PROGRAM FOR THE QUANTITATIVE AND QUALITATIVE ANALYSIS OF γ-RAY SPECTRA

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INTRODUCTION

The described computing program assures the quantitative and qualitative analysis of the spectra obtained within the neutron activation analysis method. It is meant for the laboratories interested in detecting and determining the concentration of certain elements (i.e. medicine, biology, metalurgy labs).

RESULTS AND DISCUSSIONS

The program processes regular spectrum obtained from the irradiation with neutrons within test standard terms of a sample and measured by a Ge(Li) detector. We can use both a TN 17e5 multichannel analyser and a romanian MCA 79 one, both with 1e24 channels, the interface with the computer being performed by ITC.

The program has been made and implemented on the roumanian microcomputers FELIX M118 and FELIX M216 and has a modular structure which facilitates its use and debugging. The spectrum processing by the program is performed off-line, after having been memorized on a floppy disk.

After introduction, the spectrum is dumped on display, enabling selection and extension of some spectrum windows with cross-hair facilities. The next step is to determine the background parameters (the background is supposed to be a polynomial of degree 1, 2 or 3).

Further on comes the gaussian curves fitting using the least squares method applid to the equation:

$$Y(x)=ax^3+bx^2+cx+d+\sum y_i \exp(-(x-x_{oi})^2/2\sigma_i^2) \qquad (1)$$

The fitting process can be simultaneously made on maximum 1e gaussians and starts by introduction (by the user) of an initial evaluation of parameters (it may be performed either by a cross-hair or may be taken from another spectrum analysis program of smaller resolution, for example the PRAG program).

The gaussian curves fitting is iteratively made, ending either when exceeding an iteration maximum number or when the process converges. It is accompanied by the permanent dump of the initial spectrum as well as of the one calculated after each iteration. In case the process does not converge it is recovered with a reintroduction of the gaussian initial parameters. The identification of the elements is performed using a polynomial relation between energy and channel, obtained by the calibration of the device with a standard sample.

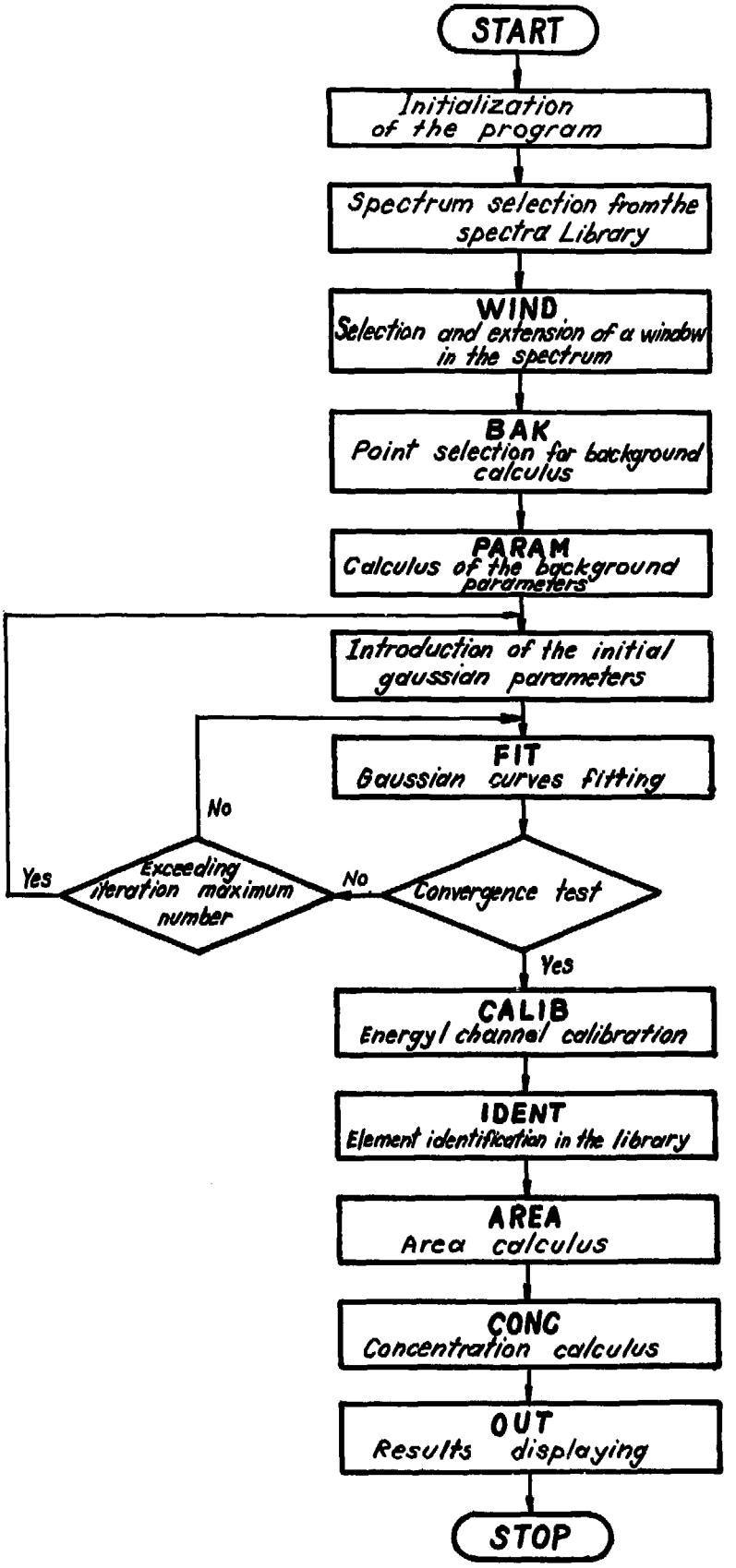
Further comes the calculus of the peak-areas (by integration) and the element identifying module, by searching in the library associated to the program.

The calculus of the elements concentration (elements pseviously identified in the sample) is made supposing that the relation betweeh them and the induced activities is known.

Finally the program puts at the user's disposal the list of the elements identified during the test, together with their concentrations, in the form of an analysis report.

REFERENCES

/1/ W.L.Zijp, Lecture notes on computerized gamma-ray spectrometry, ECN, febr.1984
/2/ V.Tepelea, E.Purice, G.Teodosiu, V.Galis, N.Mocanu, PRAG-program for antropogammametric analysis


START
Initialization of the program
Spectrum selection from the spectra Library
WIND
Selection and extension of a window in the spectrum
BAK
Point selection for background calculus
PARAM
Calculus of the background parameters
Introduction of the initial gaussian parameters
FIT
Gaussian curves fitting
Convergence test
No
Exceeding iteration maximum number
Yes
No
Yes
CALIB
Energy/channel calibration
IDENT
Element identification in the library
AREA
Area calculus
CONC
Concentration calculus
OUT
Results displaying
STOP