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ABSTRACT

A suite of three computer codes has been written to analyse the pulse height spectra from an organic scintillator neutron or gamma ray spectrometer. Data prepared by the first code are submitted to the second which unfolds the pulse height spectra. Comparison and presentation of analysed data are performed by the third code.

The spectrum unfolding process was tested by unfolding the fairly complex spectrum from the $^{9}Be(d,n)^{10}B$ reaction, which was known from other measurements. The performance of the code when unfolding monoenergetic neutron responses was comparable to the performance of codes used by other workers.

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A CODES; D CODES; U CODES; NEUTRON SPECTROMETERS; GAMMA SPECTROMETERS; ORGANIC CRYSTAL PHOSPHORS; NEUTRON SPECTRA; PULSE TECHNIQUES; PULSES

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1. INTRODUCTION

Computer codes were required for the analysis of pulse height data from an NE213 scintillator (Nuclear Enterprises Ltd, Edinburgh) for time-dependent neutron energy spectrum measurement by Whittlestone [1980a]. The problem of unfolding pulse height spectra from organic scintillators to obtain neutron energy spectra has been discussed extensively in the literature. Despite the large number of publications on the topic, the overwhelming majority of unfolding methods can be divided into two classes: the differentiation method and the FERDOR method. The former, developed by Broek and Anderson [1960], has been widely employed, for example, by Liu and Oltman [1970] and Pieroni et al. [1974]. Slaughter [1976] has adapted the method for use with microcomputers to provide on-line analysis. The simplicity and speed of calculation using the differentiation method are gained at the expense of accuracy.

There are mathematical problems associated with the differentiation process, but the main problem is the assumption that the monoenergetic neutron responses of the detector are rectangular, or can be made so by multiplication by a simple function. Many laboratories, well equipped with computers and manpower, prefer the FERDOR approach developed by Burrus and Verbinsky [1968], which attempts to solve the unfolding problem exactly by minimising the difference between the experimental pulse height spectrum and a pulse height spectrum generated by folding the trial solution energy spectrum with an accurate monoenergetic neutron response matrix. This latter method has been widely used [Simons et al. 1977; Pieroni et al. 1974; Bogart et al. 1974; Straker et al. 1971]. An improved version of FERDOR (FORIST), in which the spacing of the energy spectrum mesh can be varied along the spectrum to optimise both statistical errors and resolution, has been developed by Johnson et al. [1977].

For the present work, an unfolding code, developed by Lang [1976] for gas-filled proton recoil counters, has been adapted to unfolding spectra obtained from the NE213 scintillator.

Mechanical aspects of the three codes (AND, UNF and DPRO) used for the analysis of the experiment are explained in Sections 2-4. The first code, AND, processes monoenergetic neutron responses or experimental data into a standard form for the second code, UNF, which unfolds spectra or regenerates pulse height spectra. The UNF output is recorded on a disk data set. The

analysed data are presented by DPRO in the desired form, and generate comparisons with selected data.

It was clear that these codes should be versatile, making it easy to use different data, or carry out processing operations in various orders, according to the changing requirements during development of the experimental system. A common feature of the codes is, therefore, a structure based on free input and keyword program control using the SKAN routine of Pollard [1978]. The basic structure of the three spectrum unfolding codes comprises program segments which can be made to execute by including the appropriate keyword in the data stream. This is illustrated in Table 1. The basic functions of the program segments are presented in Tables 2, 3 and 4.

In Section 5, the development of the code UNF is outlined, and the performance of the code tested against a neutron source with a known energy spectrum. A more detailed description of the code itself is given by Lang and Whittlestone [1980]. Section 6 is concerned with the performance of UNF compared to that of other codes in unfolding monoenergetic neutron responses.

2. DATA PREPARATION FOR THE UNFOLDING CODE

The task of AND was to take all the relevant data from experiments and assemble them into the desired form for the unfolding code. The main functions of the code are summarised in Table 2. In the case of the experimental data which were to be unfolded, the processing was limited to re-forming the pulse height spectrum so that channel 1 corresponded to zero and channel 512 to the standard pulse height (in this case 3.5 $\underline{H}_e$; the unit of pulse height, $\underline{H}_e$, is the response of the detector to a 1 MeV electron*). This re-forming of the spectra saved the trouble of adjusting the amplifier gain to achieve a particular pulse height analyser calibration for every experiment. If two data blocks were repeated, measurements of the same spectrum, AND, were also used to compare them for compatibility and to add them.

Preparing the monoenergetic neutron response sets from the raw data was somewhat more involved. For a start, the efficiency was measured separately from the responses [Whittlestone 1980b]. Therefore, the response at each energy had to be scaled so that its integral above the efficiency measurement

* The $\underline{H}_e$ is identical to 'MeVe' use elsewhere [cf. Whittlestone 1980c], and accords with AAEC practice in choice of notation.

threshold equalled the efficiency at that energy. Next, in the case of responses measured by the time-of-flight technique, there was the problem of correcting for the contribution of high energy scattered neutrons to low energy neutron responses (see Appendix A).

The last function of AND, which could not be adequately covered in Table 2, was the fitting of the experimental monoenergetic neutron responses to an analytic function to make it easier to combine data from different experiments. For example, the resolution from an associated particle measurement may be more accurate than that from a time-of-flight measurement, whereas the converse could be true for the proton response. In this case, a composite response would be generated using the resolution from the former and the proton response from the latter measurement. This is discussed more fully elsewhere [Whittlestone 1980b]. The function was:

$$Y(x_i) = A.e^{T(P-x_i)} + B.e^{U(P-x_i)} + C.\mathrm{erf}\left(\frac{Q-x_i}{S}\right) \qquad (1)$$

where $Y(x_i)$ = counts in channel i,
x_i = pulse height of channel i, and
parameters A, B, C, P, Q, S, T, U give the best fit to the experimental data.

The parameters of Equation (1) were fitted to the experimental responses using an iterative conjugate gradient fitting code, VA06A [Powell 1970]. Such codes are rather temperamental, requiring some care to obtain optimum operation when fitting fairly complex functions such as Equation (1). The important features of data presentation to VA06A to ensure optimum generation were the provision of guesses very close to the final values of the parameters and the scaling of the variables in the function to make the parameters unity at the start and for each 50 or so iterations. Finding close guesses was an empirical exercise. For example, the proton response parameter, Q, was located approximately half way down the high pulse height edge of the spectrum. This provided a basis for calculating an initial value for Q. Similar rules were found to permit AND to calculate guesses for the other parameters. A flow chart of the fitting procedure is given in Figure 1.

3. THE UNFOLDING CODE

The main program, UNF, is the means by which experimental data and the wishes of the experimenter are conveyed to the large array of subroutines controlled by subroutine UNFSWX [Lang and Whittlestone 1980]. Basic operations of UNF are summarised in Table 3. Development and testing of UNF is discussed in Sections 5 and 6.

In preparation for the unfolding process, a data file is set up containing the monoenergetic neutron response set and response sets obtained by smoothing the original set in various ways. An energy mesh and the type of smoothing, if any, are selected and a response matrix generated by interpolation, one response for each energy of the neutron energy mesh. After this, all that remains is to specify how many iterations are required.

A useful feature of UNF is that it can be used to generate a pulse height spectrum from a given energy spectrum. Whittlestone [1980b] demonstrated the value of this by checking that a given set of monoenergetic neutron responses was consistent with a pulse height spectrum measured using a known energy spectrum. Another use for this feature is the generation of test data. If the pulse height spectrum of a single energy, or a pair of energies, is generated using the response matrix, then it is known that there is a solution to the problem of unfolding that pulse height spectrum. With this facility, it was possible to check the self-consistency of the unfolding process. Two such tests are discussed in Section 6.

4. THE CODE FOR DATA PRESENTATION AND COMPARISON

The code for data presentation and comparison, DPRO, is a relatively small, fast code using only a few seconds of computer time. As may be gathered from Table 4, processed data from UNF can be written, plotted or compared with previous UNF runs in numerous ways. It is possible, therefore, to evaluate quickly any improvements during the development of the unfolding code, or to assess different ways of presenting analysed energy spectra or spectra calculated by a Monte Carlo code [Rainbow and Whittlestone 1980].

5. DEVELOPMENT OF UNF

The first stage of analysis of pulse height spectra is to establish a monoenergetic neutron response matrix with a mesh appropriate to the problem. In the present case, the basic responses had been measured directly, but were far too widely spaced, hence an interpolation routine was written. As a test, a response to 4 MeV neutrons was calculated by interpolation of measurements at 3 and 5 MeV. The result was in excellent agreement with a measured response at 4 MeV.

In an attempt to ameliorate the possible effects of statistical errors when raw experimental responses were used, various types of smoothing were applied before interpolation. On testing with the unfolding part of the code, the smoothing proved to be of little benefit. It appeared that statistical errors in the input data had the effect of damping out from the solution oscillations which tended to arise in the unfolding process. These oscillations are discussed in more detail by Lang and Whittlestone [1980].

The major part of the analysis was, of course, the unfolding. Development of the code proceeded until it achieved a satisfactory performance on a test problem, which was to unfold the pulse height spectrum from neutrons obtained from a thick beryllium target bombarded by 2.3 MeV deuterons at 0° to the deuteron beam axis. In Figure 2(a), the unfolded neutron energy spectrum is compared to the spectrum measured using time-of-flight techniques. A second means of assessing the code performance was to reconstruct a pulse height spectrum by folding the neutron energy spectrum produced by UNF with the monoenergetic neutron response set. The difference between the reconstructed and original pulse height spectra for each pulse height channel was divided by the error, producing what will be called 'point χ values'; these are shown in Figure 2(b).

There are two main points to be noted. The first is that the code had difficulty in handling steps such as that at 1.4 MeV, but the solution averaged over larger energy intervals (say 0.5 to 1 MeV) is quite good. Secondly, the point χ values provided a guide as to whether the value of the spectrum in any range could be trusted. From knowledge of the monoenergetic neutron responses in terms of electron responses, one could tell, for example, that the solution at 1.4 MeV would be suspect because of the oscillation in the point χ values at a pulse height of 0.4 $\underline{H}_e$. On the other hand, it could also be claimed that the energy spectrum average over the range 1 to 1.6 MeV

would be accurate because the average value of the point x values from the pulse height spectra was small over the range 0.25 to 0.52 $\underline{H}_e$. The basis of this claim lies not so much in mathematical rigour as in experience from testing the monoenergetic response set [Whittlestone 1980b].

6. COMPARISON OF UNF WITH OTHER CODES

There are two acid tests of an unfolding code which are independent of experimental data and only slightly dependent on the particular response matrix. The first is to unfold a monoenergetic response, and the second to unfold a pair of responses separated in energy by a small amount. The first test has been applied to TRADI, which uses the differentiation method [Pieroni et al. 1974], FERDOR [Burrus and Verbinsky 1968] and UNF. Typical results are shown in Figure 3 in which the unit of resolution is indicated as a percentage of the energy (per cent FWHM). The differentiation method demonstrates the trade-off in resolution and oscillations for simplicity. The code TRADI is about 50 per cent worse than the worst of the other two on both counts. The code FERDOR achieves an excellent suppression of oscillations (amplitude 5 per cent), but at the expense of resolution (20 per cent FWHM). With oscillations of 20 per cent but resolution of 8 per cent FWHM, UNF must be considered of comparable quality to FERDOR. If more attention were paid to the tendency of UNF to over-estimate the number of neutrons at high energy, this code might perhaps emerge slightly superior in performance at this test.

The second test, to unfold the sum of two monoenergetic responses, was made on UNF and compared with a similar test reported by Beghian et al. [1965] who used the code SLOP, a predecessor of FERDOR, The results of the test are shown in Figure 4. As in the previous test, the performance of UNF, with resolution of 15 per cent FWHM average for the two peaks and oscillations of 12 per cent, was comparable with that of its competitor, with 14 per cent FWHM and oscillations of 10 per cent.

7. ACKNOWLEDGEMENTS

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J. Pollard, and Mr G.D. Trimble for their assistance with programming.

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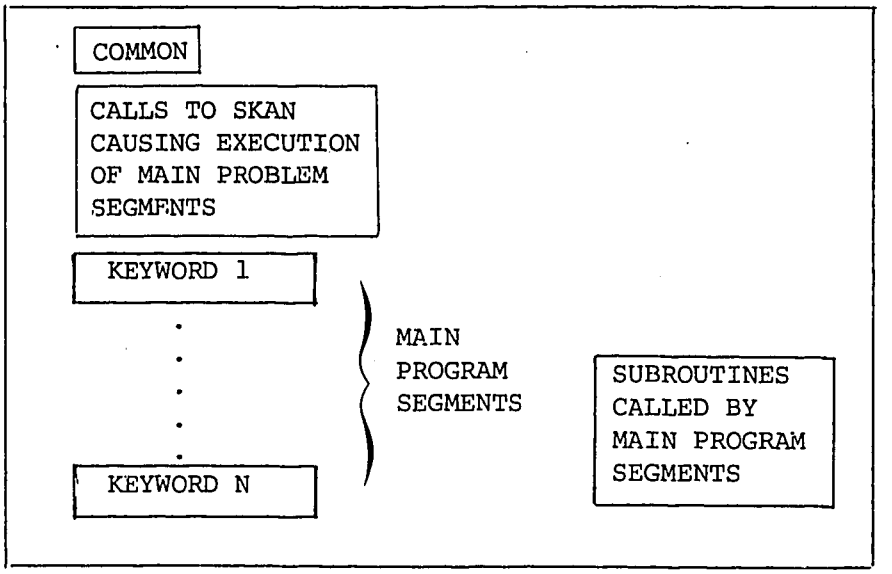
Whittlestone, S. [1980c] - Nucl. Instrum. Methods, 169:215.

TABLE 1

THE STRUCTURE OF A CODE USING THE SKAN INPUT ROUTINE

FORTRAN



Input Data Under the Control of SKAN	
Example	Explanation
$COMMON REAL*8 NAMELIST,NAME COMMON NAMELIST,NAME COMMON A,B,C,N COMMON X(100)	Variables and arrays specified for SKAN. Variables can be transferred to the FORTRAN COMMON block as shown below.
$	End $COMMON
$MOD (WRITE,NAME,2,4,6) $	Specify program control keywords. WRITE is a keyword which will cause the characters next in the data stream to be loaded into the location of the qualifying keyword NAME, which is 2 bytes, mode 4 (alphameric). The program will execute segment 6 when it encounters WRITE in the data stream.
NAMELIST TIMESPEC ENGYSPEC A 1 C 3.1 X 100*9	The variable NAMELIST is loaded with TIMESPEC and ENGYSPEC. A, C and X are loaded with 1,3.1 and 100 9's respectively.
WRITE ENGYSPEC	The program will execute segment 6 in which ENGYSPEC would be compared to the contents of NAMELIST and the desired action taken.

TABLE 2
SUMMARY OF THE FUNCTIONS OF PROGRAM SEGMENTS OF THE CODE AND

Keyword	Program Segment	Subroutines Called	Function
READ	1	READO	Read raw data.
NORM	2	EFFCAL EFINT SPINE	Read standard data file and match raw data spectrum so that channel 1=0, and channel 512=standard pulse height (MeVe). Normalise response to make the sum above the standard threshold equal to the detector efficiency at the given neutron energy. Store adjusted data in standard data file maintaining increasing order of neutron energy for monoenergetic neutron responses or increasing time for experimental data.
SETUP	3		Initialise standard data set
PLOT	4	XYPLOT [Trimble 1978]	Plot data blocks specified by IB(J) array from standard data file.
PRINT	5		Print data specified as above.
DELETE	6		Delete block IB(1) from file.
ADD	7	ADDO	Add experimental data or average responses from standard data file blocks IB(1) and IB(1)+1 and then delete block IB(1)+1.
READEX	8	REX	Read raw data. (Format different from that for READ).
DUMP	9991		Print variables named after DUMP until ENDUMP is encountered.
BACKSUB	10	BACHUS	Subtract from raw data the background estimated by matching counts above NLB for a selected higher energy data block.
FIT	11	PFIT etc.	Fit data on each of standard response file blocks IB(J) to function defined in PFIT and generate a response. Update the generated response file. An option was included to permit generating responses from parameters supplied on cards. A separate flow chart is provided for the fitting procedure.

TABLE 3
SUMMARY OF THE FUNCTIONS OF PROGRAM SEGMENTS OF THE CODE UNF

Keyword	Program Segment	Qualifying Keyword	Function
NEWMAT OLDMAT	1 2	UNSMU LINSMU LOGSMU MONLOG MONSMU	Select type of smoothing to be applied to directly measured monoenergetic neutron response functions and replace response matrix, if necessary.
RESTART	3		Continue unfolding from point where analysis stopped for another NITER iteration.
STORE	4		Put analysed data onto disc file.
WRITE	5	DATA SOL	Print pulse height or energy spectra.
PLOT	6	DATA SOL	Plot pulse height or energy spectra.
UNFOLD	7		Unfold data for NITER iterations, generate pulse height spectrum from given energy spectrum, or generate monoenergetic response at given energy, according to the parameter NCODE.
HILOAD	10		Load high energy spectrum to permit unfolding low energy spectrum in the presence of high energy flux.

TABLE 4
SUMMARY OF THE FUNCTIONS OF PROGRAM SEGMENTS OF THE CODE DPRO

Keyword	Program Segment	Qualifying Keyword	Subroutines Called	Function
WRITE	1	SOL		Print energy spectra stored in disc file blocks, IB(J), their errors and percentage errors.
WRITE	1	SOLCOMP	SQUASH SOLCHI	As above, with energy group boundaries specified by the EBOUND array. χ^2/N values from alternate blocks produced as from NORMO.
WRITE	1	DATA		Print pulse height spectrum (SWXDAT) difference from spectrum reconstructed by UNF (RECONS) and relative error.
			NORMO	If INORM=1, minimise χ^2 from SWXDAT and RECONS between channels ICHI(2J-1) and ICHI(2J).
LINPLOT LOGPLOT	2 3	SOL	LINE	Plot energy spectra from blocks IB(J) scaled so that Y(max.)=10, or by factor FNORM for experimental data and FNORM*FCAL for calculated spectra.
		SOLR		As above with curves Y+error and Y-error.
		SOLCOMP	SQUASH	As above (SOLR); alternate curves matched to previous curve between channels IC(1) to IC(2).
		DATA	LINE NORMO	Plot experimental and reconstructed pulse height spectra from blocks IB(J). Scale so that max.SWXDAT=10, RECONS scaled to minimise χ^2/N as in WRITE DATA.
		CHI		As above, but plot (SWXDAT(J)-RECONS(J))/ERROR(J).
		DIFF		As above, but plot percentage difference.
STORE	4			Store blocks IB(J) on special data file.
ENTER SAVE	5 6			Store data from cards on disc file in standard format.

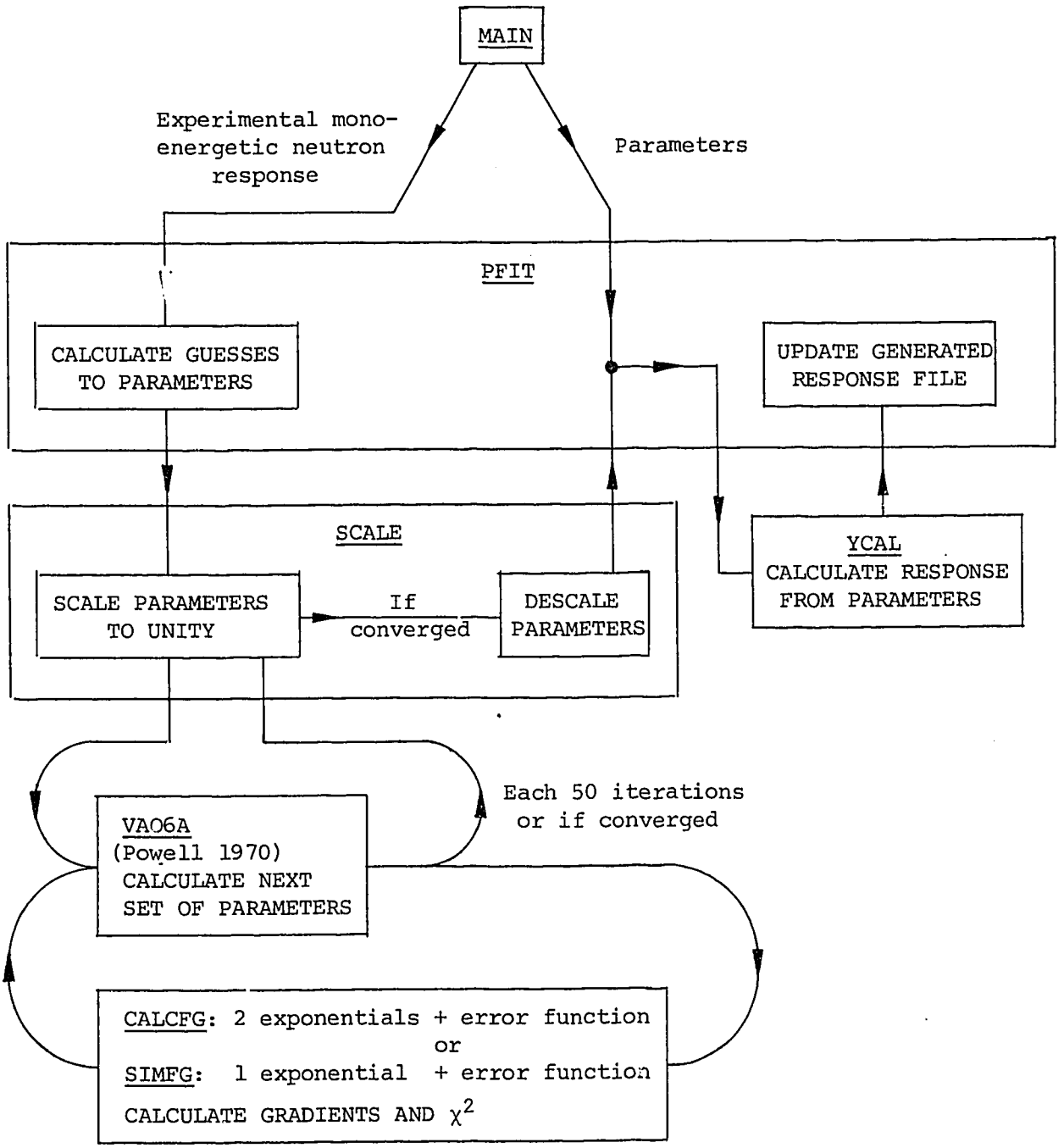
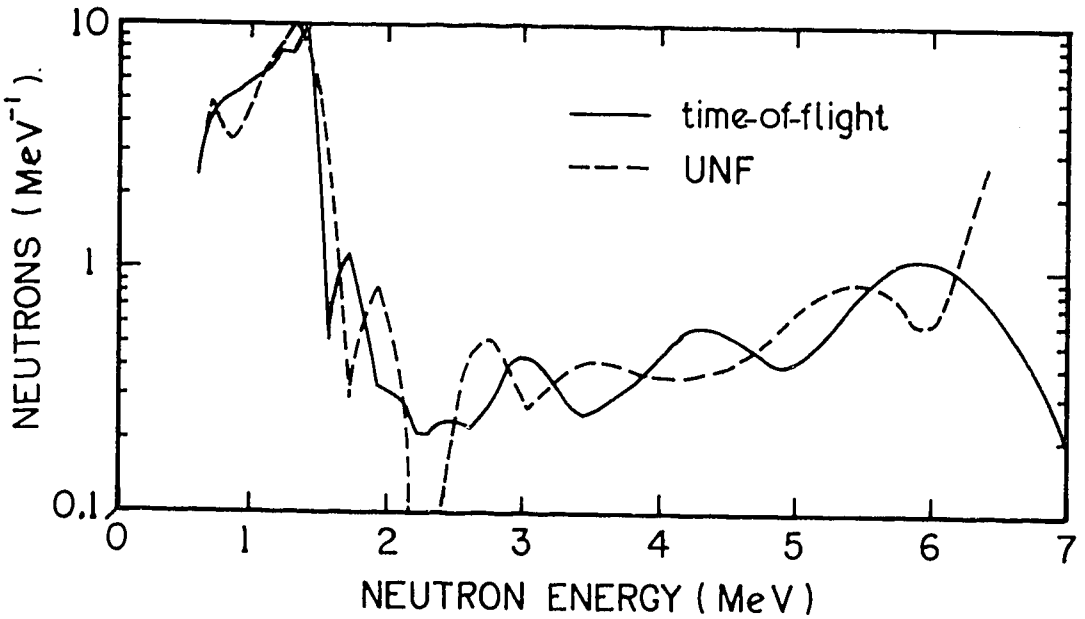
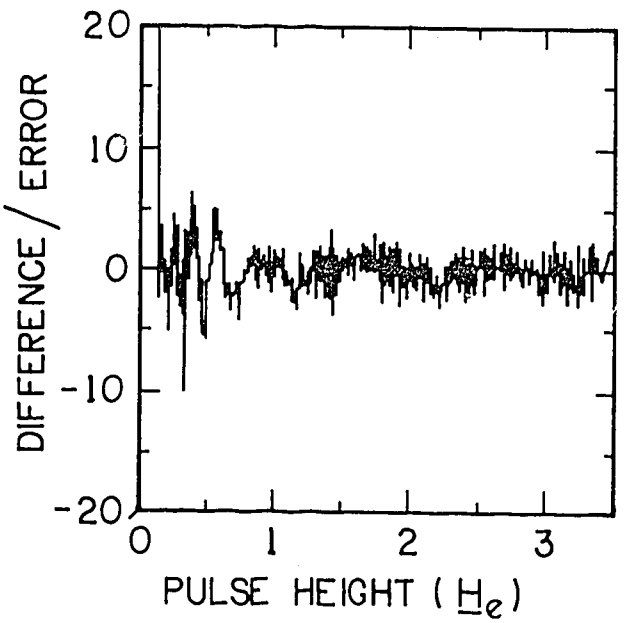


FIGURE 1. FLOW CHART OF MONOENERGETIC NEUTRON RESPONSE FITTING ROUTINE



(a) Be (d,n) SPECTRUM MEASURED BY TIME-OF-FLIGHT AND UNFOLDED USING UNF



(b) COMPARISON OF ORIGINAL AND RECONSTRUCTED PULSE HEIGHT SPECTRA

FIGURE 2. PERFORMANCE OF UNF

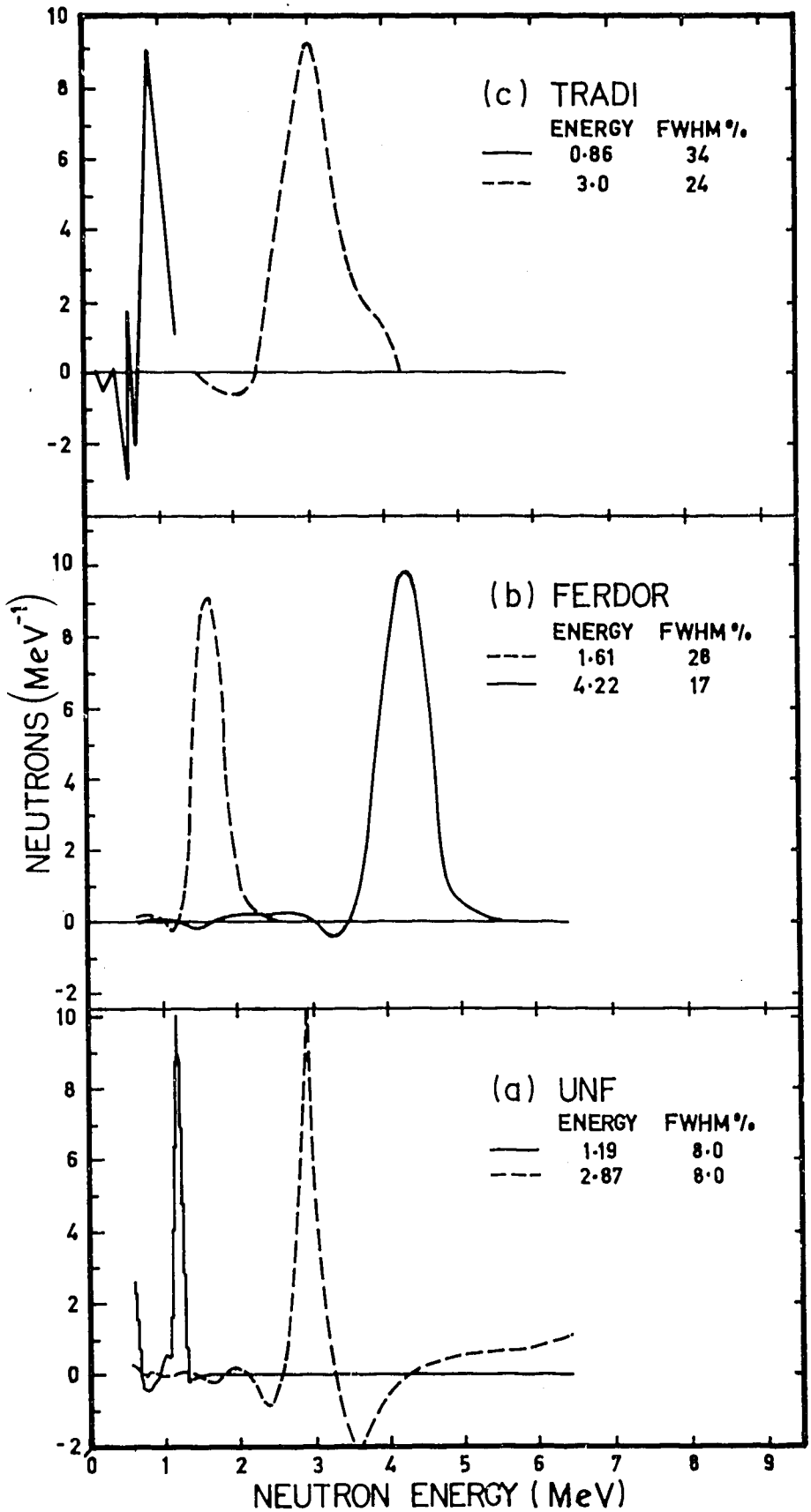


FIGURE 3. UNFOLDING MONOENERGETIC NEUTRON RESPONSES WITH DIFFERENT CODES

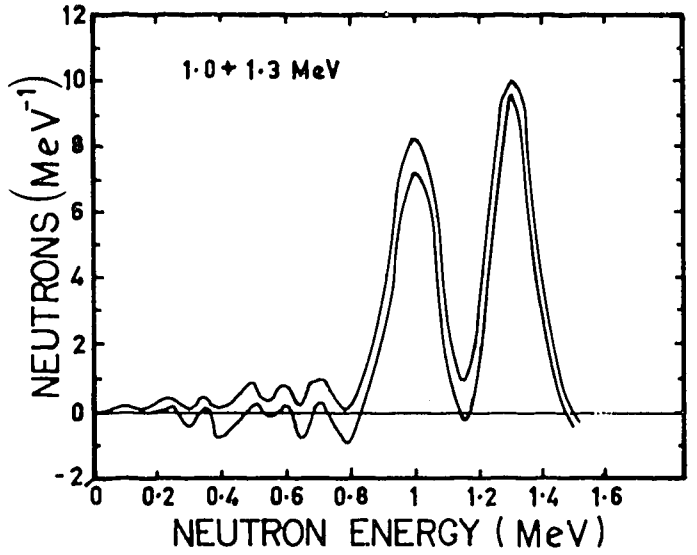


FIGURE 4. UNFOLDING THE SUM OF TWO MONOENERGETIC NEUTRON RESPONSES

APPENDIX A
MEASUREMENT OF MONOENERGETIC NEUTRON RESPONSES BY TIME-OF-FLIGHT

The monoenergetic neutron responses were measured using an elevated target facility, described in detail elsewhere [Whittlestone 1977]. The accelerator beam was pulsed and the neutron energies determined by measuring the flight time of the neutrons from the target to the detector. By analysing the pulse heights of neutron counts in a narrow range of times (a time window) after the beam pulse, a monoenergetic neutron response was obtained. The main parameters of the measurement were:

Target material:	lithium (thick)
Beam particles:	deuterons
Pulse width	3 ns FWHM
Flight path:	1.90 m
Time windows:	width 3 ns
	energy range covered: 0.535 to 6.44 MeV

The neutron source was lithium bombarded by deuterons, chosen because the neutron output from the $^{7}Li(d,n)^{8}Be$ reaction is high and the energy spectrum smooth over the range of interest. Responses of monoenergetic neutrons with energies between 0.535 and 6.44 MeV could be obtained by accumulating pulse height spectra simultaneously from several time windows.

The resolution of the measurement was limited mainly by the 3 ns minimum pulse width from the accelerator and by the choice of flight path, which was a compromise between count rate and resolution. Although the measurements could have been made with double the flight path to improve the resolution, the resultant quadrupling of the count time and increase of scattered neutron background at the low energies were unacceptable.

A second compromise on resolution versus count rate involved selection of the time window width at 3 ns, equal to the width of the beam pulse. It was considered that a reduction in resolution from about 4.2 to 3.4 ns was not worth the sacrifice of a factor of 2 in count rate obtained by reducing the window width to 1.5 ns.

Background from scattered neutrons, although smaller than that for the elevated target station, was clearly evident in the low energy responses. It was possible to evaluate and correct for this background. From experiments using the elevated target station [Whittlestone 1977], it was known that the scattered component at any particular time had a fairly narrow energy distribution, centred on an energy substantially higher than the energy defined by the time window of interest for neutrons coming directly from the target. The pulse height distribution of the scattered component at each time was therefore known quite accurately from the higher energy responses obtained at earlier times. By matching the higher pulse height part of the response to the known higher energy response, it was possible to form an accurate estimate of the contribution to low energy responses from scattered higher energy neutrons (Figure A1). This contribution could then be subtracted.

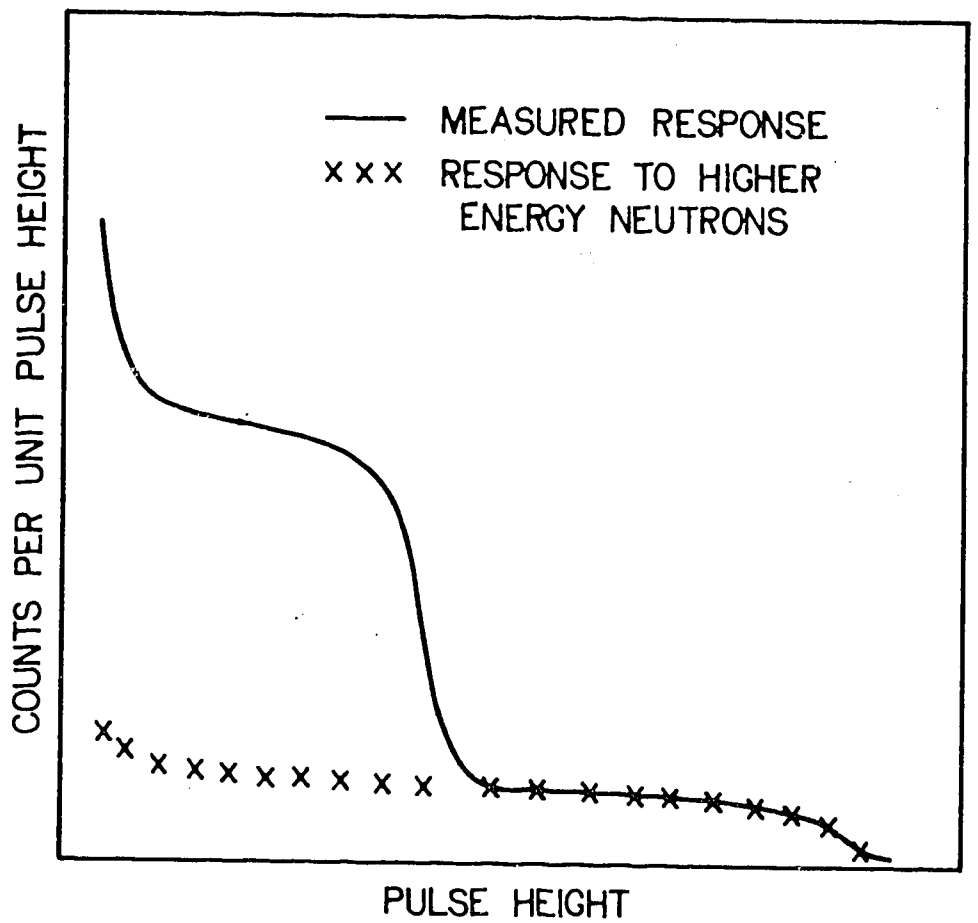


FIGURE A1. ILLUSTRATION OF BACKGROUND EVALUATION FOR MONOENERGETIC NEUTRON RESPONSES