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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

PROCEEDINGS OF THE

IAEA CONSULTANTS' MEETING ON THE

ASSESSMENT OF THE RESULTS OF THE REAL-80 PROJECT ON CROSS SECTION UNFOLDING CODES

and

PLANNING FOR CONTINUATION OF THIS PROJECT

13 - 15 June 1983

Vienna, Austria

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Programme
for
IAEA Consultants' Meeting on the
Assessment of the Results of the REAL-80 Project
on Cross Section Unfolding Codes
and
Planning for Continuation of this Project

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Monday: 14:00-17:00	Review of REAL-80	- Opening of Meeting - Approval of Agenda - Review of REAL-80 Exercise - Verification of Processing Codes
Tuesday: 09:00-12:00	Improvements due to REAL-80	- Role of Normalization Factors - Development of the EAGLE Unfolding Code - Discussion of Lessons learned from REAL-80
Tuesday: 14:00-17:00	REAL-84	- Aims of REAL-84 - Scope of REAL-84 - Self-Shielding - Uncertainties - Spectra - Availability of Input Information - Estimation of Interest by Participating Laboratories - Time Schedule - Organization and Responsibilities
Wednesday: 09:00-12:00	Future Planning	- Round Table Discussion of Future Plans - Formulation of Conclusions and Recommendations
Wednesday: 14:00-17:00	Conclusions and Recommendations	-Presentation of Conclusions and Recommendations

List of Participants

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Proceedings of the IAEA Consultants' Meeting on the Assessment of the Results of the REAL-80 Project on Cross Section Unfolding Codes and Planning for Continuation of this Project

13 - 15 June 1983
Vienna, Austria

1. Introduction

The REAL-80 project was designed to assess the ability of currently used spectrum adjustment codes to predict radiation damage. This IAEA consultants' meeting was organized to assess the results of the REAL-80 exercise and to formulate plans for continuation of this project.

This meeting formulated the REAL-84 project which is designed to improve the ability to quantify the accuracy of radiation damage calculations. It was pointed out during the meeting that a 1% change in the accuracy of damage calculations can lead to a 1% change in pressure vessel lifetime. It was generally agreed that radiation damage estimates are of limited use unless they are accompanied by an estimate of their accuracy.

A by-product of this exercise will include improvements in the available covariance information. In addition it will allow an opportunity for participants to improve their confidence in the spectrum adjustment methods and codes that they use by validating them against other methods and codes.

The meeting unanimously agreed that the REAL-84 can lead to significant improvements in the ability to predict the accuracy of radiation damage estimates and recommended that the IAEA strongly support this project.

2. Lessons from the REAL-80 exercise

2.1 Acknowledgement

The meeting expressed appreciation to the joint team of evaluators (from the Nuclear Reactor of the Technical University Budapest and the Netherlands Energy Research Foundation ECN, Petten), for their work in

preparing the final report on the REAL-80 exercise (report ECN-128; INDC(NED)-3; BME-TR-RES 6/82).

2.2 Differential vs. integral responses

The REAL-80 exercise has shown that adjusted spectra provided by the participants can have remarkable differences in shape, and still can predict correct values for reaction rates of interest (i.e. displacement rates in steel and activation rates in nickel). Most of the differences observed were attributable to poor or incomplete application of the input data rather than to the computer codes themselves.

2.3 Differences in input

The neutron spectrum adjustment procedures used in the exercise did not show deficiencies in predicting these reaction rates. It is noted, however, that some adjustment procedures are not capable to take into account all the input information (like variance-covariance information), or to make estimates of uncertainties in output spectra and in predicted reaction rates.

2.4 Differences in output correlation matrices

It was noted that the correlation matrices for the output spectra for ORR and YAYOI obtained by a generalized least squares adjustment procedure were clearly different from those obtained by a Monte Carlo procedure in combination with a SAND-type of code. Uptill now the Monte Carlo technique used did not take into account the input correlations.

2.5 Incompleteness of input information

It is recognized in neutron spectrum adjustment procedures that all of the necessary input information required for a generalized least squares adjustment procedure is not always available. This holds especially for the availability of realistic (i.e. physics based) covariance information, both for input spectra and cross section data.

Physicists are urged to develop methods for generating this missing information and to provide the data for the neutron spectra of interest and for activation and fission reactions used in neutron metrology.

2.6 Processing of cross section files

A recent study by the NDS/IAEA, Vienna (see INDC/P(83)-40, NDS/IAEA, Vienna) indicates that the combination of the complexity of current evaluations and processing codes has resulted in the situation where nearly all presently available codes for processing ENDF/B file cross section data introduce large uncertainties into multigroup cross section. The reliability of the results of the spectrum adjustment depends upon the accuracy both of the input data and their uncertainties which are large compared to the uncertainty in the evaluated data, this may invalidate the results obtained by using these data in adjustment codes.

2.7 Conversion of group structures

The REAL-80 exercise has shown that correct procedures were not always used to convert cross section data and spectrum data from one group structure to another. Different group structures gave different results due to incorrect procedures used to collapse the 100-group data provided to the participants. Consequently we recommend that future projects clearly specify collapsing procedures for the input spectrum, cross sections, and covariances. Procedures for collapsing covariance matrices are given by Mannhart.*)

The meeting recommended that the IAEA make available good procedures for conversions of one group structure to another.

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*) MANNHART, W., Status and Further Needs of Cross Section Covariance Files. Contribution to "Nuclear Data for Radiation Damage Assessment and Related Safety Aspects". Report IAEA-TECDOC-263 (IAEA, Vienna 1982), p. 47

2.8 Recommended use of covariance matrices

Neutron spectrum adjustment procedures should preferably be carried out in the presence of variance-covariance information for the input data set (comprising input spectrum data, input cross section data and input reaction rate data).

Since the goal of spectrum adjustment is usually to obtain damage rates with specified uncertainties, future exercises should require that participants consider covariance information and propagate uncertainties for their calculated damage rates.

Since it is important (and possibly even mandatory in the future) to have variance-covariance information on output spectra, the use of adjustment codes which cannot take into account covariance matrices is discouraged.

The meeting expressed the opinion that the use of neutron spectrum adjustment codes based on a generalized least squares procedure should be promoted.

2.9 Determination of input spectrum covariance

In principle, physics information should be used to determine all covariances. For neutronics calculations this is more difficult, but may be done using sensitivity studies. However, such methods are time-consuming, expensive, and not widely available. Consequently, we recommend that the IAEA sponsor an effort to further investigate this problem and to recommend standard procedures.

2.10 Consistency requirement

A spectrum adjustment procedure can only provide output information which is acceptable and realistic from a physics point of view, if the input data set shows acceptable consistency (i.e. provides a likely value of the chi-square parameter).

If the input data set shows serious inconsistency (i.e. proves an unlikely value of the chi-square parameter), then it is recommended that the input data set is analyzed in an attempt to identify the origin of the inconsistencies.

The input data set should then be modified after such an analysis by an experienced physicist who can judge whether such modifications are justifiable from a physics point of view. In the case of inconsistent reactions, the method of Yeivin, et. al.*) is recommended for determining the source of the inconsistency. Inconsistency in input spectra cannot be determined so easily and methods need to be developed for handling these cases. In general, uncertainties and covariances may not be available for input spectra and experimenters may not choose a consistent formulation.

2.11 Importance of normalization factor

The REAL-80 exercise showed that the spectrum normalization factor plays an important role in the neutron spectrum adjustment, since it may dominate in determining the energy dependent modifications. Therefore the normalization factor strongly influences the results of the adjustment procedures.

Different participants clearly used different procedures to select the normalization factor since the procedure was not specified in REAL-80. Some of the problems encountered with normalization include inconsistent input data, such as bad reaction rates or cross sections, and poorly known spectra. Optimized least-squares normalization is generally recommended as part of the adjustment, as detailed in the REAL-80 final report. For mixed-spectrum reactors, the thermal-to-fast

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*) YEIVIN, Y., WAGSCHAL, J.J., MARABLE, J.H., and WEISBIN, C.R., Relative Consistency of ENDF/B-IV and -V with Fast Reactor Benchmarks, Proc. Int. Conf. Nuclear Cross Section for Technology, Knoxville, Report CONF 79-1058-28, 1979.

neutron ratio may be incorrect such that one single normalization factor cannot be chosen. Iteration might thus be required, perhaps with initially strong correlations within a few broad energy ranges to handle this case.

2.12 Development of advanced codes

A new computer code EAGLE (Elaborated Adjustment by Generalized Least-Squares Estimates) is being developed at BME (Budapest). This code will be similar to STAY'SL with the optimized normalization procedure mentioned earlier. Whereas STAY'SL performs a linear least-squares adjustment, the EAGLE code will also calculate higher-order covariance terms, as discussed in Appendix 4 of the REAL-80 final report. The code should be available in about six months and available for use in REAL-84. ECN (Petten) will provide a version for the CDC computer and BME (Budapest) for the IBM computer.

The participants of the meeting strongly supported a recommendation that spectrum adjustments must be performed with computer codes which properly account for and propagate uncertainties. The meeting recommended that the IAEA supports the development of such advanced codes in general and of EAGLE in particular which codes will incorporate these views.

2.13 Recommendation for REAL-84

In view of the conclusions in the final report on the REAL-80 exercise it does not seem necessary to repeat the exercise with the same aim for establishing the state of the art with respect to the following questions.

- what is the quality of the adjusted neutron spectrum?
- what is the quality of an integral damage parameter?
- what is the quality of a predicted activation rate?

The meeting recommended (in agreement with the recommendations of the INDC Meeting, 16-20 May 1983, Rio de Janeiro), that a new exercise should be performed with the aim of improving the assessment of accuracies in radiation damage predictions by various laboratories, for a wide variety of applications in nuclear technology.

3. Criteria for input data for REAL-84

3.1 Introduction

Four specific applications of neutron spectra were chosen (see Section 4.2).

In order to achieve the stated objectives of REAL-84 for each of the four spectra we require the following input data:

(i) State-of-the-art estimate of the neutron spectrum to be adjusted together with a realistic (evaluated) covariance matrix;

(ii) A set of measured (integral) reaction rates determined in the field of interest together with an experimentally determined covariance matrix;

(iii) A set of fine group evaluated neutron energy response functions which includes both those relating to the measured reaction rates and those relating to the (materials) dose parameters of interest to the reactor dosimetry community. For all these response functions the best available evaluated covariance information must also be supplied.

3.2 Neutron spectra

The estimate of the neutron spectrum to be adjusted may be determined by 3-D transport calculation (i.e. by synthesis of 2D-XY and 2D-RZ deterministic codes or by explicit 3D Monte Carlo codes) or by neutron spectrometry techniques where appropriate. In the case of spectrometry the relevant covariance matrix can be determined by the experimentalists. In the case of transport calculated spectra the problem of defining the covariance matrix is more complex. However, this can be achieved by the method of sensitivity analysis (as reported by Maerker et. al.*) together with covariance information relevant to the transport calculation input data, in which propagation of uncertainties due to

- source definition
- tranmission cross sections
- geometry
- mathematical modelling (or stochastic uncertainties in the case of Monte Carlo techniques)

is treated explicitly.

The group structure of the calculated spectrum must be consistent with the criteria noted below.

3.3 Reaction Rate Measurements

The reactions whose rates are to be provided should be representative of the detector sets which are capable of being routinely employed by experimental dosimetrists in the relevant fields for the purposes of materials or reactor dosimetry. Emphasis should be given to obtaining reaction rate measurements for $^{93}Nb(n,n')^{93m}Nb$ and $^{237}Np(n,f)FP$ in view of

*) 1. MAERKER, R.E., WAGSCHAL, J.J., BROADHEAD, B.L.,"Development and demonstration of an advanced methodology for LWR dosimetry applications," Report EPRI NP-2188 (1981)

2. WAGSCHAL, J.J., MAERKER, R.E., BROADHEAD, B.L., "Surveillance dosimetry: Achievements and disappointments." Proc. 4th ASTM-EURATOM Symposium on Reactor Dosimetry, Gaithersburg, March 22-26, 1982. Report NUREG/CP 0029 Vol. 1, p.79 (Nuclear Regulatory Commission, Washington D.C., July 1982)

their importance in covering the important damage energy region in structural materials. In all cases thorough treatment of the uncertainties in such reaction rates should be documented and an appropriate covariance matrix provided. In this uncertainty analysis consideration should be given to

- self shielding effects
- thermal neutron cover efficiency
- photofission corrections (e.g. ^{237}Np, ^{238}U, ^{232}Th)
- specific counting problems (e.g. $^{93}Nb^{m}$)

It would also be desirable if evidence of benchmarking of dosimetry materials and counting techniques were provided.

It is hoped that reaction rate data can be made available for the following spectra, together with the necessary supplementary variance-covariance information.

- A prompt fission neutron spectrum (based on the work at NBS, PTB and JAERI on reference neutron spectra);

- A surveillance neutron spectrum (based on the work performed at the ORNL Pool Critical Assembly Pressure Vessel Facility);

- A fusion reactor blanket spectrum (based on the work reported in the thesis "Experimental model studies for a fusion reactor blanket" by L.J.M. Kuypers, Technische Hogeschool Eindhoven, 1976);

- An acceleration neutron spectrum (based on the work compiled by L.R. Greenwood et al).

The participants expressed their willingness to co-operate in a task force for collecting and judging the input data.

3.4 Neutron response functions

The neutron cross sections for the measured reaction rates should be provided in a fine energy group (e.g. 620 group) scheme in order to accommodate condensation to all the group schemes likely to be used by the participants with their own version of an adjustment code. The cross sections data can be based on a state-of-the-art dosimetry cross section file (e.g. IRDF82, ENDF/B). Evaluated covariance matrix information for dosimetry cross section files, however, is not easily available. It would be desirable therefore that in the absence of other effort, the IAEA should consider convening a specialists' meeting whose object should be the definition of appropriate covariance data files and processing methods for codes which in the first instance would meet the needs of REAL-84 but in the longer term provide such data for use by the reactor/materials dosimetry community as a whole.

With regard to the damage rate parameters it is desirable that as far as the quantity "displacements per atom" (DPA) is concerned, appropriate cross sections for a number of construction materials in metallic form should be provided as well as those for compounds such as Al_2O_3 (sapphire), MgO, Quartz which have applications as direct damage monitors (see further the list in section 4.3). These materials should be defined in collaboration with the ASTM E10.05 committee responsible for updating the ASTM E693-79 standard on DPA in iron as a stimulus to the production of an agreed set of DPA cross sections for a variety of structural materials.

It should be stated here that it should not be the intention of the REAL-84 exercise to comment on the applicability of displacement cross sections to materials damage mechanisms or correlations but only to provide the opportunity to make estimates of them as a consequence of spectrum adjustment. However, the subject of appropriate damage correlation parameters is one of intense technical interest and debate and the IAEA would do well to consider the setting up of a parallel international working group on the subject to coordinate effort.

3.5 Group schemes for data adjustment

It is not possible to be specific about group schemes for adjustment calculations since this will be to a large extent problem specific. However, the results of to REAL-80 exercise indicated that satisfactory results can be achieved with ≈ 30 groups (E > 0.1 MeV) and ≈ 20 groups (E < 0.1 MeV).

4. Schedule for REAL-84

4.1. Aims of REAL-84

The REAL-84 exercise will be a continuation of the REAL-80 exercise and will incorporate the experience learned from REAL-80 and will improve our ability to assess the accuracy of spectrum adjustment calculations in general and radiation damage to pressure vessels in particular. It was pointed out that a 1% change in accuracy of damage calculation can lead to a 1% change in pressure vessel life time.

The long term aims of REAL-84 will be to strive toward establishment of standardized procedures and data for use in spectrum adjustment calculations. The short term aims will be improvement in the available data, particularly spectra and cross section covariance information. In addition this exercise will allow participants to assess and validate the accuracy of the methods and codes that they are presently using.

4.2 Scope of REAL-84

Subjects

The primary scope of REAL-84 will be neutron damage in the application of nuclear technology, primarily below 20 MeV. As such it was judged that biomedical or health physics applications are outside the scope of REAL-84.

Within the scope of REAL-84 there are a number of subjects which will be considered; the two most important subjects are improvement in the available covariance data and in the methods used in adjustment codes.

Subjects which are recognized as important and relevant but which were judged not to be practical for inclusion within the time schedule of REAL-84 include detailed investigation and improvement in the treatment of foil covers and self-shielding. Although improvements in foil covers and self-shielding will not be explicitly included within the scope of REAL-84 this subject should be encouraged due to the importance of this subject work.

Participants

The initial phase of REAL-84 will involve participation by a task force which will be involved in collecting, developing and improving the data required for use in REAL-84. The result of this initial phase will be the availability of improved data, particularly covariance information, for use in adjustment codes.

The second phase of REAL-84 will involve the actual adjustment and the reporting of results. This phase will be open to all interested participants. All participants in REAL-80 will be notified about REAL-84. In addition the exercise will be advertised in Newsletters, issued by the NEA/Data Bank, RSIC, IAEA Nuclear Data Section and the Euratom Working Group on Reactor Dosimetry.

Concerning the codes to be included in REAL-84, since the objective of the exercise is to improve our ability to assess the accuracy of damage estimates, only those adjustment codes which can actually estimate the accuracy of results will be included in this exercise. Since it is felt that only codes which use covariance information to properly propagate uncertainties are able to yield a reliable accuracy estimate, only these codes will be included in the exercise.

Spectra

The spectra considered for inclusion in REAL-84 were selected based both upon the importance of the spectra to nuclear technology, as well as the availability of the necessary data within the time schedule of REAL-84. Four spectra are considered for inclusion in REAL-84; these include the following representative spectra,

(1) a prompt fission spectrum
(2) a surveillance spectrum
(3) a fusion spectrum, incident on first wall
(4) an accelerator spectrum

In addition a number of other spectra were discussed but it was felt that the required data for these spectra would not be available in time for their inclusion in REAL-84. The spectra discussed included CFRMF, ORR, YAYOI and a spallation source. The status of these spectra and their covariance information will be reviewed further and if data can be made available by the end of 1983, one or more of these spectra will be re-considered for inclusion within REAL-84.

4.3 Data required for REAL-84

Damage

It was agreed that the number of atom displacement rates (DPA) calculated in REAL-84 should be many more than those calculated in REAL-80. The materials of interest that were identified includes, Fe, Ni, Cr, Zr, Ti, V, Al(Al_2O_3), Nb, Mo, Cu, C (graphite), W and stainless steel. In addition H and He production should also be calculated.

At the present time uncertainty information is not available for most of this data. However, it was noted that since currently there is no clear understanding of the relationship between DPA and damage, the quantity DPA is currently used as a normalization, rather than absolute factor and as such uncertainties are not currently of paramount importance.

Greenwood agreed to review the available damage data and to recommend a model and data library for use in this exercise.

Spectrum covariance

The following people will be approached in an attempt to obtain spectrum covariance data: Mannhart (fission spectrum), Maerker/Thomas (surveillance), Szondi (fusion spectrum) and Greenwood (accelerator).

Activation covariance

Zsolnay, Zijp and Nolthenius will cooperate in order to provide the required activation covariance data.

Cross section covariance

The off-diagonal ENDF/B-V covariance data now available have not been tested, and their quality and consistency is uncertain. It is recognized that these data are not necessarily ideal. However, it is felt that such information constitutes a good starting point in the absence of other information. The problem of the cross-section covariance data will be considered further with the aim of providing the participants with a recommended covariance file for REAL-84. This file will be based on ENDF/B-V data wherever possible, but might be modified in many cases, to make the data more physically reasonable and consistent.

In general, the future development and testing of ENDF/B covariance data is to be encouraged. It is felt that REAL-84 is an important step in that direction.

Group structure

No common group structure was selected for representation of all data. The availability of data for each spectrum will be reviewed and an appropriate group structure selected for each spectrum. Data will be provided to users in a fine group structure and they may collapse the data to any group structure that they feel appropriate for each application (note, the guidelines presented by this committee on the minimum number of groups to be used based on the experience learned from REAL-80). In order to minimize the probability of introducing errors during group collapse participants will be provided with both data and a computer code that can be used to collapse the data.

4.4 Time schedule

The following time schedule has been established based on consideration of allowing sufficient time for: collection and development of the data required for this exercise, participants to prepare results, evaluators to analyze results.

Oct 1983	- Meeting in Budapest to review availability of required data
31 Dec 1983	- All preliminary data sent to NDS/IAEA, Vienna - Preparation and checking of EAGLE code
July 1984	- Checking and correction of preliminary data completed
Sep 1983	- Presentation of detailed REAL-84 program at 5th ASTM - Euratom Symposium - Completion of realistic covariance information
Dec 1984	- Magnetic tapes ready for distribution to participants - Distribution of final information sheet
Jan 1985	- Distribution magnetic tapes begins
Dec 1985	- Deadline for participant contributions
Sep 1986	- Consultants' Meeting (Vienna) - presentation of preliminary results of evaluation
Dec 1986	- Completion of evaluation of results
Spring 1987	- Final Report presented to 6th ASTM-Euratom Symposium

5. Final conclusion and recommendation

There was a consensus agreement by the meeting that REAL-84 can significantly contribute toward improving the ability to assess the accuracy of damage estimates.

In addition by-products of this exercise will be improvements in available covariance data as well as assessment and validation of the methods and codes used by participants. Initial contact with potential participants indicates a wide interest in this exercise.

In light of the above background information the meeting unanimously concluded that the REAL-84 is well worth undertaking and recommends that the IAEA strongly support this exercise.