DEFINING A METHODOLOGY FOR BENCHMARKING SPECTRUM UNFOLDING CODES

W. Meyer* W. H. Miller*
P. G. Kirmser** K. K. Hu**

ABSTRACT

Spectroscopy is a field of interest common to many areas of science but two narrow areas of this broad subject area are of particular interest and have been significantly developed through nuclear science and engineering. These are neutron and gamma-ray spectroscopy. The subject of this paper will be particularly devoted to neutron spectroscopy because of the author's particular interests and expertise but it is evident that a parallel development to that discussed here for neutron spectroscopy would be important in standardizing the results obtained in the analysis of gamma-ray spectra.

It has long been recognized that different neutron spectrum unfolding codes will produce significantly different results when unfolding the same measured data. In reviewing the results of such analyses it has been difficult to determine which result if any is the best representation of what was measured by the spectrometer detector. The subject of this paper is a proposal to develop a benchmarking procedure for spectrum unfolding codes. The objective of the procedure will be to begin to develop a methodology and a set of data with a well established and documented result that could be used to benchmark and standardize the various unfolding methods and codes.

It is further recognized that development of such a benchmark must involve a consensus of the technical community interested in neutron spectrum unfolding. During the Radiation Energy Spectra Unfolding Workshop the problem will be outlined, suggestions for benchmarks offered and a working group established to develop a consensus on a benchmarking procedure.

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* University of Missouri-Columbia
**Kansas State University

INTRODUCTION

The principle measurement techniques now being used for neutron spectrum determinations in the keV and MeV region rely on the detection of recoil protons produced through neutron interaction. The various devices used to detect the recoiling protons are organic liquid and solid scintillators, nuclear emulsions, gas filled counters, cloud chambers, and recoil telescopes. The latter two devices are not generally applicable for routine on line spectrum measurements because of low efficiency, large size and difficulty of operation. Gas filled counters with their low density detection medium are applicable in the keV energy region with little gamma-ray interference and are routinely used for measurements in this energy region. Nuclear emulsions are applicable to the MeV energy region but require great amounts of scanning time to measure a sufficient number of proton recoil track lengths to determine the neutron spectrum with reasonable statistics. This scanning is accomplished by individual measurement of the track lengths using a microscope. Thus nuclear emulsion techniques are not applicable to on line measuring techniques but the analysis of the data is straightforward although laborious. Such data may well serve as a suitable benchmark for standardizing measurement systems in the MeV neutron energy region. Organic liquid or solid scintillators have good neutron detection efficiency for energies in the MeV neutron energy region and are thus widely applied to reactor and accelerator neutron spectral measurements.

For those neutron spectrometry systems with on line capability, it is not possible to measure directly the energy spectrum of neutrons incident on the detector. The experimental data must be analyzed or "unfolded" to obtain the neutron spectrum from the measured complex proton recoil spectrum. To accomplish this special analysis, numerous analytical unfolding techniques and computer codes have been developed

and applied. Unfortunately only very limited efforts have been made to compare and evaluate critically the many unfolding procedures, either in terms of the validity of the basic analytic procedures used or the value of the results obtained. Such a comparison and evaluation of the accuracy as well as the validity of error estimates of the various procedures is of utmost importance if the experimental results of a neutron reflection or transmission experiment are to be used to infer nuclear cross section values or if the measured data are to be used to evaluate a transport model.

The experimental neutron spectrum results contain two components. These components are (1) the measurement of the proton recoil spectrum and (2) the unfolding of this measurement to obtain the neutron spectrum. The purpose of this paper is to open dialogue on the second of these two components and begin development of a methodology for standardizing or benchmarking the unfolding process. Further an initial benchmark is suggested and results obtained with that benchmark using several available unfolding procedures is demonstrated.

A BENCHMARKING METHODOLOGY

The response of a proton recoil detector to monoenergetic neutrons is not the single line one would expect in an ideal spectrometer but is instead a complex smear. Hence, when this detector is exposed to a polyenergetic neutron source, the complex pulse height distribution measured with a multichannel analyzer must be unfolded to obtain the energy spectrum of the incident neutrons. Various methods, as discussed below, have been used to unfold complex neutron energy spectra from the various proton recoil devices.

The expected monoenergetic neutron energy response to systems consisting entirely of carbon and/or hydrogen would be a simple rectangle if it is assumed that the only interaction is single scattering from hydrogen nuclei and that the response of the system is linear. Actually, however, this single hydrogen scattering is not the only factor contributing to the monoenergetic response and therefore the observed responses for monoenergetic neutrons are not square pulses at the high energy end but are instead slightly peaked and rounded pulses. Further deviation from the rectangular shape is caused by various nonlinear responses, detector edge effects, inelastic scattering by carbon nuclei, multiple scattering from hydrogen and carbon nuclei, smearing due to electronic noise, etc. To complicate further the distortion problem, the magnitude of the monoenergetic response distortion is an energy dependent phenomena. This follows since the neutron elastic and inelastic cross sections vary with energy, e.g., considering neutron energies above 10 MeV, the cross sections for the reactions C^{12} $(n,\alpha)Be^{9}$ and $C^{12}(n,n')3\alpha$ are large enough that they increase the low energy part of the neutron spectrum relative to the high energy part. Finally, a high gamma ray background will cause spectrum distortion due to "piled-up" gamma-rays acting like neutron induced electronic pulses.

To unfold the complex detector response to polyenergetic fast-neutrons, it is assumed by some writers of unfolding codes to be necessary to take into account all of the above distortion phenomena. If it can be assumed that the distortion effects are of minor importance, the complex response for a monoenergetic neutron can be approximated by an arithmetic procedure and this is the basis on which several of the available codes operate (see for example the work of Coolbough[1] and Toms[2]). Other codes, STUNFO[3], treat the interaction between the neutron and the detector including all distortion effects as a stochastic process

and apply Fourier analysis to obtain the unfolded neutron spectrum. However still other codes attempt to make the calculated response truly representative of the instrument response by smearing a measured response for the monoenergetic neutron in question. Knowledge gained by calculating and smearing a few responses allows smearing of a library of calculated responses without recourse to further experimental data.

Responses of both 2 x 2 and 5 x 5 inch NE-213 detectors to monoenergetic neutrons were obtained at Oak Ridge using Monte Carlo calculations and the smearing technique.[4] These calculated responses, after being smeared, accounted for the above-mentioned distortion effects (except for gamma ray interferences) and are incorporated in the FERDOR[5] unfolding code.

If a truly monoenergetic neutron source were available it would be possible of course to measure the response functions with all of the accompanying distortions. In fact such a source is not available but can be rather closely approximated using linear accelerators and time of flight techniques to eliminate much of the gamma-ray interference. Such measurements were made at ORNL in 1966.[6] However one must be concerned with the fact that such measurements may contain systematic experimental errors and are to some degree distorted by a gamma ray background.

To form improved standards for use in unfolding codes, Kirmser et. al.[7] have smoothed the Verbinski response matrix by: (a) adjusting each monoenergetic column entry using five point least-squares parabolic smoothing weighted according to the lengths of adjacent intervals in light units; (b) determining the loci of major peaks, valleys and inflection points of the

smoothed monoenergetic curves; (c) smoothing the loci using seven point parabolic smoothing moved ahead three points at a time followed by local averaging; (d) adjusting the monoenergetic column entries by stretching abscissae locally in a manner to cause the major features of the response surface to lie on smooth curves in the energy-light unit plane; and (e) adjusting the ordinates of the smoothed monoenergetic column entries to preserve the areas under the original monoenergetic column entries. These improved responses were then used to unfold oxygen penetration data. In comparing the results obtained with the smoothed and unsmoothed matrices for the oxygen data an improvement in energy resolution was obtained without increasing the number of monoenergetic curves in the response matrix.

As a first attempt to develop an unfolding code benchmark, the Kirmser smoothed ORNL 05R response functions were used as input data to several unfolding codes. A series of unfolding codes utilizing a number of different basic formulations were used in evaluating the bench marking process.

BRIEF DESCRIPTION OF THE UNFOLDING CODES USED IN THE EVALUATION

FERDOR: The widely used FERDOR code developed by Burris[5] uses a Monte Carlo calculated response matrix for the detection system. The code is described in detail elsewhere in these Proceedings.

NEUTSP: The code NEUTSP is based on the principle that the neutron spectrum is proportional to both the neutron energy and the differential of the proton energy distribution but inversely proportional to the neutron-proton cross-section as indicated in the following relation:

$$N(E) \propto \frac{E}{\sigma_{n,p}} \frac{dP(E)}{dE}$$

where N(E) and P(E) are the neutron and recoil proton energy spectra respectively and $\sigma_{n,p}$ the neutron-proton cross section. Corrections for secondary scattering of neutrons by hydrogen and for loss of protons through the end of the detector are made. Oscillations are reduced by calculating the neutron spectrum at constant energy intervals of 0.1 MeV.[2]

DUFOLD: The DUFOLD code utilizes essentially the same principle as does NEUTSP, i.e., that the neutron spectrum is directly related to the slope of the pulse-height spectrum. Here corrections for hydrogen scattering anisotropy and for edge effects are applied. In order to reduce oscillations the derivative is taken after the recoil proton spectrum has been binned with variable energy intervals (bin widths are proportional to the detector energy resolution) and fitted to a second degree polynomial relation with a least squares scheme.[1]

STUNFO: The code STUNFO, like DUFOLD and NEUTSP, does not require a measured response matrix. The code is based on the fact that the energy spectrum of a neutron source is essentially the probability density function of the energy with which neutrons are emitted. The theory of random variability is therefore used to implement the basic unfolding method. Time series analysis and Fourier analysis is subsequently applied to obtain smooth estimates of the neutron spectrum.[3]

MINREP: This unfolding procedure developed by Kirmser et. al., is discussed in detail elsewhere in these proceedings.

INITIAL BENCHMARK EVALUATION

What results do we hope to achieve with the benchmarking procedure? The answers to this question will determine the suitability of any benchmarking methodology selected. In this

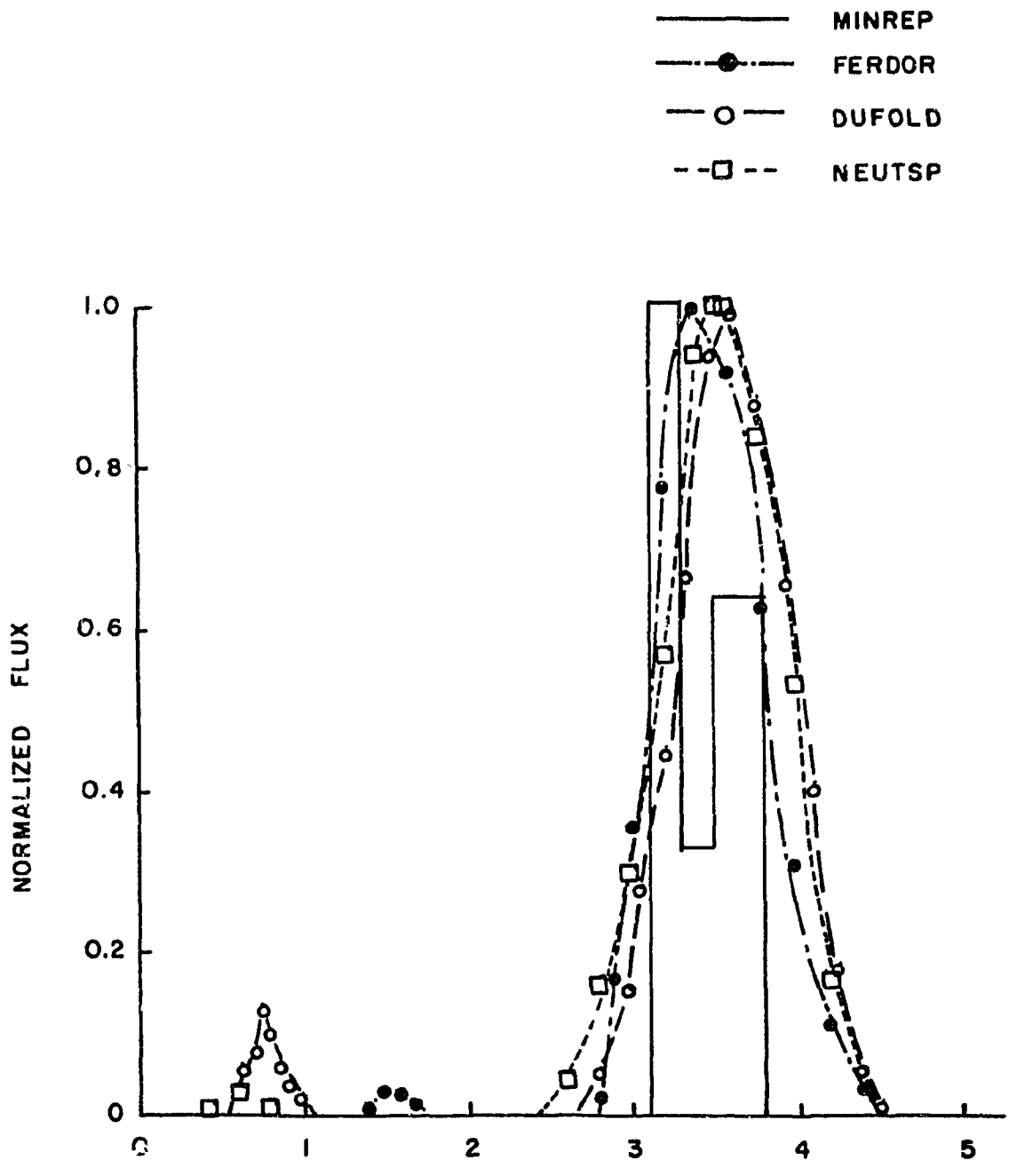
initial attempt at benchmarking, the following three determinations were sought:

1) What is the capability of the unfolding code to identify a monoenergetic benchmark?
2) What is the capability of the unfolding code to identify and separate a combination of monoenergetic benchmarks?
3) What is the capability of the unfolding code to identify the respective pulse heights of a combination of monoenergetic benchmarks?

Figures 1 and 2 present the results of two of the benchmark problems obtained with the codes FERDOR, DUFOLD and NEUTSP. Shown for comparison purposes are results obtained with MINREP (It must be noted that in this case MINREP is unfolding a portion of its own response matrix). The energy resolving and pulse height identification capabilities of the various codes are evident through comparison of Figures 1 and 2.

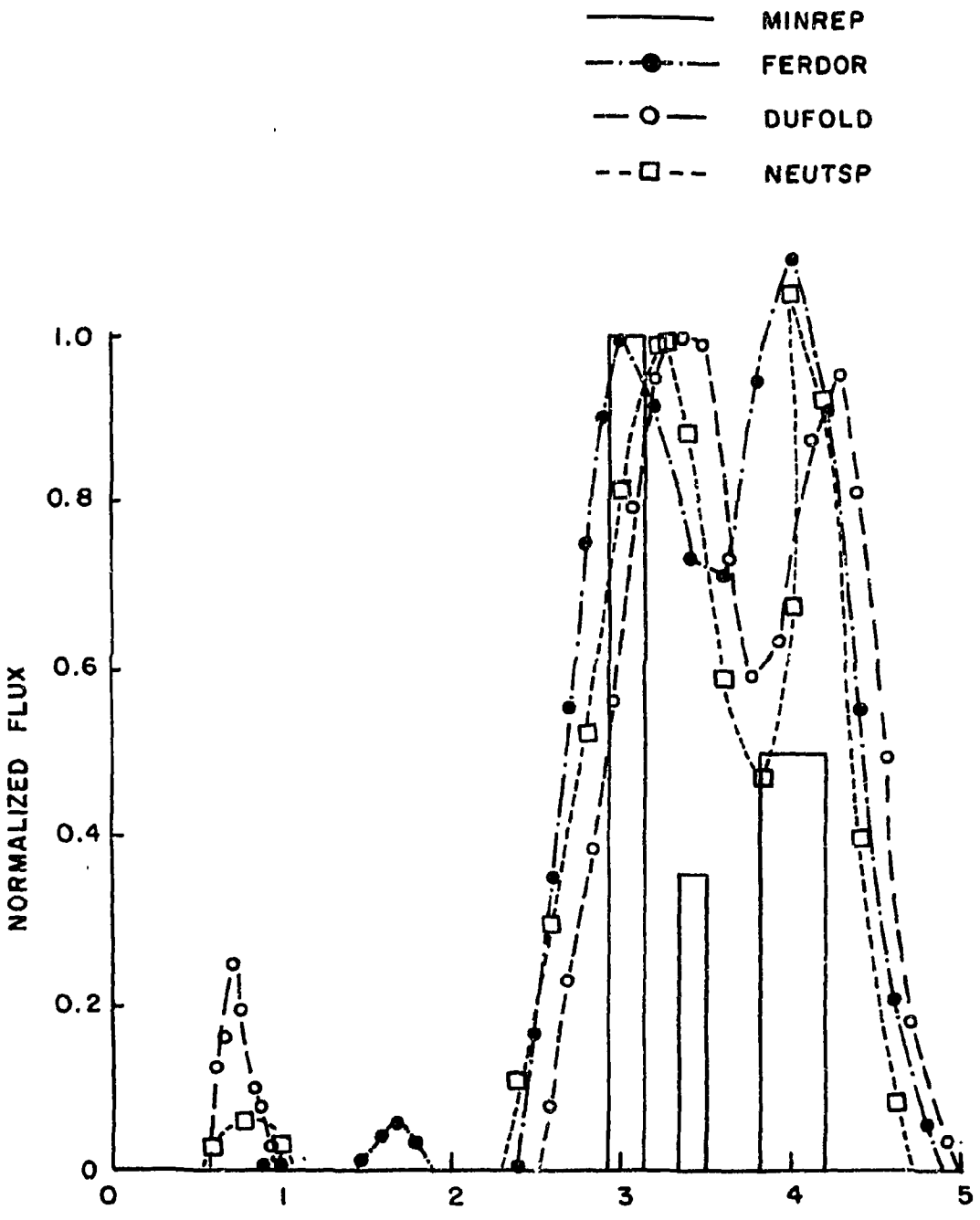
CONCLUSION

Development of an acceptable benchmarking methodology for standardizing unfolding procedures can only be achieved through a consensus of the interested technical community. An initial attempt is made here to begin to formulate the body of a benchmarking methodology applicable to neutron spectra unfolding. Clearly the total objectives of the benchmarking process remain to be derived and the adequacy of the methodology proposed here or any other methodology, will be evaluated in the light of their ability to achieve the objectives.



ENERGY	MAGNITUDE	MAGN / MeV
3.22	3	1
3.40	1	0.33
3.60	3	0.63

FIG 1 (UNFOLDING BENCHMARK* 3)



ENERGY	MAGNITUDE	MAGN/MeV
3.02	3	1
3.40	1	0.35
4.00	3	0.50

FIG 2 (UNFOLDING BENCHMARK # 5)

REFERENCES

1. M. J. Coolbaugh, R. E. Faw and W. Meyer, Fast Neutron Spectroscopy in Aqueous Media Using an NE-213 Proton Recoil Spectrometer System, USAEC Document No. COO-2049-7 (1971).

2. M. E. Toms, Nucl. Instr. Meth., 92, 61 (1971).

3. G. A. Mutone and W. Meyer, Nucl. Instr. Meth., 106, 445 (1973).

4. V. V. Verbinski, W. R. Burrus, T. A. Love, W. Zobel, N. W. Hill and R. Textor, Nucl. Instr. Meth., 65, 8 (1968).

5. W. R. Burrus, Utilization of A Priori Information in the Statistical Interpretation of Measured Distributions, Dissertation, ORNL-3742 (1964).

6. W. R. Burrus, Status of FERDOR Neutron Unscrambling with NE-213 Response Matrix, Intra Laboratory Correspondence, Oak Ridge National Laboratory, (November 2, 1967).

7. P. G. Kirmser, K. K. Hu and W. Meyer, Trans. Am. Nucl. Soc., 21, 536 (1975).