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Verification of Nuclear Cross Section

Processing Codes

by

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Summary of an Invited Paper which will be presented at the 1982 Kiamesha Lake Topical Meeting of the American Nuclear Society.

Abstract

Introduction

The International Atomic Energy Agency (IAEA) has begun a project for the intercomparison of neutron cross section processing codes in order to verify their ability to reproduce numerical results. In this report this reproducibility aspect is referred to as the "processing accuracy" of a code. This paper will discuss: the scope of this project, the most prominent areas and sources of disagreement between processing codes and the current status of this project toward improving the reliability of the output from processing codes.

The cross section processing code is merely a link between evaluated data on the one hand and transport or adjustment codes on the other hand. This fact has been used in order to simplify the verification task; specifically, the IAEA project attempts to assure that for a given input of evaluated data and physical assumptions, the output of the cross section processor is accurate. This project does not address the "evaluation accuracy" of the evaluated data (which are used as input to the processor), nor the "model accuracy" of the transport or adjustment code (which uses the output of the processor).

The objectives of this project are: (1.) to test the accuracy of processing codes, (2.) to understand and eliminate the sources of discrepancies, (3.) to arrive at the point where we have a number of cross section processing codes which can be used as "black boxes", without worry, to accurately process cross section data, for use in a variety of applications. As will be pointed out below, at the present time, we are far from the point of achieving these objectives.

Background

In 1981 a report was published (1) on a comparison (performed in 1980) between the 620 group (SAND-II structure (2)) group averaged cross sections derived from the ENDF/B-V Dosimetry Library (3) at Brookhaven and those derived at ECN Petten, Netherlands. Of the twenty-five

materials in the ENDF/B-V Dosimetry Library large differences were found in fourteen reactions. In individual reactions, in specific groups, differences were found of up to a factor of twenty (not twenty per-cent, a factor of twenty). Fig. 1 illustrates the ratio of the 620 group ^{237}Np fission cross sections calculated at Brookhaven to those calculated at Petten (1). Unfortunately this study (1) could not address the question of which of these two sets of data is correct.

In order to determine which of these two sets is correct the IAEA obtained additional multigroup data sets from a number of laboratories in the United States and Europe. Comparison of data sets generated at eight different laboratories showed general agreement and confirmed that the cross sections generated at Brookhaven were incorrect. In none of these eight sets were differences seen that were anywhere near those found in the Brookhaven/Petten comparison. However, in no case did any two of the data sets agree for all reactions in all groups to within 6%. This was a very surprising result, since generally these data sets were purported to be accurate to within a small fraction of one per-cent.

Problem Areas

The results of this comparison indicate large differences in the cross sections generated by various codes, primarily in the resolved and unresolved resonance regions. These differences will affect both the self-shielding and Doppler broadening properties of the cross sections. Similarly, recently Perez (4) has shown an inconsistency in the methods normally used to calculate group averaged cross sections in the unresolved resonance region. By calculating self-shielded cross sections in the resolved resonance region first directly from the resolved data and then by treating the data as unresolved and using the equivalent average level widths and spacings Perez found differences in excess of 30%. In addition, Perkins (5) has recently investigated the numerical stability of the methods used to generate group-to-group transfer matrices and has found that if extreme care is not used severe round-off problems can occur.

A more subtle problem area is the effect of these inconsistencies on the many relatively new applications that we are seeing which use the uncertainties quoted for the evaluated data in order either to assign confidence limits to calculational results or to improve our knowledge of spectra or cross sections (6) (e.g. unfolding procedures (7)). The results of these calculations can be very sensitive to the uncertainties assigned to the cross sections used. If the cross section processor introduces an error which is large compared to the error assigned to the evaluated data (as occurred in the comparison described herein) the results obtained using the processed cross sections and only the uncertainties assigned to the evaluated data, without folding in the errors introduced by the cross section processor, are of questionable validity.

Step by Step Verification

Attempting to eliminate this multitude of sins from processing codes in one fell swoop is too ambitious an undertaking and one that would be

almost bound to fail. Therefore the IAEA has decided to begin a step-by-step verification project in an attempt to address first the most glaring areas of disagreement, using the simplest possible test cases. Then more subtle areas of disagreement will be addressed, using progressively more complex test cases.

Following the step-by-step philosophy the area of largest disagreement that we see is in the calculation of cross sections in the resolved and unresolved regions. The simplest way to investigate this problem would be to compare the energy dependent point cross section values generated by a variety of processing codes. However, this information is not available from all processing codes. The next best, simple comparison is constant (flat-weighted), cold, unshielded cross sections using a fine group structure.

Results to Date

The experience gained in comparing 620 group cross sections generated from the ENDF/B-V Dosimetry library has led to recognizing the problems with several existing processing codes. These codes have now either been improved or abandoned. A direct result of these comparisons was the distribution by Brookhaven of a new version of the ENDF/B-V Dosimetry library in the 620 group, SAND-II structure. Fig. 2 illustrates the ratio of the 620 group ^{237}Np fission cross sections from the new version of the ENDF/B-V Dosimetry library as distributed by Brookhaven, to those calculated at Petten (7). Comparison of figs. 1 and 2 easily illustrates the improvements that have been achieved. These results indicate that we now have data which may be used as a standard for benchmark comparisons.

First Round

For the first round of comparisons the IAEA is asking all those interested in participating in this exercise to use the same evaluated data: ENDF/B-V Dosimetry Library (mod. 1), to calculate flat weighted, 0 Kelvin, unshielded cross sections using the SAND-II 620 group structure. Those who use energy-dependent cross sections (e.g. continuous energy Monte Carlo calculations) will be asked to send energy-dependent cross sections and the IAEA will convert them to multigroup form for comparison. Anyone who uses cross sections is encouraged to participate in this study.

Comparison will be simplified if the cross sections are sent in the ENDF/B format (each reaction as a section of file 3 using the histogram interpolation law) (3). However, any well documented, computer readable format is acceptable for this comparison.

The results of the comparison will be reported back to the participants. If there are any differences participants will be asked to investigate and eliminate the sources of these differences and to then re-submit their results. At the end of each round of tests the IAEA will publish the list of participants who have obtained agreement with the benchmark standard.

Subsequent rounds of testing will introduce the complications of: spectrum weighting, Doppler broadening and self-shielding. However, these complications will be introduced in a step-by-step manner so that when we see differences we can isolate the cause of the difference, which will simplify the task of remedying the problem.

Conclusions

The IAEA has begun a project which is intended to use a step-by-step approach to verifying the accuracy of cross section processing codes. Anyone who is presently using a cross section processing code is encouraged to participate in this project. To date this project has been successful in detecting and correcting problems with several cross section processing codes and in particular has directly led to improvements in the ENDF/B-V Dosimetry Library as distributed in 620 groups (3).

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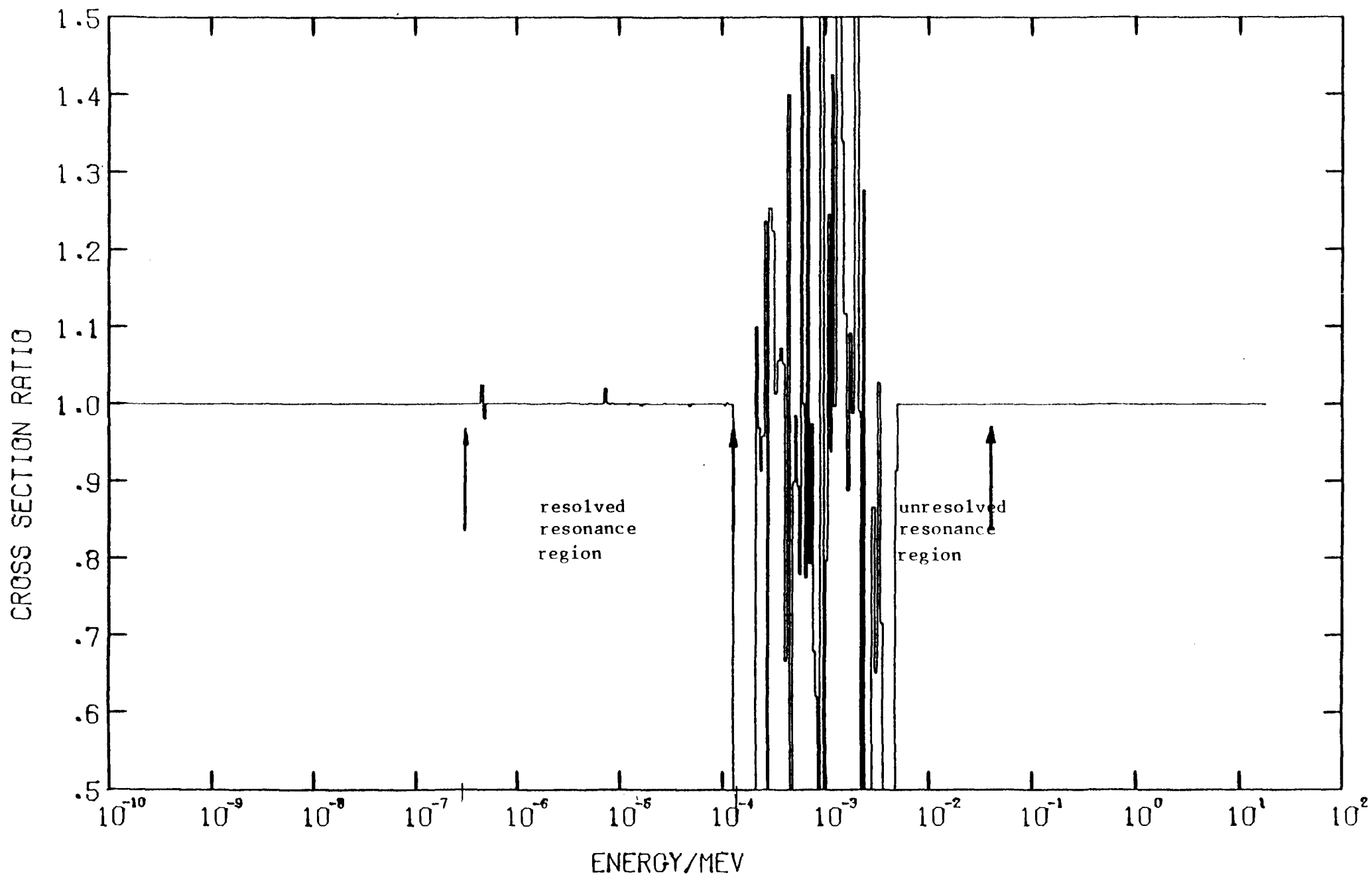


Fig. 1: CROSS SECTION RATIO FOR THE REACTION NP237(N,F)F.P.

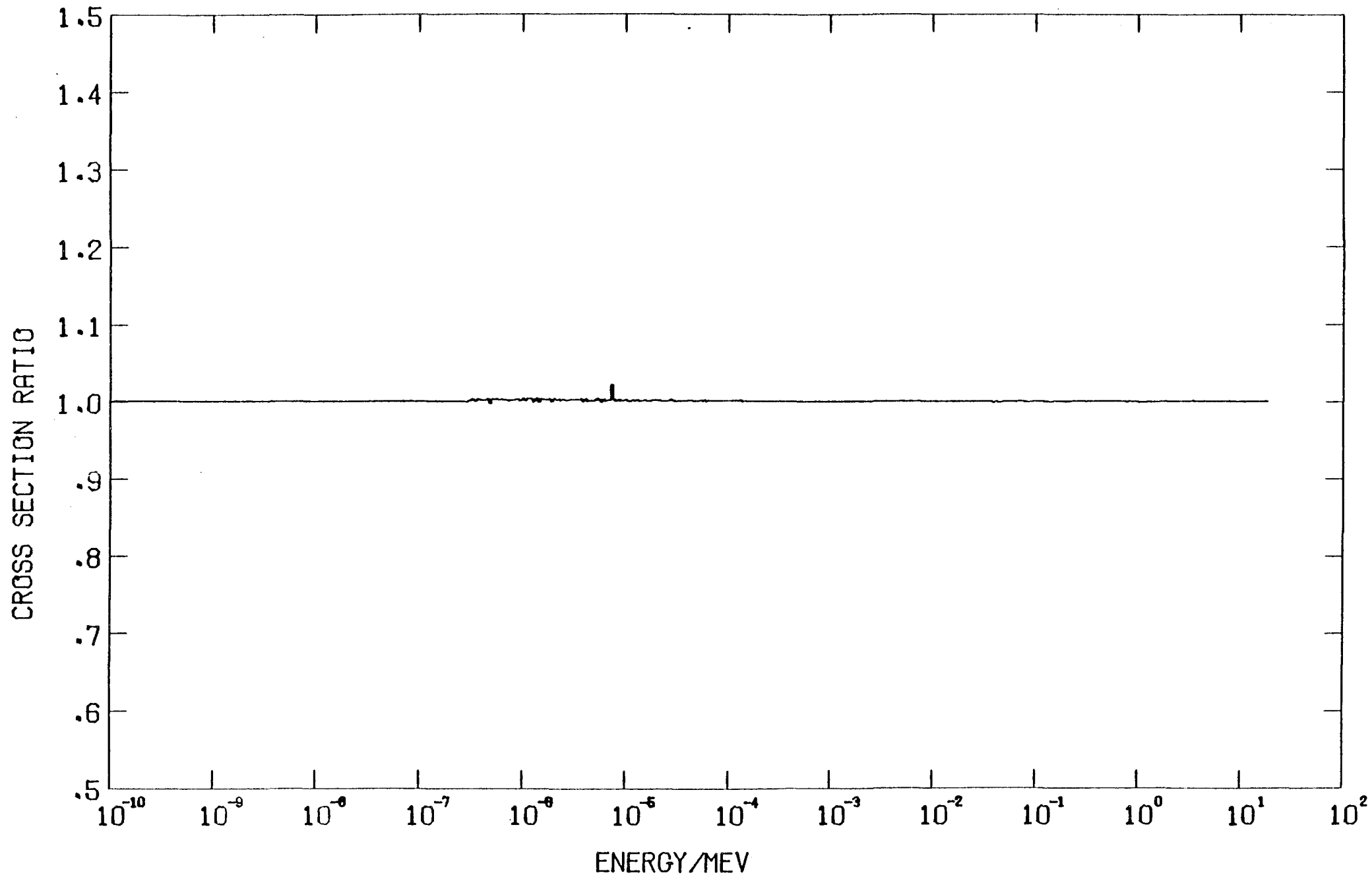


Fig. 2: CROSS SECTION RATIO FOR THE REACTION NP237(N,F)F.P. (BNL/ENTOSAN)