 Erkennungsgrenze
DIN 25 482.5 Nachweisgrenze
GTN5/CEA/EDF (France)
Nureg 0472

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Decay Corrections

- Decay correct to any date/time, either back or forward

Spectral Corrections

- Peaked Background Correction
- Random summing (high-rate counting losses)
- Library-based peak interference correction

Reporting

Choose any ORTEC Standard report option:

- Direct to printer
- Automatically written to database
- Crystal Report formatted output
- Report in HTML format. From there it can be saved as a disk file.

Calibration

Energy Calibration

- Multipoint, quadratic for energy and FWHM
- Automatic Energy Calibration (Patent No. 6,006,162)

Semi-Empirical Efficiency Calibration Fit Options:

ISOTOPIC Mode

A point source calibration is established via one of the following methods:

- Single Function Polynomial (x-Point)
- Interpolative above and below "knee"
- Quadratic above or below user-set "knee"
- Linear above or below user-set "knee"

The point source calibration is extrapolated to the physical geometry-matrix situation via point-source Kernel calculations internal to the program.

Infinite Plane Mode (for Soils and Surfaces: Uncollimated Detector)

The Beck² 1-meter methodology, with extension to large detector sizes³, as used by US DOE Environmental Measurements Laboratory (EML). The EML methodology is used to produce an efficiency curve based on detector dimensions and IEEE efficiency value. The soil density and attenuation is specified in user-editable alpha/rho files.

Soil Attenuation Factors

In soil, attenuation depends on the soil thickness and density, which is modeled by the parameter α/ρ (*where α is the reciprocal of the relaxation length, defined to be the soil thickness required to reduce the flux at a particular energy by a factor of e , and ρ is the soil density in gm/cc*). For a surface distribution α/ρ is infinite, while for uniform (natural emitters) distribution, alpha/rho is 0. Values of α/ρ ranging from 0.05 to 0.5 have been found to describe realistic fallout distributions accurately, the more aged fallout being represented by the smaller α/ρ values.

The α/ρ values are nuclide-specific and are stored in a table which may be edited by the user to reflect the measurement conditions.

Analysis Library Manager

ISOTOPIC includes a comprehensive library editor for building custom analysis libraries. The editor allows the operator to cut and paste nuclides and peaks from master libraries, add flags to individual peaks for identification (single escape peak, x-ray, or other) and analysis (key line or exclude from activity calculation), and save the library as any name. It also includes full integration of the Nuclide Navigator library tool (sold separately as model C53-B32). ISOTOPIC will use Nuclide Navigator if installed, and can read Nuclide Navigator libraries in Microsoft Access Database format (no conversion necessary), and save libraries in database format for use by Nuclide Navigator.

Quality Assurance

ISOTOPIC quality assurance complies with the demands of ANSI N13.30. For each detector the following are monitored:

- Total detector background
- Total (decay corrected) activity for all calibration nuclides
- Average FWHM ratio (spectrum to calibration standard)
- Average FW1/10M ratio (spectrum to calibration standard)
- Average peak shift from library values
- Actual peak centroid energies

Calculational Details

Summary of the ISOTOPIC Mode Methodology for Containers

The activity of an isotope in a container is given by:

$$A_{isotope} = \frac{PA_{meas} (CF_{item})(CF_{col})}{BR_{\gamma ray} (\epsilon_{det})}$$

where

- $A_{isotope}$ = activity of the isotope to be reported (Bq/ μ Ci),
- PA_{meas} = measured peak area for a reference gamma ray of the isotope (c/s),
- CF_{item} = container, matrix, and sample self-attenuation correction factors
- CF_{col} = collimator correction factor,
- $BR_{\gamma ray}$ = gamma-ray branching ratio,
- ϵ_{det} = detector efficiency measured using a NIST-traceable point source (cps per Bq, μ Ci).

When gram quantities, $Mass_{isotope}$, of reported isotopes are needed, these are given by:

$$N = \frac{A_{isotope}}{\lambda_{isotope}} \quad Mass_{isotope} = \frac{N(At)}{Av}$$

where

- N = number of atoms of a reported isotope,
- $\lambda_{isotope}$ = decay constant of a reported isotope (sec^{-1}),
- At = atomic number of the measured isotope (g/Av),
- Av = Avogadro's number.

Result Averaging of Multiple Measurements

When results of multiple measurements are combined, a weighted average is calculated according to:

$$A_{average} = \sum A_i w_i / \sum w_i$$

where

- A_i = individual activity (gram or MDA) results,
- w_i = user-defined weighting factors.

Methodology for Soils

The specific activity, A (Bq/m² or Bq/g) is related to the net peak count rate N_f by:

$$A \text{ (activity)} = \frac{N_f \text{ (net peak count rate)}}{\left(\frac{N_f}{N_0}\right) \left(\frac{N_0}{\Phi}\right) \left(\frac{\Phi}{A}\right)}$$

where

N_f/N_0 = angular correction factor of the detector at that energy for a given source distribution in the soil,

N_0/Φ = peak count rate per unit uncollided flux for a parallel beam of gamma rays of the peak energy that is incident normal to the detector face (cpm/ γ s⁻¹)

Φ/A = total uncollided flux at the peak energy arriving at the detector per unit inventory or concentration of the nuclide in the soil (γ cm⁻² s⁻¹) or (γ g⁻¹ s⁻¹).

The method of estimating calibration factors uses information about the detector and the distribution(s) of radionuclides being measured:

- Detector Efficiency (expressed as %)
- Detector Orientation (up or down)
- Detector Aspect Ratio (calculated as crystal length/crystal diameter)
- Deposition Profile Parameter (α/ρ value(s))

α/ρ is assumed to be 0 (for uniform distribution) for all natural emitters. α/ρ is assumed to be infinite (for surface only distribution) for fallout on undisturbed soil.

Beck's method is implemented in ISOTOPIC by calculating values for each of the calibration parameters. The calculation is carried out for each gamma ray of all the nuclides identified.

Collimator Correction Factors

If a container is large enough, some gamma rays will penetrate any collimator that may be surrounding the germanium detector. The collimator correction factor is heavily dependant on the diameter of the collimator, the depth of collimation, and the wall thickness of the collimator.

The collimator correction factor is determined by computing the fraction of the activity that is not shadowed by the collimator and then computing the penetration length through the collimator for the remaining activity. This is determined for each voxel of the item being measured.

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System Prerequisites

As a *CONNECTIONS-32* product, ISOTOPIC requires a Windows XP platform. Interfacing of MCB hardware to the system may be by USB, Ethernet, printer port, serial port, or ORTEC Dual-port Memory. (Check hardware literature for details). ISOTOPIC will run on any PC that supports the above Windows OS and has 20 MB of disk space.

Ordering Information

Model	Description
ISOPLUS-B32	ISOTOPIC-32 Advanced Gamma-Ray Waste Assay Analysis Software
ISOPLUS-G32	Documentation for ISOPLUS-B32
ISOPLUS-K32	Upgrade from ISO-B32 or M-1-B32 to ISOPLUS-B32
ISOPLUS-N32	ISOPLUS-B32 Network Copies
ISOPLUS-U32	Update to ISOPLUS-B32
ISOPLUS-232	2 year update subscription for ISOPLUS-B32
ISOPLUS-332	3 year update subscription for ISOPLUS-B32
ISOPLUS-432	4 year update subscription for ISOPLUS-B32
ISOPLUS-532	5 year update subscription for ISOPLUS-B32

Specifications subject to change
030409

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