IEC-115

Final report on the work of subgroup 2 of the NSC working group on Evaluation Cooperation

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Contents:

I) Work within the subgroup

Considerable work has been done on most of the topics assigned to the subgroup in the report on its initiation (NFA-FUS-90-03). In detail the following subjects have been addressed:

a) Sensitivity calculations especially for fusion reactor shielding problems (papers A 1-10).

b) Generation of covariances for evaluated cross sections of ^{56}Fe from model calculations by means of simple qualitative methods for cross sections, elastic angular distributions and total gamma-production cross-sections (papers A 9-10, 23-25).

c) Generation of covariances for ^{56}Fe cross sections evaluated from both model calculations and experimental data combined by least squares procedures (paper A 11-12).

d) Detailed comparison of evaluated ^{56}Fe cross sections and uncertainties derived by different methods with each other and with precise experimental data (papers A 11-13).

e) Derivation of an accurate set of 14 MeV cross sections for ^{56}Fe by quantitative evaluation of the experimental data base in order to provide a sensitive test for evaluated cross sections and uncertainties (paper A 14-15).

f) Work on proposals for formats for cross section types not yet describable by ENDF/B format rules, such as coupled energy-angle distributions for secondary neutrons and charged particle emission and total and energy-differential gamma-emission cross sections (papers A 16-17).

g) Derivation of cross section covariances in the resonance range (paper A 26).

In the course of this work among others the following results have been obtained.

a) Extensive sensitivity calculations have been performed for the shielding of the superconducting coils of a tokamak fusion reactor and the sensitivity of the calculations to the different cross

section types and to the various energy ranges of each cross section has been obtained in detail. Also the sensitivity of the shielding calculations to the P1 - P3 coefficient of the elastic scattering distributions was investigated and proved to be important (papers A 1-7).

b) The approximate methods for generation of covariances of cross sections from model calculations used at ORNL and IRK have been documented (papers A 8-10), compared with each other (paper A 13) and with precision experimental data (papers A 14-15) and with results from a more accurate evaluation (papers A 11-12). From this comparison it can be concluded that the approximate methods for generation of covariances used in ENDF/B-VI and EFF have provided reliable uncertainty estimates and thus can be recommended for further use.

c) The method of estimating covariances from the dispersion of different evaluations has been extended from cross sections (file 33 data) to elastic angular distributions, secondary energy distributions and total and energy differential gamma production cross sections (papers A 11-12).

d) Two formats (MF 30 and 36) (papers A 16-17) have been worked out in detail and proposed for proper dealing with covariances of coupled angle-energy distributions of secondary neutrons and charged particles and total and energy-differential gamma-production cross sections.

e) A new evaluation of all important cross sections of ^{56}Fe has been performed using all available experimental information and combining it with the EFF-2 evaluation based model calculations using quantitative Bayesian methods (papers A 11-14). It has been demonstrated that a large reduction of uncertainties (typically by factors 2-3) can be obtained in this way compared to evaluations completely based on model calculations. After two years this evaluation has been updated in 1994 by adding new accurate experimental data for a number of cross sections (paper A 22). This has resulted in considerable further reduction of the cross section uncertainties and - even more important - has fully confirmed the original evaluation within its stated uncertainties. Thus it appears that the approach developped in papers A 11-14 may be used generally for important materials in order to create accurate and easily updateable evaluations including reliable uncertainty information.

f) The problem of deriving covariances of cross sections from nuclear model calculations from uncertainties of the model parameters was investigated in some detail. As yet however results tend to seriously underestimate the cross section uncertainties (papers A 18-19). This may be partly due to the use of too restricted parameter spaces, in part due to the neglect of the inherent model deficiencies. More work on this - in principle promising method - is needed.

g) A complete set of covariances for the resonance parameters of ^{56}Fe was derived by Fröhner and put into ENDF format (file 32). There are however serious problems in the use of this information as the important potential scattering radii cannot at present be stored in the ENDF-6 format. Therefore also the existing codes

neglect the uncertainties of the potential scattering radii and thus lead to unrealistically small cross section uncertainties. In addition comparisons of cross sections in the resonance range both between different recent experiments and with the reconstructions from the resonance parameters given in the most recent evaluations have revealed considerably larger descrepancies than expected from the estimated accuracies of both the data and the resonance parameters. Thus it appears that in file 32 uncertainties of cross sections in the resonance range at present need to be supplemented by file 33 information estimated by qualitative methods.

h) As a consequence of the work described in b-e) there exist now four evaluations, EFF-2.2, ENDF/B-VI, Vienna-Obninsk and CENDL-2 with complete file 33 information (papers A 8-12) which have been compared in detail and found to agree within stated uncertainties.

i) As a result of the work for the new Vienna-Obninsk evaluation the experimental data base for ^{56}Fe has been compiled and thoroughly checked and - unless given by authors - covariance matrices were estimated for each data set. Thus a data base containing 180 data sets for 10 types of cross sections with full coavariance matrices is now available at IRK, which could be useful for further work on quantitative evaluation methods (papers A 11-12 and 22).

j) Most members of the subgroup participated in the NSC Specialist meeting and subgroup members acted as working group members and chairmen of this meeting. Thus the recommendations and conclusions of this meeting (paper A 20) summarize to a large extent the conclusions of the subgroup concerning generation and processing of covariances.

k) Based on the experience gained by the work within the subgroup, H. Vonach, coordinator, gave an overview at the Brookhaven meeting on Evaluation Methodology (paper A 21).

III) Open problems

a) Representation of covariance information in the ENDF/B-VI format

The work of the subgroup has demonstrated on the example of ^{56}Fe that the goal of generating reliable and rather complete covariance information can be obtained with reasonable effort. The actual use of this information, however, is at present severely limited by the existing processing and sensitivity codes. At present only information on cross section covariances (file 33 data) and covariances of angular distributions for elastic scattering and inelastic scattering to discrete levels (file 34 data) can be used in neutronics calculations. In order to also consider the effects of covariances of coupled energy angle distributions of secondary neutrons and total and energy-differential gamma-production cross sections considerable extensions of the present processing and sensitivity codes would be needed in order to handle the proposed new formats MF 30 and

MF 36. Likewise the processing codes for transforming file 32 information (covariances of resonances) into covariances of group cross sections have to be amended to include the covariances of all parameters especially those of the potential scattering radii. While this work is rather straightforward and should not pose major problems, it exceeds the resources available to the members of the subgroup.

b) Covariances of calculated cross sections

The problem of estimating the covariances of calculated cross sections used so far (papers A 8-12) is still rather crude and development of more rigorous methods is urgently needed. Attempts in this direction (see papers A 18-19) have shown that the consideration of the uncertainties of the model parameters is insufficient to explain the uncertainties of the theoretically calculated cross sections and an explicit inclusion of the uncertainties due to the model deficiencies is necessary for realistic uncertainties estimates. These however cannot be quantified easily. This is probably the most important, however also most difficult open question concerning the generation of reliable covariance information of evaluated nuclear data.

Appendix: List of papers originating from the work of subgroup 2

1) A. Hogenbirk
Self-Shielding in the Net Fusion Reactor Blanket and Effects of Uncertainty Calculations. Report ECN-R-90-007 (1990)

2) A. Hogenbirk, H. Gruppelaar and K.A. Verchunv
Sensitivity and Uncertainty Analysis of Net/ITER Shielding Blankets. Report ECN-RX-90-062 (1990)

3) A. Hogenbirk
Sensitivity and Uncertainty Analysis of the Nuclear Heating in the Coils of a Fusion Reactor. Report ECN-RX-90-34 (1990)

4) A. Hogenbirk
Energy Self-Shielding and SED/SAD Effects in Sensitivity Calculations of a Net Shielding Blanket. Report ECN-RX-91-038 (1991)

5) A. Hogenbirk
Extensive Sensitivity/Uncertainty Analysis of a Net Fusion Reactor Blanket. EFF-DOC-128 (1991)

6) A. Santamarina and T. Parish
Uncertainty Analysis of the Net/ITER S.C. Coil Shielding Parameters to Cross Section Data Uncertainties. Contribution to International Workshop on Fusion Neutronics, Los Angeles, June 5, 1992

7) A. Hogenbirk
New Sources of Uncertainties in Sensitivity/Uncertainty Studies, Proceedings of the 17th Symposium on Fusion Technology, September 14-18, 1992, Rome, Italy

8) A. Hogenbirk
Uncertainty Calculations made easier, Contribution to 8th International Conference on Radiation Shielding, April 24-28, 1994, Arlington, Texas, Report ECN-RX-94-035

9) A. Hogenbirk
Calculation of Design Uncertainties for the Development of Fusion Reactor Blankets taking into account Uncertainties in Nuclear Data, Contribution to Int.Conf. on Nuclear Data for Science and Technology, 9.-13.5.1994, Gatlinburg, Tennessee

10) A. Hogenbirk
Extensive neutronic Sensitivity/Uncertainty Analysis of a Fusion Reactor Shielding Blanket, Fusion Engineering and Design 24 (1994) 275-286

11) T. Parish and A. Santamarina
Sensitivity and Uncertainty Analysis of the Net Magnet Neutronic Design Parameters to Uncertainties in Cross Section Data (preprint)

12) H. Vonach et al.
Uncertainty Estimates for the Fast Neutron Cross Sections for the European Fusion File EFF 2 for ^{52}Cr, ^{56}Fe, ^{58}Ni and ^{60}Ni. EFF-DOC.85 (1990)

13) S. Tagesen and H. Vonach
Uncertainty Estimates for the EFF-files for ^{52}Cr, ^{56}Fe, ^{58}Ni and ^{60}Ni. Proc.Int.Conf. on Nuclear Data for Science and Technology, Jülich, May 12-17, 1991, Springer Berlin Ed. S. Qaim, p. 871

14) D.M. Hetrick, D.C. Larson and C.Y. Fu
Generation of Covariance Files for the Isotopes of Cr, Fe, Ni, Ca and Pb in ENDF/B-VI. Report ORNL/TM-11763 Oak Ridge (1991)

15) H. Vonach et al.
Evaluations of the Fast Neutron Cross Sections of ^{56}Fe including Complete Covariance Information. Physics Data 13-7 Fachinformationszentrum Karlsruhe (1992)

16) V. Pronyaev et al.
Updating of a Theoretical Evaluation by Experimental Data in the case of ^{56}Fe. Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data. Oak Ridge 7-9 Oct. 1992. NEA/NSC/DOC(93)3 p. 135

17) S. Tagesen and D.C. Larson
Approximate Methods for Derivation of Covariance Data. Proc. International Symposium on Evaluation methodology. Brookhaven 12.-16. October 1992 (in press)

18) H. Vonach et al.
Evaluation of 14 MeV Cross Sections for the Main Isotopes of the Structural Materials Fe, Cr and Ni. Proc.Int.Conf. on Nuclear Data for Science and Technology, Jülich, May 12-17, 1991, Springer Berlin Ed. S. Qaim, p. 906

19) A. Pavlik et al.
Evaluation of 14 MeV Cross Sections for the Main Isotopes of the Structural Materials Cr, Fe and Ni. Physics Data 13-6, Fachinformationszentrum Karlsruhe (1991)

20) D.W. Muir
Description of Covariances of Emission Spectra using ENDF File 30. Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data. Oak Ridge 7-9 Oct. 1992. NEA/NSC/DOC(93)3 p. 195

21) H. Vonach
Direct Covariance Data for Coupled Energy-angle Distributions. Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data. Oak Ridge 7-9 Oct. 1992. NEA/NSC/DOC(93)3 p. 183

22) Y. Kanda
Generation of Covariance Data from Combined Experimental and Theoretical Data. Proc. of the NSC Specialists' Meeting on Generation and Processing of Covariance Data. Oak Ridge 7-9 Oct. 1992. NEA/NSC/DOC(93)3 p. 119

23) T. Kawano et al.
Estimation of Nuclear Reaction Model Parameters for ^{59}Co, ^{58}Ni and ^{60}Ni. Proc.Int.Conf. on Nuclear Data for Science and Technology, Jülich, May 12-17, 1991, Springer Berlin Ed. S. Qaim, p. 974

24) Report of Working Group A
Generation of Covariances to meet User Needs
and
Report of Working Group B
Covariance File Formats and Processing.
Proc. of the NSC Specialists' Meeting on Generatión and Processing of Covariance Data. Oak Ridge 7-9 Oct. 1992. NEA/NSC/DOC(93)3 p. 289

25) H. Vonach
Covariances of Evaluated Nuclear Data - Present Status and prospects for the Future. Proc. International Symposium on Evaluation methodology. Brookhaven 12.-16. October 1992 (in press)

26) V.G. Pronyaev, S. Tagesen and H. Vonach
Update and Improvement of the IRK Evaluation for ^{56}Fe.
Proc.Int.Conf. on Nuclear Data for Science and Technology, Gatlinburg 9.-13.5.1994 (in press)

27) Zhao Zhixiang and Lin Tong
Uncertainty Files for Neutron Cross Sections and Elastic Angular Distributions on ^{56}Fe. EFF-DOC-266 (1993)

28) Lin Tingjin et al.
Intercomparison of Fe, Cr, Ni Neutron Data from CENDL-2, BROND-2 and ENDF/B-VI and JENDL-3. Proc.Int.Conf. on Nuclear Data for Science and Technology, Gatlinburg 9.-13.5.1994 (in press)

29) Zhao Xiang et al.
Evaluation of Neutron Induced Data on ^{56}Fe. Comm.Nucl. Data Progress, Vol. 11, 56 (1994)

30) F. Fröhner
On Uncertainty Evaluation and Fluctuations in the resolved and unresolved Resonance Regions. Proc.Int.Conf. on Nuclear Data for Science and Technology, Gatlinburg 9.-13.5.1994 (in press)