CJD: Progress Report, 2002-2004
IAEA Technical Meeting
"Co-ordination of the Network of Nuclear Reaction Data Centers"
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A.I.Blokhin, V.N.Manokhin, S.A.Maev, M.V.Mikhailukova, K.I.Zolotarev, N.A.Demin

1. Staff

Four new staff members joined during the reporting period:
Krivchikov S., post-graduate student/engineer, involved in a software development (from April 2003);
Vitvitsky R., post-graduate student/engineer, involved in a hardware development (from April 2003);
Demin N.A., PhD, scientist, a specialist in the radiation damage analysis (from September 2003);
Zolotarev F.K., post-graduate student/junior scientist, involved in nuclear data evaluation (from May 2004);

2. Data Compilation

2.1. EXFOR activity.

1. **2002-2003 (June 1):** TRANS 4127-4129 were prepared with 112 entries (17 new, 95 corrected).

2. **2003-2004 (September 1):** Three final EXFOR TRANS 4130, 4131, 4132 were sent to the NDS.
   Total numbers of ENTRIES – 55, new ENTRIES - 24, corrected ones – 31.
   Total record numbers – 21370.

3. **2004 (September 30):** EXFOR TRANS 4133 was prepared for distribution.

4. Considerable efforts were made to establish cooperation with the authors to get numerical data. On the basis of such cooperation numerical data were obtained from Khlopin Radium Institute (St.-Petersburg) on fission cross sections of heavy elements in the energy region 1 – 200 MeV, and neutron emission data from spontaneous fission of Am- and Cm isotopes. The data were obtained from Filatenkov's group and Laptev&Vorobiov's team and were introduced in EXFOR ENTRIES 41424, 41425, 41429, 41431 and 41428.
   A similar activity were made concerning the transmission data in the resonance neutron energy region for many nuclides with A=120 – 180 obtained by Grigoriev's group (IPPE+JINR cooperation), the photo-fission cross sections for 23 fissile nuclides measured by Soldatov's group (IPPE), some data concerning the high energy measurements from Gatchina.

2.2. CINDA activity.

1. **2002-2003 (June 1):** Three CINDA batches (CJD044-CJD046) with 2031 entries were transmitted to the NDS.

2. **2003-2004 (September 1):** Four CINDA batches (CJD047, CJD048, CJD049, CJD050) were prepared and distributed to the NDS (3575 CINDA entries in EXCHANGE format and 689 entries in READER format). This was possible exclusively due to the fruitful cooperation with NDS Data Section and its computer facilities.
3. During 2003-2004 CJD obtained 15 files in the EXCHANGE and READER formats from the foreign Nuclear Data Centers:

   from NNDC – 2 in EXCHANGE format, 1 in READER format (926 lines);

   from NDS – 3 in EXCHANGE format (156 lines);

   from NEA DB - 6 in EXCHANGE format, 1 in READER format (4742 lines).

4. During 2002-2004 we were engaged in checking Cinda Entry`s coded as "many". Some of them were compiled again in order to split by elements. We found that it was very useful. In process of this work some essential errors were corrected. We are going to do further checking and re-compilation, if necessary, in order to greatly diminish the number of works with code "many". In some cases the corresponding corrections were made in EXFOR entries.

3. Publications

In during 2002-2004 the three issues of the journal "Yadernye Konstanty" were prepared and printed.

4. NUCLEAR DATA EVALUATION Activity

Work performed with the participation of CJD

5. New data library ACDAM for the activation/damage calculations is compiled in the Russian Nuclear Data Center and consists from three parts:
   - *Activation/transmutation neutron cross-section base*
   - *Decay Data Library (DeDaL)*
   - *Damage Data Library (DDL)*

Activation/transmutation neutron cross-section base

The main part of the data is FENDL-2/A with selections from:

- evaluated nuclear data libraries EAF-99+ADL-3, BROND-2(3), ENDF/B-VI.3, IRDF-90, JENDL-3 (fission products), CENDL-2 (fission products);
- experimental data with using of mathematical methods of evaluations;
- empirical dependence of form of neutron threshold reaction excitation functions;
- theoretical model calculations;
- systematics of c-s around 14-MeV neutron energy;

Content:
From the element H (A=1) to Po (A=210), in the neutron energy range 10^{-5} to 20-MeV and it includes 704 target isotopes with data presentation: in ENDF-6 format.

Decay Data Library (DeDaL)

The DeDaL library is completely based on the EAF-99 Decay Data Library with the minor corrections for some nuclides.

Damage Data Library (DDL)

The DDL library is based on processing of the general purpose data files from the ENDF/B-VI.3 and BROND-2(3) libraries.

Content: DDL library is prepared for 60 elements/isotopes in the neutron energy range 10^{-5} to 20- MeV. The data for main structural elements and basic impurities involved in alloys and steels are included in the DDL in ENDF-6 format.

This work was presented on the ICFRM-11 Conference and will be published in Journal VANT, issue "Materials science and new materials" (2004) as: A.I.Blokhin, N.A.Demin, V.N.Manokhin,V.M.Chernov "New nuclear data base for transmutation, activation, gas production and radiation damage calculations for fusion reactor structural materials".

6. New version of the Russian Reactor Dosimetry File is prepared and now it is under the compilation and benchmark testing. New evaluations were made for the 26 reactions with the covariance matrices. Some of them were included into the IRDF-2002 compiled by the NDS.
7. **V-nat, V-51, V-50:** Neutron energy E_n<20 MeV; work done in collaboration with the Kurchatov Institute (Moscow) and the Institute of experimental physics (Sarov), in the frame of the ISTC project#910.
8. **Zr-90, Zr-91, Zr-92, Zr-94, Zr-96:** Neutron energy E_n<20 MeV; work done in collaboration with the Institute of Experimental Physics (Sarov), in the frame of the ISTC project#731.
9. **Pb-204, Pb-206, Pb-207, Pb-208, Bi-209:** Neutron energy E_n<20 MeV; This work was done in collaboration with the Institute of Experimental Physics (Sarov), in the frame of the ISTC project#731.
10. Enrichment of secondary gamma-ray production data produced by neutrons with energy E_n<20 MeV. Secondary gamma-ray production data are newly re-evaluated and incorporated for some nuclides needed for in the fusion application, namely for: **Al-27, Fe-nat, Cu-63, Cu-65, Zr-nat, Zr-90, Zr-91, Zr-92, Zr-94, Zr-96, Pb-nat, Pb-204, Pb-206, Pb-207, Pb-208, Bi-209;** This work was done in collaboration with the Institute of Experimental Physics (Sarov), in the frame of the ISTC project#731.
11. CJD was engaged in re-evaluation and preparation of evaluated neutron data for fission products: Ru, Pd, Mo, Nd and Sm and other isotopes for BROND-3 Library. The correction, processing and testing of new files is under way.

5. Cooperation

1. A participation in the CRP "The International Reactor Dosimetry File: IRDF-2002" organized by the IAEA NDS. Some evaluated nuclear cross sections from the Russian Reactor Dosimetry File were proposed for a new nuclear data library IRDF-2002 (see Appendix A).
2. In during of few years the cooperation between the CJD and the NuDaCe (ENEA, Bologna) continues in a field of nuclear data processing and testing. In 2004 some activity concerning the analysis the JEFF-3.0 Library was performed. In Appendix B we presented some results.

We greatly appreciated the help of V.Pronyaev, O.Schwerer, V.Zerkin and S.Dunaeva to overcome our technical problems for successful compilation into CINDA and EXFOR systems.

Appendix A.

Evaluated cross section data from russian reactor dosimetry file

K.I. Zolotarev

Cross section data for dosimetry reactions: $^{19}F(n,2n)^{18}F$, $^{24}Mg(n,p)^{24}Na$, $^{27}Al(n,p)^{27}Mg$, $^{46}Ti(n,2n)^{45}Ti$, $^{46}Ti(n,p)^{46m+g}Sc$, $^{47}Ti(n,x)^{46m+g}Sc$, $^{48}Ti(n,p)^{48}Sc$, $^{48}Ti(n,x)^{47}Sc$, $^{49}Ti(n,x)^{48}Sc$, $^{51}V(n,a)^{48}Sc$, $^{54}Fe(n,a)^{51}Cr$, $^{54}Fe(n,2n)^{53m+g}Fe$, $^{56}Fe(n,p)^{56}Mn$, $^{59}Co(n,a)^{56}Mn$, $^{58}Ni(n,p)^{58}Co$, $^{63}Cu(n,a)^{60m+g}Co$, $^{75}As(n,2n)^{74}As$, $^{93}Nb(n,n')^{93m}Nb$, $^{103}Rh(n,n')^{103m}Rh$, $^{115}In(n,n')^{115m}In$, $^{139}La(n,\gamma)^{140}La$, $^{141}Pr(n,2n)^{140}Pr$, $^{186}W(n,\gamma)^{187}W$, $^{204}Pb(n,n')^{204m}Pb$ and $^{237}Np(n,f)$ were taken to the International Reactor Dosimetry File IRDF-2002 [1] from the new version of Russian Reactor Dosimetry File. This version is the improved and extended version of the previous version of Russian Reactor Dosimetry File - RRDF-98 [2].

New evaluations of cross sections for the reactions $^{27}Al(n,p)^{27}Mg$, $^{56}Fe(n,p)^{56}Mn$, $^{58}Ni(n,p)^{58}Co$, $^{103}Rh(n,n')^{103m}Rh$, $^{115}In(n,n')^{115m}In$, $^{139}La(n,\gamma)^{140}La$, $^{139}La(n,\gamma)^{140}La$, $^{204}Pb(n,n')^{204m}Pb$, and revisions of cross section data from RRDF-98 file for the reactions $^{19}F(n,2n)^{18}F$, $^{46}Ti(n,2n)^{45}Ti$, $^{46}Ti(n,p)^{46m+g}Sc$, $^{47}Ti(n,x)^{46m+g}Sc$, $^{48}Ti(n,p)^{48}Sc$, $^{48}Ti(n,x)^{47}Sc$, $^{49}Ti(n,x)^{48}Sc$, $^{51}V(n,a)^{48}Sc$, $^{54}Fe(n,a)^{51}Cr$, $^{54}Fe(n,2n)^{53m+g}Fe$, $^{59}Co(n,a)^{56}Mn$, $^{63}Cu(n,a)^{60m+g}Co$, $^{75}As(n,2n)^{74}As$, $^{141}Pr(n,2n)^{140}Pr$, $^{237}Np(n,f)$ were carried out at the Institute of Physics and Power Engineering (IPPE), Russia, Obninsk in 2001-2003 years.

1. Summary Report of the Final Technical Meeting on “The International Reactor Dosimetry File: IRDF-2002” prepared by P.J. Griffin and R.P. Paviotti-Corcuera, Report INDC (NDS)-448, IAEA, Vienna, 2003.
2. Zolotarev, K.I., Ignatyuk, A.V.., Manokhin, V.N., et al: “RRDF−98, Russian Reactor Dosimetry File”, Report (NDS)-193, Rev.0 , IAEA, Vienna, 1999.

Appendix B.

Processing of the JEFF-3.0 library for the MCNP calculation.

A.Blokhin, M.Pescarini, R.Orsi.

1. It was performed a preliminary investigation on the JEFF-3.0 library of evaluated nuclear data files, compiled by the NEA DATA BANK. 340 elements/isotopes were tested through proper data processing with the NJOY system. The tests, where addressed to verify the self-consistency and the regular generation of processed files. In the frame of this work many problems emerged and, in particular, it was considered necessary to intervene into the evaluated data files to perform the needed corrections. The following nuclides, in particular, presented problems.

    - Na-22, Ar-36,38 and 40, Co-58 and 58m and Ni-59 present not complete evaluated data sets: namely some DADE, double differential cross sections in energy and angle for secondary neutrons and charge particles are not present;
    - The format of various cross sections files like K-nat, Ni-60, Eu-151, Os-nat, Pb-207, U-238, Pu-238,239 and 242, Cm-242 and Cf-252 were not completely correct;

Part of the needed corrections, referring to the previous two points, is contained in the NEA DATA BANK Internet site at the section "JEFF-3.0 library feedback". The nuclides K-nat, Ni-60 and Eu-151 were treated in ENEA Bologna in order to solve the problems emerged.

2. As a first step, in order to test the JEFF-3.0 library, it was decided to produce a library in ACE format, at the temperature of 300 K, for all the 340 nuclides of the evaluated library. It was decided to follow this program of work.

    - First - It was considered to generate an ACE library, based exclusively on the original files contained in the JEFF-3.0 library: without, in particular, any correction introduced at the level of evaluation;
    - Second - It was considered the possibility to produce another ACE library containing all the corrections suggested for a part of the 340 nuclides;
    - Third - It was decided to process the nuclides having URR (unresolved resonance region) data not only with the traditional UNRESR NJOY module but, in addition, with the PURR module, in order to obtain sets of probability tables to be used in transport calculations with the MCNP-4C2 and MCNPX systems. The p-tables data allow, in particular, to take better into account the self-shielding effects of resonance absorption in the fast neutron energy range in Monte-Carlo calculations.

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3. According to the recommendations of the NEA DATA BANK, the data processing of the JEFF- 3.0 library was performed with the latest version of the NJOY-99.90 system.

4. 17 evaluated data files presented the following problems.

    - Be-9 – not correct threshold energy for the Q-value;
    - F-19 – normalization problems for DE cross sections in (n,np) reaction and for DADE cross sections in (n,a) reactions;

- Na-23 – not correct reference system presentation of the (n, n'-cont) reaction, namely CM instead of LAB system;
- Al-27 – not correct format presentation for DADE cross sections;
- Si-29 – energy grid not always monotonic;
- Si-30 – not correct threshold energy for the Q-value;
- P-31 – not correct threshold energy for the Q-value;
- Ca-nat – energy grid not always monotonic;
- Sc-45 – not correct reference system presentation of the (n, n'-cont) and (n,2n) reactions, namely CM instead LAB system; not correct presentation of DE cross sections in (n,na) and (n,np) reactions;
- Ti-nat – energy grid not always monotonic;
- Mo-97 – not correct DADE cross sections for (n,xp) reaction;
- Mo-100 – not correct DADE cross sections for (n,xp), (n,xd), (n,xt) reactions;
- Ba-135 – not correct DADE cross sections for (n,na) reaction;
- U-233 – energy grid not always monotonic;
- U-234 – not correct energy balance for the total gamma-production;
- Pu-239 – not correct reference system presentation of the (n, n'-cont) reaction, namely CM instead LAB system;
- Cf-249 - not correct reference system presentation of the (n, 2n), (n,3n) and (n,fiss) reactions, namely CM instead LAB system.

Concerning the format presentation of the DADE cross sections, it was verified that the NJOY system is able to cancel the negative probabilities in the DADE data but the adjustments operated not always produce realistic (physical based) cross section trends. For this reason it is recommended to intervene inside the original evaluated data file to avoid, through proper re-evaluation, that negative values for the DADE data may be produced.