

AN APPRAISAL OF
THE NEA COLLABORATIVE PROGRAMME OF UNCERTAINTY
ANALYSIS AND SHIELDING BENCHMARK EXPERIMENTS

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1. INTRODUCTION

The collaborative programme on the application of sensitivity and uncertainty analysis in shielding calculations and the conduct of penetration benchmark experiments was initiated by the NEACRP in June 1973 with the aim of co-ordinating work on the assessment of data for shielding and exchanging results of benchmark experiments. Five meetings have been held in this programme, one of which was sponsored jointly by the IAEA and NEA at Vienna in October 1976. Whilst the original aim of generating a revised Data Request List for shielding in WRENDA has not yet been achieved, considerable progress has been made in the development of both analytical and experimental techniques.

2. THE PREPARATORY PHASE

At the beginning of the programme the ANISN/SWANLAKE codes for sensitivity analysis were not generally available in laboratories outside the USA, although it was recognised from the outset that an estimate of the sensitivity profiles was an essential requirement for the proper design of an integral benchmark experiment. A considerable amount of ground-work had to be completed however before the aim of exchanging benchmark results between European and Japanese laboratories and the subsequent intercomparisons with published American results could be realised. The achievements during this preparatory phase are summarised below.

- i) Procedures were agreed for the conduct and reporting of benchmark experiments.
- ii) A standard single-material experiment (iron) was initiated at all participating laboratories to investigate possible systematic errors, and provide a test-bed for both experimental and analytical techniques.
- iii) A common 100-group data library (which is now known as EURLIB) was generated from ENDF/B-III for the analysis of the iron benchmark experiments.
- iv) A calculational route based on the ANISN/DOT codes was adopted for the forward calculations and RADAK was chosen as the reference code for unfolding pulse-height distributions.
- v) By the time of the Paris meeting in October 1975, all the participants had implemented the ANISN/SWANLAKE codes for sensitivity analysis in one-dimensional problems, although difficulties had been encountered with convergence, and with the normalisation of forward and adjoint calculations. Two theoretical benchmarks were accordingly set up which were intended not only to validate the methods, but also to investigate the effects of using different in-house data sets for the application of sensitivity and uncertainty analysis to generic design problems.

3. THE DEVELOPMENT OF SENSITIVITY AND UNCERTAINTY ANALYSIS

Whilst six independent benchmark experiments [Refs (1) thro' (6)] had been initiated in European and Japanese laboratories by the end of 1976 it was clear that considerable difficulties were being encountered, inter alia, with the development of neutron spectrometers; and that a further period of measurement would be required before results could be compared. The thrust of the programme during this period was accordingly directed towards the application of uncertainty analysis to generic design problems in order to identify the data requirements, and to determine whether these were met by existing evaluations of differential data.

The findings in the exercise on the application of the ANISN/SWANLAKE codes to the two theoretical benchmark problems posed at the Paris meeting in 1975 were presented at the first meeting in this series to be sponsored jointly by the IAEA and

the NEA which was held at Vienna in October 1976. Both of these were typical radial shielding problems which could be modelled in one-dimension. The first problem, posed by Barre (7), was based on typical sodium-cooled FBR and the second, due to Hehn (8), was a close simulation of a typical PWR. Forward calculations with the ANISN code revealed a rather wide divergence in the values obtained for the requested target quantities but calculations of the sensitivity of these quantities to total cross-sections performed with the ANISN-SWANLAKE combination were generally in very good agreement.

The solutions submitted by McCracken (9) included an uncertainty analysis which involved the folding of sensitivity coefficients with estimates of uncertainties on the data used in the calculations. These were obtained from the compilations due to Schmidt (10) of the cross-sections for fast reactor calculations which gives estimates of the standard deviations on each cross-section, and also includes the information required to estimate the correlations between the components of the total cross-section at each energy point (the so-called partial correlations). The lack of information on energy-dependent correlations for given cross-sections was circumvented by postulating complete correlation across the whole energy range of the problem and gave rise to the concept of 'reduced' upper limit uncertainty analysis*. This work revealed the need to break down scattering matrices into their elastic and inelastic components.

By the time of the Paris meeting in November 1977, consideration had been given to the available sources of information on cross-section uncertainties. In addition to the Schmidt compilation these included:

- i) Variance-covariance matrices published by Gerstl (11) et al which were derived for CTR applications and gave no information below 2 MeV. (They were therefore of limited use for fission reactor work.)
- ii) The basic ENDF/B-IV error-correlation files for Nitrogen, Oxygen and Carbon which could be processed into multi-group covariance matrices using the PUFF code (12) or MCOVE (13).

The 15-group (E^{-1} weighted) covariance matrices published in ORNL-5318 were made available for use in the Collaborative Programme in April 1978 (14). Two problems arose in the application of these data:

- a) The group-structure is too coarse for the imposed (and in some applications unrealistic) weighting spectrum.
- b) Convergence difficulties (admittedly not insuperable) can arise in ANISN with such broad energy groups in materials with relatively poor moderating properties such as sodium and iron below the inelastic threshold.

At that stage it was already clear that:

- i) unless evaluated error-assignments were made available for the basic ENDF/B files used in compiling the EURLIB Library giving, at least, the standard deviations on the total and the partial cross-sections as a function of energy, then no significant progress could be made towards the objective of compiling a meaningful shielding request list for inclusion in WRENDA.

* Reduced in the sense that ignoring partial correlations when these are known gives rise to an unnecessarily large over-estimate of the uncertainty.

and ii) the lack of energy correlation data would be a serious limitation in practice because problems would be encountered where the target accuracy which was exceeded by the reduced upper-limit estimate could be shown to be met by introducing full variance-covariance data - this point has subsequently been demonstrated by Hall (15) in his uncertainty analysis of a generic design for a sodium-cooled FBR.

It was accordingly agreed that McCracken (Winfrith) should produce a provisional set of fine-group variance-covariance matrices for use with EURLIB based on the Oak Ridge data given in ORNL-5318. This would be achieved by expanding the 15-group data using polynomial interpolation. The corresponding matrices for oxygen, carbon and nitrogen would be provided by Hehn (IEE Stuttgart) who had implemented PUFF to process the ENDF/B-IV error files for these materials. A preliminary version of the 100-group EURLIB matrices has been published by Hall (16). With these data it is now possible to carry out uncertainty analyses in two stages:

- i) The reduced upper-limit estimates can be calculated using the standard deviations (the diagonal elements) derived from the above sources.
- ii) A full covariance matrix can be utilised to obtain 'best' estimates of the uncertainties on target quantities specified for shield design calculations.

The results of such analyses can subsequently be revised when more accurate correlation files became available within the NEA laboratories.

The current library recommended by CESWG for US shielding calculations is the 171-neutron group and the 36-gamma-ray group VITAMIN-C processed by AMPX from ENDF/B files. This set utilises the Bondarenko concept of the background cross-section (17) for spectral averaging of multi-group cross-sections for mixtures of materials. The hydrogen data in the latest version (DLC-41 VITAMIN-C) has been modified by inserting bound-in-water values for the thermal groups into the infinitely dilute cross-sections associated with the Bondarenko part of the file. The compilation of multigroup covariance matrices has also been updated with the addition of a 26-neutron group set for fast reactor benchmarks. Covariances are included for U-235, U-238, Pu-238, Pu-240, Pu-241, Na, Fe, N, O and C based on evaluated covariance files from ENDF/B-IV and private communications.

It was agreed that the next stage in the Collaborative Programme was for all participants to specify generic shielding problems which could be modelled in one-dimension for the ANISN/SWANLAKE route. Several proposals have been made, and Professor An of Tokyo University has suggested a two-dimensional shielding problem for an FBR which could be analysed initially with VIP (the two-dimensional equivalent of SWANLAKE). Hitherto, all uncertainty analysis outside the USA has been restricted to one-dimension with the exception of a feasibility study of correlated-tracking performed by Rief (18) at Ispra using a modified version of the TIMOC Monte Carlo code. This method can in principle be used for sensitivity calculations in shields with complicated geometries. The results obtained to date are limited to total cross-section sensitivities in the YAYOI gun-source experiment in which measurements were made of the scalar flux behind thin iron slabs at angles of 0° and 30° to the axis. It is difficult to assess the potential of this approach on the basis of these calculations but it is clearly important to pursue Monte Carlo perturbation methods for shields with complicated geometries which cannot be adequately treated by other methods.

4. COMPLETION OF THE IRON BENCHMARK FEASIBILITY STUDY

4.1 Status of Experiments

The results of the first three single-material experiments in iron from

Winfrith, Karlsruhe and the University of Tokyo have been published in a standard format together with the original ORNL iron experiment (19). This format has been chosen to be consistent with that laid down by the CSEWG for the reporting of benchmark experiments in the US.

The experiments conducted with a Californium-252 source in iron shells at Karlsruhe have been completed and the results have been used to validate a data-set based on the KEDAK file. The PROTEUS experiment has been completed: spectra have been measured with hydrogen-filled proportional counters and the high-energy region has been investigated with Ne-213 scintillation counters. The YAYOI experiment has been analysed with forward calculations (including the preliminary study of the sensitivity profile accomplished with correlated tracking in the Monte Carlo code TIMOC mentioned above) and further measurements have been made in sodium. Spectrum measurements have now been made in EURACOS II in collaboration with Winfrith to supplement the earlier scans with integral detectors. A series of iron/sodium mixtures has been studied in the HARMONIE facility.

4.2 Investigation of Data Adjustment Techniques

Two independent analyses have been published by European Laboratories to date: Salvatores et al (20) and McCracken (21) have both utilised the ASPIS measurements to generate adjusted data-sets for iron. These illustrate the basic decisions which must be made before adjustment of data can be undertaken, namely:

- i) How much experimental data should be included in the fit, and
- ii) Which parameters should be chosen for adjustment?

The inclusion of a small amount of experimental data, say the reaction-rates of a few activation detectors, makes the optimisation process relatively easy to achieve without excessive computational requirements. Most attempts at benchmark analysis have taken this course but there is an obvious penalty to be paid - limited refinement of data is to be expected from limited experimental information. A wide choice of parameters is available for adjustment, including the scalar cross-section of the constituents of the group total-cross-sections, the angular distribution of scatter and even, by the so-called consistent method, the scattering laws themselves.

Salvatores' analysis makes use of the consistent method to investigate the temperature in the evaporation model of inelastic scattering in the continuum energy region. He derives energy distributions of scattered neutrons which produce considerably more neutrons at energies up to 2MeV than those given by ENDF/B-IV. The amount of experimental information which is included in his fit is relatively small - typically one or two reaction-rates.

McCracken and his co-workers, on the other hand, have chosen to investigate only the scalar absorption, inelastic and elastic scattering cross-sections. They have however addressed themselves to the problem of including a very large amount of experimental information - equivalent to six or seven hundred activation detectors in the fit. This amount of information makes it possible to seek rather detailed adjustment: about two hundred scalar cross-sections are currently involved. Matthes at Ispra recently proposed a method of analysis closely related to that of McCracken et al (22).

The American work has included the published results of cross-section adjustment in experiments containing mixtures of materials. Oblow et al (23) have examined twenty-one different configurations of stainless steel, iron and sodium spanning the range of design parameters for the internal shields of the

the Clinch River FBR. They found that adjustments in 51 energy groups based on a small subset of five configurations covering a wide range of sensitivities failed to predict the results of the remaining measurements by a large margin. According to the authors, their findings were attributable in part to the transformation for the purpose of analysis from two-dimensions to one-dimension and the neglect of steel constituents such as nickel, chromium and manganese in the cross-section adjustment procedure. A further limitation was the use of a single Bonner-Ball detector which effectively measured the total flux between 1 eV and 1 MeV for all adjustments.

As a result of this work, the current capabilities of integral benchmarks have been clearly established and may be summarised as follows:

- i) each experiment can provide information on the accuracy of some partial cross-sections (and therefore on the total cross-section) in limited energy ranges;
- ii) these are determined by the spectrum and strength of the source, and the energy range over which statistically significant measurements can be made with the available detectors;
- iii) the room for manoeuvre in varying the source spectrum with the aid of filters has not been thoroughly investigated; this approach would require considerably higher powers than are available in most of the experimental facilities (with the possible exception of EURACOS-II and the ORNL-TSF), and the analysis would at least involve the prediction of the angular flux spectrum at the front surface of the slab. (This artifice obviates the need to measure the angular distribution of the flux at this starting position.)
- iv) The use of the covariance matrices derived from the ASPIS multi-group adjustments to the iron cross-section has led to a 20% reduction in the estimated uncertainty for the iron displacement-rate in the core-restraint region of the idealised FBR problem posed by Barré (7).
- v) The results obtained for iron have demonstrated the feasibility of adjusting data using benchmark penetration experiments, but the techniques utilising spectrum measurements are too cumbersome, on the one hand, whereas those based exclusively on integral measurements are too coarse, on the other. Some degree of simplification will be necessary before the former can be generally applied to a wide range of materials and there is clearly a significant amount of redundant information in the approach currently being followed at Winfrith and Ispra.

SUMMARY AND CONCLUSIONS

The participating laboratories have derived substantial benefits from the Collaborative Programme and the original objectives identified by NEACRP in June 1973 have been achieved. Progress has inevitably been slow, this reflects to some extent the general slowing down in the pace of nuclear programmes throughout the world, but it is largely due to the higher priorities accorded to commercial projects within individual laboratories.

The present situation can be summarised as follows:

- i) Capabilities have been established for one-dimensional sensitivity analysis but progress towards the compilation of a new data request list

for shielding is hampered by the lack of uncertainty assignments for the available data files.

- ii) To date, the EURLIB scheme has been used for the analysis of benchmarks in the Collaborative Programme but the VITAMIN-C scheme is now available from RSIC. Both data-sets have covariance matrices for a limited number of materials. The data for EURLIB are rudimentary but they could be expressed in a common format for comparison with VITAMIN-C. The latter includes the Bondarenko treatment whereas no provision is at present made for background effects in EURLIB; for the purpose of future collaborative NEA programmes it would be desirable to compare sensitivity analyses conducted with both sets.
- iii) There is a growing interest in the use of Monte Carlo perturbation methods for sensitivity analysis in multi-dimensional shield configurations; this approach is being explored at Ispra and Winfrith, and codes with these capabilities have been developed in the US and elsewhere; in view of the increasing use of Monte Carlo for design problems it is appropriate for the NEA to co-ordinate activities in this area.
- iv) It is generally agreed that adjustment of data is essential to derive quantitative information from benchmark experiments, and it is therefore important to reconcile the various approaches adopted within the NEA laboratories to make the best use of the available benchmark information and the experience gained in analysis without necessarily prejudging how adjusted data are utilised in practice.
- v) Good progress is being made by Matthes at Ispra with the simultaneous adjustment of iron cross-sections using measurements from different laboratories, initially the study will be confined to EURACOS and ASPIS data but it is hoped to include other experiments at a later stage.
- vi) Experimental techniques are now well established but there is a need for more multi-material data-testing benchmarks to be performed in order to investigate the range of validity of the adjusted data-sets which have been derived from measurements in single materials.

The time is now ripe for a new initiative by the NEACRP: it is therefore proposed that the NEA should sponsor a meeting in the Spring of 1980 to take up these issues and implement a further programme of collaborative work. By that time the results of the simultaneous adjustments for iron should be available from Ispra; significant progress can be anticipated with Monte Carlo perturbation methods; and comparisons of sensitivity analyses should have been made using the EURLIB covariance matrices and the VITAMIN-C data. Such a meeting would also provide an opportunity to update the compilation of benchmark results including new measurements from the US and from the European and Japanese laboratories. A provisional agenda for the meeting is given in the Appendix.

The NEACRP is accordingly invited to:

- i) note the progress made in the Collaborative Programme;
- ii) draw attention to any new work which has not been included in this review;
- and iii) endorse the proposal for a Specialists Meeting to be held in the Spring of 1980.

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APPENDIX

Proposed Topics for Discussion at the NEA Specialists Meeting to be held in the Spring of 1980

1. Sensitivity and Uncertainty Analysis

1.1 Status of Multigroup Data Sets

- a) EURLIB-IV
- b) VITAMIN-C
- c) Other sets

d) French set?

1.2 Covariance Information

- a) 15-group matrices in ORNL 5318
- b) EURLIB Covariance Matrices
- c) VITAMIN-C - 26 group matrices

1.3 Practical Examples of Sensitivity and Uncertainty Analysis Using the ANISN/SWANLAKE Route

1.4 Multi-Dimensional Sensitivity Methods

- a) Sn methods
- b) Monte Carlo methods

1.5 Compilation of Generic Problems for Analysis to Assess Shielding Data Requirements

- a) Thermal reactors
- b) Fast reactors
- ~~c) Fusion reactors and experimental plant~~

2. Shielding Benchmark Experiments

2.1 Review of Completed Experiments

2.2 Analytical Techniques

- a) Multigroup adjustment
- b) The Consistent Approach
- c) Choice of experimental information - redundancy of measured quantities
- d) Comparisons of calculation and experiment - implication for the adequacy of working data-sets

2.3 Results of Independent Analyses of Benchmark Experiments

- 2.4 Results of Simultaneous Analyses of Benchmark Experiments Performed at Different Laboratories
- 2.5 Implications for the Design of Future Benchmark Experiments
- 2.6 Future Collaborative Programme