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The 1997 IAEA intercomparison of commercially available PC-based software for alpha-particle spectrometry

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Abstract

Four commercially available, PC-based analysis programs for alpha-particle spectrometry were compared using the 1997 IAEA test spectra, i.e. AlphaVision 1.20 (EG&G Ortec, USA), Alps 4.21 (Westmeier GmbH, Germany), Winner Alpha 4.0f5 (Eurisys Mesures, France) and Genie-2000 (Canberra Industries Inc., USA). A systematic statistical study of the analysis results was performed based on *z*-scores. The results indicate that the four programs leave room for substantial improvement.

1. Introduction

With the progress in the technology of personal computers, PC-based software packages started to play a key-role in the control, acquisition and validation of the data in any nuclear experiment. Because of the range of applications of alpha-particle spectrometry, analysis software packages are among the most used software in any nuclear laboratory. They are being used in such important applications as environmental studies, low level monitoring, radioactive waste analysis and safeguards. Therefore, the IAEA decided to call a consultants' meeting in November 1997 to acquire reference spectra and compare commercially available, PC-based analysis software for alpha-particle spectrometry. In this paper, we describe the methods and results of the intercomparison. In a separate paper [1], we present the acquisition and determination of reference values for the alpha-particle spectra.

Alpha-particle spectra are usually very complex to analyze. Only a few radionuclides emit monoenergetic alpha particles and very often two or more lines from the same radionuclide overlap. Most alpha emissions have energies between 4 and 6 MeV, and with the energy resolution achievable in realistic conditions, a typical alpha-particle spectrum contains one or several groups of overlapping lines. The difficulty of the analysis depends on the

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amount of information that one tries to obtain from the spectrum and reaches its maximum when a full analysis is performed to obtain the energies and intensities of all spectral components. However, in many cases the basic information needed is the relative contribution of the component nuclides, which is often, but not always, easier to obtain.

A number of analysis programs are in use at different laboratories which allow the fitting of alpha-particle spectra with different levels of complexity, covering the range from simple peak integration to non-linear fitting algorithms. One of the many possible classifications divides them into two main groups: The first one includes a few programs which have been tested in the frame of EUROMET [2] and bilateral intercomparisons [3]. Most are in-house programs which use complex line shape models and sophisticated minimization algorithms and perform a full covariance analysis. They are general-purpose codes, optimized for high resolution spectra and, although documented, they can not be used without comprehensive prior training. The second group includes both general-purpose programs, easier to operate, and codes tailored to specific problems, e.g. uranium isotopic analysis [4]. Many programs from both groups could be used to analyze the test spectra, but this intercomparison was restricted to general-purpose, commercially available codes. That considerably reduced the number of candidate programs to be tested.

The test spectra and reference value files, as well as the software used to perform the statistical testing of the analysis results obtained, are available on the World Wide Web through URL *http://iriaxp.iri.tudelft.nl/ ~ rc/fmr/alphaspc/alphaspc.htm*.

2. Experimental

2.1. Description of the tested programs

The programs that were tested are AlphaVision 1.20 (EG&G Ortec, USA), Alps 4.21 (Westmeier GmbH, Germany), Winner Alpha 4.0f5 (Eurisys Mesures, France) and Genie-2000 (Canberra Industries Inc., USA). Evaluation copies were obtained from the manufacturers directly. The following information was obtained from the manuals.

AlphaVision can operate in three basic modes. In the first one, *regions of interest (ROIs)* can be manually set and only basic integration is performed.

The second mode, *Peak search and fit,* performs an automatic peak search, fits the peaks and gives individual information on peak areas and positions. After smoothing, a peak search is performed based on normalized first derivatives. A Gaussian function with a low-energy exponential tail is fitted to each peak with the Simplex method, in order of decreasing energy. According to the manual, the regions selected for the fitting never include more than one peak. The fitting process operates on the smoothed spectrum. After having been fitted, the contribution of the peak is subtracted from the spectrum.

The last mode, *Library Search and Fit* performs a fit using the information from the peak search as well as the data library and gives results in terms of nuclide activities or areas. In the two modes of operation which fit the spectra, the user cannot easily interact with the program to modify the results of a previous fit by adding or deleting peaks, other than by editing the library in the corresponding mode.

In *Alps*, the spectrum is divided into regions that may contain peaks and can be treated independently. For each region, a peak search is performed based on normalized first derivatives. If peaks are found, an exponential background is applied to the region such that it is always lower than the experimental channel contents. Then, the background is subtracted. The program decides if the peaks present in the region should be treated as a multiplet or not. A Gaussian function with one or two folded exponential tails is fitted to the channel contents with a linear least squares algorithm in three passes. In the first pass, the FWHM is not varied but taken from the calibration. Statistically insignificant peaks are then eliminated. A residual analysis is performed and if necessary, peaks are inserted. The fitting is repeated, allowing all parameters to be varied. Again, statistically insignificant peaks are eliminated. A final fit is then performed. After the final fit, the energy calibration is used to identify the peaks.

The manual does not define the uncertainties reported by the program. It states that the reported uncertainties are "greater than the usual 1-STD uncertainty". From the analysis results for singlet peaks, as compared to the other programs, it turns out that they are indeed; by a factor of 3.4.

In *Genie 2000*, the peak search is performed using either a library driven routine (for spectra of known contents) or by the Generalized Second Differential Method (for spectra of unknown contents). The latter was used during the current testing. Peak areas are determined either by summation (singlets) or by non-linear least squares fitting. Complex structures can be fitted as singlets or multiplets depending on the value given to a parameter, expressed in terms of FWHM. The background shape is user selectable, but some of the possible choices have no physical meaning in alpha-particle spectrometry. A modified Marquardt algorithm is used in the minimization process for fast convergence. The interactive peak fitting menu can be easily used to add or delete peaks and residual search is also available.

For *Winner Alpha*, no information is given in the manual about the line shape model or the minimization algorithm used in the fittings. However it is evident that it is planned to include them at some point in time as the headings are present, just no details. Initial values for energy calibration and peak shape parameters (FWHM and two tail parameters) must be provided before starting the analysis. An automatic peak search is possible which also marks the ROIs for subsequent area determination. Two modes of analysis are possible, fitted areas or ROI integration. If necessary, ROIs can be edited to facilitate the insertion or deletion of peaks before reanalyzing the spectrum. Modifying the ROIs requires "painting" the peaks rather than inserting or deleting a peak at cursor. The fitting process, although not documented, seems to be quite stable with respect to the initial parameter values. There is no information on the procedure used to compute the uncertainties. Output plots may include the raw data, the fits and the residuals.

2.2. Analysis procedures

Each program was tested by two users analyzing all of the IAEA test spectra [1]. In total three different users, named S, E and M exploited the analysis programs. Prior to the actual analysis of spectra, the manuals of the programs were studied for two hours.

Of the four programs tested, only Alps and Genie were designed to allow for easy analysis of spectra not acquired with software and hardware obtained from the same vendor.

As a result of this, in the case of AlphaVision, the menu options related to energy and efficiency calibration were not accessible. The energy calibration was performed with the related program "Maestro" (supplied by Ortec along with AlphaVision) and written to the spectrum file. The two programs number the channels differently, which was compensated for by offsetting the correct energies in Maestro with the slope of the calibration curve. For Winner Alpha, a special conversion of files had to be performed to label them internally as alpha-particle spectra.

For each set of spectra an internal energy calibration and, if possible, a FWHM and shape calibration was performed. Then the spectra were analyzed twice. First with all parameters, such as peak-search sensitivity and residual-search sensitivity, set to the default values or, if available, to the values suggested in the program manual. Second, with the parameters set to the user's liking, attempting to optimize for the analysis of the spectrum in each set with the best statistics. The optimization was performed using the information offered by the analysis program and its documentation, not the knowledge of the actual contents of the spectra. The optimized analysis also encompassed, if possible, manual insertion of peaks or, in the case of AlphaVision, the use of nuclide libraries tailored to the spectrum to be analyzed. This involved insertion of non-existing radionuclides in the library since only 4 peaks per radionuclide can be entered. Program and user specific remarks on applied methods are listed in Table 1.

In addition, the libraries supplied with the programs were compared with respect to ^{226}Ra and its progenies.

The statistical processing of the analysis results was performed only after all analysis runs had been completed.

Table 1
User and program specific remarks on how the analysis were performed

	AlphaVision	Alps	Genie 2000	Winner Alpha
User 1 default mode	No remarks. User "E"	No remarks. User "M"	Integrate, use continuum. User "S"	No "default" mode available User "S"
User 1 optimized mode	Realistic nuclide library employed.	Sensitivity set to maximum. Manual peak insertion employed.	Manual insertion of peaks employed.	Manual insertion of peaks employed.
User 2 default mode	Energy calibration problem compensated. User "M"	No remarks. User "S"	Fit, no continuum. User "E"	No "default" mode available. User "E"
User 2 optimized mode	Energy calibration problem compensated. Library with artificial radionuclides employed.	Sensitivity set to maximum. Low FWHM estimate employed. Manual peak insertion employed.	Manual insertion of peaks employed.	Manual insertion of peaks employed.

2.3. Direct doublet ratios in the natural uranium spectra

From the analysis results of the natural uranium spectra, the ratios and associated uncertainties of the peak areas, if reported for both components of the doublets of the ^{234}U and ^{238}U radionuclides, were computed and compared to the yield ratios found in the Table of Isotopes [5], after correction by coincidence-summing with conversion electrons as mentioned in the paper describing the reference test spectra [1]. The doublet separations are approximately 2.5 FWHM in both cases, and the components are clearly visible to the eye in the spectra with the best statistics.

2.4. Systematic statistical testing of the analysis results

2.4.1. Preliminary steps

A conversion program was written that yielded output in a standard format containing peak energies and areas, both with their absolute 1 standard deviation uncertainties. This step was not entirely trivial, because only two programs did report uncertainties in the peak positions, i.e. Alps and Genie. For the other programs, which reported energies with two digits after the decimal point, implying uncertainties of less than 0.01 keV, these uncertainties were set to 0.01 keV. Also, not all programs reported 1 standard deviation uncertainties. The reported uncertainties were converted to one standard deviation absolute uncertainties according to the definitions given in the documentation of the programs. In the case of Alps, the reported uncertainties were divided by a factor of 3.4 to achieve this.

2.4.2. Statistical comparison

A separate program was written to perform a statistical comparison based on standardized residuals or z-scores, i.e. the differences between reported values and reference values divided by their own uncertainties.

Using all cases where both a reported area and a reference area were available ("hits"), a weighted average and its uncertainty of the ratios of reference peak areas and program output peak areas were determined. The weights used were the inversed squares of the uncertainties in the area ratios, computed from reference and reported uncertainty. The computation was performed in two passes: In the first pass, the average ratio was estimated. Peaks with reference uncertainties exceeding 11% were excluded in this pass. In the second pass, outliers at the 95% confidence level were excluded from the

computation. The reported peak areas and associated uncertainties were multiplied with the average ratio before proceeding.

In the case of a "hit", two z-scores could be computed: A z-score related to the quality of area determination based on the uncertainties in the reference files

$$z_{\mathrm{ref}} = \frac{A_{\mathrm{rep}} - A_{\mathrm{ref}}}{\sqrt{2\sigma_{\mathrm{ref}}^2}}, \quad (1)$$

and a z-score related to the statistical control of the analysis program based on both the reference uncertainty and the uncertainty reported by the analysis program

$$z_{\mathrm{rep}} = \frac{A_{\mathrm{rep}} - A_{\mathrm{ref}}}{\sqrt{\sigma_{\mathrm{rep}}^2 + \sigma_{\mathrm{ref}}^2}}, \quad (2)$$

where A_{ref} and A_{rep} are the reference and reported peak area, and σ_{ref} and σ_{rep} their uncertainties, respectively. Such z-scores are expected to be normally distributed with a zero mean and a unity standard deviation, i.e. z-scores higher than 2 or lower than -2 indicate that something is wrong at the 95% confidence level.

If the reference area was missing, the reported peak was considered to be a "false hit" and only the second z-score could be computed, using zero both as the reference area and as its uncertainty. If the reported area was missing, it was considered a "miss" and only the first z-score could be computed. Missing a noisy peak or reporting a false hit with a high uncertainty in the area do not result in high z-scores and are therefore "allowed" in this test.

Some of the test spectra contained doublets with small separations. It was decided to allow the analysis programs to determine the total area of such doublets. To this end, if two peaks in the reference list matched one peak in the analysis program output, i.e. if both reference peaks were located within $1 \times \mathrm{FWHM}$ of the analysis result, the two reference peaks were merged before the computation of z-scores. This was also done if such two reference peaks were located within the position uncertainty reported by the analysis program.

A section from the comparison program output is shown in Fig. 1.

From the Z-scores, reduced sums of squares χr^2 were computed for different categories of peaks.

- Large peaks: Hits for which the ratio of reference peak area and reference peak uncertainty is larger than 10.
- Peaks with high reference uncertainty: Peaks where the reference uncertainty is significantly due to uncertainty in literature yield data.

Ratio to multiply all measured peak areas with: 1.0839 +/- 1.483 %

'TRUE' DATA AM1N.REF				ANALYSIS RESULTS AM1N.OPC				
E		A		E		A		Z-scores
val	unc	val	unc	val	unc	val	unc	rep ref
5181.0	0.1	120.3	11.0	5190.5	4.9	128.8	18.9	0.4 0.5
5233.5	0.1	1159.7	34.1	5243.8	1.7	987.6	49.1	-2.9 -3.6
5275.4	0.1	9616.5	98.1	5284.5	0.5	9433.5	180.4	-0.9 -1.3
5322.0	0.1	15.2	3.9	5331.2	7.0	87.0	16.3	4.3 13.2
5350.0	0.1	17.5	4.2	5350.0	0.1	0.0	4.6	-2.9
5388.0	0.1	226.1	15.0	5388.0	0.1	0.0	16.3	-10.7
5417.0	0.1	1.4	1.2	5417.0	0.1	0.0	1.3	-0.8
5442.9	0.1	1794.7	42.4	5449.3	0.8	1588.4	41.1	-3.5 -3.4
5469.0	0.1	5.5	2.3	5469.0	0.1	0.0	2.5	-1.7
5485.6	0.1	11508.0	107.3	5490.4	0.4	11685.0	213.1	0.7 1.2
5512.0	0.1	31.5	5.6	5526.1	5.3	302.3	42.3	6.4 34.2
5544.3	0.1	49.3	7.0	5544.3	0.1	0.0	7.6	-5.0

Fig. 1. Table of statistical results, showing e.g. a hit at 5275.4 keV and a miss at 5388 keV.

- Small peaks: Hits for which the ratio of peak area and uncertainty was less than 10.
- Any hit: All peaks belonging to the previous three categories.
- Misses
- False hits
- Total: All previous categories.

For the three "hit" categories, two χ_r^2-values were computed: one based on z_{rep} values denoted X1, and one based on z_{ref} values denoted X2.

3. Results

In Table 2, the comparison of nuclear data libraries with respect to ^{226}Ra and progeny as supplied with the programs is shown (For AlphaVision, a more extended library is available as a separate product from Ortec).

In Figs. 2 and 3, the results for the natural uranium doublet ratios are presented. The results of the statistical test, if relevant to the discussion, are presented in Figs. 4–7. The complete set of results is

Table 2
Comparison of nuclide libraries as supplied with the programs

	Alps	Genie 2000	Winner Alpha	Alpha Vision
^{226}*RA*	*1600 Y*	*1600 Y*	*1600 Y*	
	4784.5 9.445E + 01	4784.2 (0.6) 94.45 (0.05)	4784.400 94.450 (0.05)	
	4601.9 5.550E + 00	4601.4 (0.6) 5.55 (0.05)	4601.700 5.550 (0.90)	
	4340.0 6.500E-03			
	4191.0 1.000E-03			
	4160.0 2.700E-04			
RN-222	*3.823 D*	*1600 Y*	*1000 Y*	
	5489.5 9.992E + 01	5489.7 (0.3) 99.92 (0.01)	5489.200 99.920 (0.01)	
	4987.0 7.800E-02			
	4827.0 5.000E-04			
PO-218	*3.110 M*	*1600 Y*	*1000 Y*	*0.0021 Y*
	6002.4 9.996E + 01	6002.55 (0.09) 99.98 (0.002)	6002.400 99.979 (0.00)	6000.00 100
	5181.0 1.100E-03			
PO-214	*1.643E-4 S*	*1600 Y*	*1000 Y*	*0.0133 Y*
	7686.9 9.999E + 01	7686.9 (0.06) 99.9895	7686.600 99.986 (0.00)	7690.00 100
	6905.0 1.000E-02	(0.0006)		
	6610.0 5.000E-05			
PO-210	*138.38 D*	*138.38 D*	*1000 Y*	*138.38 D*
	5304.4 1.000E + 02	5304.38 (0.12) 100.00 (0.00)	5304.400 100.00 (0.00)	5304.38 100
	4524.0 1.000E-03			
PB-210				
BI-214	*19.90 M*			
	5448.0 1.132E-02			
	5512.0 8.232E-03			
	5268.0 1.218E-03			
	5184.0 1.281E-04			
	4941.0 5.250E-05			
	5023.0 4.410E-05			
BI-210	*5.013 D*			
	4649.0 7.92E-05			
	4686.0 5.28E-05			

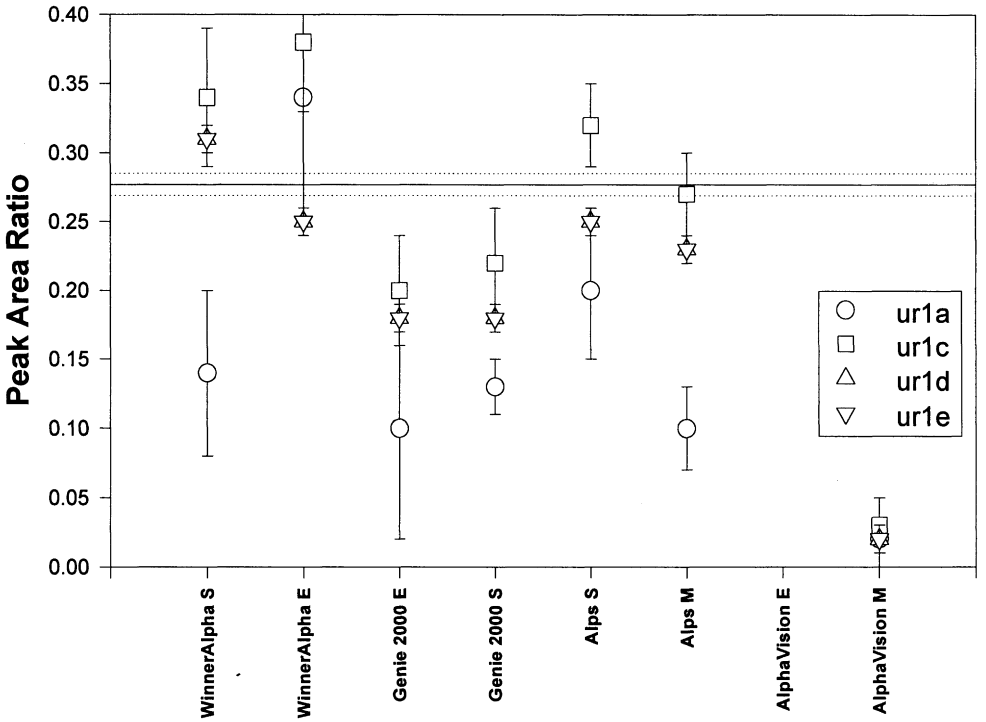

Fig. 2. Doublet ratios as found for the 4722/4775 keV doublet of ^{234}U. The horizontal line represents the target value of 0.277 ± 0.008. AlphaVision as operated by user "E" did not report the peak areas needed to compute the ratio form.

being published in an IAEA Technical Document on this intercomparison.

4. Discussion

The complete results provide a wealth of information for intercomparison purposes. In this section, only a few of the results will be presented and discussed in order to show the most important characteristics of the analysis results.

All results in this section are labeled with the first initial of the user who obtained the results.

4.1. Preliminary remarks

The tests produced a large amount of information, some of which is presented in this paper. But an accurate conclusion on the ability of the programs tested to handle a particular problem can only be drawn by the reader after defining the type of spectra and the purpose of the analysis which is to be performed. Alpha-particle spectrometry is very different from, for example, gamma-ray spectrometry. Because of the very strong asymmetry inherent to alpha peaks, the low energy tails, the relatively low energy resolution of the spectrometers and the specific emission pattern of many alpha-particle emitters, it is almost impossible to find other significant peaks from the same nuclide in a different region of the spectrum. That makes the peak deconvolution features of the programs very important, especially if chemical separation has not been performed before the measurement. A program with a good deconvolution algorithm should be preferred in this case, even if it does not find all peaks automatically, since in many cases, the peaks overlap strongly and the user must introduce the peak positions manually. On the other hand, in some applications, peak deconvolution is

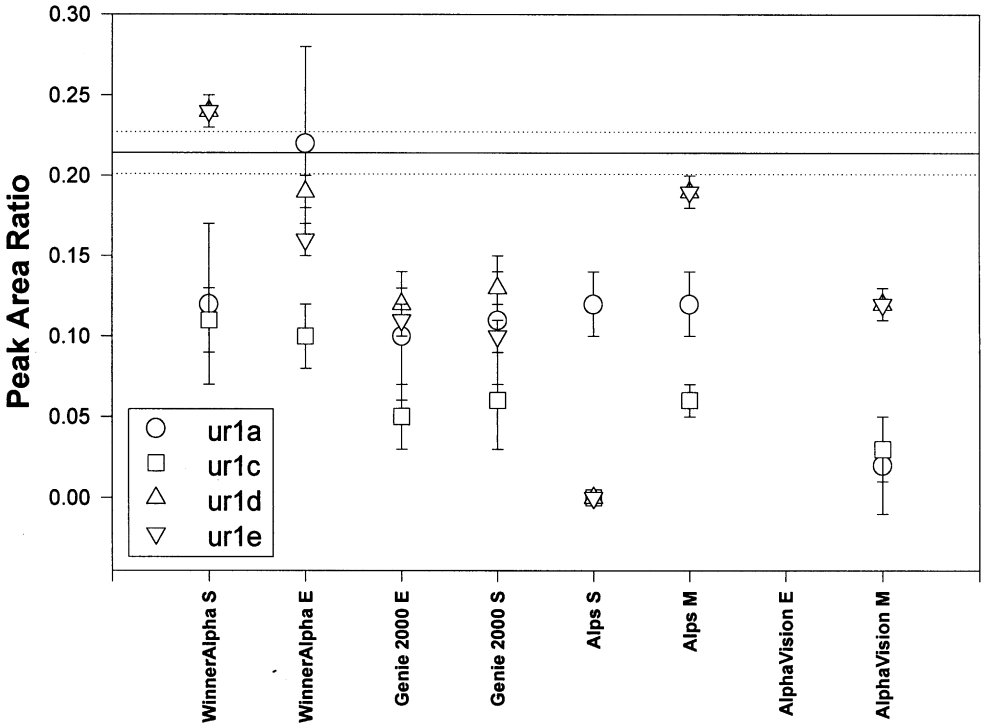

Fig. 3. Doublet ratios as found for the 4158/4918 keV doublet of ^{238}U. The horizontal line represents the target value of 0.21 ± 0.01. Missing datapoints are due to failure of the analysis programs to report the peak areas needed to compute the ratio form.

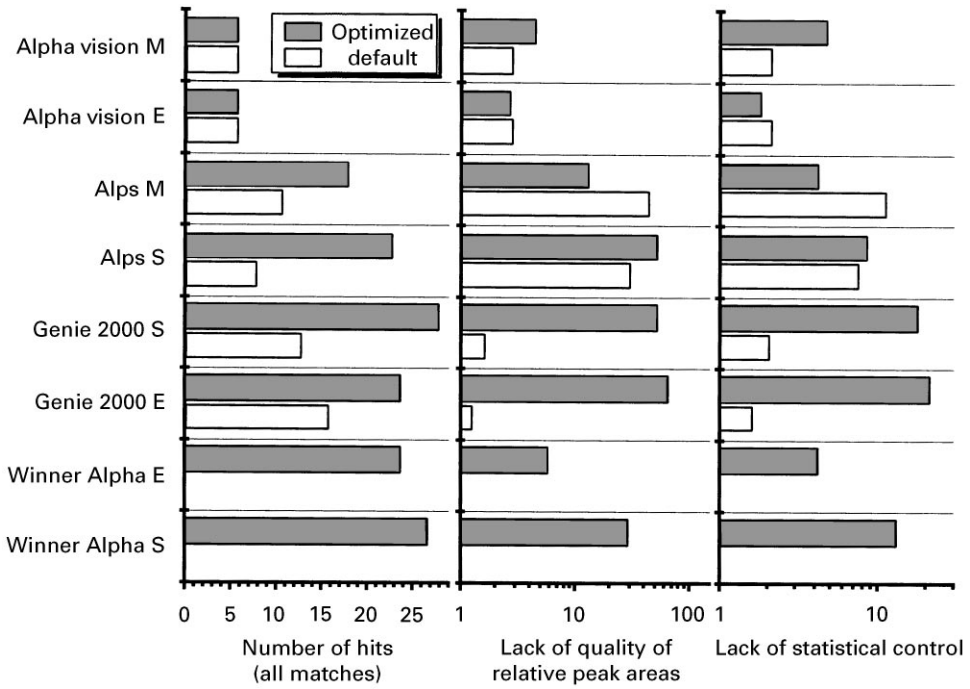

Fig. 4. All matches results for the mixed Am spectra. From left to right: number of hits, X2 and X1 values.

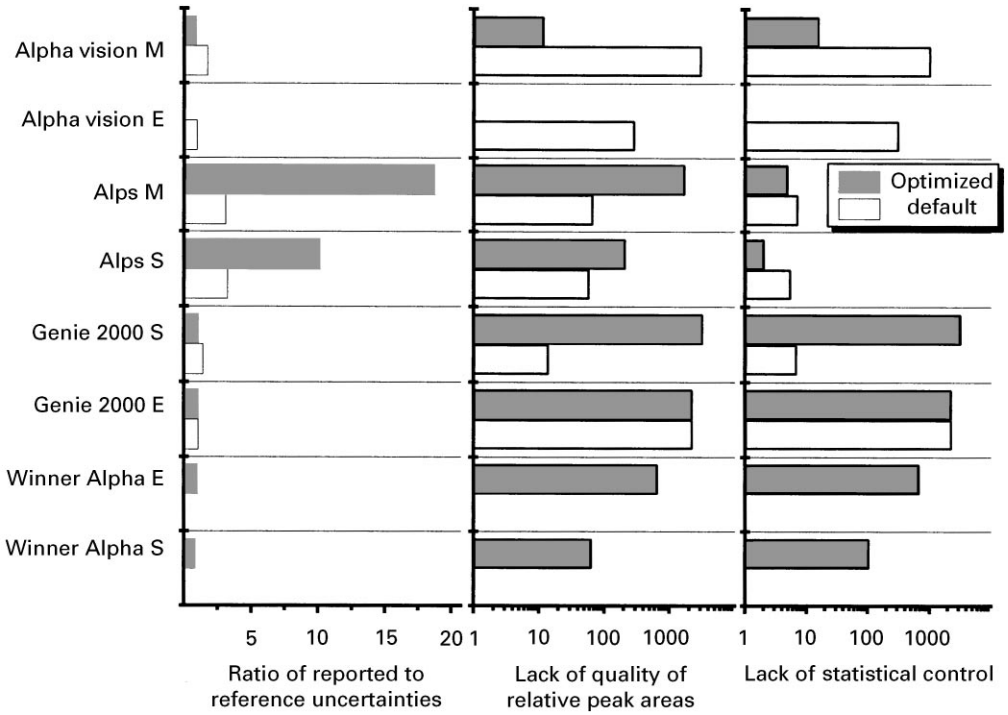

Fig. 5. All matches results for the ^{243}Am spectra. From left to right: ratio of reported to Poisson uncertainties, X2 and X1 values.

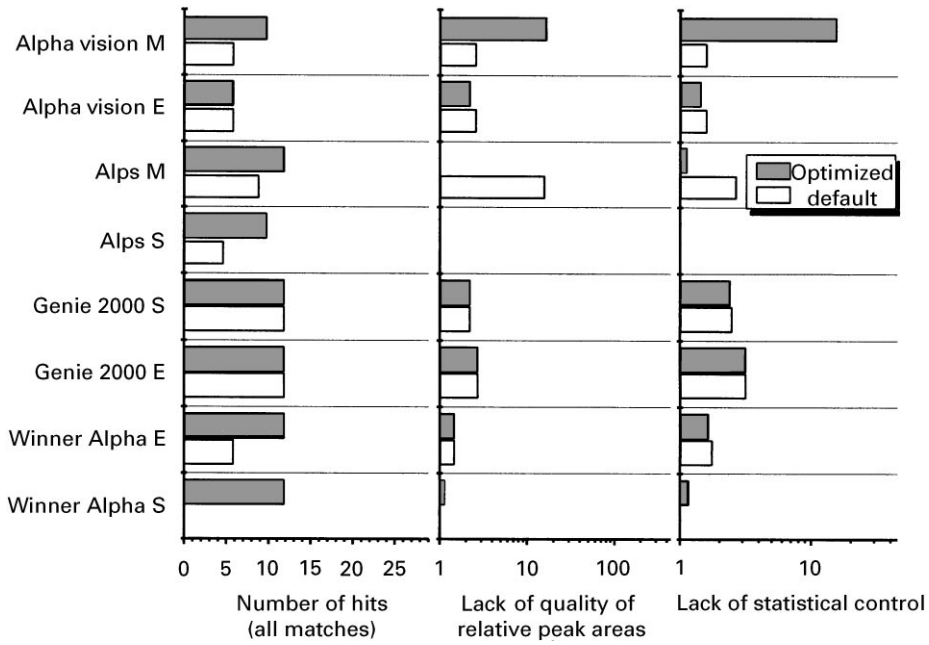

Fig. 6. Combined results for the mixed plutonium spectra: total number of hits in the "all matches" category and associated X1- and X2-values.

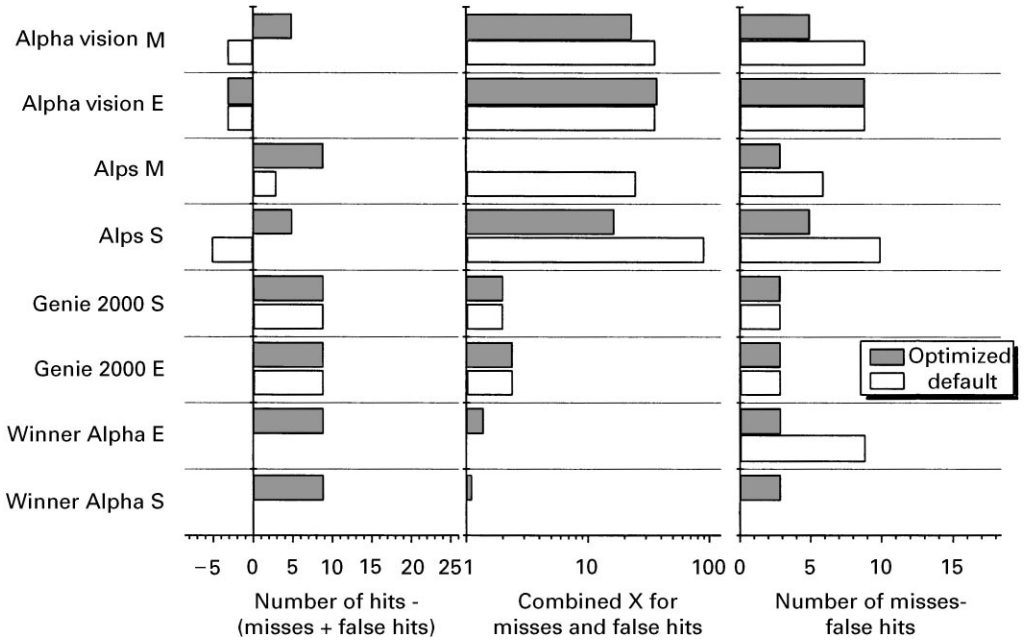

Fig. 7. Combined results for the mixed plutonium spectra: (1) The difference between number of hits and total number of misses and false hits indicating the ability to recognize true peaks, (2) *X*-values for misses and false hits indicating statistical control for deconvolution, and finally (3) the difference between number of misses and number of false hits indicating how the programs balance type 0 and type 1 errors.

not needed, as is the case in the analysis of the activity ratio $^{238}Pu/^{239+240}Pu$, where a careful tail extrapolation can provide accurate results. The best program here would be then the one which best estimates this low energy tail. Other situations exist in which the analyst is not interested in the individual peak areas, but only in the contributions of the different component nuclides. In these cases, a "nuclide- or library-oriented" analysis which includes complete information on the branching ratios and energies of the component peaks can represent a considerable advantage.

The statistical contents of the spectra also determine the choice of the optimal program. Using programs with complex line shape models and many peak parameters can be useless in spectra from environmental samples with a few counts while it is a very useful tool in the analysis of complex Pu mixtures with large peak areas. All these considerations must be taken into account to select, with the help of the data compiled in this work, the program which best adapts to the user's problem.

As was mentioned in Section 2.3 and in the paper describing the reference test spectra [1], the peak area ratios for some nuclides have been affected by significant coincidence summing between alpha particles and conversion electrons from the gamma transition depopulating the levels fed by the alpha decay. The deformations suffered by the original pulse distributions introduce additional difficulties and sources of uncertainty in the fitting of some of the spectra. This is particularly true for nuclides with high electron conversion measured with a high efficiency. However, these are conditions as found in practical laboratory work and it was decided to keep the measuring conditions as close to reality as possible.

4.2. Peak energy estimation

Only two programs reported uncertainties in the peak positions. In general, they are underestimated, and unrealistic values below 0.1 keV are reported sometimes. The problem seems to be an incomplete covariance treatment. In any case, owing to the

intrinsic non-linear behaviour of the detectors, the uncertainties in the peak positions can not be easily transformed in their equivalent energy values. The reason is that the energy loss in the detector window introduces a non-linear correction and makes it very difficult, unless a small energy region is considered.

4.3. Peak area estimation

Because of the reasons mentioned above in this paper, none of the test spectra contain singlet peaks as one would encounter in gamma-ray spectra. The separation of peaks in terms of FWHM, however, varies. To judge the capability of the programs to find peaks and determine the peak areas, the mixed Am and the ^{243}Am spectrum were used, with peak separations of about 2.5 and 5 FWHM, respectively. In the other groups of spectra, the peaks are less well separated.

The mixed Am spectra essentially consist of two groups of three peaks each. Smaller peaks are present but hardly detectable. The ^{243}Am spectrum contains one of the two groups also present in the mixed Am spectra with much better resolution and statistics, so the smaller components should be detectable. Also, in spectra with very good statistics, discrepancies between fitted and actual peak shape functions may show up as false hits with those programs that perform simple residual searches.

In this intercomparison, it was decided to test only relative peak areas within a single spectrum to allow for peak-shape model dependencies. This is essential in alpha-particle spectrometry, since contributions to the peak areas can be found in regions far from the peak maxima. However, for a single spectrum and a given analysis program, one would hope to find consistent peak areas independent of user or analysis mode. The actual renormalization factors to the known peak areas found for the AM1N spectrum are shown in Table 3. From the data, it seems that results obtained with Alps are biased depending on the mode of operation. The biases found are user-independent. It must be pointed out that this fact has no practical consequences since all peaks in the same spectrum are treated by the programs in a homogeneous manner.

The cause becomes apparent from Fig. 4. In this figure, the total numbers of hits for all three mixed Am spectra are shown. A score of six indicates two peaks found per spectrum, implying that the smaller components were overlooked or included in the total area of the triplets. Low numbers of hits correspond to low renormalization factors, resulting from the determination of total areas of triplets rather than the areas of a constituent peaks. In the case of total area determination, renormalization factors significantly smaller than unity are to be expected.

Also in Fig. 4, the quality of the relative peak area determination is shown in terms of X2-values for all matches. A perfect score of unity cannot be expected since the peaks were overlapping. From the figures, it can be seen that Genie 2000 in optimized mode finds more peaks than in default mode but at the expense of the quality of the relative peak areas, as opposed to Alps with user "M", where the quality of the results improves with the number of peaks found. From the underlying results it was concluded that Genie 2000 has difficulty with the small peaks that it reports in optimized mode, not with the large ones. Alps and Winner Alpha also scored high X2 values for the small components.

Table 3
Renormalization factors and corresponding relative uncertainties in % for the AM1N spectrum

Program	Default	Optimized	User	Default	Optimized	User
AlphaVision	0.90 (2)	0.85 (2)	M	0.90 (2)	0.89 (2)	E
Alps	0.87 (2)	0.94 (1.5)	M	0.87 (2)	0.93 (1.5)	S
Genie 2000	0.97 (1.2)	0.97 (1.2)	E	1.01 (1.2)	0.98 (1.1)	S
Winner Alpha		0.97 (1.2)	E		0.96 (0.9)	S

The problem with the analysis of small multiplet components becomes very clear from Figs. 2 and 3. Few peak area ratios for ^{234}U and ^{238}U were determined that are in agreement with the literature values.

In Fig. 5, the number of hits for the ^{243}Am spectra has been omitted, since in some cases the programs failed to report any peak areas or crashed. However, the X2-values indicating the quality of the peak areas have been plotted, indicating comparable achievements by all programs. Only Alps reported false hits for the ^{243}Am spectra. AlphaVision in optimized mode with user M yields the best peak area quality.

4.4. Peak area uncertainty estimation (*statistical control*)

In Figs. 4 and 5, X1-values representing statistical control, i.e. the ability to produce results that agree with the known true values to within the reported uncertainties, have been plotted for the "all hits" categories for the mixed Am and ^{243}Am spectra. Alps and AlphaVision (in user M optimized mode) exhibit the best control for the ^{243}Am spectra. For the mixed Am spectra, only AlphaVision is in control but at a very low number of hits. In all other cases, control is lacking, i.e. the reported uncertainties are too small (Genie 2000 as operated by user S in optimized mode sometimes even reports uncertainties below Poisson uncertainties, e.g. for 4778 keV in the UR1A spectrum it reported 83.6 ± 2.96 as peak area where the Poisson 1 s.d. uncertainty would be 9.1). In Fig. 5, the ratio of reported to reference uncertainties for the ^{243}Am spectra also has been plotted. All results seem to indicate that a full variance analysis is not performed, or at least it does not account properly for the effect of the line shape model.

4.5. Deconvolution capability

To discuss the deconvolution capability of the programs, the mixed Pu spectra were selected, since they contain a quadruplet with 2–2.5 FWHM separations. Results of interest are the numbers of hits, X1-values reflecting on statistical control, the numbers of misses and false hits and the associated X-values (X2 for misses, X1 for hits). In Figs. 6 and 7, the relevant data are plotted.

As was also observed in the mixed Am spectra, only Alps shows improved quality of peak areas with increased number of hits due to user optimization. Genie 2000 and Winner Alpha exhibit the best deconvolution capabilities with roughly the same quality of peak areas and statistical control as Alps.

From Fig. 7, it becomes clear that the programs hardly ever report false hits, but they do miss statistically significant multiplet components. This leads to the conclusion that the thresholds are set too high in the algorithms that perform residual searches looking for components that were overlooked initially.

4.6. User influence

As can be seen in all figures, the influence of the user operating the programs is very limited. Even though the difference between "default" and "optimized" modes of operation can be large, the differences between users are minor (except for Alpha Vision, where user "M" employed libraries containing non-existing radionuclides in order to get the program to fit all peaks and user "S" did not). Since the degree of experience with particular alpha-particle spectrum analysis software of the users varied, this indicates good quality of manuals and user interfaces.

5. Conclusions

Of the four programs tested, three are more or less comparable with respect to quality of peak area determination and deconvolution power: Alps, Genie 2000, and Winner Alpha. Of these three, Genie 2000 yielded the best results by a narrow margin. Exceptional are the results for the ^{243}Am spectra, where Alps performed the best in terms of statistical control, and the library-oriented AlphaVision as optimized by user "M" yielded the best peak areas. All programs have difficulty with small peaks close to large ones.

All programs exhibit lack of statistical control, especially where the deconvolution of multiplets or analysis of spectra with very good statistics are concerned: uncertainties in reported peak areas are underestimated in most cases. The same is true for the peak energy uncertainties, if reported at all.

Generally, the programs performed the same independent of the user operating them.

As a final conclusion, it is clear from the results that there is room for improvement for the developers.

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